

rch Camille Paloque Bergès o DOUGLAS A. Alexandre Hosmithauftoz utoledo. ed 10 Feb 93 Alexandre a Hocquet, 10 Fe

pate: wed, 24 Feb 93 17:21 EDTFrom: <PODOSNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>SUbject: X-Window REUROPEANTSOCIETY: for Fithe History of Science

sender@chemdLisboanderSetembropA2014

om: cares@tammy.harvard.edurate...Thu, 28 Jan 1993 15;28:31 PSTFrom: 100000 CHILE <morris@gnl2.ucdavis.edu>subject: Population Analyzis in 15823 Science Arthur Company Compan

@VAX1 LIMKC.EÖUSUbject: Semi MD=UPJPR/AMDFFLEDY/COU :21:25 R7 GFr h: By Usso

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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 -0600Fr

2008 White at: is Samery nd corpus 2 Fr Compositation and accomposition of the corpus states as the composition of the corpus states as the corpus states are the corpus states and the corpus states are the corpus states are the corpus states are the corpus states and the corpus states are the corpus states
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
             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>Dato: Wed, 10 Feb 93 16:23:41 -0600subject: parallel CHARMM?Date: Wed, 10 Feb 93 15:46:43 -0800From: rickl@biosym.comSubject: DIBUG ad Assub Proceedings of the Company of th
                  vindows for PC ..Date: Sat, 13 Feb 93 12:21:47 +0900From: Katūshi Kobayashi <ikob@les.pc.uec.ac.jp>Date:
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
Carl JugDate: Tue, 23 Feb 93 15:08:43 PSTFrom: wsonnen@alnitak.usc.edu (wayne
 a)Subject: Re: Hydrogen bond.Date:
                                                                              Wed, 24 Feb 93 17:21 EDTFrom: <PODOSNNA
nl.govSubject: X-Window terminal emulator for MacDate: Thu, 25 Feb 93 17:19:09
 l.harvard.edu (jill cheney)Subject: Computer Program to Evaluate Wigner 3j Coef
 emiempircal calculations simple oxidesFrom: sender@chemdc1.tau.ac.il (Senderow
n.deSubject: Expert Know-How wanted !!Date: 02 Mar 1993 08:13:18 -0500 (EST)Fro
 ate.Edu (Gene Carter)Subject: Co MD parameters.Date: Tue, 2 Mar 93 17:22:53 CS:
 ling Software: Does anyone have STELLA?Date: 04 Mar 1993 17:08:31 -0500 (EST)F
                                                     Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PSUVM.PSU.EDU>S
secc.fi.cnr.itSubject: MO Theory Made VisibleDate: Tue Mar 09 11:23:12 1993Date
                               Thu, 11 Mar 93 18:54 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.
  1993 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.washington.edu
MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Date: Mo
  15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdtscp@hpc.ch.man.ac.
ar 1993 13:58:36 -0400From: ZSHI@ac.dal.caSubject: Information about IBM RS6000
st Girona Seminar on Molecular SimilarityDate:
 11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom:
 3 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing AMPA
 milSubject: What about simulated annealing?Date: Wed, 24 Mar 93 14:11:32 +0100
 ject: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From:
MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mb
uk>Subject: Polyrate QueryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfil
ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@go
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an 93 13:27:12 GMTFrom: "D. Mathieu" <DEWINDT%FRSAC11.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject:

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    Date: Thu, 22 May 1997 15:29:27 -0400
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From: "Peter Shenkin" <shenkin : at : still3.chem.columbia.edu>

force constant symmetry and Gaussian 90Date: 22 Jan 93 13:06:32 UTFrom: "BD

Software for calculating zeta potential and e

I've gotten lots of private email responses on this subject, in addition to the posted responses I've seen. I've been archiving

all of these. After the dust settles, I'll post a summary to CCL.

3 Feb 93 13:04:57Subject:

**** "Deep Blue can't triumph in the game of life" (NY Times, 5/13/97)

* Peter S. Shenkin; Chemistry, Columbia U.; 3000 Broadway, Mail Code 3153 * ** NY, NY 10027; shenkin : at : columbia.edu; (212)854-5143; FAX: 678-9039

ubject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@gull.uncc.edu (Harry C. fz-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: 0 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: Mol questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvx02.loui or doubled messagesDate: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.ibm.co

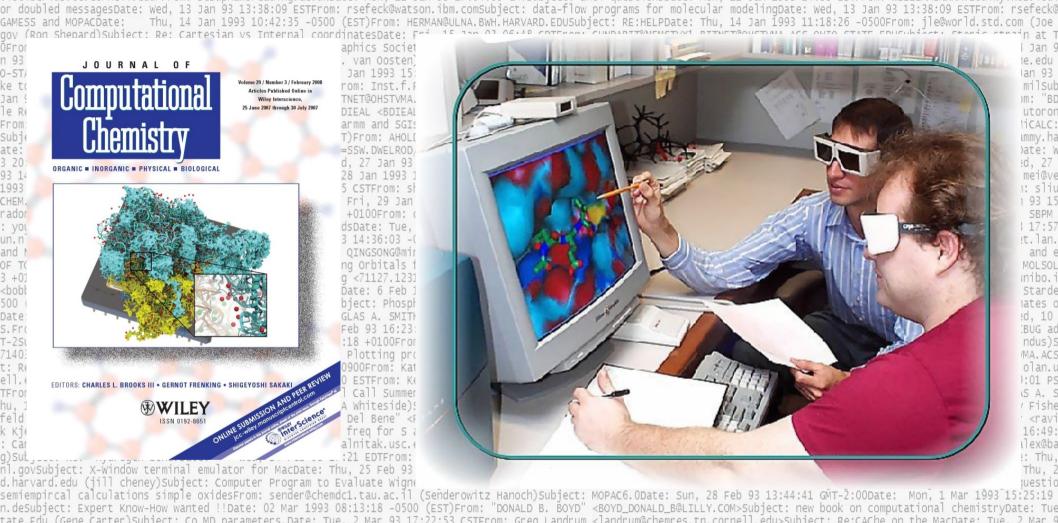
pov (Ron Shepard)Subject: Re: Cartesian vs Internal coordinatesDate: Fri, 15 Jan 93 06:48 CDTFrom: CUNDARIT%MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at 1 From: dmschn@bblt.monsanto.comSubject: next Molecular Graphics Society MeetingFrom: m.e. <harbowy@chemres.tn.cornell.edu>Subject: UHF calc's on diradicals/TSDate: Mon, 18 Jan 9 93 15:29:22 +0100From: oosten@rulhm1.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 D-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 problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" </JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed. 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" te to test a program.Date: Thu, 21 Jan 93 12:19:42 +0100From: Inst.f.Phys.Chem. I <pc1@pctc.chemie.uni-erlangen.de>Date: 21 Jan 93 07:50:00 ESTFrom: nauss@wrair-emh1.army.milSub

urrenceDate: Fri, 22 Jan 1993 13:36:26 +0000From: BDIEAL <BDIEAL@camsci.com>Subject: RÉ:: PDB on the MacDate: Thu, 21 Ján 93 17:31:46 -0500From: system@alchemy.chem.utoron

Thu, 14 Jan 1993 10:42:35 -0500 (EST) From: HERMAN@ULNA.BWH.HARVARD.EDUSubject: RE:HELPDate: Thu, 14 Jan 1993 11:18:26 -0500 From: jle@world.std.com (Joe

Subject: Re: CCL:RTFM? What FM?

*MacroModel WWW page: http://www.columbia.edu/cu/chemistry/mmod/mmod.html *





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Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@gull.uncc.edu

Lide>5 Sect: energy contribution of honds?pate: 06 Jan 1993 10:55:29 -0500 (EST)Erpm: "dwi@21]V.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: upate: Wed O MPD U3E3-1810011 arem @rine energy near the contribution of honds?pate: Thu, 7 Jan 93 19:19:39 -0100 (EST)From: "dwj@11 Ty.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F .cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMol guestionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvx02.loui

culations simple oxidesfrom: sender@chemdc1.tau.ac.il (senderowitz Hanoch)Subject: MOPAC6.ODate: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19 ect: 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@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.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 uplingtate migrate moutatronalife memory.etrus.etrus.evofs.computeers towsofvete helmiga-1:51:15 GMTFrom: jim@quanta.phy.
r 1993 02:33:09 -0800 (PST)From: Thomas Nhan stom@cassandra.em.washington.edu>Subject: PDBSource Fig. Date: Sun 14 Mar 93 1:08:13 40:000From: doe12@comp.bioz.unibas.ch.(Pe

MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Ďate: Mon. 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with 5<u>5:05 -060</u>0 (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 DIO DE PINS ZSHI@ac.dal.caSubject: Information about IBM RS6000Date: 17 Mar 93 16:18:00 EDTFrom: "STEPHEN R. HELLER" <srheller@asrr.arsusda.gov>Subject: Software Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01%EBCESCA1@OHSTVMA.ACS.OHIO-STATE.EDUSubject:

11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDDate: -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 ect: SC&A Conference speakers - thanksDaté: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrfl0128@aw

DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsrl@hpb.ch.man.ac.uk>Subject: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel uk>Subject: Polyrate QueryDāte: 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: Stéphen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDÁRIT@memstvx1.memst.eduS Computational chemistry and software

