

Density functional theory determination of an axial gateway to explain the rate and *endo* selectivity enhancement of Diels-Alder reactions by bis(oxazoline)-Cu(II)

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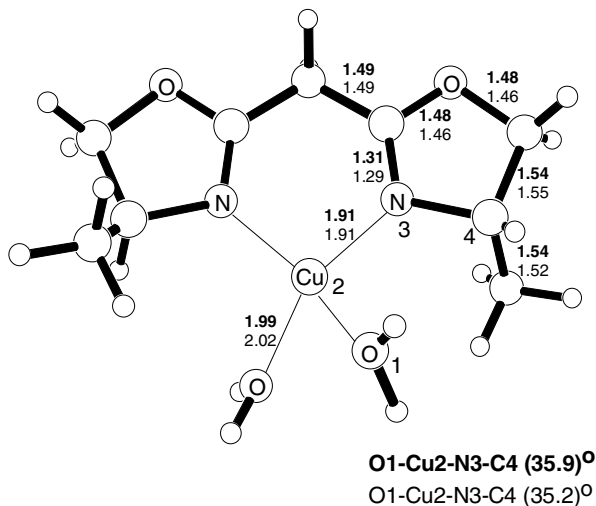
Contribution from the Center for Computational Sciences and the Department of Chemistry and Biochemistry, Duquesne University, 600 Forbes Avenue, Pittsburgh, Pennsylvania, 15282-1530.

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UB3LYP/6-31G(d) optimized ground state of methyl-bis(oxazoline)-Cu(II) coordinated to water. Bold numbers are crystallographic data for t-butyl bis(oxazoline)-Cu(II) system. Distance in Å and angles in degrees.



Cyclopentadiene in Vacuum at B3LYP/6-31G(d)

```
\Freq\UB3LYP\6-31G(d)\C5H6\JASON\13-Jun-2002\1\#\ UB
3LYP/6-31G* FREQ GEOM=CHECK\Cyclopentadiene\0,1\C\C,1,R1\C,1,R2,2,A1
\C,3,R3,1,A2,2,D0,0\C,2,R4,1,A3,3,D1,0\H,4,R5,3,A4,1,D2,0\H,5,R6,4,A5,
6,D3,0\H,3,R7,4,A6,6,D4,0\H,2,R8,5,A7,7,D5,0\H,1,R9,3,A8,8,D6,0\H,1,R1
0,2,A9,9,D7,0\R1=1.5068\R2=1.5068\R3=1.3489\R4=1.3489\R5=1.0853\R6=1.
0853\R7=1.0841\R8=1.0841\R9=1.1011\R10=1.1011\A1=103.2295\A2=109.0691\
A3=109.0707\A4=126.3296\A5=124.356\A6=126.988\A7=126.9877\A8=112.0009\
A9=112.0045\D0=-0.0042\D1=-0.0018\D2=-179.9798\D3=-0.0237\D4=-0.0004\D
5=-0.0183\D6=-59.3119\D7=-59.2917\Version=IBM-RS6000-G98RevA.3\HF=-19
4.1010581\S2=0.\S2-1=0.\S2A=0.\RMSD=6.560e-09\RMSF=2.399e-05\Dipole=-0
.1348804,0.0000346,-0.1068286\ PG=C01 [X(C5H6)]\NImag=0\
```

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole),

Raman scattering activities (A⁴/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	349.2999	521.3009	688.1490
Red. masses --	1.5521	2.3756	1.1699
Frc consts --	.1116	.3804	.3264
IR Inten --	9.6517	.0001	55.8151
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

```
Zero-point correction= .092903
(Hartree/Particle)
Thermal correction to Energy= .097046
Thermal correction to Enthalpy= .097990
Thermal correction to Gibbs Free Energy= .066305
Sum of electronic and zero-point Energies= -194.008155
Sum of electronic and thermal Energies= -194.004012
Sum of electronic and thermal Enthalpies= -194.003068
Sum of electronic and thermal Free Energies= -194.034753
```

Cyclopentadiene in PCM at B3LYP/6-31G(d)

```
FOpt\UB3LYP\6-31G(d)\C5H6\JASON\04-Jun-2003\0\#\ UB3LYP
/6-31G* OPT SCRF=(PCM,SOLVENT=8)\Cyclopentadiene\0,1\C,-0.9538607938
,-0.0002498402,-0.7555977427\C,-0.9537349687,0.0010975177,0.7496984871
\C,0.5115613508,0.0008781882,-1.0998900584\C,1.2334952498,-0.000505970
4,0.0398933391\C,0.3210786092,-0.000665566,1.19148054\H,2.3163461496,-
0.0008399133,0.1163128888\H,0.6432669689,-0.0018003401,2.2281098509\H,
0.894352814,0.001249642,-2.1143652291\H,-1.8536619675,0.0008299454,1.3
545286083\H,-1.4771278376,0.8753020584,-1.1700432499\H,-1.474412811,-0
.878067368,-1.1680502591\Version=x86-Linux-G98RevA.9\HF=-194.1063488\
S2=0.\S2-1=0.\S2A=0.\RMSD=2.535e-09\RMSF=7.657e-05\Dipole=-0.1940645,-
0.0067509,-0.1538891\PG=C01 [X(C5H6)]\@\
```

s-cis Acrylate imide at B3LYP/6-31G(d)

```
Freq\UB3LYP\6-31G(d)\C6H7N1O3\JASON\11-Jun-2002\1\
#\ UB3LYP/6-31G* FREQ GUESS=READ GEOM=CHECK\acrylimide opt.\0,1\N\C,
1,B1\O,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\C,4,B4,1,A3,2,D2,0\O,5,B5,4,A4,1,D
3,0\C,1,B6,4,A5,2,D4,0\O,7,B7,1,A6,4,D5,0\C,7,B8,1,A7,2,D6,0\C,9,B9,7,
A8,8,D7,0\H,9,B10,7,A9,8,D8,0\H,10,B11,9,A10,11,D9,0\H,10,B12,9,A11,11
,D10,0\H,4,B13,5,A12,1,D11,0\H,4,B14,5,A13,1,D12,0\H,5,B15,6,A14,2,D13
,0\H,5,B16,6,A15,2,D14,0\B1=1.41442097\B2=1.19614321\B3=1.46342491\B4
=1.53557128\B5=1.43180843\B6=1.41010883\B7=1.21435183\B8=1.49540676\B9
=1.33556234\B10=1.08593275\B11=1.08569982\B12=1.08608524\B13=1.0976526
2\B14=1.09239913\B15=1.09142543\B16=1.09603729\A1=128.95399925\A2=110.
41809608\A3=100.81836925\A4=104.68751766\A5=125.97663099\A6=122.085123
25\A7=115.23518275\A8=119.79894385\A9=119.69108305\A10=121.70069914\A1
1=120.18065449\A12=111.83266936\A13=111.85294811\A14=108.522055\A15=10
8.93750373\D1=170.77765852\D2=19.28179476\D3=-23.66035907\D4=-184.5392
6724\D5=171.53305963\D6=166.64158964\D7=-6.39073948\D8=-187.63016834\D
9=0.21528668\D10=180.45777819\D11=118.40755553\D12=-119.08605417\D13=1
42.51701501\D14=-98.46594618\Version=IBM-RS6000-G98RevA.3\HF=-513.262
8065\S2=0.\S2-1=0.\S2A=0.\RMSD=3.119e-09\RMSF=3.844e-05\Dipole=-1.9002
041,-0.245408,-2.0620295\ PG=C01 [X(C6H7N1O3)]\NImag=0\
```

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole),
Raman scattering activities (A⁴/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	59.5631	61.5914	126.5041
Red. masses --	4.3220	3.7948	3.0884
Frc consts --	.0090	.0085	.0291
IR Inten --	.2213	.1946	.4508
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
Zero-point correction=		.130600	
(Hartree/Particle)			
Thermal correction to Energy=		.139733	
Thermal correction to Enthalpy=		.140677	
Thermal correction to Gibbs Free Energy=		.095381	
Sum of electronic and zero-point Energies=		-513.132206	
Sum of electronic and thermal Energies=		-513.123074	
Sum of electronic and thermal Enthalpies=		-513.122129	

Sum of electronic and thermal Free Energies=

-513.167425

s-cis Acrylate imide PCM at B3LYP/6-31G(d)

```
|UB3LYP|6-31G(d)|C6H7N1O3|PCUSER|05-Jun-2003|0| |# UB3
LYP/6-31G(D) OPT SCRF=(PCM,SOLVENT=8) |acrylimide opt. | |0,1|N,-0.20421
61055,-0.0133746968,0.0951345826|C,-0.2078071638,0.0039226965,1.501271
6676|O,0.7275263441,0.0239517999,2.2572878679|C,-1.5627108121,-0.23500
09227,-0.4184151286|C,-2.4009256247,0.1252489702,0.8137221263|O,-1.499
7467159,-0.0343238406,1.9262691455|C,0.9657881772,0.0675201386,-0.6776
877504|O,2.0417203288,0.3685067427,-0.1900045769|C,0.7936571203,-0.233
7315804,-2.1276435755|C,1.8154157949,-0.0557403328,-2.9685873751|H,-0.
1581500715,-0.6103681525,-2.487962503|H,1.7254335707,-0.2779536117,-4.
0275957855|H,2.7688950074,0.3187678837,-2.6072893407|H,-1.7020746964,-
1.2796581007,-0.7184098412|H,-1.7856617524,0.4170722703,-1.2651680526|
H,-3.2534012558,-0.5376356747,0.9651775669|H,-2.7420326705,1.165006830
8,0.7909266003| |Version=x86-Win32-G98RevA.9|HF=-513.2784504|S2=0.|S2-1
=0.|S2A=0.|RMSD=3.425e-009|RMSF=1.065e-004|Dipole=-2.4379255,-0.325412
1,-2.4756451|PG=C01 [X(C6H7N1O3)]| |@
```

s-trans Acrylate imide at B3LYP/6-31G(d)

```
Freq\RB3LYP\6-31G(d)\C6H7N1O3\JASON\07-Jun-2002\1\
|# B3LYP/ 6-31G* FREQ GUESS=READ GEOM=CHECK\acrylimide opt.\ |0,1|N\C,
1,r1\O,2,r2,1,a1\C,1,r3,2,a2,3,d1,0\C,4,r4,1,a3,2,d2,0\O,5,r5,4,a4,1,d
3,0\C,1,r6,4,a5,2,d4,0\O,7,r7,1,a6,4,d5,0\C,7,r8,1,a7,2,d6,0\C,9,r9,7,
a8,8,d7,0\H,9,r10,7,a9,8,d8,0\H,10,r11,9,a10,11,d9,0\H,10,r12,9,a11,11
,d10,0\H,4,r13,5,a12,1,d11,0\H,4,r14,5,a13,1,d12,0\H,5,r15,6,a14,2,d13
,0\H,5,r16,6,a15,2,d14,0\ |r1=1.41614891|r2=1.19620031|r3=1.46568901|r4
=1.53355613|r5=1.43456292|r6=1.40913664|r7=1.21408553|r8=1.49471844|r9
=1.33558109|r10=1.0870814|r11=1.08635047|r12=1.08627158|r13=1.09617287
|r14=1.09130548|r15=1.09127819|r16=1.09632075|a1=128.61248123|a2=109.9
5984825|a3=100.59766929|a4=104.2673777|a5=126.5952844|a6=122.40243796\
a7=117.51737463|a8=125.95222711|a9=112.70657544|a10=121.09728314|a11=1
22.54934333|a12=111.17212938|a13=113.11071765|a14=108.38509793|a15=108
.95082248|d1=169.92843788|d2=21.22869643|d3=-26.27778558|d4=189.168148
35|d5=156.25216232|d6=166.33885597|d7=139.50094331|d8=-31.24854861|d9=
-2.09509253|d10=175.63441395|d11=118.10655511|d12=-119.29189731|d13=14
4.84277384|d14=-96.06269804\ |Version=IBM-RS6000-G98RevA.3|HF=-513.2583
913\RMSD=4.363e-09\RMSF=8.165e-05\Dipole=-1.9604671,-0.4914725,-1.9911
318 PG=C01 [X(C6H7N1O3)]\NImag=0\
```

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole),
Raman scattering activities (A⁴/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	50.5697	91.2641	133.7691
Red. masses --	5.2739	4.3277	2.3689
Frc consts --	.0079	.0212	.0250
IR Inten --	.6594	1.4415	1.5760
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Zero-point correction= .130492

(Hartree/Particle)

Thermal correction to Energy= .139618

Thermal correction to Enthalpy=	.140563
Thermal correction to Gibbs Free Energy=	.095482
Sum of electronic and zero-point Energies=	-513.127900
Sum of electronic and thermal Energies=	-513.118773
Sum of electronic and thermal Enthalpies=	-513.117829
Sum of electronic and thermal Free Energies=	-513.162909

s-trans Acrylate imide PCM at B3LYP/6-31G(d)

```
FOpt\UB3LYP\6-31G(d)\C6H7N1O3\JASON\05-Jun-2003\0\#\ UB
3LYP/6-31G(D) OPT SCRF=(PCM,SOLVENT=8)\acrylimide opt.\0,1\N,-0.0458
76295,-0.0085889914,0.0616843785\C,-0.0603610155,0.0356073186,1.470173
7812\O,0.8729835776,0.0705149236,2.2277314636\C,-1.4005438856,-0.27915
00124,-0.4438606484\C,-2.2442012205,0.1433843005,0.7616848691\O,-1.353
5226955,-0.0084296862,1.8870294507\C,1.0833023546,0.3398188568,-0.6958
216399\O,2.056681769,0.8773111353,-0.1965551354\C,1.0682204388,0.03379
01383,-2.1542608395\C,0.574674022,-1.068162029,-2.7238802655\H,1.64507
5956,0.7468888995,-2.7379844524\H,0.7138656082,-1.255628047,-3.7850583
479\H,0.0467388035,-1.8362097136,-2.1664010923\H,-1.5321905072,-1.3433
099099,-0.6651828137\H,-1.6174411225,0.3044902315,-1.3395905432\H,-3.1
133762823,-0.4939565398,0.926920421\H,-2.557223762,1.1909456008,0.7056
484057\Version=x86-Linux-G98RevA.9\HF=-513.2734667\S2=0.\S2-1=0.\S2A=
0.\RMSD=4.326e-09\RMSF=7.038e-05\Dipole=-2.4750095,-0.6672481,-2.40699
68\PG=C01 [X(C6H7N1O3)]\@
```

Acrylate imide and cyclopentadiene NC TS in vacuum at UB3LYP/6-31G(d)

```
\Freq\UB3LYP\6-31G(d)\C11H13N1O3\JASON\08-Jun-2002\1
\#\ UB3LYP/6-31G* FREQ GUESS=READ GEOM=CHECK OPTCYC=120\cypentacry_nc
opt.\0,1\C\C,1,B1\C,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\O,3,B4,4,A3,1,D2,0\
C,4,B5,3,A4,5,D3,0\C,4,B6,3,A5,5,D4,0\H,1,B7,2,A6,3,D5,0\H,1,B8,2,A7,5
,D6,0\H,2,B9,3,A8,5,D7,0\C,1,b26,8,a9,3,d8,0\C,2,b27,1,a10,8,d9,0\C,11
,b10,12,a11,3,d10,0\C,13,b11,11,a12,12,d11,0\C,11,b12,12,a13,13,d12,0\
H,13,b13,14,a14,12,d13,0\H,14,b14,12,a15,15,d14,0\H,12,b15,15,a16,11,d
15,0\H,15,b16,12,a17,13,d16,0\H,15,b17,12,a18,13,d17,0\H,11,b18,13,a19
,14,d18,0\O,7,b19,4,a20,3,d19,0\C,22,b20,7,a21,4,d20,0\O,7,b21,4,a22,3
,d21,0\H,23,b22,6,a23,4,d22,0\H,23,b23,6,a24,4,d23,0\H,6,b24,4,a25,7,d
24,0\H,6,b25,4,a26,7,d25,0\B1=1.4028891\B2=1.45135259\B3=1.42475759\B
4=1.2264739\B5=1.45806631\B6=1.39995649\B7=1.08781587\B8=1.08532323\B9
=1.08344455\b10=1.41222347\b11=1.41022603\b12=1.52330595\b13=1.0837256
1\b14=1.08385395\b15=1.08445773\b16=1.09249678\b17=1.10286687\b18=1.08
74053\b19=1.37611831\b20=1.43309907\b21=1.20026349\b22=1.09645473\b23=
1.09178362\b24=1.09320076\b25=1.09943602\b26=1.98085985\b27=2.70189774
\A1=117.68851358\A2=116.60480353\A3=120.67921651\A4=125.07168242\A5=12
3.77237461\A6=117.66421619\A7=116.46223092\A8=121.09916842\A9=96.49607
905\A10=92.857386\A11=69.88821577\A12=109.40489004\A13=39.33994293\A14
=124.82458566\A15=125.83083012\A16=124.10896684\A17=115.52007164\A18=1
08.89450947\A19=121.60372065\A20=107.85733593\A21=109.8567579\A22=129.
35526692\A23=111.68135554\A24=113.60403799\A25=111.65686123\A26=111.60
417195\D1=175.54552107\D2=177.20805872\D3=164.29374533\D4=-26.08267489
\D5=-163.6268871\D6=-24.39211121\D7=-183.73369025\d8=130.98533533\d9=1
03.58780168\d10=76.18090328\d11=-2.2052199\d12=154.77043057\d13=176.11
801317\d14=185.92578081\d15=169.60553135\d16=-140.44490409\d17=98.6659
6188\d18=197.75692569\d19=178.63047948\d20=-7.82420013\d21=-3.80750428
\d22=91.9118541\d23=-143.76401586\d24=141.92691339\d25=-96.2115612\Ve
rsion=IBM-RS6000-G98RevA.3\HF=-707.3424918\S2=0.\S2-1=0.\S2A=0.\RMSD=5
.688e-09\RMSF=3.212e-05\Dipole=-2.6363046,0.2038015,-0.3776909\ PG=C01
[X(C11H13N1O3)]\NImag=1\
```

***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole),
 Raman scattering activities (A⁴/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	-393.8664	29.1807	40.5988
Red. masses --	9.6345	6.9805	4.8074
Frc consts --	.8806	.0035	.0047
IR Inten --	21.3670	2.3675	2.2446
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000
Zero-point correction=			.226533
(Hartree/Particle)			
Thermal correction to Energy=			.239534
Thermal correction to Enthalpy=			.240478
Thermal correction to Gibbs Free Energy=			.185612
Sum of electronic and zero-point Energies=			-707.115959
Sum of electronic and thermal Energies=			-707.102958
Sum of electronic and thermal Enthalpies=			-707.102014
Sum of electronic and thermal Free Energies=			-707.156880

Acrylate imide and cyclopentadiene NC TS in PCM at UB3LYP/6-31G(d)

