se (Arne Elofsson)Subject: Re: charmm and SGIs - charmm newsgroup?Date: Sun, 24 Jan 93 15:05:30 -0500From: cnm_ramsay@emunix.em Cats/Pentred ChimistesDMautourindeenttouverture te: Wed, 27 Jan 93 14:21:29 -0700From: Jon Rusho Arusho@nitrate.chem.uta Thu.logiciedstrscientifiques.ed 5:07:10:90:11:11:01:02:05:06 STFrom: Elliot King <71127.1231@compuserve.com>subject: Call for PapersDate: Fri, 5 Feb 1993 16
AlexandreeHocquet & Frédéric Wieber Rautodesk.com (Robert A Whiteside)Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93 17:0. 49:00 Seminaire duoscentre François (Sp. Viète F Diect: Seminaire

kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u : CADD videosDate: Wed, 6 Jan 93 13:03:33 -0800From: chiremv!andromeda!jeffb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93 Re: Gaussian Flame-wars

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.

• Subject: Re: Gaussian Flame-wars

>"bugs", and the support is not so good, I don't think the spend

>that much money on customer support, given the price of the product.

• From: "Phil Hultin" < hultin., at,.cc. UManitoba. CA >

- Date: Tue, 11 Dec 2001 16:52:36 -0600

```
>I think Gaussian is a great tool, but it has a LOT of little secrets and
```

Max Valdez wrote:

I absolutely agree with this statement. I think I represent a new kind of

scientist working with tools like Gaussian. I am an experimentalist, not a computer whiz, [...] So what's the point of all this? Well, maybe people would be less prone to

jump on Gaussian (as they have over this makefile thing) if they didn't feel that the philosophy of Gaussian Inc. was similar to that of the "high priest" - only the initiates will have the secrets revealed and then only after years of study. A nice start would be to make the program work the way the manual implies that it should (or to make the manual describe how the program actually works). Even better: bring the program into the 21st century by providing a user interface that is actually user-friendly. the priests and initiates regard as "a philosophy and aesthetic of simplicity" looks quite otherwise to many of us on the outside!

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

Dr. Philip G. Hultin Associate Department Head and Associate Professor of Chemistry University of Manitoba uk>subject: Polyrate QueryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Ándreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -

1:46 -0500From: system@alchemy.chem.utoron ramsay@emunix.emich.eduSubject: CHEMiCALC: n 93 12:57:08 -0500From: watanabe@tammy.ha ted Chemistry Course Info RequestedDate: W t: Re: Periodic Table WidgetDate: Wed, 27 opulation Analysis in GaussianFrom: mei@ve Fri, 29 Jan 1993 16:47:38 -0600From: sliu and excited statesDate: Fri, 29 Jan 93 15 ntDate: 01 Feb 93 19:26:49-0500From: SBPM t: DMF dielectricDate: Mon, 1 Feb 93 17:57 e -> 2D drawing?From: QINGSONG@minmet.lan. tware for calculating zeta potential and e vin Moore <kmoore@ncsc.org>Subject: MOLSOL 17:32 +0100From: ivan@gandalf.ciam.unibo.i son.edu>Subject: Memory and CPU for Starde M (Adi Treasurywala)Subject: Coordinates o lel workstations and serversDate: Wed, 10 800From: rickl@biosym.comSubject: DIBUG ad heresa@si.fi.ameslab.gov (Theresa Windus)S er <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS 4:47:09 +0100 (WET) From: PREINERT@biolan.u for PC ..Date: Tue, 16 Feb 93 11:29:01 PS 4:15:16 -0500 (EST)From: "DR. DOUGLAS A. S 2 PSTFrom: fisher@scripps.edu (Cindy Fishe 3 11:53:05 -0500From: G. Ravishanker <ravi -scale DynamicsDate: Mon, 22 Feb 93 16:49: 6-2300From: "Alexandre MICU P16A" <alex@ba indow terminal emulator for MacDate: Thu, X-windows Server on MS-WindowsDate: Thu, 2 wang@kjemi.uio.noSubject: language guestio 1 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19 w book on computational chemistryDate: Tue ect: Re:CAChe on the MacDate: Tue, 2 Mar 9 tion?From: Jan Labanowski <jkl@ccl.net>Dat ender@chemdc1.tau.ac.il (Senderowitz Hanoc brandeis.edu (steve gallion)Subject: GROW 2 Mar 93 04:51:15 GMTFrom: jim@quanta.phy. 3 +0100From: doelz@comp.bioz.unibas.ch (Re .eduSubject: Problem with vibrational freq

3 11:49:33 GMTSubject: Re: MM2 code for UN rheller@asrr.arsusda.gov>Subject: Software

lder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic r)Subject: efg in g92From: "Christopher J : Batching files in MOPACFrom: zrfl0128@aw

n, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel

First Congress of the ISTCP (pa Fri. 19 Mar 93 14:33:18 ESTFrom: Ge

posting about PDB searching methodsDate: F

4:33 ESTFrom: WILLIAMS%XRAY2@ulkyvx02.loui Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@ 1:18:26 -0500From: jle@world.std.com (Joe .OHIO-STATE.EDUSubject: Steric strain at T calc's on diradicals/TSDate: Mon, 18 Jan 9 36 ESTFrom: landman@hal.physics.wayne.edu : Re: density problemDate: Wed, 20 Jan 93 0:00 ESTFrom: nauss@wrair-emh1.army.milsub

sian90Date: 22 Jan 93 13:06:32 UTFrom: "BD

THIS IS TESTED TO: 26 13 1993 07:20:59 - 1000 (CST) From: THOTER@VAX1.LMKC.EDUSubject: land 3 08:59:30-000 on 7/FM-04/4D . 28 // .ll=2 m.dw Roll P (D= 21/A) ADMD=TELEMAI (P (

absym.com field summary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

bi2t: El Crontemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

bi2t: El Crontemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

bi2t: El Crontemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

bi2t: El Crontemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

bi2t: El Crontemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16e1)

contemary Internals & Non-Bondspate: Tup. 2 Feb. 9: 11:12:51 (STF rom: 16

Re: ZINDO programDate: 11 Feb 1993 13:06:18 +0100From: schettle@chemix.mpi_stuttgart.mpg.desubject: Mac_summeryFrom: theresa@si.fi.ameslab.gov.com/MARCS.omio-115te: Coeing tiscums (Coeing Classic) (Coeing Class

4. iDébats ret tensions dans les deux fils

Objet d'étude inscrit dans la thématique générale des science et ordinateur (Agar, 2006, et refs. citées) Objet d'étude s'inscrit aussi dans la question de l'histoire du logiciel (Cámpbell-Kelly, 2007, 2003) (Mahoney, 2008) (Ensmenger, 2009) MAIS : histoire du <u>logiciel dans les communautés scientifiques</u> peu été développée (voir tout de même, par ex Spencer, 2015) Chimie computationnelle : science qui s'est développée à partir des années 1980, avec ordinateur comme élément constitutif Mettrema gour (certaines) des (tensions provoquées par de du la communauté soit en tensions in écessité d'un corpus qui les révèles recommunauté soitentifique choisier nécessité d'un corpus qui les révèles de la communauté soitentifique choisier nécessité d'un corpus qui les révèles les communautés soitent fiques choisier nécessité d'un corpus qui les révèles les communautés soitent de la communauté soite de la communauté de la commune de la communauté de la commune de la Décrire (esta on: complexitéra deash laon equestion ce (particulièrement 100 actuelle) l'ouverture / « openness »

Tis is dispitation

ofter well led edu subject: Re: Plottin Forbitals from 16 D/12 Camulation ate: Thu, 7 Feb 93 11:27: 5 Peb 93 1

Computational Chemistry: Un champ disciplinaire en tra

Lié à l'ordinateur, et donc à ses mutations

-mutations hardware : de big computer à personal computer (de su

llobjet big science, lointain, réservé à des spécialistes, difficile d'accès, fed

objet banal, personnel, connecté, modulable, accessible, typique de «

façons de modéliser différentes (par ex selon Lenhard): conséqu

desktop computing)

//Ordinateur 50/60//

//Ordinateur 80/90//

funded science, matériel limitant//ard@dirac.tcg.ar

matériel sur transformations épistémiques

entrepreneur », matériel de moins en moins limitant,

- AMESS and MOPACDATE: Thu, 14 Jan 1993 10:42:35 -0500 (EST) From: HERMANGULNA, BWH. HARVARD, EDUSUBJECT: RE:HELPDATE: Thu, 14 Jan 1993 11:18:26 -0500 From: 1 Jeg

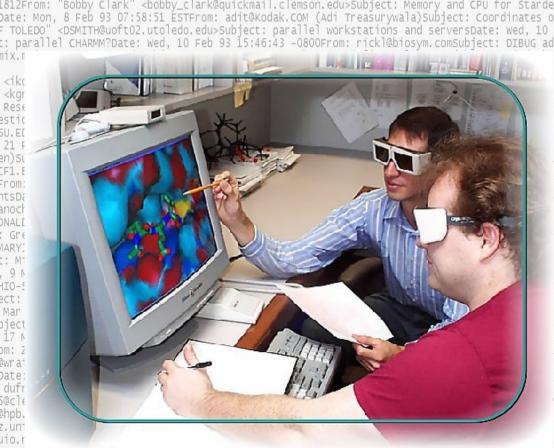
 CONSTRUCTEURS: Cherchent à promouvoir le terminal graphique pour le vendre à l'industrie

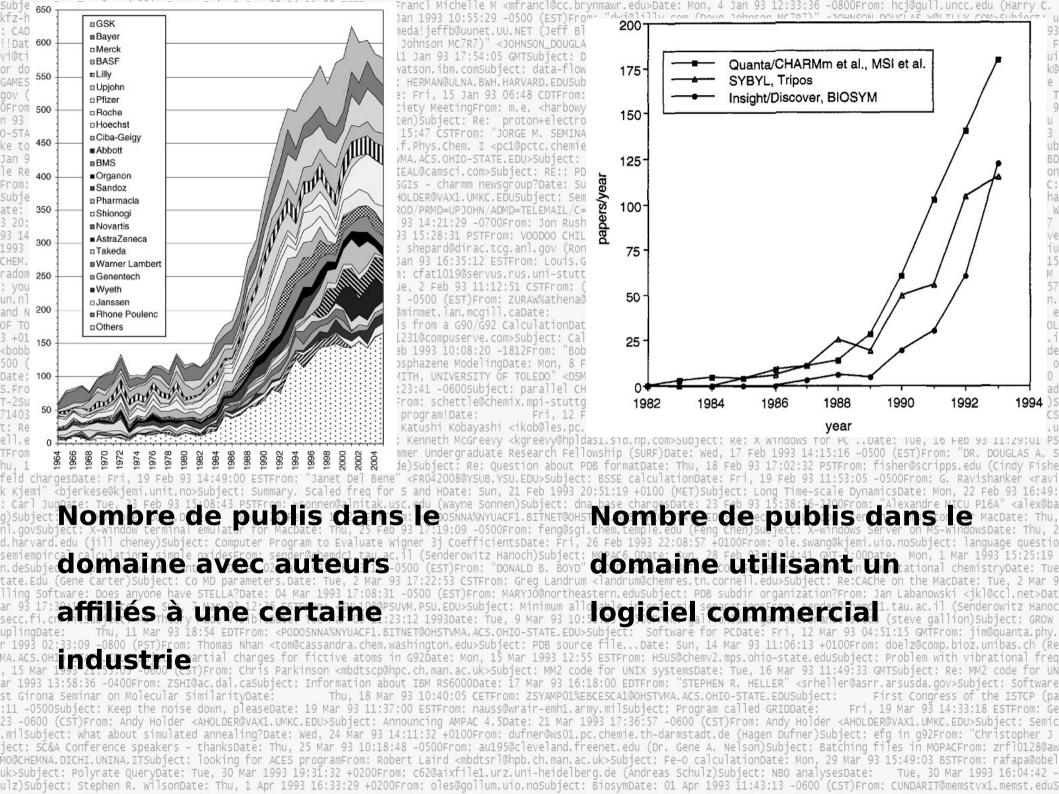
 From: dischnicobit, monsapto, comsubject: next molècular graphics society, meet ingéron: m.e. «Inspony chemies, th. competit, edu> subject: up gale s'industrie