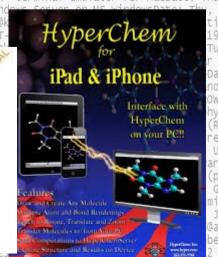


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Supercomputers: 1, Feb 93 13:28:40 ESTER Supercomputers: F.70S1 Personals Computers In 1905 at the Hydrogen bond Date: Wed, 24 Feb 93 17:21 EDTFrom:

tware: Does anyone have STEL A?Date: 04 Mar Developer & User GaussView

Gaussian, Inc. Carnegie Office Park - Building 6 Pittsburgh PA 15106 USA



PARCELLE COMPANIENCE: tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMol guestionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvx02.loui 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 ESTErom: rsefeck@ Thu, 14 Jan 1993 10:42:35 -0500 (EST) From: HERMAN@ULNA.BWH. HARVARD. EDUSUBject: RE:HELPDate: Th coordinatesDate: Fri. 15 Jan 93 06:48 CDTFrom: CUNDARIT%MEMSTVX1.BT lar Graphics Society MeetingFrom: m.e. <harbowy@chemres.tn.cornell.ed GaussView (A.B. van Oosten)Subject: Re: proton+electron=neutron?Date: Wed. ed, 20 Jan 1993 15:47 ČSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc Jan 93 I <pc1@pctc.chemie.uni-erlangen.de>Date Jan 93 HIO-STATE.EDU>Subject: ci.com>Subject: RE:: PDB on the MacDate: Thu narmm newsgroup?Date: Sun, 24 Jan 93 15:05:30 X1.UMKC.EDUSubject: Semiempirical references =UPJOHN/ADMD=TELEMAIL/C=US/@sprint.comSubject Gaussian, I 20:3 :29 -0700From: Jon Rusho <rusho@nitrate.chem Carnegie Office F 31 PSTFrom: VOODOO CHILE <morris@gnl2.ucdavi Medirac.tcg.anl.gov (Ron Shepard) Subject: exc Pittsburgh PA 15 5:35:12 ESTFrom: Louis.Grace@um.cc.umich.eduSu)19@servus.rus.uni-stuttgart.deSubject: Confe) 93 11:12:51 CSTFrom: (baell) <baell@syd.dah EST)From: ZURAW%athena@leia.polaroid.comSubj a G90/G92 CalculationDate: Thu, 4 Feb 93 11:27 buserve.com>Subject: Call for PapersDate: Fri The Social searchbare, o rep 1995 10:08:20 -1812From: "Bobby Clark" <bobby clar ack)Subject: Phosphazene ModelingDate: Mon. 8 Feb 93 07:58:51 Construction R. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: parallel workstations and serversDate: wed, 10 d, 10 Feb 93 16:23:41 -0600Subject: parallel CHARMM?Date: Wed, 10 Feb 93 15:46:43 -0800From: rickl@biosym.comSubject: DIBUG ad of Technological 13:06:18 +0100From: schettle@chemix.mpi-stuttgart.mpg.deSubject: Mac summervFrom: theresa@si.fi.ameslab.gov (Theresa windus)S Fri, 12 Feb 93 09:48:41 CETFrom: Norbert Mueller <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS Systems /UACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: X-Window terminal emulator for MacDate: Thu, Thu 25 Feb 93 17:19:09 -0500From: fendasgi.chem.temple.edu (Fend Chen)subject: x-windows server on Ms-windowsDate:

Eva Technological: Economical and Political as pects 90 fs :13:18 -0500 (EST)From: "DONALD B. BOYD" <BOYD_DONALD_B@LILLY.COM>Subject: new book on computational chemistryDate: Tue CSTFrom: Greg Landrum <landrum@chemres.tn.cornell.edu>Subject: Re:CAChe on the MacDate: Tue, 2 Mar 9 us 2 Mar 93 17:22:53 CSTFrom: Greg Landrum <Tandrum@chemres.th.cornell.edu>subject: Re:CAChe on the MacDate: Tue, 2 Mar 9 \$10\$EW@rest)From: MARYJo@northeastern.eduSubject: PDB subdir organization?From: Jan Labanowski <jkl@ccl.net>Dat Subject: Minimum allowable interatomic separationsFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoc 11:23:12 1993Date: Tue, 9 Mar 93 10:52:25 -0500From: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: GROW ACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: Softwaré for PCDate: Fri, 12 Mar 93 04:51:15 GMŤFrom: jim@ģuanta.phy. in the assandra.chem.washington.edu>Subject: PDB source file...Date: Sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re Sociology and fictive atoms in G92Date: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq History <mbdtscp@hpc.ch.man.ac.uk>Subject: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Tue, 16 Mar 93 11:49:33 GMTSubject: Tue, 16 Mar 93 Ma of Technology Information about IBM RS6000Date: 17 Mar 93 16:18:00 EDTFrom: "STEPHEN R. HELLER" <srheller@asrr.arsusda.gov>Subject: Software Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01%EBCESCA1@OHSTVMA.ACS.OHIO-STATE.EDUSubject: edited by 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDDate: Wiebe E. Bijker, EDU>Subject: Announcing AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic Thomas P. Hughes 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J and Trevor Pinch 5 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrfl0128@aw ogramFrom: Robert Laird <mbdtsrl@hpb.ch.man.ac.uk>Subject: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel :3Í:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Ándreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.eduS

Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@gull.uncc.edu (Harry C.

Subject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@qull.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 v PosDate: Led 6 C 3 13:03:33 08 transl horace and lower light have been solven accessible surfaces at 1995 to 19 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@watson.ibm.comSubject: data-flow programs for molecular modelingDate: 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@watson.ibm.comSubject: data-flow programs for molecular modelingDate: 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@watson.ibm.comSubject: data-flow programs for molecular modelingDate: 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@watson.ibm.comSubject: data-flow programs for molecular modelingDate: 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@watson.ibm.comSubject: data-flow programs for molecular modelingDate: 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@watson.ibm.comSubject: data-flow programs for molecular modelingDate: 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@watson.ibm.comSubject: data-flow programs for molecular modelingDate: 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@watson.ibm.comSubject: data-flow programs for molecular modelingDate: 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@watson.ibm.comSubject: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.ibm.comSubject: wed, 13 J Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMANGULMI, BWH, HARVARD, EDUSUBJECT: A HERDATE: Thu, 14 Jan 1993 11:18:26 -0500From: jle

Rubjeu: Rel Cardesian Ordania Confite Date: The International Confite Date: The Interna RE: PC Survey RESULTSDate: Wed, 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problembate: Wed, 20 Jan 93 gram.Date: Thu, 21 Jan 93 12:19:42 +0100From: Inst.f.Phys.Chem. I <pc1@pctc.chemie.uni-erlangen.de>Date: 21 Jan 93 07:50:00 ESTFrom: nauss@wrair-emh1.army.milSub force constant symmetry and Gaussian 90Date: 22 Jan 93 13:06:32 UTFrom: "BD : Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron Wombat Bioactivity Database: 05:30 -0500From: chm_ramsav@emunix.emich.eduSubject: CHEMiCALC: encesDate: Tue, 26 Jan 93 12:57:08 -0500From: watanabe@tammy.ha bject: Computer Assisted Chemistry Course Info RequestedDate: W





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ACS COMP Division supports CCL : emiempircal calculations simple oxidesFrom: sender@chemdc1.tau.ac.il (Se tate.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

Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PSUVM.PSU secc.fi.cnr.itSubiect: MO Theory Made VisibleDate: Tue Mar 09 11:23:12 19 Thu, 11 Mar 93 18:54 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OH 1993 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.washingt MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Da

, 15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdtscp@hpc.ch.m ar 1993 13:58:36 -0400From: ZSHI@ac.dal.caSubject: Information about IBM st Girona Seminar on Molecular SimilarityDate: :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: Announcin milSubject: What about simulated annealing?Date: Wed, 24 Mar 93 14:11:32

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: o

11:27:53 ESTFrom: Kevin Moore kmoore@ncsc.org>Subject: MOLSOL : Fri, 5 Feb 1993 16:17:32 +0100From: ivan@gandalf.ciam.unibo.i

Subject: Attack of the killer workstations

Date: Tue, 10 Dec 91 20:04:44 -0500.

From: ile \$#at#\$ world.std.com (Joe M Leonard)

n.deSubject: Expert Know-How wanted !!Date: 02 Mar 1993 08:13:18 -0500 (E Reviewing the recent discussion regarding C vs. Fortran and structured vs. spagetti coding, isn't it reasonable to consider the time of the programmer as more important that 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-thoughtout 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

.chem.utah.edu>Subject: Re: Periodic Table WidgetDate: Wed, 27 cdavis.edu>Subject: Population Analysis in GaussianFrom: mei@ve

: excited statesDate: Fri, 29 Jan 1993 16:47:38 -0600From: sliu .eduSubject: Gaussian and excited statesDate: Fri, 29 Jan 93 15 Conference AnnouncementDate: 01 Feb 93 19:26:49-0500From: SBPM d.dah.csiro.au>Subject: DMF dielectricDate: Mon. 1 Feb 93 17:57 Subject: 3D structure -> 2D drawing?From: QINGSONG@minmet.lan.