FTS\UB3LYP\6-31G(d)\C11H13N1O3\JASON\07-Jun-2003\1\#\# U
 B3LYP/6-31G* OPT=(TS,NOEIGEN,Z-MATRIX) SCRF=(PCM,SOLVENT=8)\cypentacr
 y_nc opt.\0,1\C\C,1,B1\C,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\O,3,B4,4,A3,1,D
 2,0\C,4,B5,3,A4,5,D3,0\C,4,B6,3,A5,5,D4,0\H,1,B7,2,A6,3,D5,0\H,1,B8,2,
 A7,5,D6,0\H,2,B9,3,A8,5,D7,0\C,1,b26,8,a9,3,d8,0\C,2,b27,1,a10,8,d9,0\
 C,11,b10,12,a11,3,d10,0\C,13,b11,11,a12,12,d11,0\C,11,b12,12,a13,13,d1
 2,0\H,13,b13,14,a14,12,d13,0\H,14,b14,12,a15,15,d14,0\H,12,b15,15,a16,
 11,d15,0\H,15,b16,12,a17,13,d16,0\H,15,b17,12,a18,13,d17,0\H,11,b18,13
 ,a19,14,d18,0\O,7,b19,4,a20,3,d19,0\C,22,b20,7,a21,4,d20,0\O,7,b21,4,a
 22,3,d21,0\H,23,b22,6,a23,4,d22,0\H,23,b23,6,a24,4,d23,0\H,6,b24,4,a25
 ,7,d24,0\H,6,b25,4,a26,7,d25,0\B1=1.39986488\B2=1.44900015\B3=1.42461
 268\B4=1.22936675\B5=1.46401892\B6=1.39252481\B7=1.08697325\B8=1.08504
 607\B9=1.08237084\b10=1.40802506\b11=1.41088329\b12=1.52006647\b13=1.0
 8422947\b14=1.08410418\b15=1.08453381\b16=1.09178663\b17=1.10316564\b1
 8=1.08692683\b19=1.36932634\b20=1.43886141\b21=1.20585362\b22=1.095092
 74\b23=1.09103267\b24=1.09201942\b25=1.09692517\b26=1.99946361\b27=2.6
 9800881\A1=118.49960176\A2=116.22357085\A3=120.67760154\A4=124.6408265
 2\A5=124.21912706\A6=117.69483318\A7=117.09476287\A8=120.95569966\A9=9
 5.14586413\A10=92.85537084\A11=69.98773931\A12=109.35643523\A13=39.220
 25612\A14=125.09409295\A15=125.79332704\A16=124.10825975\A17=115.70351
 706\A18=108.59149393\A19=122.19864198\A20=108.50906423\A21=110.1526016
 6\A22=129.63183195\A23=112.06559066\A24=113.45651215\A25=111.58521557\
 A26=110.93851675\D1=173.75148093\D2=174.23064765\D3=175.40616081\D4=-1
 3.03602547\D5=-161.97403039\D6=-21.83652965\D7=-182.59914301\d8=131.54
 30234\d9=103.72983255\d10=77.18094645\d11=-2.06151808\d12=155.73698867
 \d13=176.6019303\d14=187.16982647\d15=170.51130793\d16=-140.43238899\d
 17=99.00580872\d18=196.51010333\d19=180.10054911\d20=-7.98040853\d21=-
 0.92722812\d22=95.83799952\d23=-139.60547803\d24=137.17165924\d25=-101
 .21894205\Version=x86-Linux-G98RevA.9\HF=-707.3625528\S2=0.\S2-1=0.\S
 2A=0.\RMSD=3.680e-09\RMSF=2.470e-04\Dipole=-3.7047027,-0.2053666,-0.55

64855\PG=C01 [X(C11H13N1O3)]\ \@

Acrylate imide and cyclopentadiene NT TS in vacuum at UB3LYP/6-31G(d)

Freq\UB3LYP\6-31G(d)\C11H13N1O3\JASON\04-Jun-2002\1
\# UB3LYP/6-31G* FREQ GUESS=READ\cypentacry_nt opt.\0,1\C\C,1,B1\C,
2,B2,1,A1\N,3,B3,2,A2,1,D1,0\O,3,B4,4,A3,1,d2,0\C,4,B5,3,A4,5,D3,0\C,4
,B6,3,A5,5,D4,0\H,1,B7,2,A6,3,D5,0\H,1,B8,2,A7,5,D6,0\H,2,B9,3,A8,5,D7
,0\C,1,b26,8,A9,3,D8,0\C,2,b27,1,A10,8,D9,0\C,11,B10,12,A11,3,D10,0\C,
13,B11,11,A12,12,D11,0\C,11,B12,12,A13,13,D12,0\H,13,b13,14,a14,12,d13
,0\H,14,b14,12,a15,15,d14,0\H,12,b15,15,a16,11,d15,0\H,15,b16,12,a17,1
3,d16,0\H,15,b17,12,a18,13,d17,0\H,11,b18,13,a19,14,d18,0\O,7,b19,4,a2
0,3,d19,0\O,7,b20,4,a21,6,d20,0\C,23,b21,7,a22,4,d21,0\H,24,b22,6,a23,
7,d22,0\H,24,b23,6,a24,7,d23,0\H,6,b24,24,a25,7,d24,0\H,6,b25,24,a26,7
,d25,0\B1=1.4033\B2=1.4612\B3=1.4474\B4=1.2188\B5=1.465\B6=1.3984\B7=
1.0875\B8=1.0832\B9=1.0852\B10=1.4103\B11=1.4055\B12=1.5198\b13=1.0854
\b14=1.0839\b15=1.0836\b16=1.0917\b17=1.103\b18=1.0871\b19=1.203\b20=1
.3719\b21=1.4349\b22=1.0917\b23=1.0964\b24=1.0927\b25=1.0975\b26=2.043
\b27=2.4905\A1=127.8883\A2=116.7857\A3=119.6045\A4=124.4193\A5=120.715
9\A6=117.1382\A7=120.0239\A8=112.169\A9=94.984\A10=95.59\A11=70.3282\A
12=109.2466\A13=39.6892\A14=125.0647\A15=125.1424\A16=124.7587\A17=115
.9232\A18=108.5934\A19=122.4789\A20=128.1458\A21=108.7179\A22=109.344\
a23=113.5184\A24=111.9896\A25=112.825\A26=111.0519\D1=2.7796\d2=-181.6
509\D3=240.0399\D4=33.2085\D5=-155.3612\D6=-14.7976\D7=12.246\D8=129.3
366\D9=108.1339\D10=84.3967\D11=-2.4938\D12=151.5616\d13=175.2499\d14=
186.9267\d15=168.1697\d16=-142.7657\d17=95.9338\d18=193.3179\d19=31.84
48\d20=4.6466\d21=12.7813\d22=131.6225\d23=-103.7461\d24=130.2327\d25=
-107.5857\Version=IBM-RS6000-G98RevA.3\HF=-707.3326899\S2=0.\S2-1=0.\
S2A=0.\RMSD=5.660e-09\RMSF=7.213e-05\Dipole=-0.9387709,0.8865616,-2.29
26613\ PG=C01 [X(C11H13N1O3)]\NImag=1\

***** 1 imaginary frequencies (negative Signs) *****

Harmonic frequencies (cm**⁻¹), IR intensities (KM/Mole),
Raman scattering activities (A**⁴/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	-436.3440	42.0821	49.9058
Red. masses --	9.5765	4.5034	6.0674
Frc consts --	1.0743	.0047	.0089
IR Inten --	4.3152	3.8850	1.3396
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Zero-point correction= .226436
(Hartree/Particle)
Thermal correction to Energy= .239448
Thermal correction to Enthalpy= .240393
Thermal correction to Gibbs Free Energy= .185899
Sum of electronic and zero-point Energies= -707.106254
Sum of electronic and thermal Energies= -707.093241
Sum of electronic and thermal Enthalpies= -707.092297
Sum of electronic and thermal Free Energies= -707.146791

Acrylate imide and cyclopentadiene NT TS in PCM at UB3LYP/6-31G(d)

UB3LYP|6-31G(d)|C11H13N1O3|PCUSER|07-Jun-2003|1||# UB


```

3LYP/6-31G* OPT=(TS,NOEIGEN,Z-MATRIX) SCRF=(PCM,SOLVENT=8) | | cypentacry
_nt opt. | | 0,1|C|C,1,B1|C,2,B2,1,A1|N,3,B3,2,A2,1,D1,0|O,3,B4,4,A3,1,d2
,0|C,4,B5,3,A4,5,D3,0|C,4,B6,3,A5,5,D4,0|H,1,B7,2,A6,3,D5,0|H,1,B8,2,A
7,5,D6,0|H,2,B9,3,A8,5,D7,0|C,1,b26,8,A9,3,D8,0|C,2,b27,1,A10,8,D9,0|C
,11,B10,12,A11,3,D10,0|C,13,B11,11,A12,12,D11,0|C,11,B12,12,A13,13,D12
,0|H,13,b13,14,a14,12,d13,0|H,14,b14,12,a15,15,d14,0|H,12,b15,15,a16,1
1,d15,0|H,15,b16,12,a17,13,d16,0|H,15,b17,12,a18,13,d17,0|H,11,b18,13,
a19,14,d18,0|O,7,b19,4,a20,3,d19,0|O,7,b20,4,a21,6,d20,0|C,23,b21,7,a2
2,4,d21,0|H,24,b22,6,a23,7,d22,0|H,24,b23,6,a24,7,d23,0|H,6,b24,24,a25
,7,d24,0|H,6,b25,24,a26,7,d25,0| |B1=1.4038211|B2=1.45474783|B3=1.44020
497|B4=1.22541425|B5=1.4690667|B6=1.39104442|B7=1.08777277|B8=1.082114
02|B9=1.08513337|B10=1.41027899|B11=1.40633609|B12=1.51887115|b13=1.08
544281|b14=1.08435429|b15=1.08373207|b16=1.09117661|b17=1.1032095|b18=
1.08666354|b19=1.20775032|b20=1.36711697|b21=1.441772|b22=1.09084298|b
23=1.09550681|b24=1.09175975|b25=1.09555294|b26=2.02114716|b27=2.54086
6|A1=128.43832712|A2=117.57480545|A3=118.87037954|A4=126.07335497|A5=1
21.17592973|A6=116.38778304|A7=120.80895865|A8=112.24013062|A9=94.6709
3826|A10=94.35052315|A11=70.35087951|A12=109.10010774|A13=39.56578956|
a14=125.23813604|a15=125.25554259|a16=124.56887531|a17=115.91067325|a1
8=108.54903844|a19=122.39046583|a20=128.53334326|a21=109.04195434|a22=
109.36148021|a23=113.51080603|a24=112.33432356|a25=112.77718609|a26=11
0.88064979|D1=6.1478904|d2=-182.18080893|D3=229.24215489|D4=28.3464438
1|D5=-158.48698327|D6=-21.45398214|D7=10.69743441|D8=127.71266394|D9=1
08.20128047|D10=83.9505048|D11=-2.60266673|D12=152.50431027|d13=175.78
761579|d14=187.06983729|d15=168.00712742|d16=-142.45540274|d17=96.3906
3179|d18=193.62832185|d19=27.48465496|d20=6.45737094|d21=11.22241328|d
22=130.9957861|d23=-103.8449643|d24=130.81022802|d25=-106.55830801| |Ve
rsion=x86-Win32-G98RevA.9|HF=-707.3517291|S2=0.|S2-1=0.|S2A=0.|RMSD=5.
832e-009|RMSF=2.878e-004|Dipole=-1.2634771,0.933409,-3.3144255|PG=C01
[X(C11H13N1O3)] | |@

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Acrylate imide and cyclopentadiene XC TS in vacuum at UB3LYP/6-31G(d)

```

\Freq\UB3LYP\6-31G(d)\C11H13N1O3\JASON\06-Jun-2002\1
\|# UB3LYP/6-31G* FREQ GUESS=READ\acryl_cylco_ts opt. \0,1\C|C,1,r1\C
,2,r2,1,a1|N,3,r3,2,a2,1,d1,0|O,3,r4,4,a3,1,d2,0|C,4,r5,3,a4,5,d3,0|C,
4,r6,3,a5,5,d4,0|H,1,r7,2,a6,3,d5,0|H,1,r8,2,a7,5,d6,0|H,2,r9,3,a8,5,d
7,0|C,1,b26,8,a9,10,d8,0|C,2,b27,1,a10,8,d9,0|C,11,r10,12,a11,3,d10,0|
C,11,r11,1,a12,12,d11,0|C,12,r12,2,a13,11,d12,0|H,13,r13,12,a14,15,d13
,0|H,13,r14,12,a15,15,d14,0|H,14,r15,11,a16,12,d15,0|H,15,r16,12,a17,1
8,d16,0|H,12,r17,15,a18,19,d17,0|H,11,r18,14,a19,18,d18,0|O,7,b19,4,a2
0,3,d19,0|C,22,b20,7,a21,4,d20,0|O,7,b21,4,a22,3,d21,0|H,23,b22,6,a23,
4,d22,0|H,23,b23,6,a24,4,d23,0|H,6,b24,4,a25,7,d24,0|H,6,b25,4,a26,7,d
25,0|r1=1.4018|r2=1.4647|r3=1.4216|r4=1.2243|r5=1.4602|r6=1.4062|r7=1
.0848|r8=1.0869|r9=1.0822|r10=1.5161|r11=1.4114|r12=1.3902|r13=1.1035\
r14=1.0915|r15=1.0854|r16=1.0853|r17=1.0845|r18=1.0866|b19=1.3751|b20=
1.4316|b21=1.1981|b22=1.0964|b23=1.0918|b24=1.0928|b25=1.0986|b26=2.03
45|b27=2.5632|a1=119.9585|a2=115.6493|a3=120.5886|a4=125.4617|a5=123.7
64|a6=118.5468|a7=116.4501|a8=119.4389|a9=98.2813|a10=94.8042|a11=39.4
719|a12=102.364|a13=93.3195|a14=108.2886|a15=115.3704|a16=125.1956|a17
=125.5797|a18=125.744|a19=122.4702|a20=107.8365|a21=110.153|a22=129.38
71|a23=111.7101|a24=113.4598|a25=111.7032|a26=111.4161|d1=167.0265|d2=
169.104|d3=168.098|d4=-18.4473|d5=208.0734|d6=-13.9607|d7=178.8086|d8=
108.2293|d9=111.4777|d10=78.5468|d11=69.4272|d12=-68.8886|d13=-89.3444
|d14=149.4907|d15=173.9066|d16=-172.7555|d17=7.289|d18=-22.3337|d19=17
7.2844|d20=-8.6484|d21=-4.7695|d22=93.6376|d23=-142.2427|d24=139.4215\
d25=-98.7898\|Version=IBM-RS6000-G98RevA.3|HF=-707.3421788|S2=0.|S2-1=

```

0.\S2A=0.\RMSD=4.761e-09\RMSF=3.031e-05\Dipole=-2.8013023,0.3613371,-0.4396104\ PG=C01 [X(C11H13N1O3)]\NImag=1\

***** 1 imaginary frequencies (negative Signs) *****

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole),
Raman scattering activities (A⁴/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	-427.2017	31.7251	41.3083
Red. masses --	9.8519	4.9861	6.1189
Frc consts --	1.0593	.0030	.0062
IR Inten --	13.9242	3.1745	.1571
Raman Activ --	.0000	.0000	.0000
Depolar --	.0000	.0000	.0000

Zero-point correction= .226703
(Hartree/Particle)
Thermal correction to Energy= .239656
Thermal correction to Enthalpy= .240600
Thermal correction to Gibbs Free Energy= .185936
Sum of electronic and zero-point Energies= -707.115475
Sum of electronic and thermal Energies= -707.102523
Sum of electronic and thermal Enthalpies= -707.101579
Sum of electronic and thermal Free Energies= -707.156242

Acrylate imide and cyclopentadiene XC TS in PCM at UB3LYP/6-31G(d)

N-N= 1.007473097393D+03 E-N=-3.663329534173D+03 KE= 7.008620587618D+02
1\1\GINC-TUKY\FTS\UB3LYP\6-31G(d)\C11H13N1O3\JASON\07-Jun-2003\1\#\ UB
3LYP/6-31G* OPT=(TS,NOEIGEN,Z-MATRIX) SCRF=(PCM,SOLVENT=8)\acryl_cylc
o_ts opt pcm.\0,1\C\C,1,r1\C,2,r2,1,a1\N,3,r3,2,a2,1,d1,0\O,3,r4,4,a3
,1,d2,0\C,4,r5,3,a4,5,d3,0\C,4,r6,3,a5,5,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r
8,2,a7,5,d6,0\H,2,r9,3,a8,5,d7,0\C,1,b26,8,a9,10,d8,0\C,2,b27,1,a10,8,
d9,0\C,11,r10,12,a11,3,d10,0\C,11,r11,1,a12,12,d11,0\C,12,r12,2,a13,11
,d12,0\H,13,r13,12,a14,15,d13,0\H,13,r14,12,a15,15,d14,0\H,14,r15,11,a
16,12,d15,0\H,15,r16,12,a17,18,d16,0\H,12,r17,15,a18,19,d17,0\H,11,r18
,14,a19,18,d18,0\O,7,b19,4,a20,3,d19,0\C,22,b20,7,a21,4,d20,0\O,7,b21,
4,a22,3,d21,0\H,23,b22,6,a23,4,d22,0\H,23,b23,6,a24,4,d23,0\H,6,b24,4,
a25,7,d24,0\H,6,b25,4,a26,7,d25,0\|r1=1.40009658\r2=1.45487129\r3=1.42
313807\r4=1.22947132\r5=1.46541659\r6=1.39580664\r7=1.08456323\r8=1.08
711675\r9=1.08155691\r10=1.515604\r11=1.40879819\r12=1.3864774\r13=1.1
0350756\r14=1.09150424\r15=1.0854195\r16=1.08512376\r17=1.08466957\r18
=1.08630728\b19=1.36743449\b20=1.43886081\b21=1.20521023\b22=1.0948454
5\b23=1.0910124\b24=1.09190541\b25=1.0967868\b26=2.03288987\b27=2.6128
7284\a1=120.55640525\a2=115.51542699\a3=120.30847494\a4=124.91608944\a
5=123.9469277\a6=118.39326447\a7=116.93607395\a8=119.52008837\a9=98.10
023233\a10=93.92458324\a11=39.322083\a12=101.7636269\a13=92.36904646\a
14=108.4169702\a15=115.48720243\a16=125.16215274\a17=125.5849382\a18=1
25.64223279\a19=122.61607168\a20=108.52974913\a21=110.33328422\a22=129
.55040229\a23=112.05777347\a24=113.40517714\a25=111.60282677\a26=110.8
8052142\d1=168.54637725\d2=169.79965094\d3=176.21115181\d4=-12.3890229
7\d5=207.49356585\d6=-13.58186994\d7=179.74549977\d8=108.53264535\d9=1
11.22813643\d10=78.42810158\d11=69.61259673\d12=-69.09928135\d13=-90.8
5468795\d14=148.14928657\d15=174.3271595\d16=-173.3092483\d17=6.533551

```
63\d18=-22.01866299\d19=180.80566513\d20=-7.88402625\d21=-0.18631672\d
22=96.80491252\d23=-138.66412323\d24=135.99974631\d25=-102.38484662\\V
ersion=x86-Linux-G98RevA.9\HF=-707.3622138\S2=0.\S2-1=0.\S2A=0.\RMSD=7
.625e-09\RMSF=2.260e-04\Dipole=-3.7967798,-0.0062663,-0.5851118\PG=C01
[X(C11H13N1O3)]\ \@
```

Acrylate imide and cyclopentadiene XT TS in vacuum at UB3LYP/6-31G(d)