 Pharma et utilise computational chemistry comme promesse techno-scientifique om: landmanghal
- -contexte économique mais aussi politique
- ate: enapleine époque de la Ekcentrepreneurship science » us dans le domaine voisine des 9 biotechnologies (Jones) dupate: Thu, 28 Jan 1993 15:28:31 PSTFF rom: VOODOO CHILE <morris@gn]2. ucdavis. edu>Subject: Population Ana
- bouleversement des pratiques de « federally funded science » à « entrepreneurship science » : Bayh Dole act, technology transfer, pression des universités américaines sur la question du patenting, copyright... (Slaughter Roades, Popp Berman)
 - dans un domaine scientifique (chimie, pharmacie...) ou culture du brevet et du secret est forte (contrairement à « computing science », « république des informaticiens »...) (Mowery, Flichy)

Beaucoup se sont intéressés aux vigner 3 coefficient transformations de l'activité scientifique liées à ces mutations de l'ordinateur mais 500 (EST) From

n'a pas été abordé le software en tant mandant qu'outil du scientifique, outil construit par le scientifique dans ce contexte, à la frontière du scientifique, du technique, de 37:00 ESTETOM: naus l'économique et du politique (un objet +0100From au frontière, Leigh Starr), Thu, 25 Mar 93 10:18:48 -0500From: au frontière, Leigh Starr), ACES programme Robert Laird «mbdts»





July Composition of the control of t

is une is une de la physique quantique, puis la chimie théorique in complexité landmanchal physics no la chimie théorique in complexité landmanchal physics na chimie a la physique; na cration de la «pureté a la chimie a la physique; na cration de la «pureté a la chimie a la physique; na cration de la «pureté a la chimie a la physique; na cration de la chimie a la chimie a la physique; na cration de la chimie a la chimie a

1théorique Description de la constant symmetry and Gaussian90Date: 22 Jan 93 13:06:32 Univercedate: Fig. 2 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.carne@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: ti This is testpate: 36 Jan 1993 07:20:59 -0600 (CST)From: AHQLDER@VAX1.UMKC.EDUSubject: Semiempirical referencesDate: Tue, 26 Jan 93 12:57:08 -0500From: watanab 7 et l'autre de la papectroscopieyechimie physique et chimiejorganique description Reques 8:08 cMTSubject: RE: XWD-Mac conversion Date: way 27 Jan 93 14:21:29 -0700From: Jan Rusho «ruzho@nitrate chem.orah.edussubject: Re: Periodi. Table widgetDate 47 newtoniennemyde boulestetzressorts; 3 pragmatique mepistemiquement attachée à la sianFr 4:22 himie ret a sa façon historique de représenters le span Soléccules, thie explussible ates ates Date: Fri, 29 mochimie ret a sa façon historique de représenters le sa moléccules, thie explussible ates Date: Fri, 29 mochimie ret sa façon historique de représenters le sa moléccules, thie explussible ates Date: Fri, 29 mochimie ret sa façon de la constitue de la con

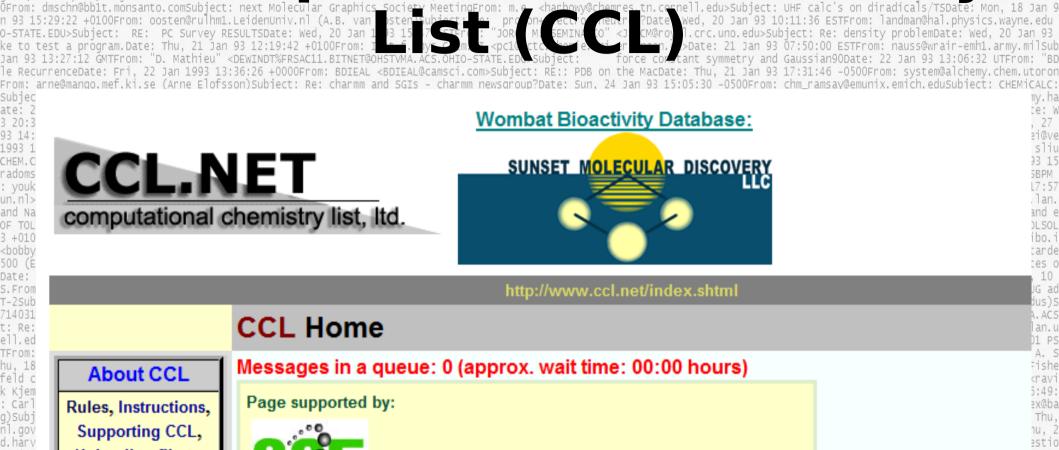
mskillindustrie et dontella complexité épistémique réside dans la paramétris ation det en paramétris ation det en pour le la scomplexité épistémique réside dans la consubject de la mon, 1 Feb la support de la monte de la mon, 1 Feb la support de la monte della monte del

all pour property of the prope

Reminal emulator for MacDate: Thu, 25 Feb 93 17:19:09 -0500From: feng@sgi.chem.temple.edu (Feng Chen)Subject: X-windows Server Program to Evaluate Wigner 31 CoefficientsDate: Fri 26 Feb 1993 22:08:57 -0100From: ple swang@ciemi.uio.modo acceptate and acceptate ac

```
Tis is dispitation
Description of the states pate: Fri. 29 Jan 93 163 12 Esteron: Louis Incedum committee is given and excited at a state of the state of 
 ne. 09 Feb 1993 21:39:58 -0500 (EST)From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" DSMITH@uoft02.utoledo.edu>Subject: parallel wor Zhob Feng (fer Artibbrooks) uluc.edu>Date: wol, 10 Feb 08.15:40:22:41 -06000 bject: parallel CHARMAZDATA: wol, 10 Feb 93.15:40:42 -0800 From Re: INDO pugramo te: 11 Feb 199 11 0018 + 10000 School School
```

-Window terminal emulator for MacDate: Thu, 25 Feb 93-17:19:09 -0500From: feng@sgi.chem.temple.edu (Feng chen)sub iDieloaits: etachteunsilomfsentolain2sebees: die gu iDieloaits: etachteunsilomfsentolain2sebees: die gun subject die gun sub



Computational Science & Engineering Online

... a laboratory without walls for scientific computing

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: 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 erius.tcs.prnell.educ John scsupham@reading.ac.ukDate: Mondill lap 93 17:57 05 CMTSubject: DMol quistions acc. No. 11 lap 1993 14:33 ESTFrom: WTW.TAMS%XPAY2@ulkyvsbled methods replied to the scsupham@reading.ac.ukDate: Mondill lap 93 17:57 05 CMTSubject: DMol quistions acc. No. 11 lap 1993 14:33 ESTFrom: WTW.TAMS%XPAY2@ulkyvsbled methods replied to the script of the script

Welcome to the CCL Website!

semiem

tate.E lling

ar 93 secc.f

upling r 1993

, 15 M ar 199

st Gir :11 -0 23 -06

.milsu

Uploading file to

CCL Site, Security

Policy, Privacy

Policy, About Us

Contact Us

Drug Discovery

Training

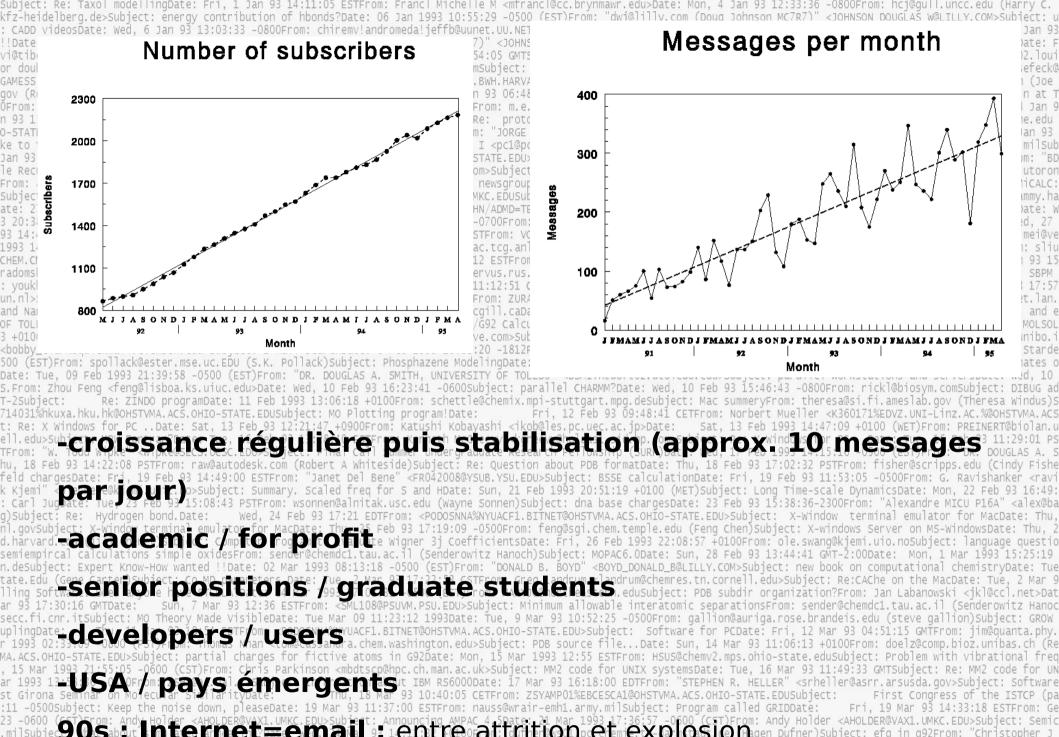
ACES GOMPHE ROBERT CATE CAMBOTS MEMBER CHARACTER AND ACES GOVERNOUS ACES GOVERNOUS MEMBERS AND ACCES GOVERNOUS MEMBERS AND ACCES GOVERNOUS AND ACCES GOV uk>Subject: Polyrate QueryDāte: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 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

1991	CCL is born	E-mail Listserver and FTP archives for computational chemists are established at OSC as a hobby project of Jan Labanowski.	om: hcj@gull.uncc.edu (Harry C. N_DOUGLAS_W@LILLY.COM>Subject: u ible surfacesDate: Thu, 7 Jan 93 out PDB searching methodsDate: Fom: 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 om: nauss@wrair-emh1.army.milSub: 22 Jan 93 13:06:32 UTFrom: "BD From: system@alchemy.chem.utoron nix.emich.eduSubject: CHEMICALC: 108 -0500From: watanabe@tammy.hatry Course Info RequestedDate: Widdic Table WidgetDate: Wed, 27 Analysis in GaussianFrom: mei@ve an 1993 16:47:38 -0600From: sliued 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 ekmoore@ncsc.org>Subject: MOLSOL)From: ivan@gandalf.ciam.unibo.ipject: Memory and CPU for Starde asurywala)Subject: Coordinates oations and serversDate: Wed, 10 ickl@biosym.comSubject: DIBUG ad fi.ameslab.gov (Theresa Windus)S L%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS					
1994	CCL gets Gopher	CCL Introduces Gopher interface to messages and its FTP site. CCL grows in number of <u>subscribers</u> and <u>messages</u> .						
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 (NSF)						
1996	CCL gets domain	Just in case, Jan Labanowski personally registers the domain $ccl.net$ 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 (buy something solid if you have money) CCL decided to operate from PCs running Linux and Apache Web Server.	LOO (WET)From: PREINERT@biolan.u Date: Tue, 16 Feb 93 11:29:01 PS 500 (EST)From: "DR. DOUGLAS A. S fisher@scripps.edu (Cindy Fishe -0500From: G. Ravishanker <ravi< th=""></ravi<>					
K K Jemn								
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>Da ar 93 17:31.991bateOhio Supercomputingsueentemject: Minimum allowable interatomic separationsFrom: sender@chemdc1.tau.ac.il (Senderowitz Hano 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 uplingDate: Thu, 11 Mar 93 18:54 EDTFrom: <podosnna%nylacf1.bitnet@ohstvma.acs.ohio-state.edu>Subject: Software for PCDate: Fri, 12 Mar 93 04:51:15 GMTFrom: jim@quanta.phy r 1993 02: Communautemdeascientifiquesigeeksbmais: pasi@computemascientists.</podosnna%nylacf1.bitnet@ohstvma.acs.ohio-state.edu></jkl@ccl.net>								
ar 1993 1:Disciplinesemergenten(journaux)s@congres.93.1):18:communautélar @imentersusda.gov>subject: software st Girona Seminar on Molecular Similaritybate: Thu, 18 Mar 93 10:40:05 CETFTOM: ZSYAMPO1%EBCESCA1@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: First Congress of the ISTCP (page 11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFTOM: nauss@wrair-emh1.army.milsubject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFTOM: Ge 23 -0600 (accessible etclouventenautous) are nestenal page 12 -0500Subject: 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								
MO@CHEMNA. uk>Subiect	DICHI.UNINA.ITSubject: looking for ACES progr : Polvrate QueryDate: Tue. 30 Mar 1993 19:31:	r 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelsoń)Subject: Batchir amFrom: Robert Laird <mbdtsrl@hpb.ch.man.ac.uk>Subject: Fe-O calculationDate: Mon, 29 Mar 32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDat 33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)F</mbdtsrl@hpb.ch.man.ac.uk>	93 15:49:03 BSTFrom: rafapa@obel :e: Tue, 30 Mar 1993 16:04:42 -					

Mainfames Mini Wasky Shors Une diversité d'acteurs: MOPACDATE: Thu, 14 Jan 1993 10:42:35 -0500 (EST) From: He Developers of Inégrative no company of the company of Hordware Super computing DUSUBJECT: RE: PC SURVEY RESULTSPATE: Wed. 20 Ja CODE PUIS LEAN OF THE PROPERTY OF THE PROPERT (Academe/Industry) mondi.ccrc.uga.eduDate: Mon, 1 Feb 1993 12:0 utilisentsercodels & Nor utilisentsercode "-Vendors 2 = 3 Vendentides HNSF, DoD : financen des projets Chamists : Re: Hydrogen bond. Date: Wed, 24 Feb 93 1

:-Supercomputers: 1 allouent des ressources de Developers Academia o-state.EDU>subject: partial charges for fictive
-Hardware vendors vendent Finfrastructure



ık>Subject: Polyrate QueryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: ılz)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: Rules

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

1EMS

oid.