_clark@quickmail.clemson.edu>Subiect: Memorv and CPU for Starde

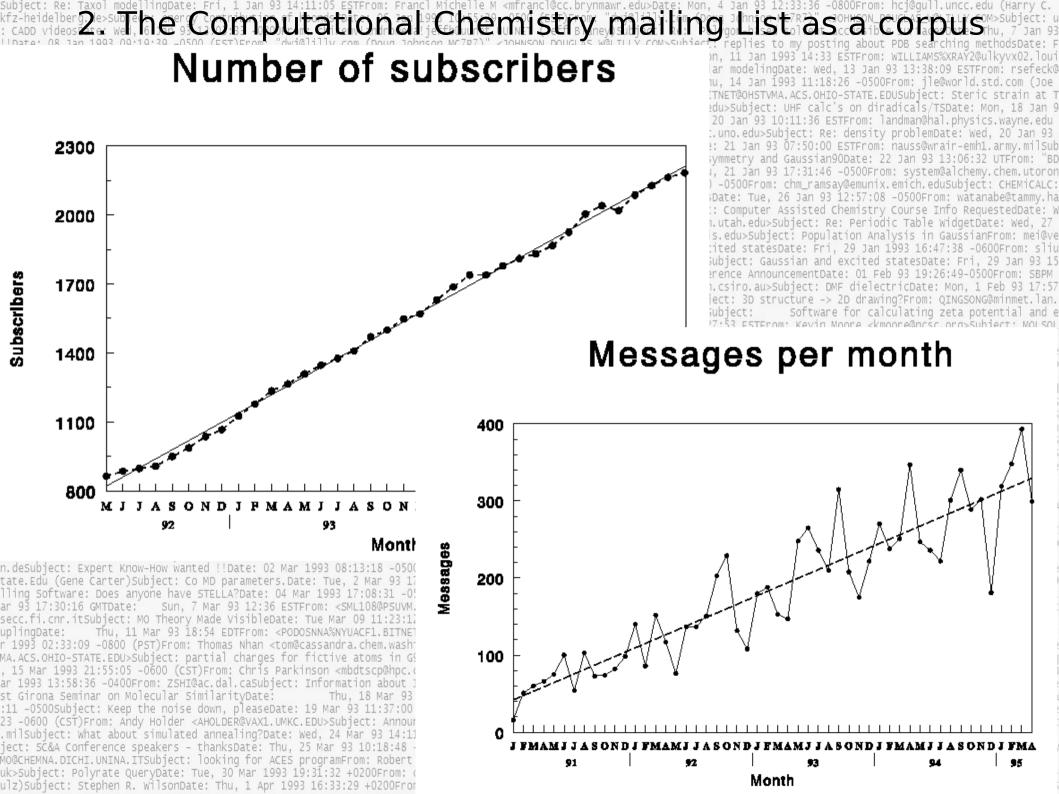
STFrom: adit@Kodak.COM (Adi Treasurywala)Subject: Coordinates o

do.edu>Subject: parallel workstations and serversDate: Wed, 10

Software for calculating zeta potential and e

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 ... iect: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -050 MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Lai Joe Leonard

jle \$#at#\$ world.std.com



ubject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@qull.uncc.edu (Harry C. fz-heidelber 2e-sutt to energy on the putation of himselfite of an 19 Chemistry energy in the publiston of himselfite of an 19 Chemistry energy in the publiston of himselfite of a subject: u capp videos 2e: well he good biston as computation at its promise of the published of t i@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@ulkyvx02.lou 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@ : 11:18:26 -0500From: jle@world.std.com (Joe CS.OHIO-STATE.EDUSubject: Steric strain at T CCL.NET IF calc's on diradicals/TSDate: Mon, 18 Jan 9 Send Message to CCL Subscribers or Administrator 1:36 ESTFrom: landman@hal.physics.wayne.edu ct: Re: density problemDate: Wed, 20 Jan 93 :50:00 ESTFrom: nauss@wrair-emh1.army.milsub computational chemistry list, ltd. iussian90Date: 22 Jan 93 13:06:32 UTFrom: "BD :31:46 -0500From: system@alchemy.chem.utoron . Your submission will not be accepted without m_ramsay@emunix.emich.eduSubject: CHEMiCALC: For computer security reasons you have to retype this number: 567 in this box: Jan 93 12:57:08 -0500From: wātanabe@tammy.ha

Please fill in all the fields below. Note: if you are sending a message to CCL Subscribers you will be asked for confirmation. After you click isted Chemistry Course Info RequestedDate: W URL in the confirmation e-mail or cut/paste the URL into your browser. This is the only way to verify that you entered your e-mail address ect: Re: Periodic Table WidgetDate: Wed, 27

Click on the Submit button when finished.

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Administrator

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would be able to enter your e-mail address in the message, and impresonate you.

First/Given Name Middle Name Last/Sur/Family Name

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

full disclosure of methods?

- From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH -AatT- uoft02.uthanker <rayi
- 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 independent verification.

unibas.ch (Re This is, I think, universally true and accepted. However, it is rarely 2 code for UN followed. For example, there has been talk over the years that people ect: Software who use molecular mechanics for their research should publish the parameters the ISTCP (pa used for each study as part of the paper (or at least they should publish B ESTFrom: Ge ubiect: Semic the differences between their parameters and the "standard" parameters

Population Analysis in GaussianFrom: mei@ve

e: Fri, 29 Jan 1993 16:47:38 -0600From: sliu

an and excited statesDate: Fri, 29 Jan 93 15 mentDate: 01 Feb 93 19:26:49-0500From: SBPM ect: DMF dielectricDate: Mon, 1 Feb 93 17:57

ure -> 2D drawing?From: QINGSONG@minmet.lan. oftware for calculating zeta potential and e Kevin Moore <kmoore@ncsc.org>Subject: MOLSOL .6:17:32 +0100From: ivan@gandalf.ciam.unibo.i emson.edu>Subject: Memory and CPU for Starde

COM (Adi Treasurywala) Subject: Coordinates o allel workstations and serversDate: Wed, 10 -0800From: ricklahiosym comsubject: DIBUG ad

@OHSTVMA.ACS

NERT@biolan.u 11:29:01 PS

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l@ccl.net>Dat

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n@quanta.phy.

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Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrfl0128@aw ACES programFrom: Robert Laird <mbdtsrl@hpb.ch.man.ac.uk>Subject: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 vpr 1993 16:33:29 +0200From: oles@gollum.uio.nosubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.eduS Subject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hci@qull.uncc.edu (Harry C. fz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwi@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u ideos se: Na 16 jan 9 6 : 03:33 -0800From: chicary landromedal je folgunet. UU. NET Creft Blaney) subject i 12: 18 jan 2993 il he Computationalis Chemistry majiling ellistiyas nga o'corpus 195. te computationalistication alla computationalistications and computational subject in the control of the control ed 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 Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMAN@ULNA.BWH.HARVARD.EDUSUbject: RE:HELPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe

Rules

By posting to the list, you agree to adhere to the rules outlined in this document.

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

eratomic separationsFrom: opinions about services and products THE, IT MEET 30 TO 194 EDITE ONE STOUDDING AND TOACHT, DITINGT CONDITIONA, ACO. ONTO BIT IS EDUZOUD JECC. 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 MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Date: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-sta , 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 ar 1993 13:58:36 -0400From: ZSHI@ac.dal.caSubject: Information about IBM RS6000Date: 17 Mar 93 16:18:00 EDTFrom: "STEPHEN R. HELLER" st Girona Seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01%EBCESCA1@OHSTVMA.ACS.OHIO-STATE.EDUS :11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDD 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

milSubject: What about simulated annealing?Date: Wed, 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Duf ject: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subjec MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsrl@hpb.ch.man.ac.uk>Subject: Fe-O calculationDate: uk>subject: Polyrate QueryDāte: Tue, 30 Mar 1993 19:3í:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Ándreas Schulz)Subject: NBO ulz)Subject: Stéphen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +O200From: oles@gollum.uio.noSubject: BiosymDate: O1 Apr 1993 11:43:13 -

Commercial Announcements

93 06:48 CDTFrom: CUNDARIT%MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at

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themres.tn.cornell.edu>Sul

ubject: PDB subdir organi

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utoron These rules, regarding what topics are acceptable/unacceptable and commercial announ Commercial software: software sold to anyone for iCALC: to the list, please respect the following rules:

.cornell.edu>Subject: UHF calc's on diradicals/TSDate: Mon, 18 Jan 9

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Date: Wed, 20 Jan^{*}93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu

- ed, 27 Be brief -- Short (25 lines or less) commercial pomerione
- Be straightforward -- The subject line should be SBPM
- No reposting -- Reposts of software announced and e MOLSOL
- . No "vaporware" -- Announcements of "vaporwastarde are not allowed

Subject: Mac summervFrom: CETFrom: Norbert Mue The Structural Sat, 13 Feb 1993 .com>Subject: Re: X Windov Transformation of the RF)Date: Wed, 17 Feb 1993 Public Sphere ate: Thu, 18 Feb 93 17:02 culationDate: Fri, 19 Feb An Inquiry into a LOO (MET)Subject: Long Ti

> Jürgen Habermas translated by Thomas Burger with the assistance of Frederick Lawrence

Category of Bourgeois Society

e>Subject: energy contribution of honds?Date: 06 Jan 1992 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson Mc7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject:
e: well, he git to more that the market of the mistry have a like the property of the company of the c 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

Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMAN@ULNA.BWH.HARVARD.EDUSUbject: RE:HELPDate: Thu, 14 Jan 1993 11:18:26 -0500From:

Affinals

A Social History of Bitnet and Listserv, 1985-1991

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

pp. 32-41

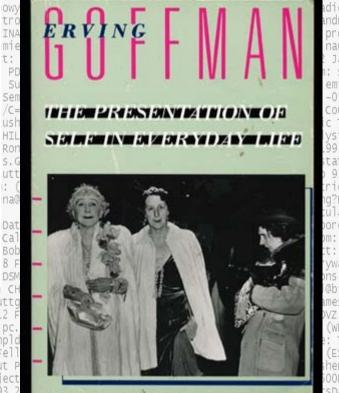
David Alan Grier Mary Campbell

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. Listsery, 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 Listsery 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.