```
Freq\UB3LYP\6-31G(d)\C11H13N1O3\JASON\31-Aug-2002\1
\#\ UB3LYP/6-31G(D) FREQ GUESS=READ GEOM=CHECK\cypentacry_xt opt.\0,
1\C\C,1,B1\C,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\O,3,B4,4,A3,1,D2,0\C,4,B5,3,
A4,5,d3,0\C,4,B6,3,A5,5,d4,0\H,1,B7,2,A6,3,D5,0\H,1,B8,2,A7,5,D6,0\H,2
,B9,3,A8,5,D7,0\C,1,b26,8,A9,10,D8,0\C,2,b27,1,A10,8,D9,0\C,11,B10,12,
A11,3,D10,0\C,11,B11,1,A12,12,D11,0\C,12,B12,2,A13,11,D12,0\H,13,B13,1
2,A14,15,D13,0\H,13,B14,12,A15,15,D14,0\H,14,B15,11,A16,12,D15,0\H,15,
B16,12,A17,18,D16,0\H,12,B17,15,A18,19,D17,0\H,11,B18,14,A19,18,D18,0\
O,7,b19,4,a20,3,d19,0\O,7,b20,4,a21,6,d20,0\C,23,b21,7,a22,4,d21,0\H,2
4,b22,6,a23,7,d22,0\H,24,b23,6,a24,7,d23,0\H,6,b24,24,a25,7,d24,0\H,6,
b25,24,a26,7,d25,0\B1=1.40274313\B2=1.44530314\B3=1.48206032\B4=1.219
16733\B5=1.46796926\B6=1.3956804\B7=1.08552141\B8=1.087059\B9=1.084356
82\B10=1.51584605\B11=1.40980328\B12=1.38770059\B13=1.1035963\B14=1.08
693765\B15=1.08554401\B16=1.08488371\B17=1.0828645\B18=1.08694805\b19=
1.20767876\b20=1.36750042\b21=1.43609354\b22=1.09633973\b23=1.09181156
\b24=1.09795464\b25=1.09381723\b26=2.04389551\b27=2.58662523\A1=126.39
441118\A2=116.59856168\A3=118.3577119\A4=115.84490366\A5=117.15767916\
A6=118.0004181\A7=117.8317119\A8=112.69189614\A9=96.86378648\A10=94.14
632061\A11=39.27984111\A12=103.28691418\A13=90.46411756\A14=107.743836
03\A15=115.44063172\A16=125.20789703\A17=125.55595038\A18=127.01677897
\A19=122.34121753\A20=127.59656155\A21=109.32591755\A22=109.40336067\A
23=111.97823842\A24=113.7076801\A25=112.06483525\A26=112.79663733\D1=-
7.99536889\D2=-172.18446413\d3=293.89459832\d4=63.69915874\D5=-144.626
98094\D6=9.76816699\D7=1.17792246\D8=105.42509469\D9=116.00445853\D10=
86.63211894\D11=69.11338957\D12=-69.98839853\D13=-88.87325549\D14=151.
12395131\D15=174.76395119\D16=-173.09584061\D17=4.67541921\D18=-21.825
73904\d19=32.45925719\d20=-16.727449\d21=-2.29035407\d22=106.06105869\
d23=-129.21783876\d24=101.20717374\d25=-135.05429835\\Version=IBM-RS60
00-G98RevA.3\HF=-707.3341681\S2=0.\S2-1=0.\S2A=0.\RMSD=6.871e-09\RMSF=
3.669e-05\Dipole=-0.5551379,0.896283,-1.860168\ \PG=C01
[X(C11H13N1O3)]\NImag=1\
```

***** 1 imaginary frequencies (negative Signs) *****

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole),
Raman scattering activities (A⁴/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1	2	3
	?A	?A	?A
Frequencies	-- -409.5597	43.9961	47.3113
Red. masses	-- 9.2697	4.4861	5.4321
Frc consts	-- .9161	.0051	.0072
IR Inten	-- 25.8887	1.9277	5.3368
Raman Activ	-- .0000	.0000	.0000
Depolar	-- .0000	.0000	.0000

```
Zero-point correction= .226478
(Hartree/Particle)
Thermal correction to Energy= .239466
```

Thermal correction to Enthalpy=	.240410
Thermal correction to Gibbs Free Energy=	.185951
Sum of electronic and zero-point Energies=	-707.107690
Sum of electronic and thermal Energies=	-707.094702
Sum of electronic and thermal Enthalpies=	-707.093758
Sum of electronic and thermal Free Energies=	-707.148218

Acrylate imide and cyclopentadiene XT TS in PCM at UB3LYP/6-31G(d)

N-N= 1.022646097763D+03 E-N=-3.693774572092D+03 KE= 7.008781729605D+02
 1\1\GINC-TUKY\FTS\UB3LYP\6-31G(d)\C11H13N1O3\JASON\13-Jun-2003\1\#\ UB
 3LYP/6-31G(D) OPT=(TS,NOEIGEN,Z-MATRIX) SCRF=(PCM,SOLVENT=8)\cypentac
 ry_xt opt.\0,1\C\C,1,B1\C,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\O,3,B4,4,A3,1,
 D2,0\C,4,B5,3,A4,5,d3,0\C,4,B6,3,A5,5,d4,0\H,1,B7,2,A6,3,D5,0\H,1,B8,2
 ,A7,5,D6,0\H,2,B9,3,A8,5,D7,0\C,1,b26,8,A9,10,D8,0\C,2,b27,1,A10,8,D9,
 0\C,11,B10,12,A11,3,D10,0\C,11,B11,1,A12,12,D11,0\C,12,B12,2,A13,11,D1
 2,0\H,13,B13,12,A14,15,D13,0\H,13,B14,12,A15,15,D14,0\H,14,B15,11,A16,
 12,D15,0\H,15,B16,12,A17,18,D16,0\H,12,B17,15,A18,19,D17,0\H,11,B18,14
 ,A19,18,D18,0\O,7,b19,4,a20,3,d19,0\O,7,b20,4,a21,6,d20,0\C,23,b21,7,a
 22,4,d21,0\H,24,b22,6,a23,7,d22,0\H,24,b23,6,a24,7,d23,0\H,6,b24,2,a2
 5,7,d24,0\H,6,b25,24,a26,7,d25,0\B1=1.40374596\B2=1.44281029\B3=1.467
 93541\B4=1.22361879\B5=1.46957948\B6=1.38610113\B7=1.08550475\B8=1.086
 51102\B9=1.08389622\B10=1.51714768\B11=1.40992471\B12=1.384933\B13=1.1
 0331502\B14=1.0894139\B15=1.08542473\B16=1.08488088\B17=1.08367545\B18
 =1.08644706\b19=1.20997257\b20=1.36617936\b21=1.44195176\b22=1.0950704
 1\b23=1.09115079\b24=1.09797399\b25=1.09241607\b26=2.0206763\b27=2.608
 68493\A1=125.54617558\A2=115.43919952\A3=118.96346489\A4=118.53604354\
 A5=119.17720804\A6=118.09581796\A7=118.21127016\A8=113.88518682\A9=97.
 96131722\A10=93.82261023\A11=39.31486784\A12=102.55449283\A13=91.32661
 67\A14=108.26507695\A15=115.6560224\A16=125.11964305\A17=125.64750883\
 A18=126.30162773\A19=122.17166919\A20=127.81017802\A21=109.42323118\A2
 2=109.47996204\A23=112.04572635\A24=113.56863448\A25=111.9541062\A26=1
 12.50273635\D1=5.37424225\D2=-179.20856073\d3=265.70747249\d4=43.32956
 159\D5=-150.96367654\D6=-9.22207083\D7=9.28140851\D8=106.71431803\D9=1
 13.71366177\D10=82.92669843\D11=69.41824449\D12=-69.64734973\D13=-89.1
 0418828\D14=150.33711647\D15=174.84479787\D16=-173.28292396\D17=3.8584
 2024\D18=-22.30624815\d19=28.96110358\d20=-12.8247343\d21=-4.41631227\
 d22=106.15579133\d23=-129.00719018\d24=103.89082518\d25=-133.0684828\
 Version=x86-Linux-G98RevA.9\HF=-707.3504339\S2=0.\S2-1=0.\S2A=0.\RMSD=
 7.670e-09\RMSF=2.014e-04\Dipole=-1.441616,1.0906825,-2.8646075\PG=C01
 [X(C11H13N1O3)]\@

Bis(oxazoline)-Cu(II) coordinated to acrylate imide in vacuum at UB3LYP/6-31G(d)

Freq\UB3LYP\6-31G(d)\C15H21Cu1N3O5(2+,2)\JASON\15-Dec-2
 002\1\#\ UB3LYP/6-31G* FREQ GUESS=MIX SCFCYC=120 SCFCON=6\Bisoxacry o
 pt.\2,2\C\Cu,1,B1\C,1,B2,2,A1\C,1,B3,2,A2,3,D1,0\N,3,B4,1,A3,2,D2,0\N
 ,4,B5,1,A4,2,D3,0\O,3,B6,1,A5,2,D4,0\O,4,B7,1,A6,2,D5,0\C,5,B8,3,A7,1,
 D6,0\C,6,B9,4,A8,1,D7,0\C,7,B10,3,A9,1,D8,0\C,8,B11,4,A10,1,D9,0\C,9,B
 12,5,A11,3,D10,0\C,10,B13,6,A12,4,D11,0\H,1,B14,2,A13,6,D12,0\H,1,B15,
 2,A14,6,D13,0\H,11,B16,7,A15,3,D14,0\H,12,B17,8,A16,4,D15,0\H,11,B18,7
 ,A17,3,D16,0\H,12,B19,8,A18,4,D17,0\H,13,B20,9,A19,5,D18,0\H,14,B21,10
 ,A20,6,D19,0\H,13,B22,9,A21,5,D20,0\H,14,B23,10,A22,6,D21,0\H,13,B24,9
 ,A23,5,D22,0\H,14,B25,10,A24,6,D23,0\O,2,B26,1,A25,3,D24,0\O,2,B27,1,A
 26,3,D25,0\H,9,B28,5,A27,3,D26,0\H,10,B29,6,A28,4,D27,0\C,28,B30,2,A29
 ,1,D28,0\O,31,B31,28,A30,2,D29,0\C,32,B32,31,A31,28,D30,0\N,31,B33,28,
 A32,2,D31,0\C,27,B34,2,A33,1,D32,0\C,34,B35,31,A34,28,D33,0\H,36,B36,3
 4,A35,31,D34,0\H,36,B37,34,A36,31,D35,0\H,33,B38,32,A37,31,D36,0\H,33,

B39, 32, A38, 31, D37, 0\C, 35, B40, 27, A39, 2, D38, 0\H, 41, B41, 35, A40, 27, D39, 0\C, 41, B42, 35, A41, 27, D40, 0\H, 43, B43, 41, A42, 35, D41, 0\H, 43, B44, 41, A43, 35, D42, 0\B1=3.376512\B2=1.495764\B3=1.495942\B4=1.295075\B5=1.294672\B6=1.316432\B7=1.315765\B8=1.497714\B9=1.499794\B10=1.466886\B11=1.468582\B12=1.527508\B13=1.527433\B14=1.099087\B15=1.097985\B16=1.090864\B17=1.090943\B18=1.091243\B19=1.091059\B20=1.095141\B21=1.095014\B22=1.095168\B23=1.095295\B24=1.094959\B25=1.094903\B26=1.956111\B27=1.951786\B28=1.093333\B29=1.092803\B30=1.236264\B31=1.306876\B32=1.462723\B33=1.39355\B34=1.254898\B35=1.486341\B36=1.090984\B37=1.093035\B38=1.089041\B39=1.091046\B40=1.460132\B41=1.083493\B42=1.343853\B43=1.085528\B44=1.085471\A1=58.401225\A2=58.392305\A3=128.115975\A4=127.979386\A5=114.430207\A6=114.488619\A7=108.095983\A8=108.067762\A9=107.772164\A10=107.679306\A11=111.674671\A12=111.570934\A13=124.95763\A14=130.318406\A15=106.973204\A16=106.873384\A17=106.976297\A18=106.980094\A19=111.218506\A20=111.237755\A21=111.264469\A22=111.318473\A23=109.954837\A24=109.842199\A25=136.452382\A26=136.128067\A27=107.742353\A28=107.825032\A29=128.087917\A30=121.842718\A31=111.117116\A32=126.809612\A33=132.732721\A34=109.607496\A35=110.811895\A36=109.990569\A37=107.182524\A38=106.922823\A39=121.815549\A40=118.642274\A41=121.030987\A42=120.815527\A43=121.75254\D1=176.670913\D2=1.793175\D3=3.037584\D4=-178.882903\D5=-177.930665\D6=177.509809\D7=177.302523\D8=179.018475\D9=178.358181\D10=-117.989771\D11=-117.033052\D12=89.32197\D13=-90.768137\D14=-117.392881\D15=-115.995875\D16=124.758549\D17=126.147123\D18=-62.261349\D19=-62.081744\D20=58.981575\D21=59.266337\D22=178.791553\D23=179.083738\D24=39.127189\D25=-142.478787\D26=121.014854\D27=121.832308\D28=176.742724\D29=-175.148529\D30=175.716218\D31=5.864245\D32=176.298708\D33=174.714573\D34=130.026041\D35=-108.299125\D36=133.169557\D37=-108.638408\D38=-172.085246\D39=-177.942971\D40=3.237181\D41=179.193453\D42=-0.311895\|V ersion=x86-Linux-G98RevA.9\HF=-2764.4857394\S2=0.751884\S2-1=0.\S2A=0.750003\RMSD=4.728e-07\RMSF=1.814e-05\Dipole=0.7224086,0.6125058,2.3747185\ \PG=C01 [X(C15H21Cu1N3O5)]\NImag=0\

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole),
Raman scattering activities (A⁴/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	23.0833	24.7507	35.1672
Red. masses --	3.3137	4.5789	5.1549
Frc consts --	0.0010	0.0017	0.0038
IR Inten --	0.0555	0.0825	4.1053
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

Zero-point correction= 0.367116
(Hartree/Particle)
Thermal correction to Energy= 0.391219
Thermal correction to Enthalpy= 0.392163
Thermal correction to Gibbs Free Energy= 0.310523
Sum of electronic and zero-point Energies= -2764.118624
Sum of electronic and thermal Energies= -2764.094521
Sum of electronic and thermal Enthalpies= -2764.093577
Sum of electronic and thermal Free Energies= -2764.175217

Bis(oxazoline)-Cu(II) coordinated to acrylate imide in PCM at UB3LYP/6-31G(d)

N-N= 2.828829915478D+03 E-N=-1.214729911356D+04 KE= 2.751664932587D+03
1|1|UNPC-UNK|SP|UB3LYP|6-31G(d)|C15H21Cu1N3O5(2+,2)|PCUSER|26-May-2003
|0|#UB3LYP/6-31G* SP SCRF=(PCM,READ,SOLVENT=8)|Bisoxacry opt. ||2,2|
C|Cu,1,3.376512|C,1,1.495764,2,58.401233|C,1,1.495941,2,58.392308,3,17
6.670943,0|N,3,1.295075,1,128.115921,2,1.793169,0|N,4,1.294672,1,127.9
79409,2,3.037551,0|O,3,1.316432,1,114.430198,2,-178.882924,0|O,4,1.315
766,1,114.488635,2,-177.930644,0|C,5,1.497715,3,108.095943,1,177.50979
6,0|C,6,1.499794,4,108.067762,1,177.302535,0|C,7,1.466886,3,107.772123
,1,179.018519,0|C,8,1.468582,4,107.679336,1,178.358173,0|C,9,1.527508,
5,111.674634,3,-117.989764,0|C,10,1.527433,6,111.570923,4,-117.032997,
0|H,1,1.099087,2,124.957657,6,89.322,0|H,1,1.097985,2,130.318397,6,-90
.768176,0|H,11,1.090864,7,106.97317,3,-117.39289,0|H,12,1.090943,8,106
.873362,4,-115.995884,0|H,11,1.091243,7,106.976321,3,124.75854,0|H,12,
1.091059,8,106.980085,4,126.147118,0|H,13,1.095141,9,111.218487,5,-62.
261408,0|H,14,1.095015,10,111.237693,6,-62.081758,0|H,13,1.095167,9,11
1.264501,5,58.981584,0|H,14,1.095294,10,111.318478,6,59.266328,0|H,13,
1.094959,9,109.954775,5,178.791561,0|H,14,1.094903,10,109.842162,6,179
.08378,0|O,2,1.956111,1,136.452397,3,39.127216,0|O,2,1.951786,1,136.12
8069,3,-142.478856,0|H,9,1.093333,5,107.742358,3,121.014858,0|H,10,1.0
92803,6,107.825028,4,121.832348,0|C,28,1.236263,2,128.087944,1,176.742
727,0|O,31,1.306876,28,121.842738,2,-175.148521,0|C,32,1.462723,31,111
.1171,28,175.716219,0|N,31,1.39355,28,126.809594,2,5.864322,0|C,27,1.2
54898,2,132.732752,1,176.298691,0|C,34,1.486341,31,109.607509,28,174.7
14564,0|H,36,1.090984,34,110.811902,31,130.026035,0|H,36,1.093035,34,1
09.990542,31,-108.29914,0|H,33,1.089041,32,107.182505,31,133.169584,0|
H,33,1.091046,32,106.922837,31,-108.638387,0|C,35,1.460132,27,121.8155
75,2,-172.085267,0|H,41,1.083494,35,118.642294,27,-177.943002,0|C,41,1
.343853,35,121.031005,27,3.237151,0|H,43,1.085528,41,120.815547,35,179
.19346,0|H,43,1.085472,41,121.752521,35,-0.311871,0|Version=x86-Win32
-G98RevA.9|HF=-2764.6716614|S2=0.752223|S2-1=0.|S2A=0.750005|RMSD=8.12
5e-005|Dipole=0.6451804,0.5068494,2.4807843|PG=C01 [X(C15H21Cu1N3O5)]

TS of methyl substituted bis(oxazoline)-Cu(II) NC Re in vacuum at UB3LYP/6-31G(d)

UB3LYP/6-31G(D) FREQ GUESS=READ GEOM=CHECK\bisoxc2_acry_nc1
opt.\2,2\C\Cu,1,B1\C,1,B2,2,A1\C,1,B3,2,A2,3,D1,0\N,3,B4,1,A3,2,D2,0\
N,4,B5,1,A4,2,D3,0\O,3,B6,1,A5,2,D4,0\O,4,B7,1,A6,2,D5,0\C,5,B8,3,A7,1
,D6,0\C,6,B9,4,A8,1,D7,0\C,7,B10,3,A9,1,D8,0\C,8,B11,4,A10,1,D9,0\C,9,
B12,5,A11,3,D10,0\C,10,B13,6,A12,4,D11,0\H,1,B14,2,A13,5,D12,0\H,1,B15
,2,A14,5,D13,0\H,11,B16,7,A15,3,D14,0\H,12,B17,8,A16,4,D15,0\H,11,B18,
7,A17,3,D16,0\H,12,B19,8,A18,4,D17,0\H,13,B20,9,A19,5,D18,0\H,14,B21,1
0,A20,6,D19,0\H,13,B22,9,A21,5,D20,0\H,14,B23,10,A22,6,D21,0\H,13,B24,
9,A23,5,D22,0\H,14,B25,10,A24,6,D23,0\O,2,B26,1,A25,3,D24,0\O,2,B27,1,
A26,3,D25,0\H,9,B28,5,A27,3,D26,0\H,10,B29,6,A28,4,D27,0\C,28,B30,2,A2
9,1,D28,0\O,31,B31,28,A30,2,D29,0\C,32,B32,31,A31,28,D30,0\N,31,B33,28
,A32,2,D31,0\C,27,B34,2,A33,1,D32,0\C,34,B35,31,A34,28,D33,0\H,36,B36,
34,A35,31,D34,0\H,36,B37,34,A36,31,D35,0\H,33,B38,32,A37,31,D36,0\H,33
,B39,32,A38,31,D37,0\C,35,B40,27,A39,2,D38,0\H,41,B41,35,A40,27,D39,0\
C,41,B42,35,A41,27,D40,0\H,43,B43,41,A42,35,D41,0\H,43,B44,41,A43,35,D
42,0\C,43,B45,41,A44,35,D43,0\C,46,B46,43,A45,41,D44,0\C,47,B47,46,A46
,43,D45,0\C,46,B48,43,A47,41,D46,0\C,47,B49,46,A48,43,D47,0\H,50,B50,4
7,A49,46,D48,0\H,50,B51,47,A50,46,D49,0\H,47,B52,46,A51,43,D50,0\H,48,
B53,47,A52,46,D51,0\H,49,B54,46,A53,43,D52,0\H,46,B55,43,A54,41,D53,0\
\B1=3.39341482\B2=1.49544248\B3=1.49626076\B4=1.29269082\B5=1.29262129
\B6=1.32024873\B7=1.31856808\B8=1.4934782\B9=1.4982244\B10=1.4645409\B
11=1.467738\B12=1.52774508\B13=1.52768963\B14=1.09933937\B15=1.0972663