Commercial software: software sold to anyone fo

Commercial Announcements

and to the list, please respect the following rules:

n at T

e.edu

lan 93 milsub

Be brief -- Short (25 lines or less) commercial pd

ly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u Re: Polygon-based solvent accessible surfacesDate: Thu,

> Be straightforward -- The subject line should be . No reposting -- Reposts of software announcen

No "vaporware" -- Announcements of "vaponwa SBPM

wed, 10 Feb 93 15:46:43 -0800From: rickl@biosym.comSubject: DIBUG ad

Subject: Mac summeryFrom: theresa@si.fi.ameslab.gov (Theresa Windus)S 3:41 CETFrom: Norbert Mueller <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS

com>Subject: Re: X Windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PS

culationDate: Fri, 19 Feb 93 11:53:05 -0500From: G. Ravishanker <rav LOO (MET)Subject: Long Time-scale DynamicsDate: Mon, 22 Feb 93 16:49 gesDate: 23 Feb 93 15:38:36-2300From: "Alexandre MICU P16A" <alex@ba

RF)Date: Wed, 17 Feb 1993 14:15:16 -0500 (EST)From: "DR. DOUGLAS A. ate: Thu, 18 Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fishe

Sat, 13 Feb 1993 14:47:09 +0100 (WET)From: PREINERT@biolan.

sDate: Fri, 5 Feb 1993 16:17:32 +0100From: ivan@gandalf.ciam.unibo.

are not allowed

<bobby_clark@quickmail.clemson.edu>Subject: Memory and CPU for Starde 3:51 ESTFrom: adit@Kodak.COM (Adi Treasurywala)Subject: Coordinates o utoledo.edu>Subject: parallel workstations and serversDate: Wed, 10

 announcements of o new chemistry software computational chemistry-related workshops and symposia.

methods

Q&A: questions and answers about solving computational chemistry problems

opinions about services and products

new methods and techniques in computational chemistry

 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

software/hardware-related issues

Topics which may appear on the list include:

Acceptable Topics

discussions. Do not reopen Pandora's box -- please.

These rules, regarding what topics are acceptable/unacceptable and commercial announties

iect: 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 D 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@av CHI.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@obe

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

HIO-STATE.EDU>Subject: X-Window terminal emulator for MacDate: Thu emuracon for macbace. Thu, 25 rep 93 17.19.09 -0500rrom. rengesyr.chem.cemple.edu (Feng Chen)Subject: X-windows Server on MS-WindowsDate: Thu.

(jill cheney)Subject: Computer Program to Eváluate Wigner 3j CoefficientsDate: Fri, 26 Feb 1993 22:08:57 +0100From: ole.swang@kjemi.uio.noSubject: language

30-16 GMTD 1-2-10), 7 Mt 91 12:36 ESTEROM (MI 108@STVM PSU EDUT biect: Minimum alfawable interations For separations For sender chemotic transport of the sender of the se 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.washington.edu>Subject: PDB source file...pate: Sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Res.oHISTUTETS); Chrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational frequency in the control of the con

L5 Mar 1⊋941) SE 05 ≥0666 (1974) Formi≳hFís 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 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 Seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMPO1%EBCESCA1@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: STENSION SE ACA: demique Commerciani.army.milsubject: Program called GRIDDate: (CST)From: Anov Holder < AHOLDER@VAXI.OMRC.EDUSUBJECC.AMOUNCING AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST)From: Anov Holder <

Formes et themes dusde batmilies and ministration of parameters. Date: Tue, 2 Mar. 1 (Gender Green) Subject: MOPAC6. Obate: Sun, 28 Feb 93 13:14:41 GMT-2:00Date: Mon. 1 Mar. 1 Formes et themes dusde batmilies and ministration of quit peut i (Gene Carter) Subject: Co MD parameters. Date: Tue, 2 Mar. 93 17:22:53 CSTFFOM: Greg Landrum «landrum@chemres.th.cornell.edu>Subject: Re:CAChe on the MacDate: Software: Does anyone have STELLA?Date: 04 Mar 1993 17:08:31 -0500 (EST)From: MARYJO@northeastern.eduSubject: PDB subdir organization?From: Jan Labanowski <

17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic

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. Therg.de>subject: energy contribution of hbonds?Date: 06 Jan 1903 10:55:29 -0500 (EST)From: "dwi@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u

DETERMINE TO D:33</break(180 From the accessible surfacesDate: Thu, 7 Jan 93

B. Jan 1903 1903 9-1000 1500 From: Dwarf During Month MCRO Compression of the accessible surfacesDate: The property of the accessible replies to my posting about PDB searching methodsDate: F « threaded conversation » est une forme de conversation asynchrone WILLIAMS XXRAY 2 Gulky VX 02. 1 ou publique unique et propre a Internet > mailing list, anewsgroups; jusqual e

Commission of the control of the con

DUSSIDECT RESPONDED TO THE WELL AND STORE WELL AND SUPERIOR SUPERI

full disclosure of methods?

. Re: full disclosure of methods?

• Re: full disclosure of methods?

Re: full disclosure of methods

- From: 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 discl of parameters:

> Besides, who ever said we had to reveal all our secrets and make

> readily available and accessible? When software copyrights and p of - > really provide adequate protection, maybe I will agree with that 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 alg The point that interests me however, is the question of software co

and patents to which Dr. Smith alludes. I have been trying to get for what can be copyrighted and patented and I get a different answ 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 "evolve" into a new program?

I will summarize to the net any e-mail sent to me, but I think that

Mark discu

>brir

folic

who u used

algo

into

make for an interesting discussion and it would be as interesting t

Initial Message Reply

93 15:05:30 -0500From: chm_ramsav@emunix.emich.eduSubject: CHEMiCALC

I referencesDate: Tue, 26 Jan 93 12:57:08 -0500From: watanabe@tammy.ha t.comSubject: Computer Assisted Chemistry Course Info RequestedDate: nitrate.chem.utah.edu>Subject: Re: Periodic Table WidgetDate: Wed, 27 2.ucdavis.edu>Subject: Population Analysis in GaussianFrom: mei@ve

Subject: excited statesDate: Fri, 29 Jan 1993 16:47:38 -0600From: sliu c.umich.eduSubject: Gaussian and excited statesDate: Fri, 29 Jan 93 1: .ulbiect: Conference AnnouncementDate: 01 Feb 93 19:26:49-0500From: aell@syd.dah.csiro.au>Subject: DMF dielectricDate: Mon. 1 Feb 93 17:5 .comSubject: 3D structure -> 2D drawing?From: QINGSONG@minmet.lan.

93 11:27:53 ESTFrom: Kevin Moore <kmoore@ncsc.org>Subject: MOLSOL

5 Feb 1993 16:17:32 +0100From: ivan@gandalf.ciam.unibo.i

Software for calculating zeta potential and e

Reply

Reply Reply Reply

14 Jan 1993 10:42:35 -0500 (EST) From: HERMAN@ULNA. BWH. HARVARD. EDUS ubject: RE: HELPDate: Thu, 14 Jan 1993 11:18:26 -0500 From: Shepard)Subject: Re: Cartesian vs Internal coordinatesDate: F Controverse scientifique Jan 93 06:48 CDTFrom: CUNDARIT%MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: <harbowv@chemres.tn.cornell.edu>Subiect: UHF calc's on diradicals/ full disclosure of methods? utilegmpourmalnihistorien;mer@ohstvma From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH -AatT- uoft02.ut oblige les acteurs à se • 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 >Let me address the more fundamental issue that this topic >brings forth. I share Graham Hurst's concerns. One of the Re: full disclosure of methods? <DSMITH@uoft02.utoledo.edu>Subject: Re: Plotting Orbitals - Sociologie pragmatique • From: st-amant { *at * } cgl.ucsf.edu (Alain St-Amant) des épreuves : la situation Subject: Re: full disclosure of methods? Date: Sat, 26 Jun 93 12:21:56 -0700 e: x windows for pc ...pate: sat, 13 Feb 93 12:21:47 +0900From: katushi dejcriser (tensions): permeter Douglas Smith recently wrote in the current discussion on the disclosure of parameters: chargespate: Fri, 19 Feb 93 14:49:00 ESTFrom: > 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. : Thu, I'll assume that Dr. Smith is referring to the specific algorithms that are changements de implemented that make the program more efficient but do not affect the final uestio results. In which case, I might agree. 25:19 Of course, I couldn't disagree more if he is referring to some development e: Tue in the methodology that actually affects the final results in any way. structure et rend The point that interests me however, is the question of software copyrights ret>Dat and patents to which Dr. Smith alludes. I have been trying to get a feel Hanoc for what can be copyrighted and patented and I get a different answer from GROW everyone. Can only specific code be copyrighted or can the structure and ch (Re algorithms be copyrighted as well? How 'modified' should code be before ll fred 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 58:36 -0400From: ZSHI@ac.dal.caSubject: Information about "evolve" СР (ра 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

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@memst

ik>Subject: Polyrate QueryDate: Tue, 30 Mar 1993 19:31:32 +0200From:

-0800From: chiremy!andromeda!jeffb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu,

eveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zr

bdtsrl@hpb.ch.man.ac.uk>Subject: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03

c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate:

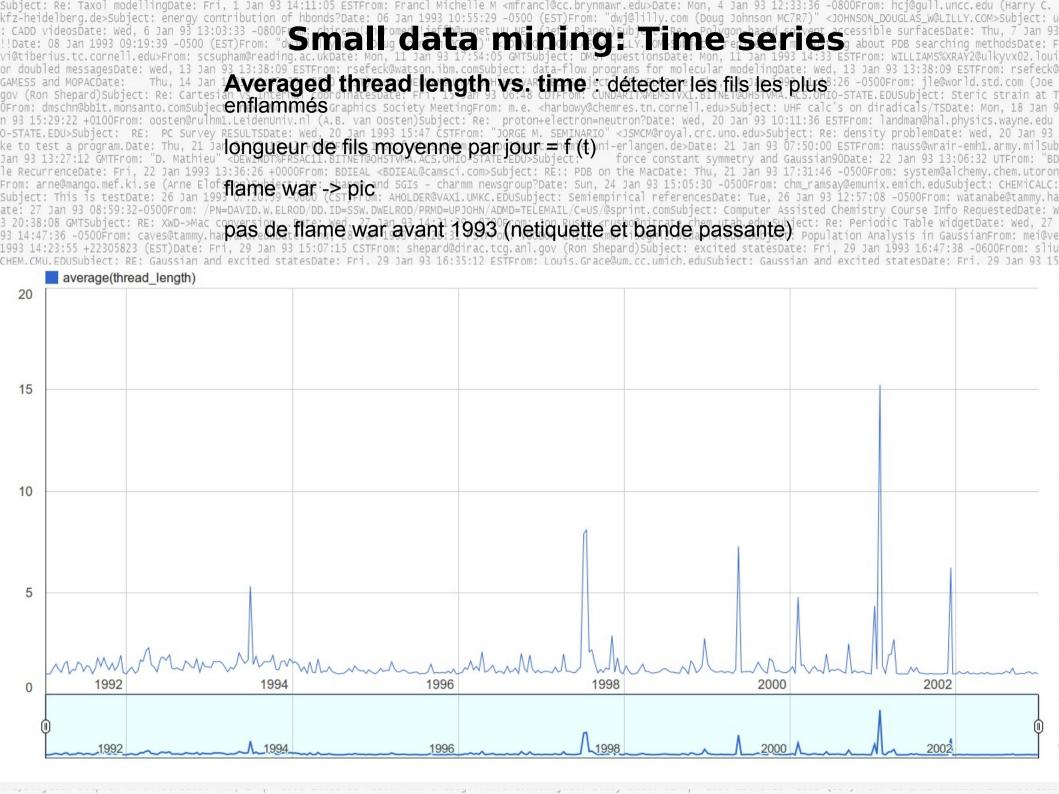
19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate:
edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMol questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvx02.lou
: 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