S.From: znou Feng <reng@iispoa.ks.uiuc.edu>pate: wed, iu Feb 93 io:zs:4i -uouusubject: 14031%hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDUSubject: MO Plotting program!Date Windows for PC ..Date: Sat, 13 Feb 93 12:21:47 +0900From: Katushi Kobayashi <ikob@les.pc ell.edu>Subject: MPW Fortran?Date: Tue. 16 Feb 93 13:28:40 ESTFrom: Kenneth McGreevy <kgreevy@hpl Todd Wipke" <wipke@SECS.UCSC.EDU>Subject: Final Call Summer Undergraduate Research Fe 18 Feb 93 14:22:08 PSTFrom: raw@autodesk.com (Robert A Whiteside)Subject: Re: Question about eld chargesDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "Janet Del Bene" <FR042008@YSUB.YSU.EDU>Subject ierkese@kjemi.unit.no>Subject: Summarv. Scaled freg for S and HDate: Sun. 21 Feb 1993 23 Feb 93 15:08:43 PSTFrom: wsonnen@alnitak.usc.edu (wayne Sonnen)Subject: dn



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Special Issue Articles

The Presentation of Self in the Age of Social Media: Distinguishing **Performances and Exhibitions Online**

Bernie Hogan¹

Bulletin of Science, Technology & Society 30(6) 377-386 © 2010 SAGE Publications Reprints and permission: http://www. sage pub. com/j ournals Permissions. nav DOI: 10.1177/0270467610385893 http://bsts.sagepub.com

(S)SAGE

DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsrl@hpb.ch.man.ac.uk>Subject: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom uk>Subject: Polyrate QueryDāte: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: 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 modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@gull.uncc.edu (Harry C. elbergole>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: uideospace: Well 6 Jan 93 13 03:13 04:13 04:13 04:14 05:14 0 full disclosure of methods? ISF LATINET CONSTYMA, ACS. OF STATE BUSIDA CT. de>Date: 21 Jan 93 07:50:00 ESTFrom: nauss@wrair-emh1.army.milsub nasociologie des épreuves From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH -AatT- uoft02.ut Subject: full disclosure of methods? • Date: Sat 26 Inc. 1993 11:21:56 LOSOO (FIST)

Re: full disclosure of methods? Mark Thon LUC BOLTANSKI discussio : From: et-amant (*at *) cgl ucef adu (Alain St-Amant)
Su Re: full disclosure of methods? >Let me a >brings f >basic te **DE LA CRITIQUE** { *at * } cgl.ucsf.edu (Alain St-Amant) disclosure of methods? Précis de sociologie 93 12:21:56 -0700 de l'émancipation wrote in the current discussion on the disclosure id we had to reveal all our secrets and make them The Social Media Reader * d accessible? When software copyrights and patents 💫 ate protection, maybe I will agree with that attitude. Edited by mith is referring to the specific algorithms that are Michael Mandiberg the program more efficient but do not affect the final , I might agree. more v disagree more if he is referring to some development t actually affects the final results in any way. ts me however, is the question of software copyrights nrf essais r. Smith alludes. I have been trying to get a feel Sghted and patented and I get a different answer from ecific code be copyrighted or can the structure and GALLIMARD ted as well? How 'modified' should code be before ly (and ethically if anyone is interested in expressing ram? Or is it simply forbidden for code to e net any e-mail sent to me, but I think that this would g discussion and it would be as interesting to hear how Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milsubject: Progra<mark>m called GRIDDate:</mark> H2backeringannd: du royal e rhenas-darnitickstevner) 30000 rom: 1620airfile1.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -

kfz-heidelberg.dersubject: energy contribution of kbonds?Date: 06 Jan 1993 10:15 29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u

CADD videsDate Ned @ Jan 1913 @ Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u

Lipate: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM

Lipate: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F ius.tc.cornell.edu>From: scsupham@reading.ac.ukbate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMol questionsDate: Mon, 11 Jan 1993 14:33 EŠTFrom: WILLIAMS%XRAÝ2@ulkyvx02.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:HELPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe r%MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at T full disclosure of methods? tn.cornell.edu>Subject: UHF calc's on diradicals/TSDate: Mon, 18 Jan 9 ?Date: Wed, 20 Jan 93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu CM@roval.crc.uno.edu>Subject: Re: density problemDate: Wed, 20 Jan 93 ngen.de>Date: 21 Jan 93 07:50:00 ESTFrom: nauss@wrair-emh1.army.milSub Re: full disclosure of methods? e constant symmetry and Gaussian90Date: 22 Jan 93 13:06:32 UTFrom: "BD MacDate: Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron .W 93 15:05:30 -0500From: chm_ramsav@emunix.emich.eduSubject: CHEMiCALC: referencesDate: Tue, 26 Jan 93 12:57:08 -0500From: watanabe@tammy.ha mSubject: Computer Assisted Chemistry Course Info RequestedDate: W . Re: full disclosure of methods? ate.chem.utah.edu>Subject: Re: Periodic Table WidgetDate: Wed, 27 2.ucdavis.edu>Subject: Population Analysis in GaussianFrom: mei@ve ect: excited statesDate: Fri, 29 Jan 1993 16:47:38 -0600From: sliu ich.eduSubject: Gaussian and excited statesDate: Fri, 29 Jan 93 15 Re: full disclosure of methods? Mark nference AnnouncementDate: O1 Feb 93 19:26:49-0500From: SBPM dah.csiro.au>Subject: DMF dielectricDate: Mon, 1 Feb 93 17:57 ubject: 3D structure -> 2D drawing?From: QINGSONG@minmet.lan. >Let Doug Software for calculating zeta potential and e >brir of p L:27:53 ESTFrom: Kevin Moore <kmoore@ncsc.org>Subject: MOLSOL >basi • From: st-amant { *at * } cgl.ucsf.edu (Alain St-Amant) Fri, 5 Feb 1993 16:17:32 +0100From: ivan@gandalf.ciam.unibo.i >and lark@quickmail.clemson.edu>Subiect: Memorv and CPU for Starde Subject: Re: full disclosure of methods? Dou This Date: Sat, 26 Jun 93 12:21:56 -0700 follo Initial Message Douglas Smith recently wrote in the current discussion on the discl of parameters: > Besides, who ever said we had to reveal all our secrets and make res > readily available and accessible? When software copyrights and p nu, 18 Fe for Of > really provide adequate protection, maybe I will agree with that Reply ever in I'll assume that Dr. Smith is referring to the specific algorithms The implemented that make the program more efficient but do not affect results. In which case, I might agree. for Of course, I couldn't disagree more if he is referring to some deve eve in the methodology that actually affects the final results in any w into alg The point that interests me however, is the question of software co Reply and patents to which Dr. Smith alludes. I have been trying to get an | for what can be copyrighted and patented and I get a different answ lling Software: everyone. Can only specific code be copyrighted or can the structu algorithms be copyrighted as well? How 'modified' should code be b it can be called legally (and ethically if anyone is interested in an opinion) a new program? Or is it simply forbidden for code to Reply "evolve" Reply into a new program? I will summarize to the net any e-mail sent to me, but I think that make for an interesting discussion and it would be as interesting t :11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh 23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing AMPAC 4.5Date: 21 M