```

\B16=1.09117589\B17=1.09112708\B18=1.09142531\B19=1.09109569\B20=1.094
76545\B21=1.09470495\B22=1.09519378\B23=1.0953998\B24=1.09544507\B25=1
.09494084\B26=1.92841305\B27=1.93590371\B28=1.09339177\B29=1.09254583\
B30=1.24250888\B31=1.31604223\B32=1.45961585\B33=1.37212462\B34=1.2781
805\B35=1.47772303\B36=1.09154803\B37=1.09416812\B38=1.08903757\B39=1.
09172901\B40=1.40818598\B41=1.08215781\B42=1.39875963\B43=1.08500819\B
44=1.08364956\B45=2.1293775\B46=2.34777517\B47=1.36968066\B48=1.393793
84\B49=1.49589393\B50=1.09346276\B51=1.10368054\B52=1.08474038\B53=1.0
8385028\B54=1.085147\B55=1.08494137\A1=58.4078728\A2=58.43864977\A3=12
8.15031654\A4=127.9017884\A5=114.3103537\A6=114.40508978\A7=108.046995
57\A8=107.93312206\A9=107.58421847\A10=107.48089496\A11=111.53540461\A
12=111.49326097\A13=122.12822055\A14=133.06151804\A15=107.02169226\A16
=106.9085166\A17=107.06509445\A18=107.0503325\A19=110.88731295\A20=111
.17769335\A21=111.27549385\A22=111.29682284\A23=110.03190697\A24=109.8
667374\A25=135.13473985\A26=134.84935906\A27=107.48689822\A28=107.8095
9927\A29=125.95753852\A30=120.71667894\A31=110.10424972\A32=127.441470
83\A33=129.47533768\A34=109.60410586\A35=110.4959993\A36=110.29827328\
A37=107.40004181\A38=107.18323708\A39=123.55033883\A40=118.67276751\A4
1=121.7165134\A42=117.973324\A43=118.88978053\A44=110.57963299\A45=98.
418964\A46=71.47997866\A47=99.63532\A48=39.03319986\A49=115.34797458\A
50=108.32280318\A51=162.42849262\A52=126.00345284\A53=124.87395689\A54
=96.62520206\D1=173.28160561\D2=0.87307321\D3=3.2291321\D4=-179.065295
54\D5=-177.93734819\D6=178.25683477\D7=176.99577427\D8=178.36268104\D9
=178.25486479\D10=-118.07679246\D11=-116.56895051\D12=-94.06760919\D13
=85.76131305\D14=-117.39267311\D15=-115.44169698\D16=124.80184874\D17=
126.69993607\D18=-62.16467033\D19=-61.63701529\D20=58.86928194\D21=59.
59561264\D22=178.46899898\D23=179.42741822\D24=42.90414342\D25=-139.73
025392\D26=121.33196145\D27=122.45342979\D28=-175.81208416\D29=-176.29
909964\D30=175.80259551\D31=5.14383661\D32=159.52126157\D33=172.273399
5\D34=133.74944686\D35=-105.05348571\D36=135.51887827\D37=-106.2040063
7\D38=-152.65213867\D39=177.29661578\D40=2.00532308\D41=156.36659361\D
42=9.36712518\D43=-104.08956289\D44=3.70924024\D45=94.2590566\D46=74.2
7832507\D47=-97.67218634\D48=127.98526095\D49=-113.73994001\D50=-81.44
104273\D51=-178.03108533\D52=85.87122381\D53=-160.46756377\Version=HP
-PARisc-HPUX-G98RevA.11\HF=-2958.594269\S2=0.751909\S2-1=0.\S2A=0.7500
03\RMSD=8.024e-09\RMSF=4.380e-05\Dipole=0.6433151,0.7414459,1.5959569\
PG=C01 [X(C20H27Cu1N3O5)]\NImag=1\

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*****      1 imaginary frequencies (negative Signs) *****
Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
Raman scattering activities (A**4/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal
coordinates:

```

	1	2	3
	?A	?A	?A
Frequencies --	-248.1153	14.6159	25.4354
Red. masses --	8.7736	4.6626	3.8060
Frc consts --	0.3182	0.0006	0.0015
IR Inten --	277.2392	0.0223	0.0928
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

```

Zero-point correction= 0.462400
(Hartree/Particle)
Thermal correction to Energy= 0.490853
Thermal correction to Enthalpy= 0.491797
Thermal correction to Gibbs Free Energy= 0.399272

```

Sum of electronic and zero-point Energies=	-2958.131869
Sum of electronic and thermal Energies=	-2958.103416
Sum of electronic and thermal Enthalpies=	-2958.102472
Sum of electronic and thermal Free Energies=	-2958.194997

TS of methyl substituted bis(oxazoline)-Cu(II) NC *Re* in PCM at UB3LYP/6-31G(d)

```
UB3LYP/6-31G(D) SP SCRF=(PCM,READ,SOLVENT=CH2CL2) | | ncrepnc opt. |
| 2, 2 | C | Cu, 1, 3.39237 | C, 1, 1.495855, 2, 58.474141 | C, 1, 1.496363, 2, 58.351938,
3, 174.650494, 0 | N, 3, 1.292765, 1, 128.090017, 2, 0.86314, 0 | N, 4, 1.292801, 1, 12
7.990716, 2, 3.435866, 0 | O, 3, 1.31998, 1, 114.346872, 2, -179.319072, 0 | O, 4, 1.3
18531, 1, 114.32356, 2, -177.488961, 0 | C, 5, 1.495215, 3, 107.996134, 1, 177.4861
71, 0 | C, 6, 1.497965, 4, 108.004717, 1, 178.232296, 0 | C, 7, 1.465786, 3, 107.53759
4, 1, 178.156102, 0 | C, 8, 1.467255, 4, 107.577264, 1, 179.231466, 0 | C, 9, 1.527771
5, 111.512793, 3, -116.759602, 0 | C, 10, 1.527009, 6, 111.675415, 4, -119.39669,
0 | H, 1, 1.099116, 2, 123.382901, 6, 90.055319, 0 | H, 1, 1.097531, 2, 131.870611, 6,
-89.914409, 0 | H, 11, 1.091225, 7, 107.013854, 3, -116.231879, 0 | H, 12, 1.090813,
8, 106.967319, 4, -118.251933, 0 | H, 11, 1.091195, 7, 107.06981, 3, 125.943177, 0 |
H, 12, 1.09143, 8, 107.003017, 4, 123.927821, 0 | H, 13, 1.094655, 9, 111.048161, 5,
-61.821646, 0 | H, 14, 1.094666, 10, 110.947404, 6, -62.374643, 0 | H, 13, 1.095337,
9, 111.191218, 5, 59.290201, 0 | H, 14, 1.095553, 10, 111.241021, 6, 59.065913, 0 | H
, 13, 1.095015, 9, 110.032906, 5, 179.104925, 0 | H, 14, 1.094969, 10, 109.887329, 6
, 178.860738, 0 | O, 2, 1.918578, 1, 136.394575, 3, 39.329712, 0 | O, 2, 1.943112, 1, 1
33.954285, 3, -139.080186, 0 | H, 9, 1.093013, 5, 107.734504, 3, 122.464327, 0 | H, 1
0, 1.092801, 6, 107.63045, 4, 119.878175, 0 | C, 28, 1.24229, 2, 125.417594, 1, 165.
656333, 0 | O, 31, 1.315643, 28, 120.605501, 2, -170.212571, 0 | C, 32, 1.458678, 31,
110.442348, 28, 175.274178, 0 | N, 31, 1.373052, 28, 127.545323, 2, 10.327651, 0 | C
, 27, 1.277554, 2, 131.885022, 1, -169.636793, 0 | C, 34, 1.478021, 31, 109.92169, 2
8, 175.971536, 0 | H, 36, 1.091577, 34, 110.793696, 31, 129.161305, 0 | H, 36, 1.0940
25, 34, 109.90484, 31, -109.781718, 0 | H, 33, 1.089283, 32, 107.40816, 31, 132.547
723, 0 | H, 33, 1.091304, 32, 107.128719, 31, -109.312985, 0 | C, 35, 1.409266, 27, 12
2.79291, 2, 177.004928, 0 | H, 41, 1.081866, 35, 119.096226, 27, -179.873068, 0 | C,
41, 1.3966, 35, 121.476077, 27, -1.140802, 0 | H, 43, 1.084831, 41, 118.191772, 35,
-161.405185, 0 | H, 43, 1.083183, 41, 119.19772, 35, -12.968666, 0 | C, 43, 2.149597
, 41, 110.332055, 35, 98.654959, 0 | C, 46, 2.347888, 43, 98.54741, 41, -3.867142, 0
| C, 46, 1.392758, 43, 99.225015, 41, -74.518513, 0 | C, 47, 1.369117, 46, 71.415359
, 43, -94.090721, 0 | C, 47, 1.496472, 46, 39.002656, 43, 97.450389, 0 | H, 50, 1.1035
83, 47, 108.398245, 46, 113.939675, 0 | H, 50, 1.09355, 47, 115.246396, 46, -127.77
258, 0 | H, 46, 1.084855, 43, 96.107428, 41, 160.288556, 0 | H, 47, 1.084724, 46, 162.
403021, 43, 82.027332, 0 | H, 49, 1.084008, 47, 126.106161, 46, 178.346061, 0 | H, 48
, 1.085064, 46, 125.132955, 43, -85.353199, 0 | | Version=x86-Win32-G03RevB.03 |
State=2-A | HF=-2958.7799243 | S2=0.751846 | S2-1=0. | S2A=0.750003 | RMSD=5.729
e-005 | Dipole=0.7382782, 0.5153701, 1.6788347 | PG=C01 [X(C20H27Cu1N3O5)] | |
@
```

TS of methyl substituted bis(oxazoline)-Cu(II) NC *Si* in vacuum at UB3LYP/6-31G(d)

```
UB3LYP/6-31G* FREQ GUESS=READ GEOM=CHECK\ \bisoxc2_acry_nc opt
.\ \ 2, 2 | C | Cu, 1, B1 | C, 1, B2, 2, A1 | C, 1, B3, 2, A2, 3, D1, 0 | N, 3, B4, 1, A3, 2, D2, 0 | N, 4
, B5, 1, A4, 2, D3, 0 | O, 3, B6, 1, A5, 2, D4, 0 | O, 4, B7, 1, A6, 2, D5, 0 | C, 5, B8, 3, A7, 1, D6
, 0 | C, 6, B9, 4, A8, 1, D7, 0 | C, 7, B10, 3, A9, 1, D8, 0 | C, 8, B11, 4, A10, 1, D9, 0 | C, 9, B12
, 5, A11, 3, D10, 0 | C, 10, B13, 6, A12, 4, D11, 0 | H, 1, B14, 2, A13, 6, D12, 0 | H, 1, B15, 2,
A14, 6, D13, 0 | H, 11, B16, 7, A15, 3, D14, 0 | H, 12, B17, 8, A16, 4, D15, 0 | H, 11, B18, 7, A
17, 3, D16, 0 | H, 12, B19, 8, A18, 4, D17, 0 | H, 13, B20, 9, A19, 5, D18, 0 | H, 14, B21, 10, A
20, 6, D19, 0 | H, 13, B22, 9, A21, 5, D20, 0 | H, 14, B23, 10, A22, 6, D21, 0 | H, 13, B24, 9, A
23, 5, D22, 0 | H, 14, B25, 10, A24, 6, D23, 0 | O, 2, B26, 1, A25, 3, D24, 0 | O, 2, B27, 1, A26
, 3, D25, 0 | H, 9, B28, 5, A27, 3, D26, 0 | H, 10, B29, 6, A28, 4, D27, 0 | C, 28, B30, 2, A29, 1
, D28, 0 | O, 31, B31, 28, A30, 2, D29, 0 | C, 32, B32, 31, A31, 28, D30, 0 | N, 31, B33, 28, A3
```


2, 2, D31, 0\C, 27, B34, 2, A33, 1, D32, 0\C, 34, B35, 31, A34, 28, D33, 0\H, 36, B36, 34, A35, 31, D34, 0\H, 36, B37, 34, A36, 31, D35, 0\H, 33, B38, 32, A37, 31, D36, 0\H, 33, B39, 32, A38, 31, D37, 0\C, 35, B40, 27, A39, 2, D38, 0\H, 41, B41, 35, A40, 27, D39, 0\C, 41, B42, 35, A41, 27, D40, 0\H, 43, B43, 41, A42, 35, D41, 0\H, 43, B44, 41, A43, 35, D42, 0\C, 43, B45, 41, A44, 35, D43, 0\C, 46, B46, 43, A45, 41, D44, 0\C, 46, B47, 43, A46, 41, D45, 0\C, 48, B48, 46, A47, 43, D46, 0\C, 47, B49, 46, A48, 43, D47, 0\H, 50, B50, 47, A49, 46, D48, 0\H, 50, B51, 47, A50, 46, D49, 0\H, 46, B52, 43, A51, 41, D50, 0\H, 47, B53, 46, A52, 43, D51, 0\H, 49, B54, 48, A53, 46, D52, 0\H, 48, B55, 46, A54, 43, D53, 0\B1=3.39237042\B2=1.49585512\B3=1.496364\B4=1.29276523\B5=1.29280004\B6=1.31998008\B7=1.31853139\B8=1.49521496\B9=1.49796447\B10=1.46578684\B11=1.46725421\B12=1.52777137\B13=1.52700948\B14=1.09911601\B15=1.09753099\B16=1.09122527\B17=1.09081331\B18=1.0911944\B19=1.09142982\B20=1.09465458\B21=1.09466585\B22=1.09533695\B23=1.09555343\B24=1.09501452\B25=1.09496907\B26=1.91857895\B27=1.94311138\B28=1.09301329\B29=1.09280106\B30=1.2422902\B31=1.31564358\B32=1.45867779\B33=1.37305112\B34=1.2775537\B35=1.47802013\B36=1.0915766\B37=1.09402582\B38=1.08928353\B39=1.09130449\B40=1.40926621\B41=1.08186522\B42=1.39660005\B43=1.08483142\B44=1.08318268\B45=2.14959654\B46=2.34788824\B47=1.39275748\B48=1.42922825\B49=1.49647264\B50=1.10358188\B51=1.09354982\B52=1.08485623\B53=1.08472414\B54=1.08400693\B55=1.08506485\A1=58.47413462\A2=58.35190801\A3=128.09003456\A4=127.99074202\A5=114.34686343\A6=114.32352305\A7=107.99616168\A8=108.00472766\A9=107.53757974\A10=107.57725212\A11=111.51278504\A12=111.67542141\A13=123.38290745\A14=131.87060872\A15=107.01382084\A16=106.96735957\A17=107.06980941\A18=107.00302871\A19=111.04814673\A20=110.94737941\A21=111.19120671\A22=111.24103801\A23=110.03291691\A24=109.88737783\A25=136.39458431\A26=133.95429197\A27=107.73453708\A28=107.63048974\A29=125.41760155\A30=120.60545883\A31=110.44229471\A32=127.54535892\A33=131.88502209\A34=109.92172864\A35=110.79374405\A36=109.90483826\A37=107.40817534\A38=107.12870693\A39=122.79288914\A40=119.0961843\A41=121.47605222\A42=118.19170943\A43=119.1977304\A44=110.3320419\A45=98.54742114\A46=99.22501489\A47=109.90793724\A48=39.00267955\A49=108.39827292\A50=115.24639403\A51=96.10738703\A52=162.40300167\A53=125.03943658\A54=125.13293758\D1=174.65046264\D2=0.86312702\D3=3.43589525\D4=-179.31900535\D5=-177.4889561\D6=177.48622486\D7=178.23229694\D8=178.15609232\D9=179.23148137\D10=-116.7595867\D11=-119.39670518\D12=90.05533048\D13=-89.91440862\D14=-116.23193405\D15=-118.25197195\D16=125.94315103\D17=123.92780808\D18=-61.82168355\D19=-62.37464135\D20=59.29016886\D21=59.0658632\D22=179.10487323\D23=178.86074006\D24=39.32972344\D25=-139.0801412\D26=122.46433298\D27=119.87816924\D28=165.65639367\D29=-170.21254591\D30=175.27413276\D31=10.32752928\D32=-169.63678611\D33=175.97163068\D34=129.16136589\D35=-109.78166523\D36=132.54768428\D37=-109.31308506\D38=-182.99505177\D39=-179.87306918\D40=-1.14080424\D41=-161.40518314\D42=-12.9687046\D43=98.65497763\D44=-3.86717954\D45=-74.51854532\D46=93.21371802\D47=97.45042197\D48=113.93968951\D49=-127.77248494\D50=160.28848682\D51=82.02752496\D52=-176.54785979\D53=-85.35320179\Version=HP-PARisc-HPUX-G98RevA.11\HF=-2958.5966259\S2=0.751919\S2-1=0.\S2A=0.750003\RMSD=4.141e-09\RMSF=3.229e-05\Dipole=0.6132388,0.5956211,1.541325\ PG=C01[X(C20H27Cu1N3O5)]\NImag=1\

***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
 Raman scattering activities (A**4/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal
 coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	-231.8427	17.5159	19.0627

Red. masses --	8.8989	4.3700	4.3086
Frc consts --	0.2818	0.0008	0.0009
IR Inten --	256.7427	0.0255	0.1447
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

Zero-point correction=	0.462428
(Hartree/Particle)	
Thermal correction to Energy=	0.490955
Thermal correction to Enthalpy=	0.491899
Thermal correction to Gibbs Free Energy=	0.399052
Sum of electronic and zero-point Energies=	-2958.134198
Sum of electronic and thermal Energies=	-2958.105671
Sum of electronic and thermal Enthalpies=	-2958.104727
Sum of electronic and thermal Free Energies=	-2958.197574

TS of methyl substituted bis(oxazoline)-Cu(II) NC Si in PCM at UB3LYP/6-31G(d)