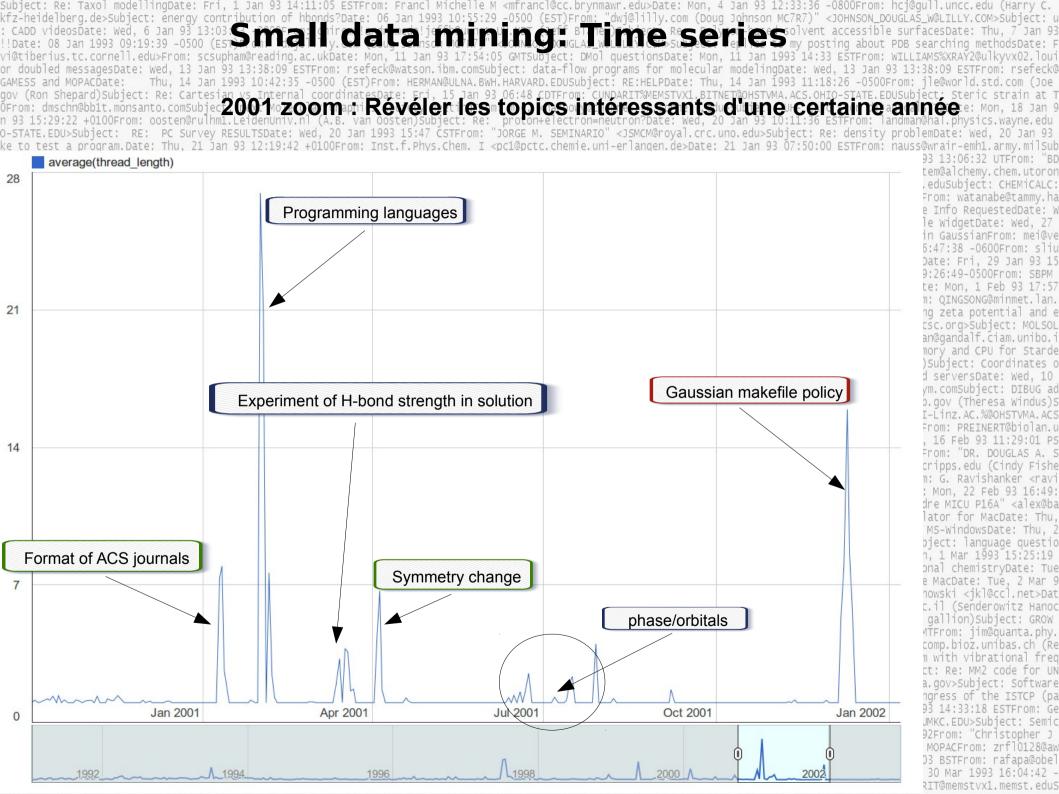
Dizaines de milliers de messages organisés et lexte 3 10:1date of la autel e pour le la company de l

Analyse quantitative: Small data mining

Sociala Metwork analysis and excited statespath Fri 79 Jan 93 16:35:12 ESTFrom: Louis. Grace@um.cc.umich.eduSubject: Gaussian and Sociala. Network analysis for charlot gard and excited statespath. Fri 79 Jan 93 16:35:12 ESTFrom: Louis. Grace@um.cc.umich.eduSubject: Gaussian and Social Analysis for Conference Announcement of the Conference

Nouveauté : utiliser ces techniques avec le « thread » comme unité





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: eggy contribution of hboris?Date: 06 Jan 1991 10:55:29 -05% (EST)Er m: "drj@j\]jy.com (Doug Johnson Mc7RA" <10HNSON DOUGLASEW@LILLY.COM>Subject: CADD videosDate: Wed, 6 Jan 1903 14:00 Call DV Sfl.Spate: Thu, 7 Jan 9 !Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson Mc7RA" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: !!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R) < JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: Fig. 12 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@ulkyvx02.loui or doubled messagesDate: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@GMMESS 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 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 TOFTOM: dmschn@bblt.monsanto.comsubject: next Molecular Graphics Society MeetingFrom: m.e. <a href="https://doi.org/10.2016/1

constant symmetry and Gaussian9ODate: 22 Jan 93 13:06:32 UTFrom: "BD MacDate: Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron Qui poste dans quels fils ?: comSubject: Computer Assisted Chemistry Course Info RequestedDate: V trate.chem.utah.edu>Subject: Re: Periodic Table WidgetDate: Wed, 27
nAnalyseideoreseauxin GaussianFrom: mei@ve bject: excised statesbate: Fri, 79 Jan 1993 16:47:38 -0600From: SITU USOCIAUX GPERMETED Statesbate: Fri, 29 Jan 93 15:ect: Conference Announcement Date: 101 Feb 25:19:26:49:0500From: SBPM: Gardtographier less fils etiles 17:57:Jacomphier Statesbate: (icie 2001) Ulating zeta potential and exciteurs :Atetfrom: Norbert Musiler <k360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS MESSAGES)14:47:09 +0100 (WET)from: PREINERT@biolan.u com>Subject: Re: x Windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PS
F) Date: Wed, 17 Feb 1993 14:15:16 -0500 (EST) From: "DR. DOUGLAS A. S
then in the point of the property majoritécdes offisonputapetitstypate: mon 1 mit 1993 15:25:19 majoritécdes offisonputapetitstypate: Tue nemres.tn.cornell.edu>Subject: Re:CAChe on the MacDate: Tue, 2 Mar 9 Subject: PDB subdir organization?From: Jan Labanowski <jkl@ccl.net>Dat teratomic separationsFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoc OFrom: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: GROW Software for PCDate: Fri, 12 Mar 93 04:51:15 GMTFrom: jim@quanta.phy. Date: Sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re : HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq (systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN

From: "STEPHEN R. HELLER" <srheller@asrr.arsusda.gov>Subject: Software

57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic :h-darmstadt.dé (Hagen Dúfner)Subject: efg in g92From: "Christopher J (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrfl0128@aw t: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel ireas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 te: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edus

HSTVMA.ACS.OHIO-STATE.EDUSubject: iect: Program called GRIDDate:

is.tc.cornell.edu>From: scsupham@reading.ac.ukĎate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMol questionsDate: Mon, 11 Jan 1993 14:33 EŠTFrom: WILLIAMS%XRAÝ2@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@ or doubled messagesbate, wed, is sail as 15.36.09 Estitiom. Is ecknowned to mode the mode thingbate, wed, is sail as 15.36.09 Estitiom. Is ecknowned messagesbate. Wed, is sail as 15.36.09 Estitiom. Is ecknowned messagesbate. Thu, 14 Jan 1993 11:18:26 -0500 (EST) from: HERMANQULNA.BWH.HARVARD.EDUSUbject: RE:HELPDATE: Thu, 14 Jan 1993 11:18:26 -05000 (EST) from: Jegov (Joe 1908) (Joe posteurs en commun 93 13:06:32 UTF les principaux acteurs sont Programming languages)ate acher policy era (5 y rom Format of ACS journals 57 th-da (Dr it: reas

aussi caractérisés par les wed. Filsxauxquelsi, is an 1993 16:47:38 -0600From: sliu Contribuentibate: 01 Feb 93 19:26:49-0500From: SBPM Subject: 3D structure -> 2D drawing?From: QINGSONG@minmet.lan. Software for calculating zeta potential and e 93 11:27:53 ESTFrom: Kevin Moore <kmoore@ncsc.org>Subject: MOLSOL ersDate: Fri, 5 Feb 1993 16:17:32 +0100From: ivan@gandalf.ciam.unibo.i <bobbv_clark@quickmail.clemson.edu>Subject: Memorv and CPU for Starde 38:51 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 eSubject: Mac summeryFrom: theresa@si.fi.ameslab.gov (Theresa Windus)S 18:41 CETFrom: Norbert Mueller <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS familles thématiques de threads. tte et de posteurs 16 -0500 (EST) From: "DR. DOUGLAS A. S MET)Subject: Long Time-scale DynamicsDate: Mon, 22 Feb 93 16:49: Programming languages Gaussian makefile policy Symmetry change phase/orbitals

small datacomuning well extended the complete of the complete Evolution de trois keywords (graphics, linux, supercomputer) en fonction du « graphics » and « supercomputer » : époque du supercomputi « linux » : époque du desktop computing évolution des débats dans la liste exemple du hardware : disparition de "graphics" et "supercompute années 90, corrélativement à l'apparition de "linux" separd sur passage de "supercomputing" à "desktop modelling"