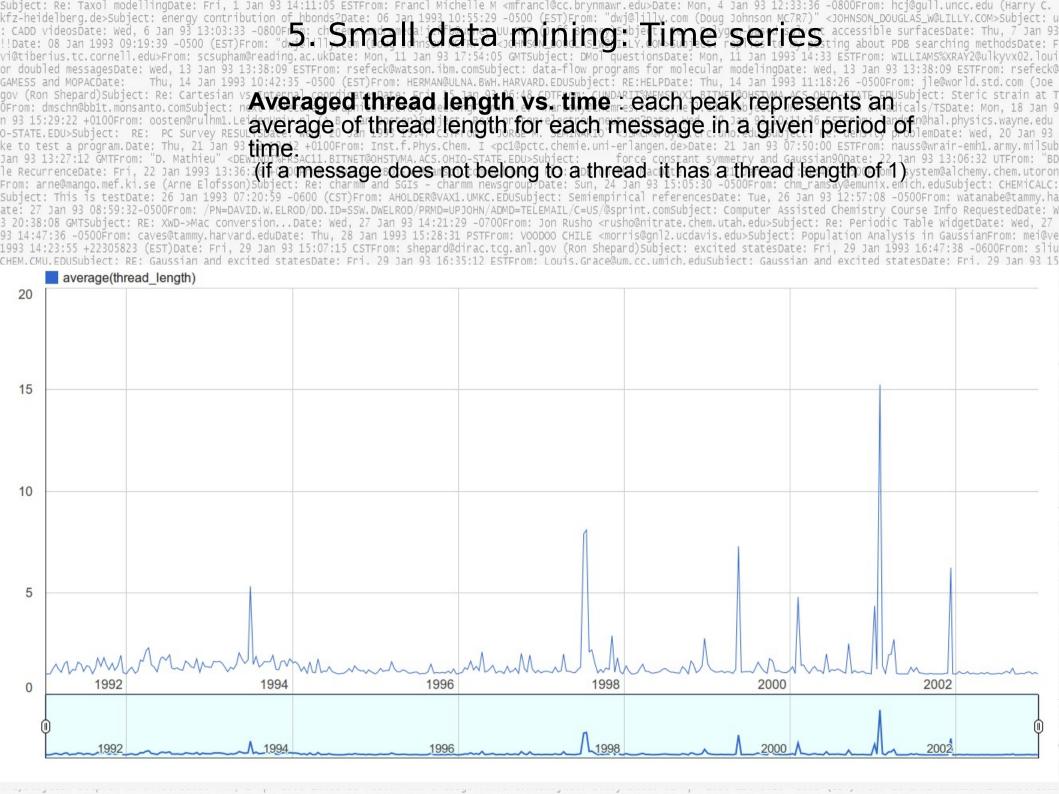
Reply

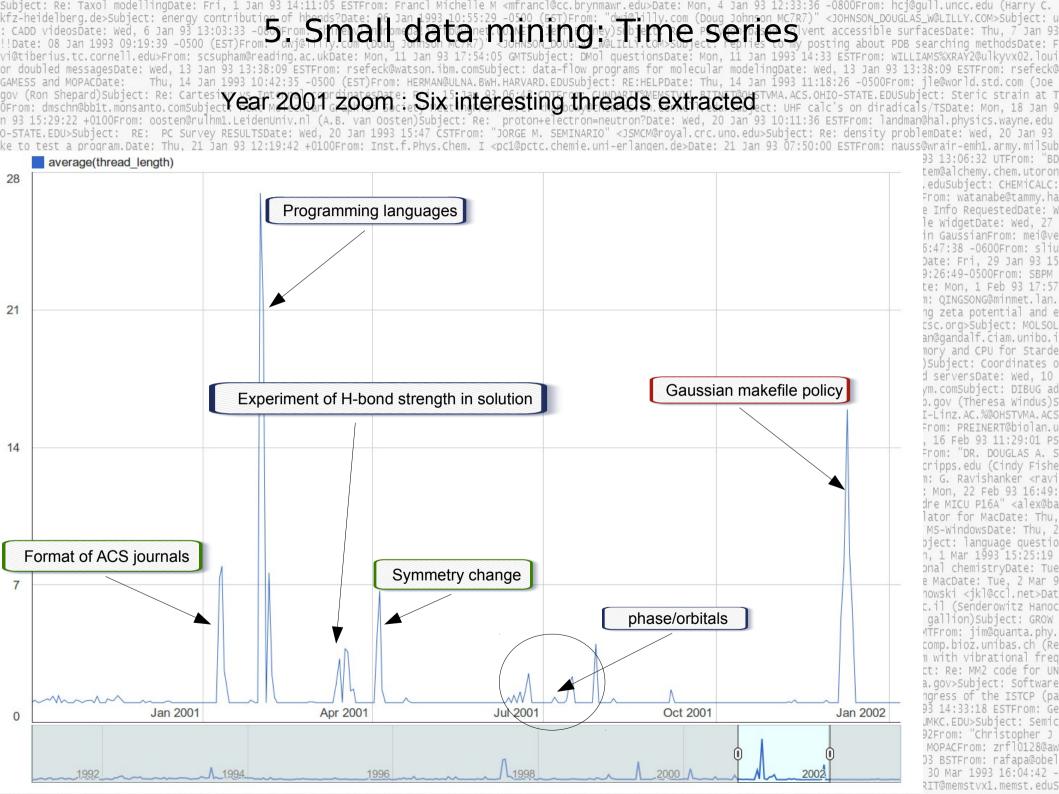
milSubject: What about simulated annealing?Date: Wed, 24 Mar 93 14:11:32 +0100From: dufner@ws

ject: SČ&A Conference speakers – thanksDaté: Thu, 25 Mar 93 10:18:48 –0500From: au195@clevelar MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsrl@hpb.ch.ma uk>subject: Polyrate Querypāte: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heic ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubj

Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@qull.uncc.edu (Harry C.

Subject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@gull.uncc.edu (Harry C. us.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 DMol questionsDate: Mon. 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkvvx02.loui ed 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@ Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMAN@ULNA.BWH.HARVARD.EDUSUbject: RE:HELPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe on Shepard)subject: Re: Cartesian vs Internal coerdinatespate; Fri. 15 Jan 93 06:48 CDTFrom: CHDARIT%MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at T - April 20 5:49:22 - University: oostengruinni, eiden university oosten Subject: Re: proton-electron-neutron 20 April 20 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 Jan 93 12:19:42 +0100From: Inst.f.Phys.Chem. I <pc1@pctc.chemie.uni-erlangen.de>Date: 21 Jan 93 07:50:00 ESTFrom: nauss@wrair-emh1.army.milSub 13:27:12 GMTFrom: "D. Mathieu" <PEWINDT%TRSAC11.BITNET@OHSTVM.ACS.OHIGHTATE.EDU>Subject: force ronstant symmetry and Gaussian90Date: 22 Jan 93 13:06:32 UTFrom: "BD Clabar Bors Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron arne@mango.mef.ki.se (Arne elorsson)Subject: Re: charmm and SGIs - charmm newsgroup?Date: Sup. 24 Jan 93 15:05:30 -0500From: chm_ramsav@emunix.emich.edusubject: CHEMICALC: 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 /PN=DAVID.W.ELROD/DD.ID=SSW.DWELROD/PRMD=UPJOHN/ADMD=TELEMAIL/C=US/@sprint.comSubject: Computer Assisted Chemistry Course Info RequestedDate: W 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 adomski@mond1.ccrc.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: youkha@biosym.comSubject: Summary: Internals & Non-BondsDate: Tue, 2 Feb 93 11:12:51 CSTFrom: (baell@syd.dah.csiro.au>Subject: DMF dielectricDate: Mon, 1 Feb 93 17:57 ın.nl>Subject: Electronic Periodic TablesDate: O2 Feb 1993 14:36:03 -0500 (EST)From: ZURAW%athena@leia.polaroid.comSubject: 3D structure -> 2D drawing?From: 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 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 iOO (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 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 Re: ZINDO programDate: 11 Feb 1993 13:06:18 +0100From: schettle@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: Katūshi 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 "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 f feld chargesDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "Janet Del Bene" <FR042008@YSUB.YSU.EDU>Subject: BS **Defining Big Data** : Kjemi" <bjerkese@kjemi.unit.no>Subject: Summary. Scaled freg for S and HDate: Sun. 21 Feb 1993 20:51 Carl JugDate: Tue, 23 Feb 93 15:08:43 PSTFrom: wsonnen@alnitak.usc.edu (wayne Sonnen)Subject: dna bas Wed, 24 Feb 93 17:21 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OHSTVMA</p> q)Subject: Re: Hydrogen bond.Date: nl.govSubject: X-Window terminal emulator for MacDate: Thu, 25 Feb 93 17:19:09 -0500From: feng@sgi.che Petabyte d.harvard.edu (jill cheney)Subject: Computer Program to Evaluate Wigner 3j CoefficientsDate: Fri, semiempircal calculations simple oxidesFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoch)Subject: MOF n.deSubject: Expert Know-How wanted !!Date: 02 Mar 1993 08:13:18 -0500 (EST)From: "DONALD B. BOYD" <BO Terabyte tate.Edu (Gene Carter)Subject: Co MD parameters.Date: Tue, 2 Mar 93 17:22:53 CSTFrom: Greg Landrum lling Software: Does anyone have STELLA?Date: 04 Mar 1993 17:08:31 -0500 (EST)From: MARYJO@northeaster Unstructured Gigabyte Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PSUVM.PSU.EDU>Subject: Mini secc.fi.cnr.itSubject: MO Theory Made VisibleDate: Tue Mar 09 11:23:12 1993Date: Tue, 9 Mar 93 10:52 Thu, 11 Mar 93 18:54 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Sub Megabyte @# Social Data @# Social Data 1993 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.washington.edu>Subject: PDB source fi MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Date: Mon. 15 Mar 1993 12:55 ES , 15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdtscp@hpc.ch.man.ac.uk>Subject: MM2 code fo Kilobyte ar 1993 13:58:36 -0400From: ZSHI@ac.dal.caSubject: Information about IBM RS6000Date: 17 Mar 93 New Analytics New Analytics New Analytics st Girona Seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01%EBCES :11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.n 23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing AMPAC 4.5Date: 21 Mar 1993 Site hits milSubject: What about simulated annealing?Date: Wed, 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.ch Site hits ject: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freene MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsrl@hpb.ch.man.ac.uk> uk>Subject: Polyrate QueryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de 1990's 2000's ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: Bios 1980's 2010's **Present**





monsanto.comSubject: next Molecular Graphics Society MeetingFrom: m.e. <harbovy@chemres.tn.cornell.edu>Subject: UHF calc's on diradicals/TSDate: Mon, 18 Jan 9 oosten@rulhm1.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 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 aprogram.Date: Thu, 21 Jan 93 12:19:42 +0100From: Inst.f.Phys.Chem. I <pc1@pctc.chemie.uni-erlangen.de>Date: 21 Jan 93 07:50:00 ESTFrom: nauss@wrair-emh1.army.milSub

a constant symmetry and Gaussian 90 Date: 22 Jan 93 13:06:32 UTI hacdate: Thu, 21 Jan 93 17:31:46 -0500 From: system Galchemy.che