```

1 | 1 | UNPC-UNK | SP | UB3LYP | 6-31G(d) | C20H27Cu1N3O5 (2+, 2) | PCUSER | 09-Jun-2003
| 0 | # UB3LYP/6-31G* SP SCRF=(PCM,READ,SOLVENT=CH2CL2) | xc si pcm sp. |
2, 2 | C | Cu, 1, 3.3934 | C, 1, 1.4954, 2, 58.4079 | C, 1, 1.4963, 2, 58.4386, 3, 173.2816
, 0 | N, 3, 1.2927, 1, 128.1503, 2, 0.8731, 0 | N, 4, 1.2926, 1, 127.9018, 2, 3.2291, 0 | O
, 3, 1.3202, 1, 114.3104, 2, -179.0653, 0 | O, 4, 1.3186, 1, 114.4051, 2, -177.9373, 0
| C, 5, 1.4935, 3, 108.047, 1, 178.2568, 0 | C, 6, 1.4982, 4, 107.9331, 1, 176.9958, 0 |
C, 7, 1.4645, 3, 107.5842, 1, 178.3627, 0 | C, 8, 1.4677, 4, 107.4809, 1, 178.2549, 0 |
C, 9, 1.5277, 5, 111.5354, 3, -118.0768, 0 | C, 10, 1.5277, 6, 111.4933, 4, -116.569,
0 | H, 1, 1.0993, 2, 122.1282, 5, -94.0676, 0 | H, 1, 1.0973, 2, 133.0615, 5, 85.7613, 0
| H, 11, 1.0912, 7, 107.0217, 3, -117.3927, 0 | H, 12, 1.0911, 8, 106.9085, 4, -115.44
17, 0 | H, 11, 1.0914, 7, 107.0651, 3, 124.8018, 0 | H, 12, 1.0911, 8, 107.0503, 4, 126.
6999, 0 | H, 13, 1.0948, 9, 110.8873, 5, -62.1647, 0 | H, 14, 1.0947, 10, 111.1777, 6, -
61.637, 0 | H, 13, 1.0952, 9, 111.2755, 5, 58.8693, 0 | H, 14, 1.0954, 10, 111.2968, 6,
59.5956, 0 | H, 13, 1.0954, 9, 110.0319, 5, 178.469, 0 | H, 14, 1.0949, 10, 109.8667, 6
, 179.4274, 0 | O, 2, 1.9284, 1, 135.1347, 3, 42.9041, 0 | O, 2, 1.9359, 1, 134.8494, 3,
-139.7303, 0 | H, 9, 1.0934, 5, 107.4869, 3, 121.332, 0 | H, 10, 1.0925, 6, 107.8096, 4
, 122.4534, 0 | C, 28, 1.2425, 2, 125.9575, 1, -175.8121, 0 | O, 31, 1.316, 28, 120.716
7, 2, -176.2991, 0 | C, 32, 1.4596, 31, 110.1042, 28, 175.8026, 0 | N, 31, 1.3721, 28, 1
27.4415, 2, 5.1438, 0 | C, 27, 1.2782, 2, 129.4753, 1, 159.5213, 0 | C, 34, 1.4777, 31,
109.6041, 28, 172.2734, 0 | H, 36, 1.0915, 34, 110.496, 31, 133.7494, 0 | H, 36, 1.094
2, 34, 110.2983, 31, -105.0535, 0 | H, 33, 1.089, 32, 107.4, 31, 135.5189, 0 | H, 33, 1.
0917, 32, 107.1832, 31, -106.204, 0 | C, 35, 1.4082, 27, 123.5503, 2, -152.6521, 0 | H
, 41, 1.0822, 35, 118.6728, 27, 177.2966, 0 | C, 41, 1.3988, 35, 121.7165, 27, 2.0053
, 0 | H, 43, 1.085, 41, 117.9733, 35, 156.3666, 0 | H, 43, 1.0836, 41, 118.8898, 35, 9.3
671, 0 | C, 43, 2.1294, 41, 110.5796, 35, -104.0896, 0 | C, 46, 2.3478, 43, 98.419, 41,
3.7092, 0 | C, 47, 1.3697, 46, 71.48, 43, 94.2591, 0 | C, 46, 1.3938, 43, 99.6353, 41, 7
4.2783, 0 | C, 47, 1.4959, 46, 39.0332, 43, -97.6722, 0 | H, 50, 1.0935, 47, 115.348, 4
6, 127.9853, 0 | H, 50, 1.1037, 47, 108.3228, 46, -113.7399, 0 | H, 47, 1.0847, 46, 162
.4285, 43, -81.441, 0 | H, 48, 1.0839, 47, 126.0035, 46, -178.0311, 0 | H, 49, 1.0851,
46, 124.874, 43, 85.8712, 0 | H, 46, 1.0849, 43, 96.6252, 41, -160.4676, 0 | | Version
=x86-Win32-G03RevB.03 | State=2-A | HF=-2958.7770416 | S2=0.7519 | S2-1=0. | S2A
=0.750003 | RMSD=9.344e-005 | Dipole=0.6494741, 0.8029453, 1.755112 | PG=C01 [
X(C20H27Cu1N3O5)] | | @

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TS of methyl substituted bis(oxazoline)-Cu(II) XC Re in vacuum at UB3LYP/6-31G(d)

```

UB3LYP/6-31G* FREQ GUESS=READ GEOM=CHECK\\bisoxc2_acry_xc1 op
t. \\2, 2\C\Cu, 1, B1\C, 1, B2, 2, A1\C, 1, B3, 2, A2, 3, D1, 0\N, 3, B4, 1, A3, 2, D2, 0\N,
4, B5, 1, A4, 2, D3, 0\O, 3, B6, 1, A5, 2, D4, 0\O, 4, B7, 1, A6, 2, D5, 0\C, 5, B8, 3, A7, 1, D

```

6,0\C,6,B9,4,A8,1,D7,0\C,7,B10,3,A9,1,D8,0\C,8,B11,4,A10,1,D9,0\C,9,B1
2,5,A11,3,D10,0\C,10,B13,6,A12,4,D11,0\H,1,B14,2,A13,5,D12,0\H,1,B15,2
,A14,5,D13,0\H,11,B16,7,A15,3,D14,0\H,12,B17,8,A16,4,D15,0\H,11,B18,7,
A17,3,D16,0\H,12,B19,8,A18,4,D17,0\H,13,B20,9,A19,5,D18,0\H,14,B21,10,
A20,6,D19,0\H,13,B22,9,A21,5,D20,0\H,14,B23,10,A22,6,D21,0\H,13,B24,9,
A23,5,D22,0\H,14,B25,10,A24,6,D23,0\O,2,B26,1,A25,3,D24,0\O,2,B27,1,A2
6,3,D25,0\H,9,B28,5,A27,3,D26,0\H,10,B29,6,A28,4,D27,0\C,28,B30,2,A29,
1,D28,0\O,31,B31,28,A30,2,D29,0\C,32,B32,31,A31,28,D30,0\N,31,B33,28,A
32,2,D31,0\C,27,B34,2,A33,1,D32,0\C,34,B35,31,A34,28,D33,0\H,36,B36,34
,A35,31,D34,0\H,36,B37,34,A36,31,D35,0\H,33,B38,32,A37,31,D36,0\H,33,B
39,32,A38,31,D37,0\C,35,B40,27,A39,2,D38,0\H,41,B41,35,A40,27,D39,0\C,
41,B42,35,A41,27,D40,0\H,43,B43,41,A42,35,D41,0\H,43,B44,41,A43,35,D42
,0\C,41,B45,35,A44,27,D43,0\C,46,B46,41,A45,35,D44,0\C,46,B47,41,A46,3
5,D45,0\C,48,B48,46,A47,41,D46,0\C,47,B49,46,A48,41,D47,0\H,50,B50,47,
A49,46,D48,0\H,50,B51,47,A50,46,D49,0\H,46,B52,41,A51,35,D50,0\H,47,B5
3,46,A52,41,D51,0\H,49,B54,48,A53,46,D52,0\H,48,B55,46,A54,41,D53,0\\\B
1=3.38936564\B2=1.49594838\B3=1.49660358\B4=1.29270642\B5=1.29293722\B
6=1.31976747\B7=1.31845681\B8=1.49494876\B9=1.49807434\B10=1.46582419\
B11=1.46753741\B12=1.5276114\B13=1.52720547\B14=1.09935894\B15=1.09714
247\B16=1.09106132\B17=1.09093274\B18=1.09133978\B19=1.09127604\B20=1.
09478428\B21=1.09448475\B22=1.09529583\B23=1.09552665\B24=1.09501228\B
25=1.09496748\B26=1.92101939\B27=1.9417967\B28=1.09320612\B29=1.092706
04\B30=1.24226741\B31=1.315152\B32=1.45856051\B33=1.37388916\B34=1.278
81665\B35=1.47859231\B36=1.09161527\B37=1.09382595\B38=1.0894001\B39=1
.09113309\B40=1.41012118\B41=1.08173347\B42=1.39425168\B43=1.08281026\
B44=1.08477009\B45=3.21062497\B46=2.34793674\B47=1.36805437\B48=1.4313
5131\B49=1.51191504\B50=1.10302826\B51=1.0943471\B52=1.08471604\B53=1.
08471753\B54=1.08545617\B55=1.08399905\A1=58.50276349\A2=58.43055595\A
3=128.0372165\A4=127.93653254\A5=114.39410005\A6=114.38727641\A7=108.0
5560355\A8=107.99477208\A9=107.56801712\A10=107.5506777\A11=111.604478
46\A12=111.59736729\A13=121.45182255\A14=133.72596332\A15=107.04798367
\A16=106.9275826\A17=107.02378826\A18=107.01356408\A19=111.07148581\A2
0=110.99291682\A21=111.20656284\A22=111.24231882\A23=110.03353641\A24=
109.86727977\A25=135.16904015\A26=135.35502035\A27=107.65101302\A28=10
7.71662702\A29=125.7517467\A30=120.54350636\A31=110.59597341\A32=127.6
0749897\A33=132.20246491\A34=109.98284146\A35=110.70319446\A36=109.869
62466\A37=107.3611524\A38=107.11530382\A39=123.2908086\A40=118.7690135
3\A41=122.29063862\A42=119.00824566\A43=119.03958605\A44=94.0356627\A4
5=62.77717931\A46=84.01858007\A47=108.78564918\A48=38.4870078\A49=108.
16142066\A50=115.79184424\A51=114.07800353\A52=159.10853992\A53=124.74
981575\A54=126.31791359\D1=172.41052445\D2=0.96731249\D3=3.31820033\D4
=-179.04339826\D5=-177.81167335\D6=178.05698448\D7=177.60053874\D8=178
.63889496\D9=178.95791716\D10=-118.01108834\D11=-118.24107052\D12=-94.
6266632\D13=85.3470996\D14=-117.622852\D15=-117.14256738\D16=124.55561
111\D17=125.02970557\D18=-62.02413942\D19=-62.07358516\D20=59.09418131
\D21=59.3115658\D22=178.92911904\D23=179.10344594\D24=42.40344778\D25=
-139.7141517\D26=121.2509366\D27=120.95168137\D28=-190.16419266\D29=-1
71.86332173\D30=-184.1308415\D31=8.65116102\D32=187.42586026\D33=-183.
42042798\D34=127.69278821\D35=-111.35410371\D36=131.03899984\D37=-110.
88628234\D38=-184.05050086\D39=-179.60395253\D40=-1.92939687\D41=-158.
3479386\D42=-7.88081574\D43=88.02606046\D44=-123.13429318\D45=164.6895
6287\D46=65.70290805\D47=97.50177781\D48=114.88983107\D49=-125.9795963
9\D50=37.86428606\D51=131.41440407\D52=-182.27752193\D53=-114.89866092
\Version=HP-PARisc-HPUX-G98RevA.11\HF=-2958.5964029\S2=0.751919\S2-1=
0.\S2A=0.750003\RMSD=3.122e-09\RMSF=2.953e-05\Dipole=0.5951757,0.63139
16,1.483695\ PG=C01 [X(C20H27Cu1N3O5)]\NImag=1\\

***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole),
 Raman scattering activities (A⁴/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal
 coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	-209.4250	16.9375	19.7295
Red. masses --	8.5503	4.8990	4.2980
Frc consts --	0.2209	0.0008	0.0010
IR Inten --	325.3023	0.0256	0.1527
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

Zero-point correction= 0.462303
 (Hartree/Particle)
 Thermal correction to Energy= 0.490919
 Thermal correction to Enthalpy= 0.491864
 Thermal correction to Gibbs Free Energy= 0.398697
 Sum of electronic and zero-point Energies= -2958.134100
 Sum of electronic and thermal Energies= -2958.105484
 Sum of electronic and thermal Enthalpies= -2958.104539
 Sum of electronic and thermal Free Energies= -2958.197706

TS of methyl substituted bis(oxazoline)-Cu(II) XC Re in PCM at UB3LYP/6-31G(d)

1 | 1 | UNPC-UNK | SP | UB3LYP | 6-31G(d) | C20H27Cu1N3O5 (2+, 2) | PCUSER | 09-Jun-2003
 | 0 | # UB3LYP/6-31G* SP SCRF=(PCM,READ,SOLVENT=CH2CL2) | | bisoxc2_acry_xc
 1 opt. | | 2, 2 | C | Cu, 1, 3.389366 | C, 1, 1.495948, 2, 58.502773 | C, 1, 1.496603, 2, 58.
 430575, 3, 172.410503, 0 | N, 3, 1.292707, 1, 128.037214, 2, 0.967296, 0 | N, 4, 1.29
 2938, 1, 127.936513, 2, 3.318209, 0 | O, 3, 1.319768, 1, 114.394146, 2, -179.043367
 , 0 | O, 4, 1.318457, 1, 114.38732, 2, -177.811676, 0 | C, 5, 1.494949, 3, 108.055629,
 1, 178.057013, 0 | C, 6, 1.498075, 4, 107.994762, 1, 177.600542, 0 | C, 7, 1.465824, 3
 , 107.568057, 1, 178.638857, 0 | C, 8, 1.467538, 4, 107.550708, 1, 178.95794, 0 | C, 9
 , 1.527611, 5, 111.60448, 3, -118.01106, 0 | C, 10, 1.527205, 6, 111.597331, 4, -118
 .241053, 0 | H, 1, 1.099359, 2, 121.451828, 6, 91.273702, 0 | H, 1, 1.097143, 2, 133.7
 25976, 6, -88.752473, 0 | H, 11, 1.091061, 7, 107.047997, 3, -117.622849, 0 | H, 12, 1
 .090933, 8, 106.927523, 4, -117.14257, 0 | H, 11, 1.09134, 7, 107.023741, 3, 124.55
 5571, 0 | H, 12, 1.091276, 8, 107.01357, 4, 125.029726, 0 | H, 13, 1.094784, 9, 111.07
 1497, 5, -62.024173, 0 | H, 14, 1.094485, 10, 110.992909, 6, -62.073622, 0 | H, 13, 1.
 095296, 9, 111.206575, 5, 59.094169, 0 | H, 14, 1.095526, 10, 111.242366, 6, 59.311
 57, 0 | H, 13, 1.095012, 9, 110.033536, 5, 178.92909, 0 | H, 14, 1.094967, 10, 109.867
 223, 6, 179.103483, 0 | O, 2, 1.921019, 1, 135.169025, 3, 42.403478, 0 | O, 2, 1.94179
 7, 1, 135.354996, 3, -139.714161, 0 | H, 9, 1.093206, 5, 107.651005, 3, 121.250915,
 0 | H, 10, 1.092706, 6, 107.716582, 4, 120.951687, 0 | C, 28, 1.242268, 2, 125.7517, 1
 , 169.835784, 0 | O, 31, 1.315152, 28, 120.543481, 2, -171.863332, 0 | C, 32, 1.45856
 , 31, 110.595972, 28, 175.869181, 0 | N, 31, 1.373889, 28, 127.607535, 2, 8.651237,
 0 | C, 27, 1.278817, 2, 132.202419, 1, -172.574185, 0 | C, 34, 1.478592, 31, 109.9828
 66, 28, 176.579518, 0 | H, 36, 1.091615, 34, 110.703196, 31, 127.692796, 0 | H, 36, 1.
 093826, 34, 109.869605, 31, -111.354145, 0 | H, 33, 1.0894, 32, 107.361129, 31, 131
 .038998, 0 | H, 33, 1.091133, 32, 107.115302, 31, -110.886216, 0 | C, 35, 1.410122, 2
 7, 123.290792, 2, 175.949472, 0 | H, 41, 1.081733, 35, 118.769055, 27, -179.603934
 , 0 | C, 41, 1.394252, 35, 122.290602, 27, -1.929334, 0 | H, 43, 1.08281, 41, 119.0082
 06, 35, -158.348017, 0 | H, 43, 1.084769, 41, 119.039591, 35, -7.880855, 0 | C, 41, 3.
 210625, 35, 94.035639, 27, 88.026105, 0 | C, 43, 2.196149, 41, 110.623805, 35, 94.3
 13899, 0 | C, 46, 1.368054, 41, 84.018578, 35, 164.689559, 0 | C, 47, 1.390367, 43, 98
 .565069, 41, 69.353489, 0 | C, 46, 1.497117, 41, 73.569623, 35, -82.619972, 0 | H, 50

, 1.103029, 46, 108.811623, 41, 178.780615, 0 | H, 50, 1.094347, 46, 114.933098, 41, 59.731366, 0 | H, 46, 1.084716, 41, 114.07802, 35, 37.864269, 0 | H, 47, 1.084717, 43, 95.040272, 41, -165.562335, 0 | H, 49, 1.085457, 47, 125.283715, 43, 84.297766, 0 | H, 48, 1.083999, 46, 126.317968, 41, -114.898677, 0 | | Version=x86-Win32-G03R evB.03 | State=2-A | HF=-2958.7782302 | S2=0.751966 | S2-1=0. | S2A=0.750003 | RMS D=9.406e-005 | Dipole=0.7071834, 0.4717494, 1.5786115 | PG=C01 [X(C20H27Cu1N3O5)] | | @

TS of methyl substituted bis(oxazoline)-Cu(II) XC Si in vacuum at UB3LYP/6-31G(d)

```
# UB3LYP/6-31G*  FREQ  GUESS=READ  GEOM=CHECK\ \bisoxc2_acry_xc  opt
.\ \2,2\C\Cu,1,B1\C,1,B2,2,A1\C,1,B3,2,A2,3,D1,0\N,3,B4,1,A3,2,D2,0\N,4
,B5,1,A4,2,D3,0\O,3,B6,1,A5,2,D4,0\O,4,B7,1,A6,2,D5,0\C,5,B8,3,A7,1,D6
,0\C,6,B9,4,A8,1,D7,0\C,7,B10,3,A9,1,D8,0\C,8,B11,4,A10,1,D9,0\C,9,B12
,5,A11,3,D10,0\C,10,B13,6,A12,4,D11,0\H,1,B14,2,A13,6,D12,0\H,1,B15,2,
A14,6,D13,0\H,11,B16,7,A15,3,D14,0\H,12,B17,8,A16,4,D15,0\H,11,B18,7,A
17,3,D16,0\H,12,B19,8,A18,4,D17,0\H,13,B20,9,A19,5,D18,0\H,14,B21,10,A
20,6,D19,0\H,13,B22,9,A21,5,D20,0\H,14,B23,10,A22,6,D21,0\H,13,B24,9,A
23,5,D22,0\H,14,B25,10,A24,6,D23,0\O,2,B26,1,A25,4,D24,0\O,2,B27,1,A26
,4,D25,0\H,9,B28,5,A27,3,D26,0\H,10,B29,6,A28,4,D27,0\C,28,B30,2,A29,1
,D28,0\O,31,B31,28,A30,2,D29,0\C,32,B32,31,A31,28,D30,0\N,31,B33,28,A3
2,2,D31,0\C,27,B34,2,A33,1,D32,0\C,34,B35,31,A34,28,D33,0\H,36,B36,34,
A35,31,D34,0\H,36,B37,34,A36,31,D35,0\H,33,B38,32,A37,31,D36,0\H,33,B3
9,32,A38,31,D37,0\C,35,B40,27,A39,2,D38,0\H,41,B41,35,A40,27,D39,0\C,4
1,B42,35,A41,27,D40,0\H,43,B43,41,A42,35,D41,0\H,43,B44,41,A43,35,D42,
0\C,41,B45,35,A44,27,D43,0\C,43,B46,41,A45,35,D44,0\C,47,B47,43,A46,41
,D45,0\C,46,B48,41,A47,35,D46,0\C,46,B49,41,A48,35,D47,0\H,50,B50,46,A
49,41,D48,0\H,50,B51,46,A50,41,D49,0\H,47,B52,43,A51,41,D50,0\H,48,B53
,47,A52,43,D51,0\H,49,B54,46,A53,41,D52,0\H,46,B55,41,A54,35,D53,0\ \B1
=3.39287448\B2=1.49549221\B3=1.49616685\B4=1.29279212\B5=1.29266014\B6
=1.32007819\B7=1.3184958\B8=1.49402799\B9=1.49817169\B10=1.46485977\B1
1=1.46767892\B12=1.52783214\B13=1.52762881\B14=1.09924159\B15=1.097396
22\B16=1.09118112\B17=1.09106441\B18=1.0913602\B19=1.09115192\B20=1.09
486435\B21=1.0947054\B22=1.09521379\B23=1.09539846\B24=1.09522718\B25=
1.09493754\B26=1.92885356\B27=1.93733907\B28=1.09339349\B29=1.09264049
\B30=1.2423034\B31=1.3158332\B32=1.46017783\B33=1.37292507\B34=1.27935
758\B35=1.47838468\B36=1.09159969\B37=1.09416798\B38=1.08897982\B39=1.
09177912\B40=1.40915169\B41=1.08207928\B42=1.39515071\B43=1.08281635\B
44=1.08503248\B45=3.1963252\B46=2.18653519\B47=1.39076537\B48=1.367796
39\B49=1.49765032\B50=1.09429867\B51=1.1029314\B52=1.08480356\B53=1.08
548449\B54=1.08401248\B55=1.08467888\A1=58.40885415\A2=58.42429129\A3=
128.1615778\A4=127.92344876\A5=114.29822628\A6=114.39165724\A7=108.028
29513\A8=107.95946109\A9=107.58298604\A10=107.50983829\A11=111.5262989
5\A12=111.54207028\A13=122.73379433\A14=132.47333259\A15=107.01884795\
A16=106.92409299\A17=107.07200192\A18=107.03559618\A19=111.00472072\A2
0=111.18843719\A21=111.23796915\A22=111.29079148\A23=110.04745308\A24=
109.86038566\A25=135.39951302\A26=134.68937503\A27=107.57610363\A28=10
7.77721582\A29=125.97815602\A30=120.80562976\A31=110.0748475\A32=127.4
0986264\A33=129.49983751\A34=109.58508126\A35=110.46282221\A36=110.265
91883\A37=107.39213861\A38=107.16361558\A39=123.90626197\A40=118.51887
7\A41=122.19856851\A42=118.95148422\A43=118.87583428\A44=97.12170257\A
45=110.29195928\A46=98.58316974\A47=84.3838179\A48=73.32709502\A49=114
.65585841\A50=108.70679196\A51=95.25233658\A52=125.25373617\A53=126.34
032392\A54=113.97600923\D1=174.00883871\D2=0.95555157\D3=3.1769416\D4=
-179.02536249\D5=-177.92407204\D6=178.10424894\D7=177.22468789\D8=178.
180094\D9=178.44023954\D10=-117.65138739\D11=-117.04950192\D12=90.6219
5582\D13=-89.52343113\D14=-116.92530147\D15=-115.99588431\D16=125.2460
```