ubject: Re: Taxol modellingDate: Fri, fz-heidelberg.de>Subject: energy contr CADD videosDate: Wed, 6 Jan 93 13:03: !Date: 08 Jan 1993 09:19:39 -0500 (EST i@tiberius.tc.cornell.edu>From: scsuph	ribution of hbonds?pate: 06:33 - Simall art T)From Simall art	Franci Michelle M <mrranci Jan 1993 10:55:29 -0500 (E Jantaan, Indi</mrranci 	acc.brynmawr.edu>bate st)from: "dwi@lilly.c f(\$1.42)\$11eX	i: Mon, 4 Jan 93 12:33: om (Doug Johnson MC7R7 L je men alla	36 -0800From: hcj@gull.unco)" <johnson_douglas_w@lilly at accessible surfacesDate sting about PDB searching</johnson_douglas_w@lilly 	i.edu (Harry C. 7.COM>Subject: u a: Thu, 7 Jan 93 g methodsDate: F
r doubled messagesDate: Wed, 13 Jan 9: AMESS and MOPACDate: Thu, 14 Jan 19 ov (Ron Shepard)Subject: Re: Cartesiar	3 13:38:09 ESTFrom: rsefect 993 10:42:35 -0500 (EST)From	(@watson.ibm.comSubject: dat @watson.ibm.comSubject: dat. .m: HERMAN@ULNA.BWH.HARVARD.	act: DMOT questionsDa a-flow programs for m EDUSubiect: RE:HELPDa	nce: Mon, 11 Jan 1993 1 Molecular modelingDate: Molecular 14 Jan 1993 1	4:33 ESTFROM: WILLIAMS%XKAN Wed, 13 Jan 93 13:38:09 E 1:18:26 -0500From: ile@wor	72@u1KyVXU2.10u1 STFrom: rsefeck@ ld.std.com (Joe
From Four of the six thr.	reads highligh	ted in: 2001 m.e. <n. "lorge="" m.="" m.<="" re.="" sten="" subject="" th=""><th>arbowy@cnemres.tn.cor lectron=neutron?Date: semINARTO" <15MCM@rov</th><th>MeII.edu>Subject: UHF Wed, 20 Jan 93 10:11:</th><th>calc's on diradicals/TSDate 36 ESTFrom: landman@hal.phy • Re• density problemDate•</th><th>e: Mon, 18 Jan 9 ysics.wayne.edu Wed 20 Jan 93</th></n.>	arbowy@cnemres.tn.cor lectron=neutron?Date: semINARTO" <15MCM@rov	MeII.edu>Subject: UHF Wed, 20 Jan 93 10:11:	calc's on diradicals/TSDate 36 ESTFrom: landman@hal.phy • Re• density problemDate•	e: Mon, 18 Jan 9 ysics.wayne.edu Wed 20 Jan 93
e to test a program Date: Thu, 21 Jan an 9 C: Une Tigne Corre e RecurrenceDate: Fri, 22 Jan 1993 13: rom: arne@mango.mef.ki.se (Arne Elofs:	93 12:19:42 +0100From: Ins PSONDC & BUNTOIN :56:26 +0000From: BDIEAL <e son)Subject: Re: charmm and</e 	it,f.Phys.Chem.I. <pc]@pctc. readoplutôtoqu BDIEAL@camsci.com>Subject.R SGIs - charmm newsgroup?Da</pc]@pctc. 	Themie, uni-erlangen, d I UNE ANNÉE E:: PDB on the MacDat te: Sun. 24 Jan 93 15	le>Date: 21 Jan 93 07:5 tant symmetry and Gaus e: Thu, 21 Jan 93 17:3 :05:30 -0500From: chm	0:00 ESTFrom: nauss@wrair-6 sian90Date: 22 Jan 93 13:00 1:46 -0500From: system@alch	emhl.army.milSub 5:32 UTFrom: "BD nemy.chem.utoron iect: CHEMiCALC:
ubje Classer, les fils (iC te: Classer, les fils (iC 20:38:08 GMTSubject: RE: XWD->Mac cor	i ceux de l'anr	née 2001) par k	eywords	rencesDate: Tue, 26 Ja Subject: Computer Assis	n 93 12:57:08 -0500From: Wa ted Chemistry Course Info F	atanabe@tammy.na RequestedDate: W
3 14:47:36 -0500From: caves@tammy.harv 993 !!Software (Est) com r HEM.CMO.EDUSUDJECT RE: @ausstan de adomski@mondl.ccrc.uga edupate: Mon	vard.eduDate: Thu, 28 Jan 1 mercial 7.07:11 Sup the 1993 12:04:28 +0100Fr	993 15:28:31 PSTFrom: VOODO Port dora Copen port 16:33:12 Open com: cfat10198servus rus uni	CHILE <morris@gnl2. "(permet<sup="">bjecbuile desubiect) -stuttgart desubiect)</morris@gnl2.>	ucdavis.edu>Subject: P t: excited statesDate: h.eduSubject: Gaussian	opulation Analysis in Gauss Fri, 29 Jan 1993 16:47:38 and excited statesDate: Fr	sianFrom: mei@ve -0600From: sliu ri, 29 Jan 93 15 -0500From: SRPM
youkha@biosym.comSubject: Summary: 1 n.nl=s@etrevelerrceuXak nd NanotechnologiesDate: Wed, 3 Feb 9 F TOLEDO" <dsmith@uoft02.utoledo.edu>S</dsmith@uoft02.utoledo.edu>	Internals & Non-RondsDate: Qui Sont les4pl 3 10:46:20 MSTFFOM: 0INSOR	Tue, 2 Feb 93 11:12:51 CSTF US Intéressant G@minmet. lan, mcgill, capate:	rom: (бaell) <baell@s Siena@leia.polaroid.c 3 Feb 93 13:</baell@s 	yd.dah.csiro.au>Subjec omSubject: 3D structur 04:57Subject: Sof	t: DMF dielectricDate: Mon. e -> 2D drawing?From: QINGS tware for calculating zeta	, 1 Feb 93 17:57 50NG@minmet.lan. potential and e
bobby de les catégorise 00 (EST)From: spollack@ester.mse.uc.EC vate: Tue, 09 Feb 1993 21:39:58 -0500 (.From: Zhou Feng <feng@lisboa.ks.uiuc.< td=""><td>ert par style de DU (s.K. Pollack)Subject: F (EST)From: "DR. DOUGLAS A. .edu>Date: Wed, 10 Feb 93 1</td><td>rtopico:om>subject rtopico:08:20 -1812From Phosphazene ModelingDate: ModelingDate: ModelingDate: ModelingDate: ModelingDate: ModelingDate: parali</td><td>t: Call for PapersDat : "Bobby Clark" <bobb 1, 8 Feb 93 07:58:51 ' <dsmith@uoft02.utol lel CHARMM?Date: Wed,</dsmith@uoft02.utol </bobb </td><td>e: Fri, 5 Feb 1993 16: y_clark@quickmail.clem ESTFrom: adit@Kodak.CO edo.edu>Subject: paral 10 Feb 93 15:46:43 -0</td><td>17:32 +0100From: TVan@ganda son.edu>Subject: Memory and M (Adi Treasurywala)Subject lel workstations and server 800From: rickl@biosym.comSu</td><td>air.ciam.unibo.i d CPU for Starde t: Coordinates o rsDate: Wed, 10 ubject: DIBUG ad</td></feng@lisboa.ks.uiuc.<>	ert par style de DU (s.K. Pollack)Subject: F (EST)From: "DR. DOUGLAS A. .edu>Date: Wed, 10 Feb 93 1	rtopico:om>subject rtopico:08:20 -1812From Phosphazene ModelingDate: ModelingDate: ModelingDate: ModelingDate: ModelingDate: ModelingDate: parali	t: Call for PapersDat : "Bobby Clark" <bobb 1, 8 Feb 93 07:58:51 ' <dsmith@uoft02.utol lel CHARMM?Date: Wed,</dsmith@uoft02.utol </bobb 	e: Fri, 5 Feb 1993 16: y_clark@quickmail.clem ESTFrom: adit@Kodak.CO edo.edu>Subject: paral 10 Feb 93 15:46:43 -0	17:32 +0100From: TVan@ganda son.edu>Subject: Memory and M (Adi Treasurywala)Subject lel workstations and server 800From: rickl@biosym.comSu	air.ciam.unibo.i d CPU for Starde t: Coordinates o rsDate: Wed, 10 ubject: DIBUG ad
-2Subject: Re: ZINDO programDate: 14031%hkuxa.hku.hk@OHSTVMA.ACS.OHIO-ST : Re: X Windows for PCDate: Sat, 1: .ll.edu>Subject: MPW Fortran?Date: Tue, From: "W. Todd Wipke" <wipke@secs.ucso u. 18 Feb 93 14:22:08 PSTFrom: raw@aut Bubblelines</wipke@secs.ucso 	TATE.EDUSubject: MO Plottir 3 Feb 93 12:21:47 +0900From . 16 Feb 93 13:28:40 ESTFrom	n: Katushi Kobayashi <ikob@l om: Kenneth McGreevv <koreev< td=""><td>, 12 Feb 93 09:48:41 es.pc.uec.ac.jp>Date: /@hpldas1.sid.hp.com></td><td>CETFrom: Norbert Muell Sat, 13 Feb 1993 1 Subject: Re: X Windows</td><td>er <k360171%edvz.uni-linz.a 4:47:09 +0100 (WET)From: PF for PCDate: Tue. 16 Feb</k360171%edvz.uni-linz.a </td><td>AC.%@OHSTVMA.ACS REINERT@biolan.u b 93 11:29:01 PS</td></koreev<></ikob@l 	, 12 Feb 93 09:48:41 es.pc.uec.ac.jp>Date: /@hpldas1.sid.hp.com>	CETFrom: Norbert Muell Sat, 13 Feb 1993 1 Subject: Re: X Windows	er <k360171%edvz.uni-linz.a 4:47:09 +0100 (WET)From: PF for PCDate: Tue. 16 Feb</k360171%edvz.uni-linz.a 	AC.%@OHSTVMA.ACS REINERT@biolan.u b 93 11:29:01 PS
	▼ Granularity □	300 Separate Lines for Terms	1			
software support method	open commercial	_	<i>′</i>			
CCL2001_890(formatACSjour;		•		• • • •	• • •	22
CCL2001 813(gaussianmakef;		• • •	00 00 0	• • •	∞ ∞ ●	46
CCL2001_556(programmingla;	• • • •	•	•	• • • •	• • •	25
CCL2001 465(symmetrychang;			•			4
lz)Subject: Stephen R. WilsonDate: Thu	u, 1 Apr 1993 16:33:29 +020	OFrom: oles@gollum.uio.noSu	oject: BiosymDate: 01	Apr 1993 11:43:13 -06	00 (CST)From: CUNDARIT@mems	stvx1.memst.eduS

e:Ir9939:13debuts: de la cione warz (la bandwidth est rare) : Ser Spice file est la première de l'histoire: contexte de communauté scientifique en train de se définir, de stratégies éditoriales,

commerciales; de startégies bureaucratiques nouvelles conquirafonte réagirm Res

2001cchamp bien établi, a traverse plusieurs

crises (liées au marché de l'emploi et à l'apparition

d'autres promesses technoscientifiques, comme la

bioinformatique), un logiciel particulier (Gaussian)

accapare l'attention par son succès et les débats

guill provoque

Tis is tisp: LEO O U Coto :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 93 16:33:12 ESTFrom: Louis Tree@um.cc.umickedus kject: Gaussian and excited statesDate: Fri, 29 Jan 93 16:33:12 ESTFrom: Louis Tree@um.cc.umickedus kject: Gaussian and excited for the complete of the complete

POR SECURE SECURE SECURE SECURE SECURES SECURE

uggere: Tue, 2005 93 2:0043 PSTErom; wsonnen@alnitak.u.m.edu (nayne sonnen)subject: Una base chargesDate: 23 F67 93 15:38:36-2300From: Malexandre MI t A: Hydrogen block of well A let (17:21 0) 17. < Pot Swings (18:25 0) Ad A respectively of the letter of

Kolomo Carlo Carlo

```
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
ÕFrom: 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
n 93 15:29:22 +0100From: oosten@rulhm1.LeidenUniv.nl (A.B. van Oosten)Šubject: Re: proton+electron=neutron?Date: Wed, 20 Jan 93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu
0-STATE.EDU>Subject: RE: PC Survey RESULTSDate: Wed, 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problemDate: Wed, 20 Jan 93
ke to test 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
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: w
3 20:38:08 GMTSubject: RE: XWD->Mac conversion...Date: Wed, 27 Jan 93 14:21:29 -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 15:28:31 PSTFrom: VOODOO CHILE <morris@gnl2.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)Sŭbject: 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@mondl.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: SBPM
: youkha@biosym.comSubject: Summary: Internals & Non-BondsDate: Tue, 2 Feb 93 11:12:51 CSTFrom: (baell) <baell
un nl>Subject: Electronic Periodic TablesDate: 02 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
OF TOLEDO" <DSMIŤH@uoft02.utoledo.edu>Subject: Re: Plotting Orbitals from a G90/Ğ92 CalculationDate: Thu, 4 Feb 93 11:27:53 ESTFrom: Kevin Moore <kmoore@ncsc.org>Subject: MOLSOL
3 +0100 (NET)Date: 05 Feb 93 09:28:33 ESTÉrom: Elliot King <71127.1231@compuserve.com>Subject: Call for PapersDate: Eri. 5 Feb 1993 16:17:32 +0100From: ivan@gandalf.ciam.unibo.i
                                    Evleth, June 25th
```

Subject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brvnmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hci@qull.uncc.edu (Harry C. kfz-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 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: "dwi@lillv.com (Doug Johnson MC7R7)" <JOHNSON DOUGLAS W@LILLV.COM>Subject: replies to my posting about PDB searching methodsDate: F /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 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@

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

Adamo, June 28th Holder, June 25th Fernandes, July 1st Graham Hurst, June Wipke, June 29th Leonard, June 30th Smith, June 26th States, June 26th

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: 02 Mar 1993 08:13:18 -0500 (EST)From: "DONALD B. BOYD" <BOYD_DONALD_B@LILLY.COM>Subject: new book on computational chemistryDate: Tue tate.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: MARYJŌ@northeastern.eduSubject: PDB subdir organizātion?From: Jan Labanowski <jkl@ccl.net>Dat