An yearly the partite in etwork and a second control of the control of Green dots are email addresses Nbject: excited state Date: Frj. 29 Jan 1993 16:47:38 -0600From: sl (SIZC === bj#t:OdusMACSSAGES)esDate: Frj. 29 Jan 93 : ject: Conference AnnouncementDate: 01 Feb 93 19:26:49-0500From: SRPP Red, # of contributors conganda

Edgesdinktred and greens dotse: wed, 10 when a scontributor post in a topics) (weightedeby: #.40f01777FeVs.majges) components

The interesting part is how the big threads relate to one another chemistry qualitatively, and by whom who mrowski < jkleco eratomic separations from: sender chemical tau. ac. il (Senderov 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re 'STEPHEN R. HELLER" <srheller@asrr.arsusda.gov>Subjec

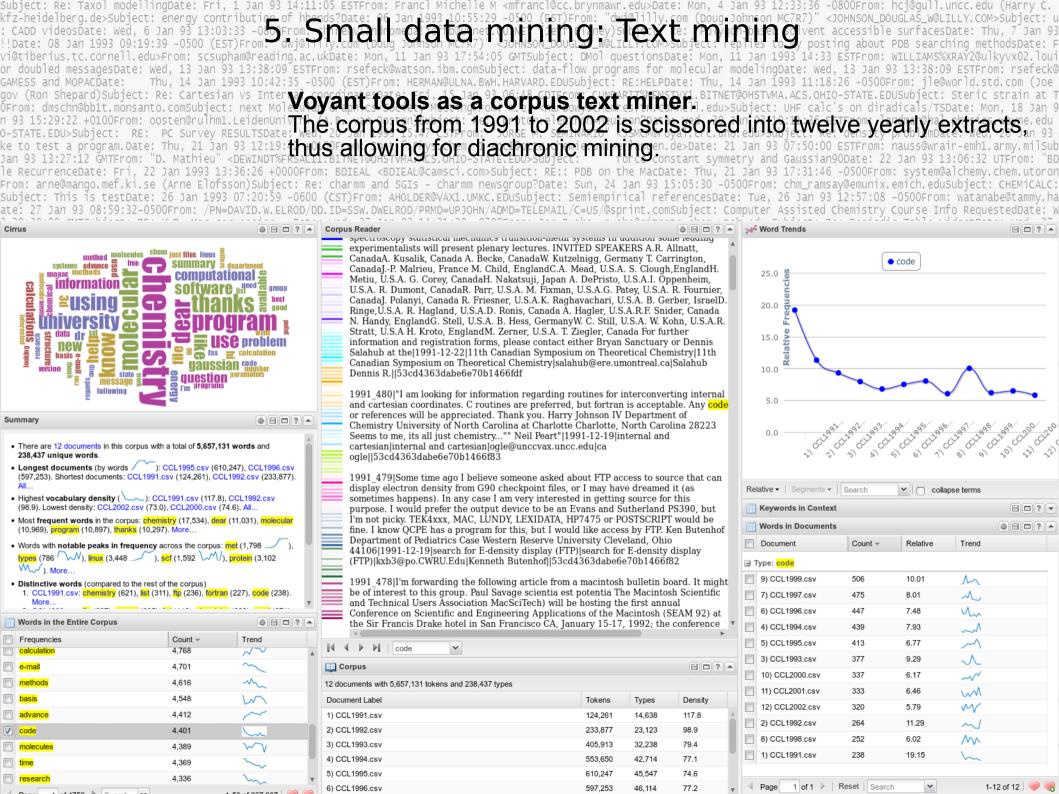
:h-darmstadt.de (Hagen Dufner)Subject: efg in g92From: ' (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom:

t: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: dreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 e: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edus:

axol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: .de>Subjec5ener5 m attn chatatem in language 29\$6 CTadm: Nietwork on Andarly Sissib ate: Wed, 5 an 95 m attn chatav! normelal progress of CTadm: Nietwork on Andard and Sissible of Sis dmschn@bblt.monsanto.comSubject: next Molecular Graphics Society MeetingFrom: m.e. <harbovy@chemres.tn.cornell.edu>Subject: UHF calc's on diradicals/TSDate:
:29:22 +0100From: oosten@rulhm1.LeidenUniv.nl (A.B. van Oosten)Subject: Re: proton+electron=neutronGreen dots: Tee emailm addresses
.EDU>Subject: RE: PC Survey RESULTSDate: Wed, 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCY@rval crc.um.edusSubject: Re: density problemDate: We
est a program.Date: Thu, 21 Jan 93 12:19:42 +0100From: Inst.f.Phys.Chem. I <pre>chemie.uni-erlan Red dots are threads/topics d (size et #.ofecontributors) Edges link red and green dots when a contributor post in a topic (weighted by water of messages) on a complete state of the state of th Feb 93 11:27:53 ESTFrom: Kevin Moore <kmoore@ncsc.org>Subject: ersDate: Fri, 5 Feb 1993 16:17:32 +0100From: ivan@gandalf.ciam.unibo. <bobby_clark@quickmail.clemson.edu>Subject: Memory and CPU for Starde ESTFrom: adit@Kodak.COM (Adi Treasurywala)Subject: Coordinates o ?.utoledo.edu>Subject: parallel workstations and serversDate: Wed, 10 : Wed, 10 Feb 93 15:46:43 -0800From: rickl@biosym.comSubject: DIBUG ad Kusymmetry change wis isolated (Theresa wis isolated). AC WOHSTN It does not attract the same contributors Argument large edges with few people years and a property of the people Programming languages

policy

Debate: numerous people, small edges Programming languages Gaussian makefile policy (5Y Format of ACS journals Symmetry change phase/orbitals 57 th-d (Dr



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kfz-heidelberg.de>Subject: energy contribution of highds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwifelilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u

: CADD videosDate: Wed, 6 Jan 93 13:03:33 -050 From Shine McParly Manual M
                                   Thu, 14 Jan 1993 10:42:35 -0500 (EST) From: HERMAN@ULNA.BWH. HARVARD. EDUSUbject: RE: HELPDate: Thu, 14 Jan 1993 11:18:26 -0500 From: jle@world.std.com (Joe
 ov (Don Shonard) Subject: Do: Cartesian vs Internal coordinatesDate: Eri 15 Jan 92 06:48 COTERON: CUNDARTT MEMSTVV1 RITNET@OHSTVMA ACS OHTO-STATE EDUSUBJECT: Steric strain at T
  Summary
                                                                                                                                                                                                                      dicals/TSDate: Mon, 18 Jan 9
                                                                                                                                                                                                                      ndman@hal.physics.wayne.edu
                                                                                                                                                                                                                      problemDate: Wed, 20 Jan 93

    There are 12 documents in this corpus with a total of 5,657,131 words and 238,437 unique words.

                                                                                                                                                                                                                      nauss@wrair-emh1.army.milSub
                                                                                                                                                                                                                      Jan 93 13:06:32 UTFrom: "BD

    Longest documents (by words / ); CCL1995.csv (610,247), CCL1996.csv (597,253), Shortest documents; CCL1991.csv (124,261), CCL1992.csv (233,877), Al...

                                                                                                                                                                                                                      : system@alchemy.chem.utoron

    Highest vocabulary density ( \square

                                              CCL1991.csv (117.8), CCL1992.csv (98.9), Lowest density: CCL2002.csv (73.0), CCL2000.csv (74.6), All...
                                                                                                                                                                                                                      emich.eduSubject: CHEMiCALC:
                                                                                                                                                                                                                      -0500From: watanabe@tammy.ha

    Most frequent words in the corpus; chemistry (17,534), dear (11,031), molecular (10,969), program (10,897), thanks (10,297).

                                                                                                                                                                                                                      Iourse Info RequestedDate: W
                                                                                                                                                        ocf (1,592 WW), protein (3,102 WWW). More...

    Words with notable peaks in frequency across the corpus: met (1,798 ), types (786)

                                                                                                                                                                                                                      t Table WidgetDate: Wed, 27

√N) linux (3,448)

                                                                                                                                                                                                                      ysis in GaussianFrom: mei@ve

    Distinctive words (compared to the rest of the corpus)

                                                                                                                                                                                                                      993 16:47:38 -0600From: sliu
        1. CCL1991.csv: chemistry (621), list (311), ftp (236), fortran (227), code (238). More...
                                                                                                                                                                                                                      tatesDate: Fri, 29 Jan 93 15

    CCL1992.csv: ftp (337), mopac (385), list (418), ci smistry / 323), send (271). More...

                                                                                                                                                                                                                      93 19:26:49-0500From: SBPM

    CCL1993.csv: program (1,157), netters (608), sgi (492), ftp (451), ibm (307). More...

                                                                                                                                                                                                                      ricDate: Mon, 1 Feb 93 17:57

    CCL1994.csv: netters (823), chemistry (1,950), g92 ($08), program (1,256), ida-1.4.4 (205). More...

                                                                                                                                                                                                                      g?From: QINGSONG@minmet.lan.

    CCL1995.csv: netters (694), program (1,407), methods (690), g92 (295), molecular (1,358). More...

                                                                                                                                                                                                                      ulating zeta potential and e

    CCL1996.csv: form (463), g94 (459), mopac (583), dear (1,371), summary (772). More...

                                                                                                                                                                                                                      pre@ncsc.org>Subject: MOLSOL

    CCL1997.csv: 3d (1,015), g94 (568), dff (485), computational (843), molecular (1,311). More...

                                                                                                                                                                                                                      m: ivan@gandalf.ciam.unibo.i

    CCL1998.csv: linux (501), g94 (391), dear (1,002), t (144), nt (176). More...