215\D17=126.14778434\D18=-61.58657987\D19=-61.8297882\D20=59.38719763\
D21=59.42228629\D22=179.07102721\D23=179.24826148\D24=-143.90903135\D2
5=34.33974758\D26=121.56405162\D27=121.97051695\D28=-176.8248297\D29=-
175.66827561\D30=175.49495679\D31=5.77173438\D32=159.96438092\D33=172.
13939541\D34=134.35511178\D35=-104.47392296\D36=136.14287911\D37=-105.
56806144\D38=-152.22689594\D39=177.6691739\D40=2.33586027\D41=155.5013
6737\D42=5.82403157\D43=-90.00530247\D44=-97.33203704\D45=-70.50264704
\D46=-165.71917592\D47=81.70134853\D48=-59.53305547\D49=181.33982668\D
50=164.51520929\D51=-84.2407884\D52=115.08453265\D53=-38.63122437\\Ver
sion=HP-PARisc-HPUX-G98RevA.11\HF=-2958.594885\S2=0.751903\S2-1=0.\S2A
=0.750003\RMSD=5.262e-09\RMSF=4.859e-05\Dipole=0.6184208,0.7120265,1.5
281476\ PG=C01 [X(C20H27Cu1N3O5)]\NImag=1\\

***** 1 imaginary frequencies (negative Signs) *****
Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
Raman scattering activities (A**4/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal
coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	-211.3363	15.7259	23.0794
Red. masses --	8.5199	4.6444	4.7569
Frc consts --	0.2242	0.0007	0.0015
IR Inten --	332.3793	0.0501	0.5672
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

Zero-point correction= 0.462368
(Hartree/Particle)

Thermal correction to Energy=	0.490873
Thermal correction to Enthalpy=	0.491817
Thermal correction to Gibbs Free Energy=	0.399131
Sum of electronic and zero-point Energies=	-2958.132517
Sum of electronic and thermal Energies=	-2958.104012
Sum of electronic and thermal Enthalpies=	-2958.103068
Sum of electronic and thermal Free Energies=	-2958.195754

TS of methyl substituted bis(oxazoline)-Cu(II) XC Si in PCM at UB3LYP/6-31G(d)

1 | 1 | UNPC-UNK | SP | UB3LYP | 6-31G(d) | C20H27Cu1N3O5 (2+, 2) | PCUSER | 10-Jun-2003
| 0 | # UB3LYP/6-31G* SP SCRF=(PCM,READ,SOLVENT=CH2CL2) | | xcsipcm pcm sp.
| | 2, 2 | C | Cu, 1, 3.3929 | C, 1, 1.4955, 2, 58.4089 | C, 1, 1.4962, 2, 58.4243, 3, 174.00
88, 0 | N, 3, 1.2928, 1, 128.1616, 2, 0.9556, 0 | N, 4, 1.2927, 1, 127.9234, 2, 3.1769, 0
| O, 3, 1.3201, 1, 114.2982, 2, -179.0254, 0 | O, 4, 1.3185, 1, 114.3917, 2, -177.9241
, 0 | C, 5, 1.494, 3, 108.0283, 1, 178.1042, 0 | C, 6, 1.4982, 4, 107.9595, 1, 177.2247,
0 | C, 7, 1.4649, 3, 107.583, 1, 178.1801, 0 | C, 8, 1.4677, 4, 107.5098, 1, 178.4402, 0
| C, 9, 1.5278, 5, 111.5263, 3, -117.6514, 0 | C, 10, 1.5276, 6, 111.5421, 4, -117.049
5, 0 | H, 1, 1.0992, 2, 122.7338, 6, 90.622, 0 | H, 1, 1.0974, 2, 132.4733, 6, -89.5234,
0 | H, 11, 1.0912, 7, 107.0188, 3, -116.9253, 0 | H, 12, 1.0911, 8, 106.9241, 4, -115.9
959, 0 | H, 11, 1.0914, 7, 107.072, 3, 125.246, 0 | H, 12, 1.0912, 8, 107.0356, 4, 126.1
478, 0 | H, 13, 1.0949, 9, 111.0047, 5, -61.5866, 0 | H, 14, 1.0947, 10, 111.1884, 6, -6
1.8298, 0 | H, 13, 1.0952, 9, 111.238, 5, 59.3872, 0 | H, 14, 1.0954, 10, 111.2908, 6, 5
9.4223, 0 | H, 13, 1.0952, 9, 110.0475, 5, 179.071, 0 | H, 14, 1.0949, 10, 109.8604, 6,
179.2483, 0 | O, 2, 1.9289, 1, 135.3995, 4, -143.909, 0 | O, 2, 1.9373, 1, 134.6894, 4,
34.3397, 0 | H, 9, 1.0934, 5, 107.5761, 3, 121.5641, 0 | H, 10, 1.0926, 6, 107.7772, 4,
121.9705, 0 | C, 28, 1.2423, 2, 125.9782, 1, -176.8248, 0 | O, 31, 1.3158, 28, 120.805
6, 2, -175.6683, 0 | C, 32, 1.4602, 31, 110.0748, 28, 175.495, 0 | N, 31, 1.3729, 28, 12

7.4099, 2, 5.7717, 0 | C, 27, 1.2794, 2, 129.4998, 1, 159.9644, 0 | C, 34, 1.4784, 31, 1.09.5851, 28, 172.1394, 0 | H, 36, 1.0916, 34, 110.4628, 31, 134.3551, 0 | H, 36, 1.0942, 34, 110.2659, 31, -104.4739, 0 | H, 33, 1.089, 32, 107.3921, 31, 136.1429, 0 | H, 33, 1.0918, 32, 107.1636, 31, -105.5681, 0 | C, 35, 1.4092, 27, 123.9063, 2, -152.2269, 0 | H, 41, 1.0821, 35, 118.5189, 27, 177.6692, 0 | C, 41, 1.3952, 35, 122.1986, 27, 2.3359, 0 | H, 43, 1.0828, 41, 118.9515, 35, 155.5014, 0 | H, 43, 1.085, 41, 118.8758, 35, 5.824, 0 | C, 41, 3.1963, 35, 97.1217, 27, -90.0053, 0 | C, 43, 2.1865, 41, 110.292, 35, -97.332, 0 | C, 47, 1.3908, 43, 98.5832, 41, -70.5026, 0 | C, 46, 1.3678, 41, 84.3838, 35, -165.7192, 0 | C, 46, 1.4977, 41, 73.3271, 35, 81.7013, 0 | H, 50, 1.0943, 46, 114.6559, 41, -59.5331, 0 | H, 50, 1.1029, 46, 108.7068, 41, 181.3398, 0 | H, 47, 1.0848, 43, 95.2523, 41, 164.5152, 0 | H, 48, 1.0855, 47, 125.2537, 43, -84.2408, 0 | H, 49, 1.084, 46, 126.3403, 41, 115.0845, 0 | H, 46, 1.0847, 41, 113.976, 35, -38.6312, 0 | | V
ersion=x86-Win32-G03RevB.03 | State=2-A | HF=-2958.7773415 | S2=0.751951 | S2-1=0. | S2A=0.750003 | RMSD=8.135e-005 | Dipole=0.570138, 0.7415887, 1.6289304 |
PG=C01 [X(C20H27Cu1N3O5)] | | @

***t*-butyl Bis(oxazoline)-Cu(II) coordinated to acrylate imide in PCM at UB3LYP/6-31G(d)**

Freq\UB3LYP\6-31G(d)\C21H33Cu1N3O5(2+, 2)\MADURA\18-Jun-2
003\1\#\ UB3LYP/6-31G(D) FREQ GUESS=MIX SCFCON=7 SCFCYC=120\Bisoxacry
opt.\2, 2\C\Cu, 1, B1\C, 1, B2, 2, A1\C, 1, B3, 2, A2, 3, D1, 0\N, 3, B4, 1, A3, 2, D2, 0
\N, 4, B5, 1, A4, 2, D3, 0\O, 3, B6, 1, A5, 2, D4, 0\O, 4, B7, 1, A6, 2, D5, 0\C, 5, B8, 3, A7,
1, D6, 0\C, 6, B9, 4, A8, 1, D7, 0\C, 7, B10, 3, A9, 1, D8, 0\C, 8, B11, 4, A10, 1, D9, 0\C, 9
, B12, 5, A11, 3, D10, 0\C, 10, B13, 6, A12, 4, D11, 0\H, 1, B14, 2, A13, 6, D12, 0\H, 1, B1
5, 2, A14, 6, D13, 0\H, 11, B16, 7, A15, 3, D14, 0\H, 12, B17, 8, A16, 4, D15, 0\H, 11, B18
, 7, A17, 3, D16, 0\H, 12, B19, 8, A18, 4, D17, 0\O, 2, B20, 1, A19, 3, D18, 0\O, 2, B21, 1,
A20, 3, D19, 0\H, 9, B22, 5, A21, 3, D20, 0\H, 10, B23, 6, A22, 4, D21, 0\C, 22, B24, 2, A2
3, 1, D22, 0\O, 25, B25, 22, A24, 2, D23, 0\C, 26, B26, 25, A25, 22, D24, 0\N, 25, B27, 22
, A26, 2, D25, 0\C, 21, B28, 2, A27, 1, D26, 0\C, 28, B29, 25, A28, 22, D27, 0\H, 30, B30,
28, A29, 25, D28, 0\H, 30, B31, 28, A30, 25, D29, 0\H, 27, B32, 26, A31, 25, D30, 0\H, 27
, B33, 26, A32, 25, D31, 0\C, 29, B34, 21, A33, 2, D32, 0\H, 35, B35, 29, A34, 21, D33, 0\
C, 35, B36, 29, A35, 21, D34, 0\H, 37, B37, 35, A36, 29, D35, 0\H, 37, B38, 35, A37, 29, D
36, 0\C, 14, B39, 10, A38, 6, D37, 0\H, 40, B40, 14, A39, 10, D38, 0\H, 40, B41, 14, A40,
10, D39, 0\H, 40, B42, 14, A41, 10, D40, 0\C, 14, B43, 10, A42, 6, D41, 0\H, 44, B44, 14,
A43, 10, D42, 0\H, 44, B45, 14, A44, 10, D43, 0\H, 44, B46, 14, A45, 10, D44, 0\C, 14, B4
7, 10, A46, 6, D45, 0\H, 48, B48, 14, A47, 10, D46, 0\H, 48, B49, 14, A48, 10, D47, 0\H, 4
8, B50, 14, A49, 10, D48, 0\C, 13, B51, 9, A50, 5, D49, 0\H, 52, B52, 13, A51, 9, D50, 0\H
, 52, B53, 13, A52, 9, D51, 0\H, 52, B54, 13, A53, 9, D52, 0\C, 13, B55, 9, A54, 5, D53, 0\
H, 56, B56, 13, A55, 9, D54, 0\H, 56, B57, 13, A56, 9, D55, 0\H, 56, B58, 13, A57, 9, D56,
0\C, 13, B59, 9, A58, 5, D57, 0\H, 60, B60, 13, A59, 9, D58, 0\H, 60, B61, 13, A60, 9, D59
, 0\H, 60, B62, 13, A61, 9, D60, 0\B1=3.365338\B2=1.495046\B3=1.495333\B4=1.2
95432\B5=1.295016\B6=1.317333\B7=1.31642\B8=1.502121\B9=1.503551\B10=1
.467134\B11=1.468597\B12=1.561867\B13=1.562406\B14=1.098742\B15=1.0982
03\B16=1.092335\B17=1.092176\B18=1.088009\B19=1.087837\B20=1.96397\B21
=1.961747\B22=1.0934\B23=1.093067\B24=1.234302\B25=1.309143\B26=1.4609
88\B27=1.394902\B28=1.252799\B29=1.485463\B30=1.090861\B31=1.093146\B3
2=1.089052\B33=1.091188\B34=1.461805\B35=1.083439\B36=1.343455\B37=1.0
85489\B38=1.085523\B39=1.540664\B40=1.094463\B41=1.096953\B42=1.095292
\B43=1.544574\B44=1.094527\B45=1.094976\B46=1.09654\B47=1.540543\B48=1
.094483\B49=1.09638\B50=1.098584\B51=1.54459\B52=1.096701\B53=1.094465
\B54=1.095077\B55=1.54047\B56=1.096594\B57=1.098217\B58=1.094494\B59=1
.541072\B60=1.095311\B61=1.094416\B62=1.096753\A1=58.367985\A2=58.3462
42\A3=128.167099\A4=128.003615\A5=114.497737\A6=114.581347\A7=107.6029
12\A8=107.646786\A9=106.976774\A10=106.952326\A11=112.929638\A12=112.7
95374\A13=126.242014\A14=128.988622\A15=106.737324\A16=106.703671\A17=
106.932168\A18=106.902764\A19=136.330656\A20=136.018761\A21=108.099667
\A22=108.125981\A23=127.588576\A24=121.778947\A25=111.118945\A26=127.0

40909\A27=132.323641\A28=109.58229\A29=110.898896\A30=110.009617\A31=107.249136\A32=107.015417\A33=121.697869\A34=118.757058\A35=120.912477\A36=120.838092\A37=121.681976\A38=111.789283\A39=109.868293\A40=111.894889\A41=112.662849\A42=107.641656\A43=109.868136\A44=112.646484\A45=111.585141\A46=109.900025\A47=109.983038\A48=111.310459\A49=112.015083\A50=107.614835\A51=111.658542\A52=109.859802\A53=112.661631\A54=109.861293\A55=111.449599\A56=111.966665\A57=110.010903\A58=111.88252\A59=112.69944\A60=109.79814\A61=111.931321\D1=178.286276\D2=7.371205\D3=7.871695\D4=-175.098137\D5=-174.603544\D6=171.281512\D7=171.704224\D8=176.478469\D9=176.291724\D10=-109.227219\D11=-109.485112\D12=84.63525\D13=-95.441453\D14=-106.189215\D15=-106.251953\D16=136.35123\D17=136.237283\D18=40.480437\D19=-140.32152\D20=130.584597\D21=130.102832\D22=176.535587\D23=-175.351697\D24=175.518486\D25=5.826051\D26=176.199372\D27=174.357305\D28=130.627924\D29=-107.671967\D30=133.890406\D31=-107.889705\D32=-171.59324\D33=-178.660232\D34=2.446817\D35=179.23416\D36=-0.372865\D37=59.422194\D38=178.045557\D39=-63.146424\D40=59.113626\D41=-179.487849\D42=176.431818\D43=-64.581232\D44=57.090272\D45=-61.897022\D46=-177.804416\D47=-58.681666\D48=63.755056\D49=-178.906491\D50=57.491226\D51=176.82212\D52=-64.206115\D53=-61.223349\D54=-57.611577\D55=64.87079\D56=-176.804686\D57=60.087563\D58=59.261268\D59=178.18627\D60=-63.111725\\Version=HP-PARisc-HPUX-G98RevA.11\HF=-3000.3674793\S2=0.751839\S2-1=0.\S2A=0.750003\RMSD=9.359e-08\RMSF=3.832e-05\Dipole=0.7261379,0.6673435,2.8257483\ PG=C01 [X(C21H33Cu1N3O5)]\NImag=0\

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole),
Raman scattering activities (A⁴/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	16.7455	22.3078	28.6293
Red. masses --	3.8686	4.6545	4.4475
Frc consts --	0.0006	0.0014	0.0021
IR Inten --	0.3612	0.6580	3.3083
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

Zero-point correction= 0.536578 (Hartree/Particle)
Thermal correction to Energy= 0.568513
Thermal correction to Enthalpy= 0.569457
Thermal correction to Gibbs Free Energy= 0.472340
Sum of electronic and zero-point Energies= -2999.830902
Sum of electronic and thermal Energies= -2999.798966
Sum of electronic and thermal Enthalpies= -2999.798022
Sum of electronic and thermal Free Energies= -2999.895140

TS of *t*-butyl substituted bis(oxazoline)-Cu(II) NC *Re* in vacuum at UB3LYP/6-31G(d)

Freq\UB3LYP\6-31G(d)\C26H39Cu1N3O5(2+,2)\MADURA\31-Mar-2
003\1\#\ UB3LYP/6-31G(D) FREQ GUESS=READ GEOM=CHECK\bisoxc2_acry_nctu
bal opt.\2,2\C\Cu,1,B1\C,1,B2,2,A1\C,1,B3,2,A2,3,D1,0\N,3,B4,1,A3,2,D
2,0\N,4,B5,1,A4,2,D3,0\O,3,B6,1,A5,2,D4,0\O,4,B7,1,A6,2,D5,0\C,5,B8,3,
A7,1,D6,0\C,6,B9,4,A8,1,D7,0\C,7,B10,3,A9,1,D8,0\C,8,B11,4,A10,1,D9,0\
C,9,B12,5,A11,3,D10,0\C,10,B13,6,A12,4,D11,0\H,1,B14,2,A13,6,D12,0\H,1
,B15,2,A14,6,D13,0\H,11,B16,7,A15,3,D14,0\H,12,B17,8,A16,4,D15,0\H,11,
B18,7,A17,3,D16,0\H,12,B19,8,A18,4,D17,0\O,2,B20,1,A19,3,D18,0\O,2,B21