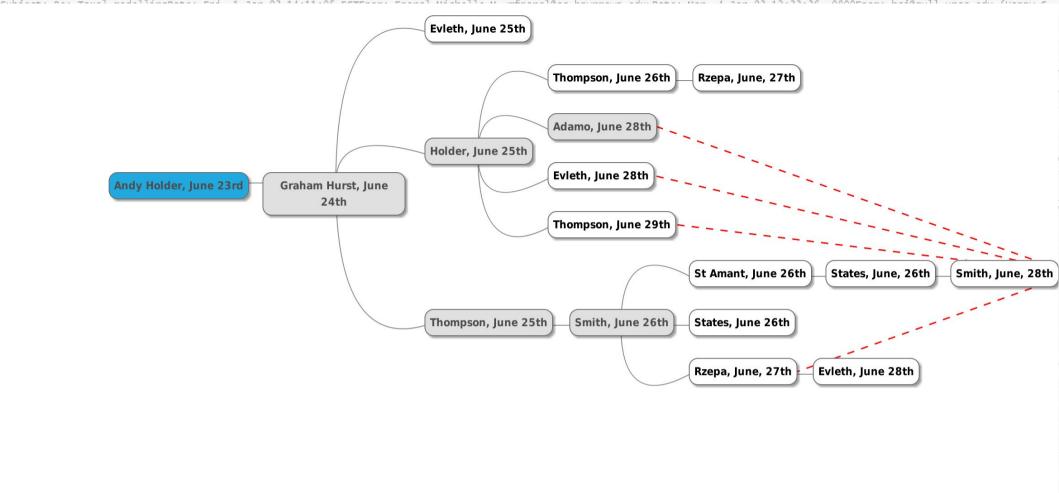
Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PSUVM.PSU.EDU>Subject: Minimum allowable interatomic separationsFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoc secc.fi.cnr.itSubject: MO Theory Made VisibleDate: Tue Mar 09 11:23:12 1993Date: Tue, 9 Mar 93 10:52:25 -0500From: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: GROW 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

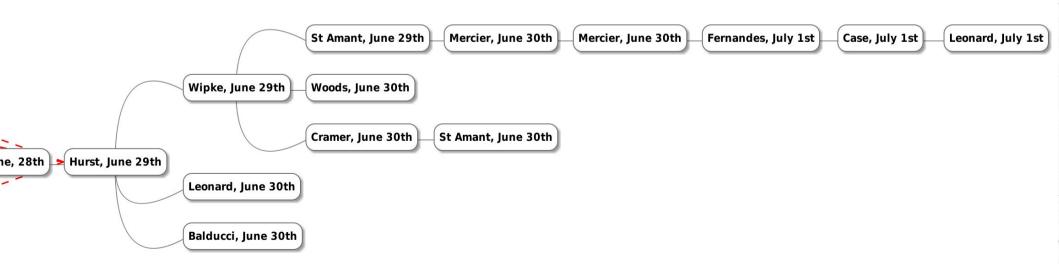
MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Date: Mon. 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq , 15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdtscp@hpc.ch.man.ac.uk>Subject: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN

ar 1993 13:58:36 -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 First Congress of the ISTCP (pa st Girona Seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01%EBCESCA1@OHSTVMA.ACS.OHIO-STATE.EDUSubject: 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: SČ&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

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





pov (Ron Shepard) Subject: Re: (artesian vs Internal coordinatespate: Fri 15 Jan 93 06:48 COTFORM: (UNDARTSMENSTVX). BITNET®OHSTWM, ACS. OHIO-STATE. EDUSUbject: Steric strain at 7 Jeronic discribibly drivers. The control of the con

• From: Andy Holder < AHOLDER %! at !% VAX1.UMKC.

ct: 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. eidelberg.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 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 13:03:39 -0500 (EST)From: "dvjogoom (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: FDF in the Company of the Comp

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

watson.ibm.comSubject: data-flow programs for molecular modelingDate: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@

• Subject: SAM1 reference

carl Jud

secc.fi.cr

23 -0600 (.milSubjec • Date: Wed, 23 Jun 1993 17:44:29 -0500 (CDT)

method now has an official reference. It is as follows:

Dewar, M. J. S.; Jie, C.; Yu, G. Tet. 1993, 23, 5003.

This is primarily a listing of results for the new method for a vast array of systems. It also compares quite favorably with AM1 and PM3. A more complete paper describing the model will be forthcoming

Hi netters. For those of you interested, Michael Dewar's new SAM1

from my lab in the next year. Professor Dewar felt it important to

commence par un message anodin : Andy Holder annonce la publication d'un article donnant les résultats obtenus, pour différents systèmes moléculaires, avec une nouvelle méthode semi-empirique de chimie quantique « SAM1 » troll: Graham Hurst: « this post disturbs me...» - problème : « it will be impossible to independently reproduce these results [....] If the method has not yet been published, then the results should not have been accepted for publication since they cannot be verified. [...] Is the SAM1 method sufficiently described in this sub paper, Ma (Ord 136 publications and it rue, references) mile to manual low and independent <u>verification</u> of the reported results? »

V (Ron Snepard Subject: Re: Carestan VS Internal Coordinates Date: Fri, 15 Jan 93 10:38 CDIFFOM: COMBACI MAMBOSTATIC CONSUSPECT: UPT Calc's on diradicals/TSDate: Mon, 18 Jan 93 15:29:22 +0100From: oosten@rulhm1.LeidenUniv.ml (A.B. van oosten)Subject: Re: proton+electron=neutron?Date: Wed, 20 Jan 93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu
STATE.EDUS-Subject: RE: proturvey RESULTSDate: Wed, 20 Jan 1993 15:27:55 From: "JORGE M. SEMINARIO" (JSMCM@royal.crc.uno.edu>subject: Re: density problemDate: Wed, 20 Jan 1993 15:27:12 GM | Promo U. Matchieu Sewinolas Result. Sain New Journal Combacine (Protuct Results) Problem Pr

NO (EST)From: spollack@ester.mse.uc.EDU (S.K. Pollack)Subject: Phosphazene ModelingDate: Mon, 8 Feb 93 07:58:51 ESTFrom: aditCkmail.Clemson.edu>Subject: Memory and CPU for Stark (DO) (EST)From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" (DSMITH@uoft02.utoledo.edu>Subject: parallel workstations and serversDate: Wed, 10 Feb 93 16:23:41 -0600Subject: parallel CHARMM?Date: Wed, 10 Feb 93 15:46:43 -0800From: tacl@biosym.comsubject: DIBUG (Dibugent) 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; 4031%hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: MO Pictting program!Date: Fri. 12 Feb 93 09:48:41 CSTFrom: Norbeyt Mueller <k360171%EDVZ.UNI-Linz AC. %@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: MO Pictting program!Date: Fri. 12 Feb 93 09:48:41 CSTFrom: Norbeyt Mueller <k360171%EDVZ.UNI-Linz AC. %@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: MO Pictting program!Date: Fri. 12 Feb 93 09:48:41 CSTFrom: Norbeyt Mueller <k360171%EDVZ.UNI-Linz AC. %@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: MO Pictting program!Date: Fri. 12 Feb 93 09:48:41 CSTFrom: Norbeyt Mueller <k360171%EDVZ.UNI-Linz AC. %@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: MO Pictting program!Date: Fri. 12 Feb 93 09:48:41 CSTFrom: Norbeyt Mueller <k360171%EDVZ.UNI-Linz AC. %@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: MO Pictting program!Date: Fri. 12 Feb 93 09:48:41 CSTFrom: Norbeyt Mueller <k360171%EDVZ.UNI-Linz AC. %@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: MO Pictting program!Date: Fri. 12 Feb 93 09:48:41 CSTFrom: Norbeyt Mueller <k360171%EDVZ.UNI-Linz AC. %@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: Molecular Ac. %@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: Molecular Ac. %@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: Molecular Ac. & CONTROL & CO

positions, interrogations des acteurs émergent

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 Fish de ChargesDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "Janet Del Bene" <FR042008@YSUB.YSU.EDU>Subject: BSSE calculationDate: Fri, 19 Feb 93 11:53:05 -0500From: G. Ravishanker <ra* jemi"

jemi"

jemi"

spiral pugdate: 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" alexa
ubject: Re: HCONTEADU DISCUSSION DTFroles Office Sonten Subject: dna base chargesDate: 23 Feb 93 15:38:36-2300From; "Alexandre MICU P16A" alexa
ubject: Re: HCONTEADU DISCUSSION DTFroles Office Sonten Subject: Alexa (Feb 93 15:38:36-2300From; "Alexandre MICU P16A" alexa
ubject: Re: HCONTEADU DISCUSSION DTFroles Office Sonten Subject: Resultance (Fri) (Feb 93 15:38:36-2300From; "Alexandre MICU P16A" alexa
ubject: Resultance (Fri) (Feb 93 15:38:36-2300From; "Alexandre MICU P16A" alexa
ubject: Resultance (Fri) (Feb 93 15:38:36-2300From; "Alexandre MICU P16A" alexa
ubject: Resultance (Fri) (Feb 93 15:38:36-2300From; "Alexandre MICU P16A" alexa
ubject: Resultance (Fri) (Feb 93 15:38:36-2300From; "Alexandre MICU P16A" alexa
ubject: Resultance (Fri) (Feb 93 16:49)
ubject: Resultance (Fri)

empircal calculations simple oxidesfrom: sender@chemocl.tau.ac.il (Senderowitz Hanoch)Subject: MOPAC6.ODate: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25: Subject: Expert Know-How wanted !!Date: 02 Mar 1993 08:13:18 -0500 (EST)From: "DONALD B. BOYD" <BOYD_DONALD_B@LILLY.COM>Subject: new book on computational chemistryDate: .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 g 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> 3 17:30:16 GMTDate: Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PSUVM.PSU.EDU>Subject: Minimum allowable interatomic separationsFrom: sender@chemdcl.tau.ac.il (Senderowitz Ha file) file for the computation of th

ingDate: 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.pp3 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 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 formation of the subject of the subject in the subject of the subject in the subject

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: Softw.
irona Seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01%EBCESCA1@OHSTVMA.ACS.OHIO-STATE.EDUSUbject: First Congress of the ISTCP
-0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emhl.army.milSubject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom:
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: Select: What about simulated annealing?Date: Wed 24 Mar 93 14:11:32 +0100From: dufner@ws01 no chemie th-darmstadt de (Hagen Dufner)Subject: efg in g92From: "Christopher

ISUBJECT: What about simulated annealing?Date: Wed, 24 Mar 93 14:11:32 +0100From: dufher@ws01.pc.chemie.th-darmstadt.de (Hagen Dufher)Subject: erg in g92From: "Christopher J t: 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 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 Subject: Polvrate Ouervoate: 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 -

```
**Modered messagesbate: wed, 13 Jan 93 13:38:09 ESTFrom: Tsefteck@watson.1Dm.ComSubject: data-flow programs for molecular modelingDate: Med, 13 Jan 93 13:38:09 ESTFrom: Fsefteck@watson.1Dm.ComSubject: Thi, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (joe ov (Ron Shepard)Subject: Re: LED93 11:18:26 -0500From: jle@world.std.com (joe ov (Ron Shepard)Subject: Re: Cartesian vs Internal coordinatesDate: Fri, 15 Jan 93 06:48 CDTFrom: CUNDARIT%MEMSTVX1.BITNET@OHSTWMA.ACS.OHIO-STATE.EDUSUbject: Steric strain at Tsrom: dmschn@bblt.monsanto.comSubject: next Molecular Graphics Society Meetingprom: m.e. <a href="https://doi.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.org/10.1016/journal.o
```

ckmail.clemson.edu>subject: E-mail.cearchōate: 6 Feb 1993 10:03:20 -1812From: "Bobby clark" <bobby_clark@clark object: 6 Jemson 3 Subject: Marcry and cpu for the second control of the second control

pate: Ethiogue jepublication of simportance peer review of less eresultats de

méthodes nat propriétaires reproper ne 19:00 ont la passiche partier et de ject «X-open in a scientific

dans entreprise (développement de logiciels)

Fil de discussion 1993

<u>Un message pivot</u> : Douglas Smith, 26/06/93

- répond point par point à l'Italian ponde déal d'réel
- T.: "good science is that of reproducibility and independent verification" OK mais rarement suivi : <u>paramètres</u> en MM, nota MM2, MacroModel, Hyperchem...
- control of the contro
- readily available and accessible? When software copyrights and patents really provide adequate protection, maybe I will agree with that attitude"
- literature" ALORS: "where do they belong? Comparison of these results with "standard" and commonly available "academic" results is healthy and stimulating.