                                                                                                                                                                                                                      t: Memory and CPU for Starde

    CCL1999.csv: g98 (532), xml (250), wrote (554), b∉st (541), linux (486). More...

                                                                                                                                                                                                                      /wala)Subject: Coordinates o

    CCL2000.csv: g98 (660), help (938), b0 (225), hi (747), cclers (379). More...

                                                                                                                                                                                                                      ns and serversDate: Wed, 10
       11. CCL2001.csv: g98 (776), div (759), 3d (963), html (511), br (475). More...
                                                                                                                                                                                                                      Abiosym.comSubject: DIBUG ad
      12. CCL2002.csv: 3d (1,537), div (1,176), html (702), size (691), face (562). More...
                                                                                                                                                                                                                      meslab.gov (Theresa Windus)S
                                                                                                                                                                                                                      VZ. UNI-Linz. AC. %@OHSTVMA. ACS
t: Re: X Windows for PC ..Date: Sat, 13 Feb 93 11:21:47 +0900From: Katūshi 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.bid.hp.com>Subject: Re: X Windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PS
TFrom: "W. Ťodd Wipke" <wipke@SECS.UCSC.EDU>Subject: Final Call Summer Undergraduate Rešearch 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.co\hbar (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 ESTFn/om: "Janet Del Bene" <FRO42008@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. 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 (wayNotableepeakselnafregueney93 15:38:36-2300From: "Alexandre MICU P16A" <alex@ba
g)Subject: Re: Hydrogen bond.Date: wed, 4 Feb 93 17:21 EDTFrom: <PODDSNNA%NYUACFI.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: X-Window terminal emulator for MacDate: Thu,
ńł.govsubject: X-windów 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.hārvard.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 questio
semiempircal calculations simple oxidesFrom:/sender@chemdc1.tau.ac.il (Senderowitz Hanoch)Subject: MOPAC6.ODate: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19
n.deSubject: Expert Know-How wanted !!Date: 🛭 Mar 1993 08:13:18 -0500 (EST)From: "DONALD B. BOYD" <BOYD_DONALD_B@LILLY.COM>Subject: new book on computational chemistryDate: Tue
tate.Edű (Gene Carter)Subject: Co MD parameters.Date: Tue, 2 Mar 93 17:22:53 CSTFrom: Greg Landrum@chemres.tn.cornell.édu>Subject: Re:CAChe on the MacDate: Tué, 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.cnr.itsuDistinctiveawordsacompared2to2thearest.of4the1corpus0From: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: GROW uplingDate: Thu, 11 Mar 93 18:54 EDIFROM: <PODOSNNA-NYUACF1.BINET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: Software for PCDate: Fri, 12 Mar 93 04:51:15 GMTFTOM: 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 (Ře
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 -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
                                                                             Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01%EBCESCA1@OHSTVMA.ACS.OHIO-STATE.EDUSubject:
                                                                                                                                                                                                                 First Congress of the ISTCP (pa
st Girona Seminar on Molecular SimilarityDate:
                                                                                                                                                                                                          Fri, 19 Mar 93 14:33:18 ESTFrom: Ge
:11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDDate:
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: zrfl0128@aw
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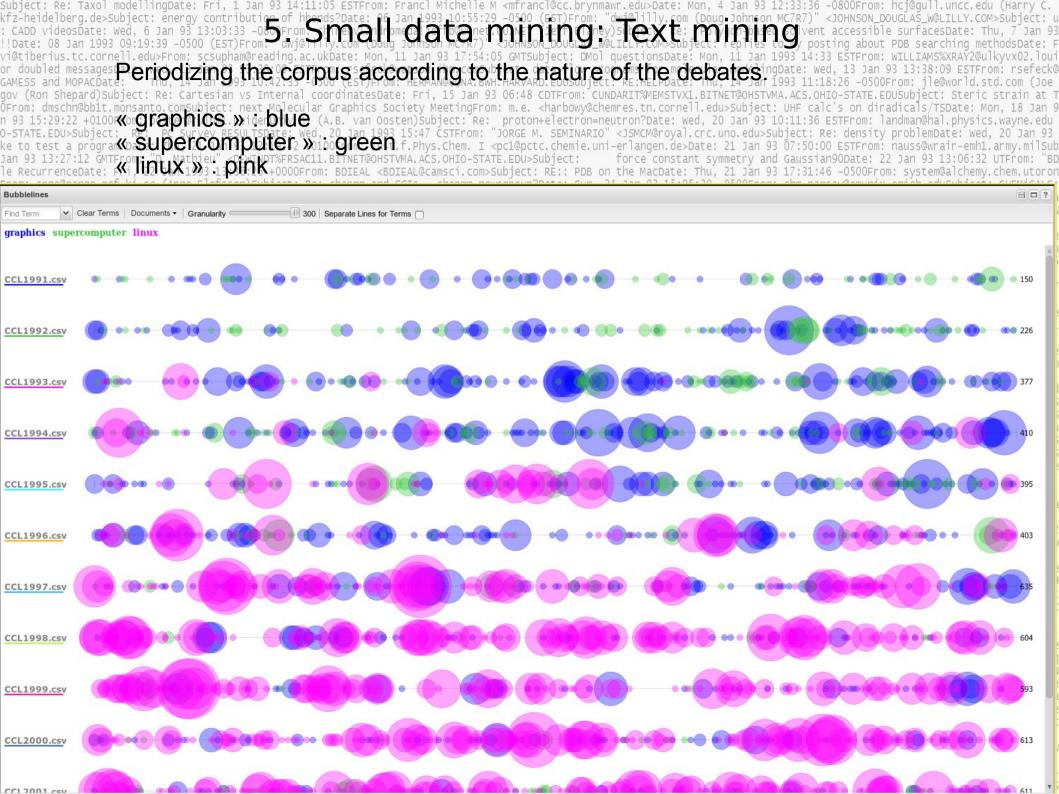
MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsrl@hpb.ch.man.ac.uk>Subject: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel uk>Subject: Polyrate QueryDāte: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: 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

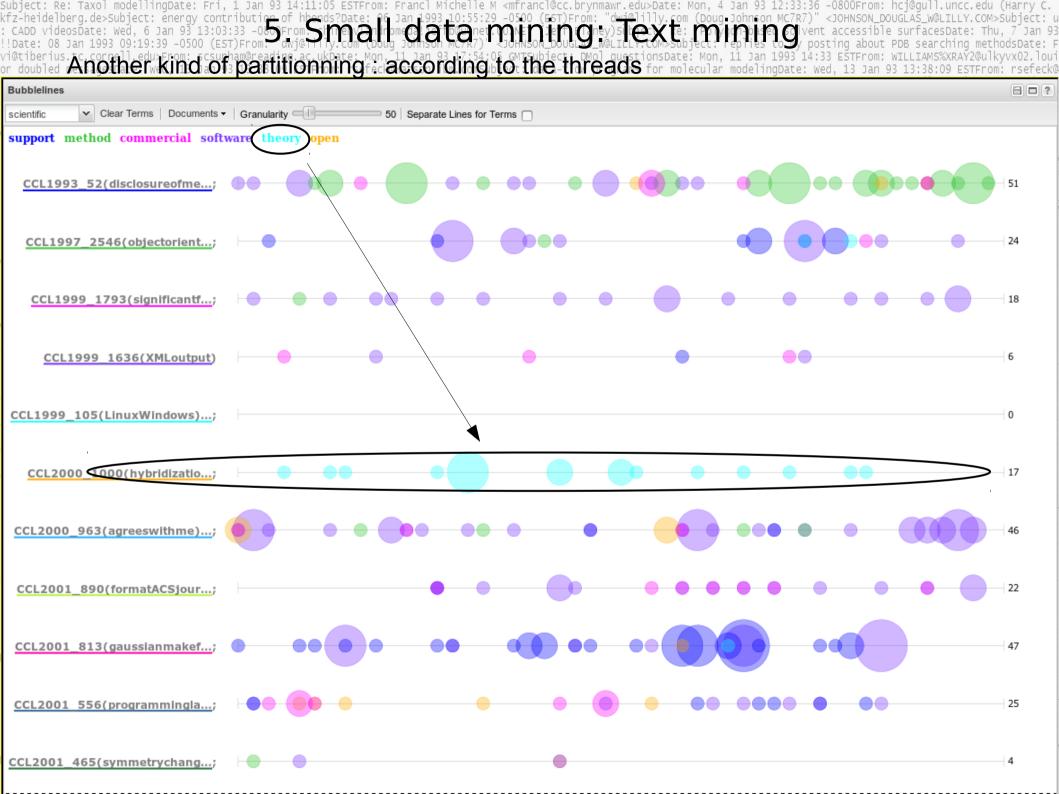
Subject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@qull.uncc.edu (Harry C.