, 1, A20, 3, D19, 0\H, 9, B22, 5, A21, 3, D20, 0\H, 10, B23, 6, A22, 4, D21, 0\C, 22, B24, 2, A23, 1, D22, 0\O, 25, B25, 22, A24, 2, D23, 0\C, 26, B26, 25, A25, 22, D24, 0\N, 25, B27, 22, A26, 2, D25, 0\C, 21, B28, 2, A27, 1, D26, 0\C, 28, B29, 25, A28, 22, D27, 0\H, 30, B30, 28, A29, 25, D28, 0\H, 30, B31, 28, A30, 25, D29, 0\H, 27, B32, 26, A31, 25, D30, 0\H, 27, B33, 26, A32, 25, D31, 0\C, 29, B34, 21, A33, 2, D32, 0\H, 35, B35, 29, A34, 21, D33, 0\C, 35, B36, 29, A35, 21, D34, 0\H, 37, B37, 35, A36, 29, D35, 0\H, 37, B38, 35, A37, 29, D36, 0\C, 37, B39, 35, A38, 29, D37, 0\C, 35, B40, 37, A39, 38, D38, 0\C, 40, B41, 37, A40, 35, D39, 0\C, 42, B42, 40, A41, 37, D40, 0\C, 41, B43, 40, A42, 37, D41, 0\H, 44, B44, 41, A43, 40, D42, 0\H, 44, B45, 41, A44, 40, D43, 0\H, 40, B46, 37, A45, 35, D44, 0\H, 41, B47, 40, A46, 37, D45, 0\H, 43, B48, 42, A47, 40, D46, 0\H, 42, B49, 40, A48, 37, D47, 0\C, 13, B50, 9, A49, 5, D48, 0\H, 51, B51, 13, A50, 9, D49, 0\H, 51, B52, 13, A51, 9, D50, 0\H, 51, B53, 13, A52, 9, D51, 0\C, 13, B54, 9, A53, 5, D52, 0\H, 55, B55, 13, A54, 9, D53, 0\H, 55, B56, 13, A55, 9, D54, 0\H, 55, B57, 13, A56, 9, D55, 0\C, 13, B58, 9, A57, 5, D56, 0\H, 59, B59, 13, A58, 9, D57, 0\H, 59, B60, 13, A59, 9, D58, 0\H, 59, B61, 13, A60, 9, D59, 0\C, 14, B62, 10, A61, 6, D60, 0\H, 63, B63, 14, A62, 10, D61, 0\H, 63, B64, 14, A63, 10, D62, 0\H, 63, B65, 14, A64, 10, D63, 0\C, 14, B66, 10, A65, 6, D64, 0\H, 67, B67, 14, A66, 10, D65, 0\H, 67, B68, 14, A67, 10, D66, 0\H, 67, B69, 14, A68, 10, D67, 0\C, 14, B70, 10, A69, 6, D68, 0\H, 71, B71, 14, A70, 10, D69, 0\H, 71, B72, 14, A71, 10, D70, 0\H, 71, B73, 14, A72, 10, D71, 0\B1=3.37757401\B2=1.49522318\B3=1.49558434\B4=1.29324279\B5=1.29398066\B6=1.32036701\B7=1.31891346\B8=1.50008842\B9=1.50255766\B10=1.46541781\B11=1.46764069\B12=1.56237814\B13=1.5617447\B14=1.09929371\B15=1.09702206\B16=1.09256671\B17=1.09244797\B18=1.08790063\B19=1.08789093\B20=1.92510327\B21=1.9506967\B22=1.09304149\B23=1.09225857\B24=1.24079538\B25=1.3171671\B26=1.45705017\B27=1.37349708\B28=1.27566897\B29=1.47733428\B30=1.09174124\B31=1.0938759\B32=1.08949865\B33=1.09112914\B34=1.41032677\B35=1.08172967\B36=1.39791614\B37=1.08504549\B38=1.08327469\B39=2.13239932\B40=3.13694904\B41=1.39398458\B42=1.42805757\B43=1.49623854\B44=1.1035211\B45=1.09344062\B46=1.08498075\B47=1.08470826\B48=1.08372105\B49=1.08505004\B50=1.5407819\B51=1.09553504\B52=1.09454338\B53=1.09663868\B54=1.54047981\B55=1.09625899\B56=1.09737072\B57=1.09466806\B58=1.54438952\B59=1.09675009\B60=1.09451524\B61=1.09508165\B62=1.54429723\B63=1.0950975\B64=1.0964104\B65=1.09468105\B66=1.54053251\B67=1.09530037\B68=1.09561292\B69=1.09806474\B70=1.5408676\B71=1.09467183\B72=1.09691095\B73=1.09522913\A1=58.53673136\A2=58.36133069\A3=128.19134268\A4=127.81698646\A5=114.31346947\A6=114.59667706\A7=107.52035096\A8=107.41119253\A9=106.8250769\A10=106.71711065\A11=113.14027778\A12=112.92214464\A13=120.90062933\A14=134.17222028\A15=106.82923258\A16=106.69223189\A17=106.94947149\A18=107.00835539\A19=135.38908374\A20=134.91568484\A21=107.9079048\A22=108.03895646\A23=125.39954306\A24=120.49505888\A25=110.6313507\A26=127.73558585\A27=131.68126712\A28=110.07888571\A29=110.73605475\A30=109.9161276\A31=107.42526158\A32=107.18195795\A33=122.71786665\A34=119.22212741\A35=121.34563856\A36=118.04276798\A37=118.98806577\A38=110.5829278\A39=88.21170872\A40=99.53819404\A41=109.91998882\A42=39.04695551\A43=108.41596547\A44=115.24956183\A45=96.475057\A46=162.37589821\A47=125.05459091\A48=125.09998312\A49=111.80971689\A50=112.68420612\A51=109.84871341\A52=111.8635728\A53=109.88784068\A54=111.37537195\A55=111.97405112\A56=109.93697561\A57=107.69505234\A58=111.6210834\A59=109.87207821\A60=112.72050018\A61=107.61298474\A62=112.59120838\A63=111.5607041\A64=109.94146584\A65=109.80483811\A66=109.79597331\A67=111.50590388\A68=111.77825644\A69=111.95934067\A70=109.83113273\A71=111.95289832\A72=112.67240711\D1=171.74126681\D2=7.23627666\D3=9.76832388\D4=-174.34425985\D5=-172.95866139\D6=172.34549299\D7=171.63347465\D8=175.85354677\D9=175.85172707\D10=-109.584389\D11=-109.06124398\D12=86.6869503\D13=-93.4538554\D14=-106.64036098\D15=-105.30114898\D16=135.93875651\D17=137.22686482\D18=41.51072534\D19=-138.88650456\D20=130.4297941\D21=130.72721977\D22=169.06408909\D23=-172.62962507\D24=175.74487699\D25=7.80921136\D26=-169.93111696

\D27=177.29010722\D28=126.83920936\D29=-112.23364225\D30=130.52691742\
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 D35=-160.63513457\D36=-13.03652174\D37=98.7941946\D38=102.87316396\D39=
 -73.74246675\D40=92.85019279\D41=97.60545598\D42=113.91739668\D43=-127
 .72105393\D44=161.04476592\D45=81.01070145\D46=-175.86469472\D47=-85.4
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 909\D52=-62.20864167\D53=-58.31305562\D54=63.93947291\D55=-177.5307199
 8\D56=-179.81418474\D57=57.14680943\D58=176.38320829\D59=-64.59679648\
 D60=-178.3339765\D61=-63.92011988\D62=57.63263623\D63=177.04530962\D64
 =-60.63836475\D65=-177.12132459\D66=-57.81983844\D67=64.04482656\D68=6
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 HP-PARisc-HPUX-G98RevA.11\HF=-3194.4764913\S2=0.751888\S2-1=0.\S2A=0.7
 50003\RMSD=4.477e-09\RMSF=3.050e-05\Dipole=0.7960866,1.0156018,2.25663
 49\ PG=C01 [X(C26H39Cu1N3O5)]\NImag=1\

***** 1 imaginary frequencies (negative Signs) *****
 Harmonic frequencies (cm**⁻¹), IR intensities (KM/Mole),
 Raman scattering activities (A**⁴/AMU), Raman depolarization ratios,
 reduced masses (AMU), force constants (mDyne/A) and normal
 coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	-243.1189	19.5491	20.0510
Red. masses --	9.0192	4.4799	4.2143
Frc consts --	0.3141	0.0010	0.0010
IR Inten --	255.7288	0.0738	0.1352
Raman Activ --	0.0000	0.0000	0.0000
Depolar --	0.0000	0.0000	0.0000

Zero-point correction= 0.632523
 (Hartree/Particle)
 Thermal correction to Energy= 0.668630
 Thermal correction to Enthalpy= 0.669574
 Thermal correction to Gibbs Free Energy= 0.562664
 Sum of electronic and zero-point Energies= -3193.843969
 Sum of electronic and thermal Energies= -3193.807862
 Sum of electronic and thermal Enthalpies= -3193.806917
 Sum of electronic and thermal Free Energies= -3193.913828

t-butyl substituted bis(oxazoline)-Cu(II) NC Re in PCM at UB3LYP/6-31G(d)

1 | 1 | UNPC-UNK | SP | UB3LYP | 6-31G(d) | C26H39Cu1N3O5 (2+, 2) | PCUSER | 10-Jun-2003
 | 0 | # UB3LYP/6-31G* SP SCRF=(PCM,READ,SOLVENT=CH2CL2) | | tbutncrepcm sp.
 | | 2, 2 | C | Cu, 1, 3.3776 | C, 1, 1.4952, 2, 58.5367 | C, 1, 1.4956, 2, 58.3613, 3, 171.74
 13, 0 | N, 3, 1.2932, 1, 128.1913, 2, 7.2363, 0 | N, 4, 1.294, 1, 127.817, 2, 9.7683, 0 | O
 , 3, 1.3204, 1, 114.3135, 2, -174.3443, 0 | O, 4, 1.3189, 1, 114.5967, 2, -172.9587, 0
 | C, 5, 1.5001, 3, 107.5204, 1, 172.3455, 0 | C, 6, 1.5026, 4, 107.4112, 1, 171.6335, 0
 | C, 7, 1.4654, 3, 106.8251, 1, 175.8535, 0 | C, 8, 1.4676, 4, 106.7171, 1, 175.8517, 0
 | C, 9, 1.5624, 5, 113.1403, 3, -109.5844, 0 | C, 10, 1.5617, 6, 112.9221, 4, -109.061
 2, 0 | H, 1, 1.0993, 2, 120.9006, 6, 86.687, 0 | H, 1, 1.097, 2, 134.1722, 6, -93.4539, 0
 | H, 11, 1.0926, 7, 106.8292, 3, -106.6404, 0 | H, 12, 1.0924, 8, 106.6922, 4, -105.30
 11, 0 | H, 11, 1.0879, 7, 106.9495, 3, 135.9388, 0 | H, 12, 1.0879, 8, 107.0084, 4, 137.
 2269, 0 | O, 2, 1.9251, 1, 135.3891, 3, 41.5107, 0 | O, 2, 1.9507, 1, 134.9157, 3, -138.
 8865, 0 | H, 9, 1.093, 5, 107.9079, 3, 130.4298, 0 | H, 10, 1.0923, 6, 108.039, 4, 130.7
 272, 0 | C, 22, 1.2408, 2, 125.3995, 1, 169.0641, 0 | O, 25, 1.3172, 22, 120.4951, 2, -1
 72.6296, 0 | C, 26, 1.4571, 25, 110.6314, 22, 175.7449, 0 | N, 25, 1.3735, 22, 127.735
 6, 2, 7.8092, 0 | C, 21, 1.2757, 2, 131.6813, 1, -169.9311, 0 | C, 28, 1.4773, 25, 110.0

789, 22, 177.2901, 0 | H, 30, 1.0917, 28, 110.7361, 25, 126.8392, 0 | H, 30, 1.0939, 28, 109.9161, 25, -112.2336, 0 | H, 27, 1.0895, 26, 107.4253, 25, 130.5269, 0 | H, 27, 1.0911, 26, 107.182, 25, -111.398, 0 | C, 29, 1.4103, 21, 122.7179, 2, 173.3394, 0 | H, 35, 1.0817, 29, 119.2221, 21, -179.8344, 0 | C, 35, 1.3979, 29, 121.3456, 21, -1.4423, 0 | H, 37, 1.085, 35, 118.0428, 29, -160.6351, 0 | H, 37, 1.0833, 35, 118.9881, 29, -13.0365, 0 | C, 37, 2.1324, 35, 110.5829, 29, 98.7942, 0 | C, 35, 3.1369, 37, 88.2117, 38, 102.8732, 0 | C, 40, 1.394, 37, 99.5382, 35, -73.7425, 0 | C, 42, 1.4281, 40, 109.92, 37, 92.8502, 0 | C, 41, 1.4962, 40, 39.047, 37, 97.6055, 0 | H, 44, 1.1035, 41, 108.416, 40, 113.9174, 0 | H, 44, 1.0934, 41, 115.2496, 40, -127.7211, 0 | H, 40, 1.085, 37, 96.4751, 35, 161.0448, 0 | H, 41, 1.0847, 40, 162.3759, 37, 81.0107, 0 | H, 43, 1.10837, 42, 125.0546, 40, -175.8647, 0 | H, 42, 1.0851, 40, 125.1, 37, -85.4054, 0 | C, 13, 1.5408, 9, 111.8097, 5, 59.2074, 0 | H, 51, 1.0955, 13, 112.6842, 9, 59.4106, 0 | H, 51, 1.0945, 13, 109.8487, 9, 178.3632, 0 | H, 51, 1.0966, 13, 111.8636, 9, -62.9219, 0 | C, 13, 1.5405, 9, 109.8878, 5, -62.2086, 0 | H, 55, 1.0963, 13, 111.3754, 9, -58.3131, 0 | H, 55, 1.0974, 13, 111.9741, 9, 63.9395, 0 | H, 55, 1.0947, 13, 109.937, 9, -177.5307, 0 | C, 13, 1.5444, 9, 107.6951, 5, -179.8142, 0 | H, 59, 1.0968, 13, 111.6211, 9, 57.1468, 0 | H, 59, 1.0945, 13, 109.8721, 9, 176.3832, 0 | H, 59, 1.0951, 13, 112.7205, 9, -64.5968, 0 | C, 14, 1.5443, 10, 107.613, 6, -178.334, 0 | H, 63, 1.0951, 14, 112.5912, 10, -63.9201, 0 | H, 63, 1.0964, 14, 111.5607, 10, 57.6326, 0 | H, 63, 1.0947, 14, 109.9415, 10, 177.0453, 0 | C, 14, 1.5405, 10, 109.8048, 6, -60.6384, 0 | H, 67, 1.0953, 14, 109.796, 10, -177.1213, 0 | H, 67, 1.0956, 14, 111.5059, 10, -57.8198, 0 | H, 67, 1.0981, 14, 111.7783, 10, 64.0448, 0 | C, 14, 1.5409, 10, 111.9593, 6, 60.6987, 0 | H, 71, 1.0947, 14, 109.8311, 10, 178.7139, 0 | H, 71, 1.0969, 14, 111.9529, 10, -62.4279, 0 | H, 71, 1.0952, 14, 112.6724, 10, 59.8391, 0 | | Version=x86-Win32-G03RevB.03 | State=2-A | HF=-3194.6513478 | S2=0.751886 | S2-1=0. | S2A=0.750003 | RMSD=4.489e-005 | Dipole=0.9717243, 1.0876843, 2.4923463 | PG=C01 [X(C26H39Cu1N3O5)] | |@

Population analysis of methyl substituted bis(oxazoline)-Cu(II)

			116	117	118	119	120	
			(A) --O	(A) --O	(A) --O	(A) --V	(A) --V	
16	2	Cu	1S	0.00060	0.00058	-0.00003	0.00003	-0.00172
17			2S	0.00280	0.00286	-0.00069	0.00036	-0.00414
18			2PX	-0.00050	-0.00101	-0.00071	-0.00024	-0.00292
19			2PY	0.00510	0.00363	0.00038	-0.00139	-0.00312
20			2PZ	-0.00552	-0.00144	-0.00144	0.00230	-0.01346
21			3S	-0.00628	-0.00576	-0.00049	0.00000	0.02356
22			3PX	0.00144	0.00147	0.00152	0.00008	0.00477
23			3PY	-0.01360	-0.00908	-0.00002	0.00352	0.00788
24			3PZ	0.01307	0.00343	0.00278	-0.00421	0.02826
25			4S	0.01717	0.02923	-0.01465	0.00618	0.01771
26			4PX	-0.00155	-0.01347	-0.00571	-0.00523	-0.03407
27			4PY	0.02169	0.01998	0.00861	-0.00737	-0.01742
28			4PZ	-0.03623	-0.00955	-0.01366	0.02367	-0.11438
29			5S	0.01166	-0.00449	-0.01324	0.01496	0.15783
30			5PX	0.02484	-0.00219	0.00600	-0.00327	0.00932
31			5PY	0.02371	0.00866	-0.00886	-0.04224	-0.00195
32			5PZ	0.01502	0.02041	-0.00661	0.00785	-0.05689
33			6XX	0.17312	0.13505	0.00382	-0.00140	-0.01343
34			6YY	-0.20081	-0.04188	-0.01091	0.01145	0.03337
35			6ZZ	0.02704	-0.09377	0.00766	-0.01040	-0.02237
36			6XY	0.20344	0.16766	-0.02645	0.01477	-0.01519
37			6XZ	-0.01358	0.02435	0.04562	-0.02924	-0.02505
38			6YZ	-0.14486	0.03122	0.02879	-0.02777	-0.01450
39			7XX	0.08597	0.07043	0.00163	-0.00015	-0.00338
40			7YY	-0.10390	-0.01801	-0.00659	0.00537	0.01711

41	7ZZ	0.01399	-0.05023	0.00334	-0.00504	-0.00835
42	7XY	0.10040	0.08511	-0.01297	0.00685	-0.00658
43	7XZ	-0.00478	0.01448	0.02360	-0.01357	-0.01169
44	7YZ	-0.07682	0.01857	0.01479	-0.01266	-0.00598
45	8F 0	0.00204	0.00210	0.00057	-0.00091	0.00065
46	8F+1	0.00287	-0.00075	-0.00021	0.00040	0.00097
47	8F-1	-0.00096	-0.00119	0.00023	-0.00060	0.00008
48	8F+2	0.00006	0.00120	-0.00099	0.00177	0.00183
49	8F-2	-0.00087	0.00167	-0.00092	0.00167	0.00119
50	8F+3	-0.00066	-0.00053	-0.00115	0.00146	0.00154
51	8F-3	-0.00122	0.00099	0.00020	-0.00030	0.00023

1\1\GINC-CANGREJO1\SP\UB3LYP\6-31G(d)\C20H27Cu1N3O5(2+,2)\JASON\18-Jul-2003\0\#\ UB3LYP/6-31G* POP=FULL\Nc re methyl popfull\2,2\C\Cu,1,3.3924\C,1,1.4959,2,58.4741\C,1,1.4964,2,58.3519,3,174.6505,0\N,3,1.2928,1,128.09,2,0.8631,0\N,4,1.2928,1,127.9907,2,3.4359,0\O,3,1.32,1,114.3469,2,-179.319,0\O,4,1.3185,1,114.3235,2,-177.489,0\C,5,1.4952,3,107.9962,1,177.4862,0\C,6,1.498,4,108.0047,1,178.2323,0\C,7,1.4658,3,107.5376,1,178.1561,0\C,8,1.4673,4,107.5773,1,179.2315,0\C,9,1.5278,5,111.5128,3,-116.7596,0\C,10,1.527,6,111.6754,4,-119.3967,0\H,1,1.0991,2,123.3829,6,90.0553,0\H,1,1.0975,2,131.8706,6,-89.9144,0\H,11,1.0912,7,107.0138,3,-116.2319,0\H,12,1.0908,8,106.9674,4,-118.252,0\H,11,1.0912,7,107.0698,3,125.9432,0\H,12,1.0914,8,107.003,4,123.9278,0\H,13,1.0947,9,111.0481,5,-61.8217,0\H,14,1.0947,10,110.9474,6,-62.3746,0\H,13,1.0953,9,111.1912,5,59.2902,0\H,14,1.0956,10,111.241,6,59.0659,0\H,13,1.095,9,110.0329,5,179.1049,0\H,14,1.095,10,109.8874,6,178.8607,0\O,2,1.9186,1,136.3946,3,39.3297,0\O,2,1.9431,1,133.9543,3,-139.0801,0\H,9,1.093,5,107.7345,3,122.4643,0\H,10,1.0928,6,107.6305,4,119.8782,0\C,28,1.2423,2,125.4176,1,165.6564,0\O,31,1.3156,28,120.6055,2,-170.2125,0\C,32,1.4587,31,110.4423,28,175.2741,0\N,31,1.3731,28,127.5454,2,10.3275,0\C,27,1.2776,2,131.885,1,-169.6368,0\C,34,1.478,31,109.9217,28,175.9716,0\H,36,1.0916,34,110.7937,31,129.1614,0\H,36,1.094,34,109.9048,31,-109.7817,0\H,33,1.0893,32,107.4082,31,132.5477,0\H,33,1.0913,32,107.1287,31,-109.3131,0\C,35,1.4093,27,122.7929,2,-182.9951,0\H,41,1.0819,35,119.0962,27,-179.8731,0\C,41,1.3966,35,121.4761,27,-1.1408,0\H,43,1.0848,41,118.1917,35,-161.4052,0\H,43,1.0832,41,119.1977,35,-12.9687,0\C,43,2.1496,41,110.332,35,98.655,0\C,46,2.3479,43,98.5474,41,-3.8672,0\C,46,1.3928,43,99.225,41,-74.5185,0\C,48,1.4292,46,109.9079,43,93.2137,0\C,47,1.4965,46,39.0027,43,97.4504,0\H,50,1.1036,47,108.3983,46,113.9397,0\H,50,1.0935,47,115.2464,46,-127.7725,0\H,46,1.0849,43,96.1074,41,160.2885,0\H,47,1.0847,46,162.403,43,82.0275,0\H,49,1.084,48,125.0394,46,-176.5479,0\H,48,1.0851,46,125.1329,43,-85.3532,0\Version=x86-Linux-G03RevB.03\State=2-A\HF=-2958.5954862\S2=0.751966\S2-1=0.\S2A=0.750003\RMSD=7.026e-05\Dipole=0.576172,0.5205459,1.4622533\PG=C01 [X(C20H27Cu1N3O5)]\@