 And, not to tweak Mark Thompson, who freely distributes Argus, what about Gaussian? [accès ou pas au code source]

<u>message pivot</u> : Douglas Smith, 26/06/

manque transparence méthode (paramètres)

comsubject: Summary: Internals & Nop-BondsDate: Tue, 2 Feb 93 11:12:51 CSTFrom: (baell)

logiciels propriétaires -05 diffusion et code source

rotection et rétribution travail de programmation

3 15:08:43 PSTFrom: wsonnen@alnitak.usc.edu (wayne Sonnen)Subject: dna base chargesDate: 23 Feb. 93 15:38:36-2300From: >>> Versequestionsossurack.Bsoftware.copyrightsinand.

patents »; « actual trend in commercializing computationa

: partial charges for fictive atoms in G92bate: Mon. 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.edusubject: F Miggardi message: deisynthese de Hurst mapaise la con

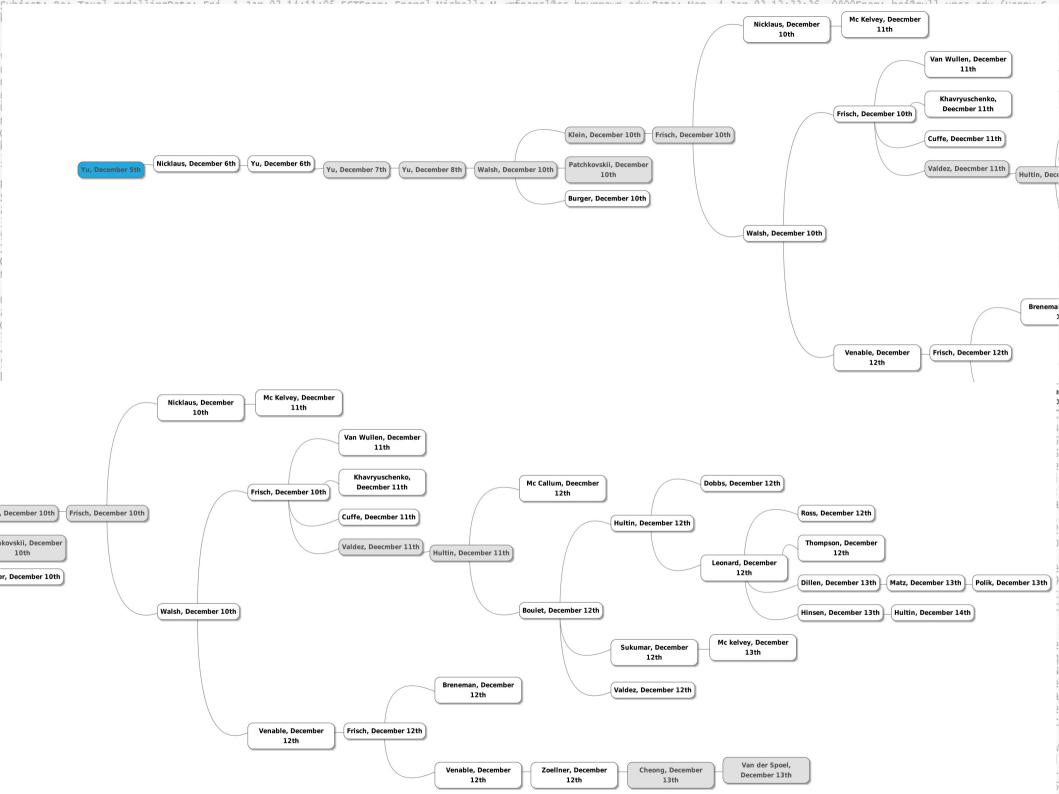
```
Subject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brvnmawr.edu>Date: Mon. 4 Jan 93 12:33:36 -0800From: hci@gull.uncc.edu (Harry C.
kfz-heidelberg.de>Subject: energy contribution of hbonds?pate: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwi@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u
 CADD videosDate: Wed, 6 Jan 93 13:03:33 -0800From: chiremv!andromeda!jeffb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93
 !Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwi@lillv.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 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@
                          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
dov (Ron Shepard)Subiect: Re: Cartesian vs Internal coordinatesDate: Fri, 15 Jan 93 06:48 CDTFrom: CUNDARIT%MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at T
ÕFrom: 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
n 93 15:29:22 +0100From: oosten@rulhm1.LeidenUniv.nl (A.B. van Oosten)Šubject: Re: proton+electron=neutron?Date: Wed, 20 Jan 93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu
0-STATE.EDU>Subject: RE: PC Survey RESULTSDate: Wed, 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problemDate: Wed, 20 Jan 93
ke to test 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
Jan 93 13:27:12 ĞMTFrom: "D. Máthieu" <DEWINDT%FRSAC11.BITNET@OHSTVMA.AĆS.OHIO-STATĖ.EDU>Subject: force constant symmetry and Gaussian90Date: 22 Jan 93 13:06:32 UTFrom: "BD
le RecurrenceDate: Fri, 22 Jan 1993 13:3526-0000Frcm: RDIFAL ADTEAL Marson filsuhiele RÉCIRDE MacCate Dré 22001:31:46 -0500From: system@alchemy.chem.utoron
From: arne@mango.mef.ki.se (Arne ElofsscStiftucture adeil-enfiladeadeurDécentbré52001m_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: w
3 20:38:08 GMTSubject: RE: XWD->Mac conversion...Date: Wed, 27 Jan 93 14:21:29 -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 15:28:31 PSTFrom: VOODOO CHILE <morris@gnl2.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)Sŭbject: 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
                                                                                                                Van Wullen, Decemb
                                                                                                               Cuffe, Deecmber 11th
                                                                                                                                                Hultin December 12th
                                                                                                                                                                       Thompson, Decemb
                                               Yu December 8th
                                                                                                                          Hultin, December 11th
                                                                                                                                     Boulet, December 12th
                                                                                                                                                            Mc kelvey, Dece
                                                                                                                Frisch, December 12th
ar 93 17:30:16 GMTDate:
```

d.harvard.edu (jill cheney)Subject: Computer Program to Evaluate Wigner 3i CoefficientsDate: Fri. 26 Feb 1993 22:08:57 +0100From: ole.swang@kjemi.ujo.noSubject: language guestio 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: 02 Mar 1993 08:13:18 -0500 (EST)From: "DONALD B. BOYD" <BOYD_DONALD_B@LILLY.COM>Subject: new book on computational chemistryDate: Tue tate.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: MARYJŌ@northeastern.eduSubject: PDB subdir organizātion?From: Jan Labanowski <jkl@ccl.net>Dat 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 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 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: 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 11:49:40 GMTSubject: Re: MM2 code for UNIX systemsDate: Tue, 16 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

st Girona Seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01%EBCESCA1@OHSTVMA.ACS.OHIO-STATE.EDUSubject: First Congress of the ISTCP (pa 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.armv.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: SČ&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

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



il de discussion 2001 : GAUSSIAN commence partun message anodin (Jen-Shiang Yu, PhD Taiwan) annonce 9d9: un est combenchmarkec benchmark per pour 5Picom: kevir Moore choose of Subsection annonce of the combenchmarkec benchmark per pour 5Picom: kevir Moore choose of Subsection annonce of the combench of the comben bricole les machines desktop computing) .hk@hstma.aca.ohio-state.edusubjet: Mo Plotting proc.am!Date: Fri. 12 Feb 93 09:48:41 CETFron: Norbert Mueller enchaînement: desopremiers messages (voir schema: 24) chargesDate: Fri, 19 jeb 14:49:00 steme "Janet Del Jene" str. 42008@ysub. ysu. EDU> subject: Bss. calc. Lation ate: Fri, 19 jeb 3 11:13:05 -0500From: G. Ravis Janker will subject strain ate: Fri, 19 jeb 3 11:13:05 -0500From: G. Ravis Janker bei subject str. 40 jeb 3 11:13:05 -0500From: G. Ravis Janker bei subject sub

of makefile or the instructions is violation to the licence agreement. »

Gaussian, Inc. (MarFrisch) hpc.ch. man. ac. uk

17:30:16 GMTdtéroulement : Estfram «SM 10:80 ESTFram »SM 10:80 ESTFram «SM 10:80 ESTFram «SM 10:80 ESTFram »SM 10:80 EST

de discussion 2001 : GAUSSIAN ect: RE: PC Survey RESULTSDAte: Wed, 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edy>subject: Re: density problemate, wed, 2 OUNCELLOS COUNCELLOS COUNC tensions avec la licence, différences de Gaussian avec le monde du libre Gaussian restateun blogiciel apropriétaire de qui dans seus persont code isource lisible (par souci de transparence épistémique) mais la licence est TRES restrictive - pas d'initiative dans la compilatio - pas de publication d'output PW Fortran?Date: Tue, 16 Feb 93 13:28:40 ESTFrom: Kenneth McGreevy < kgreevy@npidas1.sid.hp.com>subject: Re: X Windows for PC ..Date: Tue, 16 Feb 93 11:2

On string Cs. peuton compiler: Graussian Fedure (SSUP). Le 17 matériel -05 prévus epar Cogespate: Fr., 19 Feb. 92 14:49:00 ESTFrom: "Janet Del Bene" (FRO1008@YSUBYSU.EDU>Subject: BSSB calcular propered (19 Feb. 93 11:13:05 -0:00From: G. Ravishinker (19 Feb. 93 11:13:05 -0:00From: G. Ravishinker (19 Feb. 93 15:08:8) PSTFrom: wsonnen@apritak.usc.edu (wayne sonnen)subject dha base chargespate: 23 Feb. 93 15:38:36-2300From: "Alexandre Micu P16A" < brack to be the property of the prope ert 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 charist. aperformance: ddug calcul?: (software) = etrureproductibilité: (méthode E.EDU>Subject: partial charges for fictive atoms in G92Date: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.edusubject: Pro Refus. (de of alas contribution adeuklaje communauté et // rquestion 33 du différentes catégories d'utilisateurs (lead users, end users...

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. 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 Citation (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_w@LILLY.COM>Subject: u. v. Jan 93 IC. itation (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_w@LILLY.COM>Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93 i@tiberius.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, or doubled messagesDate: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@ GAMESS and MOPACDate: Thu, 14 Jan 1993 10:42:35 -0500 (EST)From gov (Ron Shepard)Subject: Re: Cartesian vs Internal coordinatesDat From: dmschn@bb1t.monsanto.comSubject: next Molecular Graphics So 93 15:29:22 +0100From: oosten@rulhm1.LeidenUniv.nl (A.B. van Oos EDU>Subject: RE: PC Survey RESULTSDate: Wed, 20 Jan 1993 to test a program pate: Thu 21 Jan 93 12:19:42 +0100From: Inst Carlos Of Mittlessecrets Instantal Security Secrets (Secure 1) Secure 12:42 +0100From (Secure 1) Secure 12:42 +0 and mando met kgs (Urne Elofsson)Subject: Re: charmm and 1993 07:20:59 -0600 (CST)From: A From: "Phil Hultin" <hultin.,at,.cc.UManitoba.CA> 27 Jan 93 08:59:32-0500From: /PN=DAVID.W.ELROD/DD.ID=SSW.DWEL 20:38:08 GMTSubject: RE: XWD->Mac conversion...Date: Wed, 27 Jan 14:47:36 -0500From: caves@tammy.harvard.eduDate: Thu, 28 Jan 19 « the support is not so crc.uga.eduDate: Mon, 1 Feb 1993 12:04:28 +0100Frc **2006**/m) mSubject: Summary: Internals & Non-BondsDate: ubject: Electronic Periodic TablesDate: O2 Feb 1993 14:36:0 d NanotechnologiesDate: Wed. 3 Feb 93 10:46:20 MSTFrom: QINGSONG TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: Re: Plotting Orbita +0100 (NET) pate: 05 Feb 93 (12:33 VSm: Elliot King <71127. oCOMPULE New Hizby VS - mail searchpate: 6 F) (EST)From: spollack@ester.mse.uc.EDU (S.K. Pollack)Subject: Pr EXPERIMENTALIST(EST)From: "DR. DOUGLAS A. S. Fom: "DR. DOUGLAS A. S. Fom: Prom. Prom Re: ZINDO programDate: 11 Feb 1993 13:06:18 +0100 4031%hkuxa.hku.hk@oHSTVMA.ACS.OHIO-STATE.EDUSubject: MO Plotting Re: X Windows for PC F. Data: Sat, 13 Feb 93 12:21:47 +0900From: 1 (4du People on tran?rat promeb to 3:28:40 ESTFrom rom: V. Tood wipke wipkeeses. UCSC. EDU>Subject: Final call Su jump on Gaussian Com (Robert A Whitesi <bjerkese@kjemi.unit.no>Subject: Summary. Scaled freq for carl JugDate: Tue, 23 Feb 93 15:08:43 PSTFrom: wsonnen@alnitak.u Subject: Re: Hydrogen bond Date: Wed, 24 Feb 93 17:21 EDTFr . X/Stoctmakeethe program Thu, 25 Feb havatodumakeeythee program Evaluate w work the way the manual 18 implies that it should >> i.cnr.itSubject: MO Theory Made VisibleDate: Tue Mar 09 11:2 1993 02:33:09 -0800 (PST) From: Thomas Nhan tom@cassandr A. « a a user Interface that is actually user friendly shu, 18 Mar :11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37

23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Ar milSubject: What about simulated annealing?Date: Wed, 24 Mar 93 1 ject: SC&A Conference speakers – thanksDate: Thu, 25 Mar 93 10:18: MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Rob..