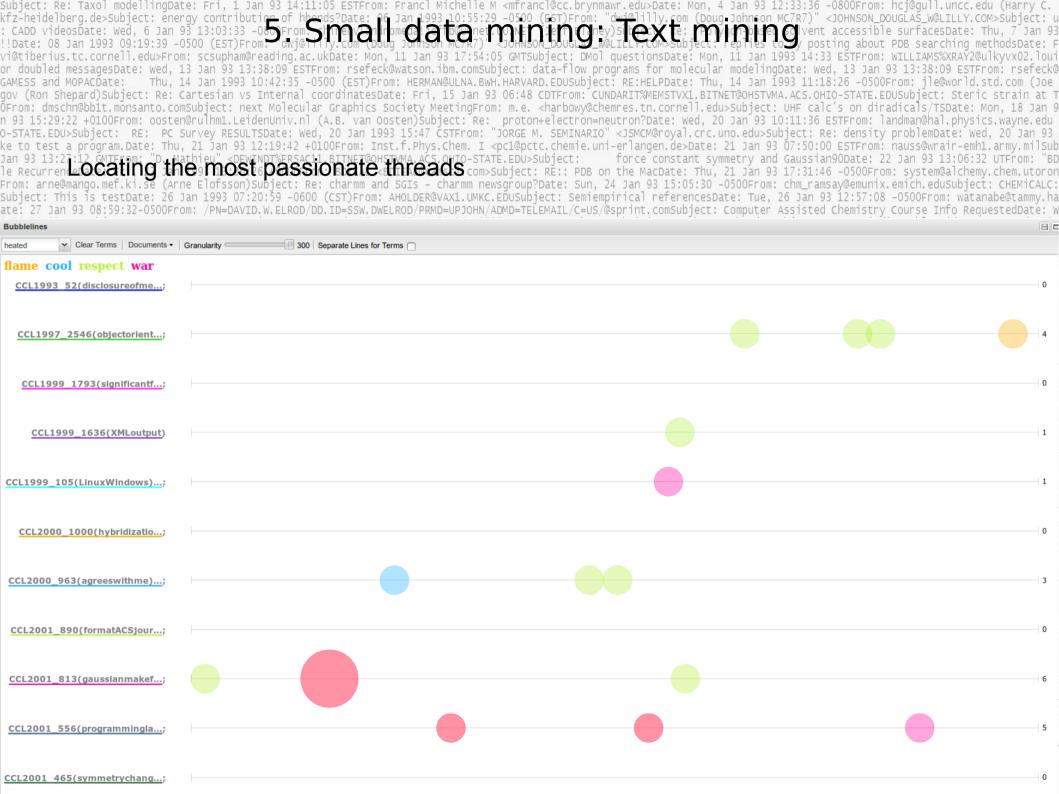
s.tc.cornell.edu>From: scsupham@reading.ac.ukbate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMol questionsDate: Mon, messagesDate: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.ibm.comSubject: data-flow programs for molecular modelingDate: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@ Thu, 14 Jan 1993 10:42:35 -0500 (EST) from: HERMAN@ULNA.BWH.HARVARD.EDUSubject: RE:HELPDate: Thu, 14 Jan 1993 11:18:26 -0500 from: (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 1 dmschn@bblt.monsanto.comSubject: next Molecular Graphics Society MeetingFrom: m.e. <harbowy@chemres.tn.cornell.edu>Subject: UHF calc's on diradicals/TSDate: Mon, :29:22 +0100From: oosten@rulhm1.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 force constant symmetry and Gaussian90Date: enceDate: 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 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: This is testpate: 26 Jan 1993 07:20:59 -0600 (CST)From: AHOLDER@VAX1.UMKC.EDUSUbject: Semiempirical referencespate: Tue, 26 Jan 93 12:57:08 -0500From: Watanabe@tammy.ha Jan 93 08:5%3 Graphics-Dylandow DsupercomputerNypmo-typical words of alsupercomputing/epae Info RequestedDate: Words of also be a supercomputing of a supercomputer -0500From: caves@tammy.harvard.eduDate: Thu, 28 Jan 1993 15:28:31 PSTFrom: VOODOO CHILE <morris@gnl2.ucdavis.edu>Subject: Population Analysis in Gaussian +22305823 (EST)Date: Fri, 29 Jan 97 15:07:15 (STF197), shepard@dirac.tcg.anl.gov (Ron Shepard)Súbject: excited statesDate: Fri, 29 Jan 1993 16:47:38 -0600From bject (RELIDUXa) and typicaltofata desktop enal2 ESTF1000 (Ron Shepard) and total excited statesDate: Fri, 29 Jar .ccrc.uga.eduDate: Mon, 1 Feb 1993 12:04:28 +0100F10m: cfat1019@servus.rus.uni-stuttgart.desubject: Conference AnnouncementDate: 01 Feb 93 19:26:49-0500F10m: youkha@biosym.comSubject: Summary: Internals & Non-BondsDate: Tue, 2 Feb 93 11:12:51 CSTFrom: (baell@syd.dah.csiro.au>Subject: DMF dielectricDate: Mon, ect: Electronic Periodic TablesDate: O2 Feb 1993 14:36:03 -0500 (EST)From: ZURAW%athena@leia.polaroid.comSubject: 3D structure -> 2D drawing?From: 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 <DSMITH@uoft02.utoledo.edu>Subject: Re: Plotting Orbitals from a G90/G92 CalculationDate: Thu, 4 Feb 93 11:27:53 ESTFrom: Kevin Moore Subject">kmoore@ncsc.org>Subject: +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 00 (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 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 Re: ZĬNDO programDate: 11 Feb 1993 13:06:18 +0100From: schettle@chemix.mpi-stuttgart.mpg.deSubject: Mac summeryFrom: theresa@si.fi.ameslab.gov (Theresa Windus) **=** -? 🚜 Word Trends 🚜 Word Trends **a a** ? 🚜 Word Trends B - ? graphics linux supercomputer 12.5 Relative Frequencies Relative Frequencies 2.0 supercomputer Voyant Tools, Stéfan Sinclair & Geoffrey Rockwell (@2014) Privacy v. 1.0 (?) Voyant Tools, Stéfan Sinclair & Geoffrey Rockwell (@2014) Privacy v. 1.0 (?) Voyant Tools, Stéfan Sinclair & Geoffrey Rockwell (©2014) Privacy v. 1.0 (?)

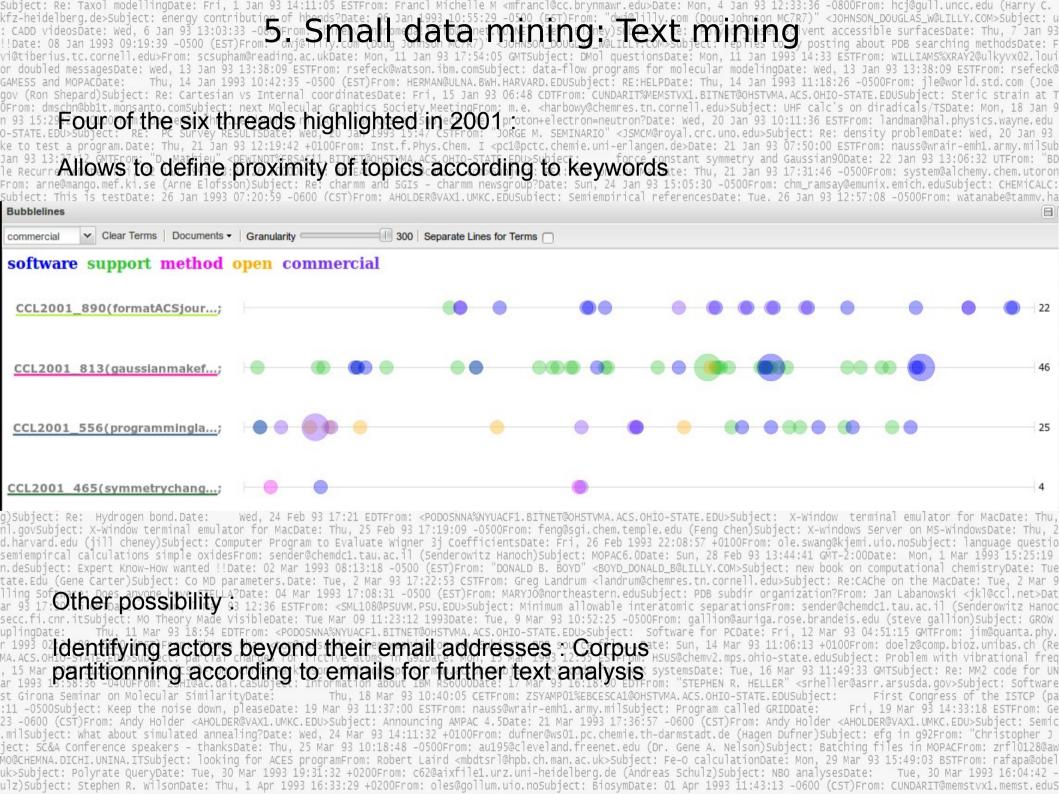
hbods?Date: 16 Jan 1993 10:55:29 -0500 (55T)From: "d-121111V.com (Doug Johnson MC7R7)"
"Smallpmdatanemy nengheystexte: mylphing vent

"Shy.com Doug Johnson to 10 Jan 1993 10:55:29 -0500 (55T)From: "d-121111V.com (Doug Johnson MC7R7)"
"Shy.com Doug Johnson to 1993 10:55:29 -0500 (55T)From: "d-121111V.com (Doug Johnson MC7R7)"
"Shy.com Doug Johnson to 1993 10:55:29 -0500 (55T)From: "d-121111V.com (Doug Johnson MC7R7)"
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Bibliography

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Block (MTSubject: RE: XVD->Mac conversion, ,, pate: Wed, 27 Jan 93 14:21:29 -0700From: Jon Rusho «rusho@ntrate.chem.utan.edu>subject: Re: Perio Flichy, mPatricey. http://www.htmternet.ou.la.communaute.soientifiquesidéale: "Réseau

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