Re: Gaussian Flame-wars

Subject: Re: Gaussian Flame-wars

Date: Tue, 11 Dec 2001 16:52:36 -0600

Max Valdez wrote:

>I think Gaussian is a great tool, but it has a LOT of little secrets and >"bugs", and the support is not so good, I don't think the spend >that much money on customer support, given the price of the product.

I absolutely agree with this statement. I think I represent a new kind of scientist working with tools like Gaussian. I am an experimentalist, not a computer whiz, [...]

So what's the point of all this? Well, maybe people would be less prone to jump on Gaussian (as they have over this makefile thing) if they didn't feel that the philosophy of Gáussian Inc. was similar to thắt of the "high priest" - only the initiates will have the secrets revealed and then only after years of study. A nice start would be to make the program work the way the manual implies that it should (or to make the manual describe how the program actually works). Even better: bring the program into the 21st century by providing a user interface that is actually user-friendly. What the priests and initiates regard as "a philosophy and aesthetic of simplicity" looks quite otherwise to many of us on the outside!

Dr. Philip G. Hultin Associate Department Head and Associate Professor of Chemistry University of Manitoba Winnipeg, MB, Canada R3T 2N2 (vox) 204-474-9814 (fax) 204-474-7608 mailto:hultin.,at,.cc.umanitoba.ca http://www.umanitoba.ca/chemistry/

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

la question de la maintenance (Frisch) avive les tensions: logiciels des attentes de clients : le fil embraye sur le sujet de la maintenance (ou absence de maintenance), payante (ou pas), de qualité (ou pas)

liscussion 2001: GAUSSIAN

mail.clemson.edu>subject: 5-mail.searchoate: 6 Feb 1993 10:08:20 -1812From: "Bobby clark" dobby clark@quickmail.clemson.edu>subject: Memory and cou f Cecier conduit polàck) discuterie Malinquestion 07de1 Elf-accessibilitéeas (Hultin) or

mxztuser-friendliness: 3, 10 fc black 6600 box. 3, stuzgz zg. desQUIb 93 utiliseresales ames logiciels (différents types d'utilisateurs : développeurs ou utilisateurs)

9:00 ESTFrom: "If Col Bene" <FR042008@YSUB_YSU.EDU>Subject: BSSE_calculationDate: Fri. 19 Feb. 93:11:5105 - 8:00

Samura differences Daentre Felouverture Me et Die accessibilité;

compétences nécessaires pour modéliser, parallèl

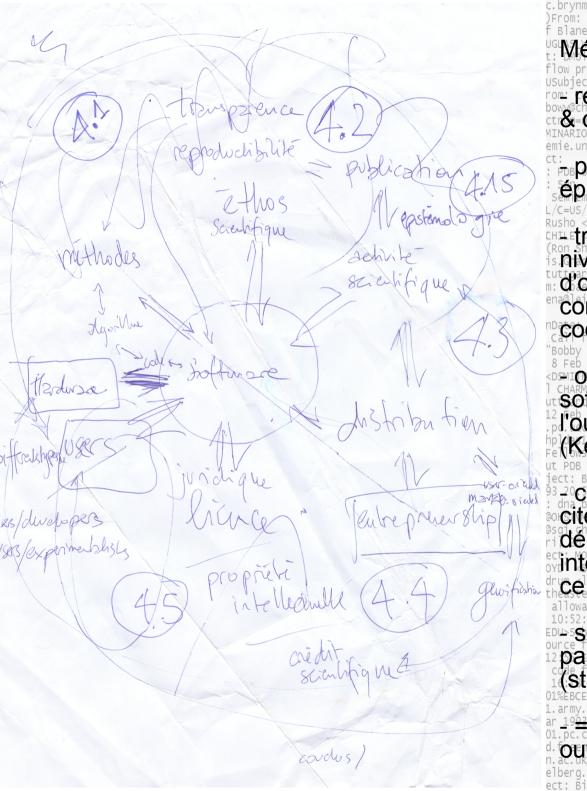
Comparaison fil 1993 et fil 2001

friendliness)

- TE.EDU>Subject: RE: PC Survey RESULTSDATE: Wed, 20 Jan 1992 15:47 CSTFFOR: "JORGE M. SMINARIO" «JSKCM@royal.crc.uno du Subject: Re: density problembate: Wed, 20 test a prografient of the problem of the
- 38:08 GMTSubject: RE: XWD->Mac conversion...Date: Wed, 27 Jan 93:14:21:29 -0700From: Jon Rusho crusho@nitrate.chem.utah.edu>subject: Re: Periodic Table WidgetDate: WidgetDate: WidgetDate: Re: Periodic Table WidgetDate: WidgetDate: Re: Periodic Table WidgetDate: WidgetDate: Re: Periodic Table WidgetDate: Re: Re: XWD->Mac Conversion...Date: Wed, 27 Jan 93:14:21:29 -0700From: Jon Rusho Crushown Laboration La
- LEDO" OSMITICOPYRIGHT: brevets from Ces calenape 10993; sedes iquestions if selections if selections if selections if selections if selections in the content of the content in the conten
- Jugdate: Tue 23 Feb 93 15:08:43 PSTFrom: wsonnen@alritak.usc.edu (wayne sonnen)subject: dna base chargesdate: 23 Feb 93 15:38:36-2300From: "Alexandre MTCU P16A"
 ject: Re _ Hudra popset a ped, 24 Feb 1 Colores September Popset a ped 15:38:36-2300From: "Alexandre MTCU P16A"
 vsubject: x-urray popset a ped 15:08:43 PSTFrom: wsonnen@alritak.usc.edu (wayne sonnen)subject: dna base chargesdate: 23 Feb 93 15:38:36-2300From: "Alexandre MTCU P16A"
 vsubject: x-urray popset popset ped 15:08:43 PSTFrom: wsonnen@alritak.usc.edu (wayne sonnen)subject: dna base chargesdate: 23 Feb 93 15:38:36-2300From: "Alexandre MTCU P16A"
 vsubject: x-urray popset ped 15:08:43 PSTFrom: wsonnen@alritak.usc.edu (wayne sonnen)subject: dna base chargesdate: 23 Feb 93 15:38:36-2300From: "Alexandre MTCU P16A"
 vsubject: x-urray popset ped 15:08:43 PSTFrom: wsonnen@alritak.usc.edu (wayne sonnen)subject: dna base chargesdate: 23 Feb 93 15:38:36-2300From: "Alexandre MTCU P16A"
 vsubject: x-urray popset ped 15:08:43 PSTFrom: "Alexandre MTCU P16A"
 vsubject: x-urray popset ped 15:08:43 PSTFrom: "Alexandre MTCU P16A"
 vsubject: x-urray popset ped 15:08:43 PSTFrom: "Alexandre MTCU P16A"
 vsubject: x-urray popset ped 15:08:43 PSTFrom: "Alexandre MTCU P16A"
 vsubject: x-urray popset ped 15:08:43 PSTFrom: "Alexandre MTCU P16A"
 vsubject: x-urray popset ped 15:08:43 PSTFrom: "Alexandre MTCU P16A"
 vsubject: x-urray popset ped 15:08:43 PSTFrom: "Alexandre MTCU P16A"
 vsubject: x-urray ped 15:08:43 PSTFrom: "Alexandre MTCU
- Edu (Gene Carter) Subject: Co MD Paris 1993 08-33:18 -0500 (EST) From: "DONALD B. 1970" < BOYD DONALD BELLLY. COM> Subject: new book on computational chemistry Date (Gene Carter) Subject: Co MD Paris Steen time of the computational chemistry Date (Gene Carter) Subject: Co MD Paris Steen time of the computation of th

```
Multiples tensions:
         EDUSSUBJECT: RE: PC SURVEY RESULTSDATE: Wed. 20 Jan 1993 15:47 CSTEROM: "JORGE N. SEMINARIO" < JSMCMOR MAIL CC. SAME OF THE CONSTRUCTION OF THE SEMINARIO" < JSMCMOR MAIL CC. SAME OF THE CONSTRUCTION OF THE SEMINARIO" < JSMCMOR MAIL CC. SAME OF THE CONSTRUCTION OF THE SEMINARIO" < JSMCMOR MAIL CC. SAME OF THE CONSTRUCTION OF THE SEMINARIO" < JSMCMOR MAIL CC. SAME OF THE CONSTRUCTION OF THE SEMINARIO OF THE CONSTRUCTION OF THE CONSTRUCTION OF THE SEMINARIO OF THE CONSTRUCTION OF THE 
          de leuradistribution AL SBDI
           de leur maintenance
           defleurautilisation 18 Jan
Questions des acteurs :
sur ce que peut et doit être l'activité scientifique (normes
vérification de la et med l'reproductibilité charm poublication sofrom et le tres lab de la peer-
reviewing, productions scientifiques comme bien commun)
                Todstukr «wipklesucsc. Edra ports summer entre Researm éthodes ved, 17et 1993 1 og iciels m: "Dres
implémentant
1 jugnate: Tue, 23 Feb 93 15:08:43 PSTFFGM: wsonnergalnitak.usc.edu. (wayne sonnen)subject: dna base chargespate: 23 Feb 93 15:38:36-2300
ject Sulnydiban bitormeed deep rétribuution non duit that the lander code gendow
vsub Sulnydiban telling in the code of the contract of the contract of the code of the 
          sur le brevet, la propriété intellectuelle, la licence
          ect: Expert Know-How wanted !!Date: 02 Mar 1903 08:13:18 -0500 (EST) From: "DONALD B. BOYD" ROYD_DONALD BOLTLLY.COM>Subject: new book on computational Surfice and Isation 2008 of Computational Surfice Production of Chief Surfice Cherches
```

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 IICHI.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 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 -



Méthode et programme sont entremeles reproductibilité vs reconnaissance (pu &-diffusion de code) 11:36 ESTECOM: - paramétrisation => transparence épistémique n'est qu'idéale sho <rusho@nitrate.chem.utah.edu>subject: Re: Periodic Table WidgetDate:
--transparence épistémique Ananiveau pub niveau code source : deux formes d'ouverture différentes et en pratique compliquées (publi : peer-reviewing, code: ouvert mais pas modifiable) ouverture du code =/ ouverture du software (possibilité de compiler : ... l'ouverture dépend aussi du hardware cité de la science (rétribution=publi) vs cité industrielle (software=commodity) --débats sur =/ formes propriété intellectuelle + licensing policy qui façonne software bien public (contribution) par/pour la communauté) ou bien privé (stabilité garantie) ; question du support - =/ catégories de users + empowe ouverture = accessibilité

Multiples tensions: au niveau de la construction des logiciels de leur distribution AL < BD de leur maintenance defleurautilisation 28 Jan Questions des acteurs : sur ce que peut etidoit être l'activité scientifique (normes «ridéales » c. lo idéal sud ouverture de la science, la transparence, vérification de la et med 1 reproductibilité charm publications of rom: et abiosympeer de la constant de la con reviewing, productions scientifiques comme bien commun) To Sturr wink lesucsc. Edrapports summer entre Researm éthodes Wed, 1 et 1993 1 logiciels m: "DR les implémentant l jugdate: Tue, 23 Feb 93 15:08:43 PSTFrom: wsonnergalnitak.usc.edu (wayne sonnen)subject: dna base chargesdate: 23 Feb 93 15:38:36-2300 ject Sturydrom bif ormeedde retributtipo mandulation tugesgivant ordetem of the production of the contraction of the contra Surilles brevet, sha coron fetéemintellectuelles, la lorice de conservation de la surille de la company de la comp s. OHIO-STATE. EDU> Subject: partial charges for fictive atoms in G920ate: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS Perspectives cauar de mars dech maretude: de de Casson om

ouverture comme valeur problématique dépend contexte

biographies de logiciels (autres sources)

et arène