Population analysis of *t*-butyl substituted bis(oxazoline)-Cu(II)

		141	142	143	144	145		
		(A) --O	(A) --O	(A) --V	(A) --V	(A) --V		
16	2	Cu	1S	-0.00063	0.00014	0.00024	0.00168	-0.00031
17			2S	-0.00229	0.00125	0.00127	0.00338	0.00068
18			2PX	-0.00033	-0.00028	0.00106	-0.00144	-0.00715
19			2PY	-0.00302	-0.00081	-0.00210	-0.00174	-0.00376
20			2PZ	0.00042	-0.00060	-0.00076	-0.00670	-0.01587
21			3S	0.00748	-0.00059	-0.00242	-0.02402	0.00627
22			3PX	-0.00054	0.00067	-0.00173	0.00131	0.01558

23	3PY	0.00730	0.00129	0.00492	0.00179	0.00680
24	3PZ	-0.00104	0.00138	0.00054	0.01394	0.03548
25	4S	-0.01418	0.01982	0.01107	-0.03227	0.03180
26	4PX	-0.01161	-0.00185	0.01265	-0.02415	-0.05685
27	4PY	-0.01856	-0.00954	-0.01411	-0.02781	-0.03903
28	4PZ	0.00204	-0.00417	-0.01387	-0.05802	-0.11947
29	5S	0.02122	0.01590	0.01636	-0.17486	0.08448
30	5PX	-0.00628	0.00037	-0.00098	0.02424	0.00687
31	5PY	0.01413	-0.00619	-0.04802	0.01203	0.00921
32	5PZ	0.01836	-0.00897	0.02221	0.00188	-0.12351
33	6XX	-0.11279	0.00891	0.00524	0.00589	0.04942
34	6YY	0.08867	0.01740	0.01923	-0.03192	-0.00845
35	6ZZ	0.02401	-0.02704	-0.02498	0.02904	-0.04275
36	6XY	0.07747	-0.05690	-0.03266	0.00625	-0.01530
37	6XZ	-0.08276	-0.02273	-0.01452	0.01963	0.03687
38	6YZ	0.06278	-0.00570	-0.00624	0.02130	0.00699
39	7XX	-0.05928	0.00490	0.00262	-0.00059	0.02264
40	7YY	0.04655	0.01001	0.00839	-0.01669	-0.00257
41	7ZZ	0.01133	-0.01321	-0.01209	0.01028	-0.01829
42	7XY	0.03934	-0.02899	-0.01524	0.00299	-0.00557
43	7XZ	-0.04381	-0.01232	-0.00689	0.00933	0.01619
44	7YZ	0.03614	-0.00352	-0.00333	0.01019	0.00251
45	8F 0	-0.00100	0.00070	0.00141	-0.00127	0.00245
46	8F+1	0.00033	-0.00050	-0.00106	0.00076	0.00067
47	8F-1	0.00225	0.00005	0.00012	0.00043	0.00054
48	8F+2	0.00004	-0.00027	-0.00052	-0.00036	0.00168
49	8F-2	-0.00141	-0.00066	-0.00073	0.00135	0.00147
50	8F+3	0.00114	-0.00091	-0.00129	0.00097	0.00013
51	8F-3	-0.00073	-0.00117	-0.00189	0.00155	0.00098

1 | 1 | UNPC-UNK | SP | UB3LYP | 6-31G(d) | C26H39Cu1N3O5(2+,2) | PCUSER | 18-Jul-2003
| 0 | # UB3LYP/6-31G* POP=FULL | | tbutncre pop=full. | | 2,2 | C | Cu,1,3.3776 | C,
1,1.4952,2,58.5367 | C,1,1.4956,2,58.3613,3,171.7413,0 | N,3,1.2932,1,128.
1913,2,7.2363,0 | N,4,1.294,1,127.817,2,9.7683,0 | O,3,1.3204,1,114.3135,2
,-174.3443,0 | O,4,1.3189,1,114.5967,2,-172.9587,0 | C,5,1.5001,3,107.5204
,1,172.3455,0 | C,6,1.5026,4,107.4112,1,171.6335,0 | C,7,1.4654,3,106.8251
,1,175.8535,0 | C,8,1.4676,4,106.7171,1,175.8517,0 | C,9,1.5624,5,113.1403
,3,-109.5844,0 | C,10,1.5617,6,112.9221,4,-109.0612,0 | H,1,1.0993,2,120.9
006,6,86.687,0 | H,1,1.097,2,134.1722,6,-93.4539,0 | H,11,1.0926,7,106.829
2,3,-106.6404,0 | H,12,1.0924,8,106.6922,4,-105.3011,0 | H,11,1.0879,7,106
.9495,3,135.9388,0 | H,12,1.0879,8,107.0084,4,137.2269,0 | O,2,1.9251,1,13
5.3891,3,41.5107,0 | O,2,1.9507,1,134.9157,3,-138.8865,0 | H,9,1.093,5,107
.9079,3,130.4298,0 | H,10,1.0923,6,108.039,4,130.7272,0 | C,22,1.2408,2,12
5.3995,1,169.0641,0 | O,25,1.3172,22,120.4951,2,-172.6296,0 | C,26,1.4571,
25,110.6314,22,175.7449,0 | N,25,1.3735,22,127.7356,2,7.8092,0 | C,21,1.27
57,2,131.6813,1,-169.9311,0 | C,28,1.4773,25,110.0789,22,177.2901,0 | H,30
,1.0917,28,110.7361,25,126.8392,0 | H,30,1.0939,28,109.9161,25,-112.2336
,0 | H,27,1.0895,26,107.4253,25,130.5269,0 | H,27,1.0911,26,107.182,25,-11
1.398,0 | C,29,1.4103,21,122.7179,2,173.3394,0 | H,35,1.0817,29,119.2221,2
1,-179.8344,0 | C,35,1.3979,29,121.3456,21,-1.4423,0 | H,37,1.085,35,118.0
428,29,-160.6351,0 | H,37,1.0833,35,118.9881,29,-13.0365,0 | C,37,2.1324,3
5,110.5829,29,98.7942,0 | C,35,3.1369,37,88.2117,38,102.8732,0 | C,40,1.39
4,37,99.5382,35,-73.7425,0 | C,42,1.4281,40,109.92,37,92.8502,0 | C,41,1.4
962,40,39.047,37,97.6055,0 | H,44,1.1035,41,108.416,40,113.9174,0 | H,44,1
.0934,41,115.2496,40,-127.7211,0 | H,40,1.085,37,96.4751,35,161.0448,0 | H
,41,1.0847,40,162.3759,37,81.0107,0 | H,43,1.0837,42,125.0546,40,-175.86
47,0 | H,42,1.0851,40,125.1,37,-85.4054,0 | C,13,1.5408,9,111.8097,5,59.20

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.36423892E+00
EXCITATION FACTOR 0.94169738E-03
ZERO-POINT DIFFERENCE FACTOR 0.27020242E+02
TELLER-REDLICH PRODUCT RATIO 0.10069872E+01
(S2/S1) F 0.10916674E+02

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RELATIONSHIPS BETWEEN ISOTOPOMERS 10 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.36306004E+00
EXCITATION FACTOR 0.93689517E-03
ZERO-POINT DIFFERENCE FACTOR 0.29932740E+02
TELLER-REDLICH PRODUCT RATIO 0.10035244E+01
(S2/S1) F 0.11672107E+02

QUIVER output of methyl substituted bis(oxazoline)-Cu(II) NC Re TS

=====

RELATIONSHIPS BETWEEN ISOTOPOMERS 2 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.90792497E+00
EXCITATION FACTOR 0.35917112E-07
ZERO-POINT DIFFERENCE FACTOR 0.12451809E+01
TELLER-REDLICH PRODUCT RATIO 0.10138557E+01
(S2/S1) F 0.11478996E+01

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RELATIONSHIPS BETWEEN ISOTOPOMERS 3 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.91014114E+00
EXCITATION FACTOR 0.35373656E-07
ZERO-POINT DIFFERENCE FACTOR 0.12376692E+01
TELLER-REDLICH PRODUCT RATIO 0.10178873E+01
(S2/S1) F 0.11466335E+01

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RELATIONSHIPS BETWEEN ISOTOPOMERS 4 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.91103439E+00
EXCITATION FACTOR 0.35284997E-07
ZERO-POINT DIFFERENCE FACTOR 0.12439147E+01
TELLER-REDLICH PRODUCT RATIO 0.10200897E+01
(S2/S1)F 0.11506200E+01

=====

RELATIONSHIPS BETWEEN ISOTOPOMERS 5 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.90829846E+00
EXCITATION FACTOR 0.35374870E-07
ZERO-POINT DIFFERENCE FACTOR 0.12469216E+01
TELLER-REDLICH PRODUCT RATIO 0.10165323E+01
(S2/S1)F 0.11503563E+01

=====

RELATIONSHIPS BETWEEN ISOTOPOMERS 6 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.92088429E+00
EXCITATION FACTOR 0.35361996E-07
ZERO-POINT DIFFERENCE FACTOR 0.12211428E+01
TELLER-REDLICH PRODUCT RATIO 0.10292015E+01
(S2/S1)F 0.11369238E+01

=====

RELATIONSHIPS BETWEEN ISOTOPOMERS 7 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.36987429E+00
EXCITATION FACTOR 0.35525611E-07
ZERO-POINT DIFFERENCE FACTOR 0.26606361E+02
TELLER-REDLICH PRODUCT RATIO 0.10348951E+01
(S2/S1)F 0.10827405E+02

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RELATIONSHIPS BETWEEN ISOTOPOMERS 8 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.37105590E+00
EXCITATION FACTOR 0.32644998E-07
ZERO-POINT DIFFERENCE FACTOR 0.27746549E+02
TELLER-REDLICH PRODUCT RATIO 0.10406535E+01

(S2/S1)F 0.11220373E+02

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RELATIONSHIPS BETWEEN ISOTOPOMERS 9 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.36818673E+00
EXCITATION FACTOR 0.32956602E-07
ZERO-POINT DIFFERENCE FACTOR 0.27362670E+02
TELLER-REDLICH PRODUCT RATIO 0.10316297E+01
(S2/S1)F 0.11076380E+02

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RELATIONSHIPS BETWEEN ISOTOPOMERS 10 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.36756690E+00
EXCITATION FACTOR 0.32668574E-07
ZERO-POINT DIFFERENCE FACTOR 0.29852196E+02
TELLER-REDLICH PRODUCT RATIO 0.10265768E+01

QUIVER output of *t*-butyl substituted bis(oxazoline)-Cu(II) NC Re TS

=====

RELATIONSHIPS BETWEEN ISOTOPOMERS 2 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.90078903E+00
EXCITATION FACTOR 0.22330327E-10
ZERO-POINT DIFFERENCE FACTOR 0.12515632E+01
TELLER-REDLICH PRODUCT RATIO 0.10072111E+01
(S2/S1)F 0.11497237E+01

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RELATIONSHIPS BETWEEN ISOTOPOMERS 3 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.90395464E+00
EXCITATION FACTOR 0.21896639E-10
ZERO-POINT DIFFERENCE FACTOR 0.12299122E+01
TELLER-REDLICH PRODUCT RATIO 0.10121264E+01
(S2/S1)F 0.11385944E+01

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RELATIONSHIPS BETWEEN ISOTOPOMERS 4 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.90235677E+00
EXCITATION FACTOR 0.21804533E-10
ZERO-POINT DIFFERENCE FACTOR 0.12503761E+01
TELLER-REDLICH PRODUCT RATIO 0.10115071E+01
(S2/S1)F 0.11520780E+01

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RELATIONSHIPS BETWEEN ISOTOPOMERS 5 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.90162818E+00
EXCITATION FACTOR 0.21869161E-10
ZERO-POINT DIFFERENCE FACTOR 0.12503131E+01
TELLER-REDLICH PRODUCT RATIO 0.10103360E+01
(S2/S1)F 0.11512072E+01

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RELATIONSHIPS BETWEEN ISOTOPOMERS 6 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.91199902E+00
EXCITATION FACTOR 0.21866931E-10
ZERO-POINT DIFFERENCE FACTOR 0.12198677E+01
TELLER-REDLICH PRODUCT RATIO 0.10206946E+01
(S2/S1)F 0.11328763E+01

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RELATIONSHIPS BETWEEN ISOTOPOMERS 7 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.36418789E+00
EXCITATION FACTOR 0.21929043E-10
ZERO-POINT DIFFERENCE FACTOR 0.27914042E+02
TELLER-REDLICH PRODUCT RATIO 0.10203825E+01
(S2/S1)F 0.11129083E+02

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RELATIONSHIPS BETWEEN ISOTOPOMERS 8 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.36450806E+00
EXCITATION FACTOR 0.20397828E-10
ZERO-POINT DIFFERENCE FACTOR 0.28050012E+02
TELLER-REDLICH PRODUCT RATIO 0.10236264E+01
(S2/S1) F 0.11261447E+02

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RELATIONSHIPS BETWEEN ISOTOPOMERS 9 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.36398227E+00
EXCITATION FACTOR 0.20274075E-10
ZERO-POINT DIFFERENCE FACTOR 0.27279441E+02
TELLER-REDLICH PRODUCT RATIO 0.10214032E+01
(S2/S1) F 0.11017702E+02

=====

RELATIONSHIPS BETWEEN ISOTOPOMERS 10 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.36256497E+00
EXCITATION FACTOR 0.20124252E-10
ZERO-POINT DIFFERENCE FACTOR 0.30855990E+02
TELLER-REDLICH PRODUCT RATIO 0.10145938E+01
(S2/S1) F 0.12015661E+02

QUIVER output of cyclopentadiene

=====

RELATIONSHIPS BETWEEN ISOTOPOMERS 2 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.92398576E+00
EXCITATION FACTOR 0.58629252E+00
ZERO-POINT DIFFERENCE FACTOR 0.12332923E+01
TELLER-REDLICH PRODUCT RATIO 0.10002708E+01
(S2/S1) F 0.11446810E+01

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RELATIONSHIPS BETWEEN ISOTOPOMERS 3 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.92324673E+00

EXCITATION FACTOR 0.58366165E+00
ZERO-POINT DIFFERENCE FACTOR 0.12361395E+01
TELLER-REDLICH PRODUCT RATIO 0.99986864E+00
(S2/S1) F 0.11484651E+01

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RELATIONSHIPS BETWEEN ISOTOPOMERS 4 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.92344621E+00
EXCITATION FACTOR 0.58261521E+00
ZERO-POINT DIFFERENCE FACTOR 0.12387503E+01
TELLER-REDLICH PRODUCT RATIO 0.99930066E+00
(S2/S1) F 0.11501822E+01

=====

RELATIONSHIPS BETWEEN ISOTOPOMERS 5 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.92345018E+00
EXCITATION FACTOR 0.58310009E+00
ZERO-POINT DIFFERENCE FACTOR 0.12387312E+01
TELLER-REDLICH PRODUCT RATIO 0.99930451E+00
(S2/S1) F 0.11501692E+01

=====

RELATIONSHIPS BETWEEN ISOTOPOMERS 6 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.92324427E+00
EXCITATION FACTOR 0.58310021E+00
ZERO-POINT DIFFERENCE FACTOR 0.12361420E+01
TELLER-REDLICH PRODUCT RATIO 0.99986638E+00
(S2/S1) F 0.11484660E+01

=====

RELATIONSHIPS BETWEEN ISOTOPOMERS 7 / 1

I am here now 1

TEMPERATURE 298.1500
RATIO OF PRODUCT OF FREQUENCIES 0.38547722E+00
EXCITATION FACTOR 0.58261438E+00
ZERO-POINT DIFFERENCE FACTOR 0.25459274E+02
TELLER-REDLICH PRODUCT RATIO 0.99921608E+00
(S2/S1) F 0.10496702E+02

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RELATIONSHIPS BETWEEN ISOTOPOMERS      8      /      1

I am here now                          1

TEMPERATURE                             298.1500
RATIO OF PRODUCT OF FREQUENCIES        0.38582553E+00
EXCITATION FACTOR                       0.54815859E+00
ZERO-POINT DIFFERENCE FACTOR            0.26521466E+02
TELLER-REDLICH PRODUCT RATIO            0.99828085E+00
(S2/S1) F                                0.10886149E+02
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=====
RELATIONSHIPS BETWEEN ISOTOPOMERS      9      /      1

I am here now                          1

TEMPERATURE                             298.1500
RATIO OF PRODUCT OF FREQUENCIES        0.38583226E+00
EXCITATION FACTOR                       0.55109766E+00
ZERO-POINT DIFFERENCE FACTOR            0.26525169E+02
TELLER-REDLICH PRODUCT RATIO            0.99829771E+00
(S2/S1) F                                0.10887822E+02
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RELATIONSHIPS BETWEEN ISOTOPOMERS     10      /      1

I am here now                          1

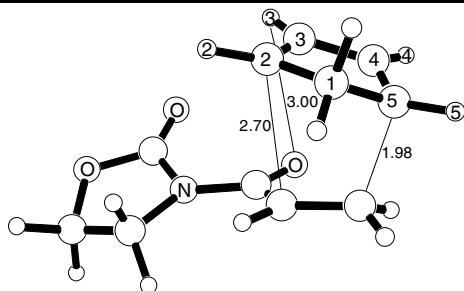
TEMPERATURE                             298.1500
RATIO OF PRODUCT OF FREQUENCIES        0.38547310E+00
EXCITATION FACTOR                       0.55109955E+00
ZERO-POINT DIFFERENCE FACTOR            0.25461571E+02
TELLER-REDLICH PRODUCT RATIO            0.99920597E+00
(S2/S1) F                                0.10497479E+02
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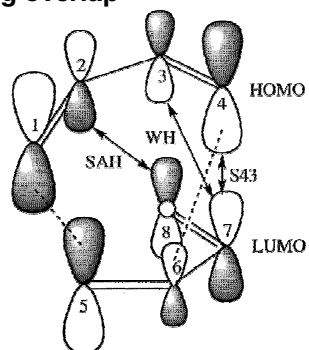
Calculated SKIEs (k_H/k_D or k_{12C}/k_{13C}) for the Diels-Alder reaction of acrylate imide and cyclopentadiene compared to the methyl substituted bis(oxazoline)-Cu(II) and t-butyl substituted bis(oxazoline)-Cu(II) catalyzed system. SKIEs calculated at the B3LYP/6-31G* level of theory

Isotopomer	Parent NC TS	Methyl NC TS	t-butyl NC TS
C1	0.997	0.999	1.014
C2	1.009	1.002	1.032
C3	0.998	1.000	1.017
C4	1.001	1.001	1.017
C5	1.034	1.031	1.051

H2	0.985	0.970	0.964
H3	0.966	0.972	0.985
H4	0.997	0.983	1.007
H5	0.900	0.900	0.891



Mulliken bonding overlap



Me substituted

TS	NC- <i>Re</i>	NC- <i>Si</i>	XC- <i>Re</i>	XC- <i>Si</i>
S43	-0.000333	-0.000321	-0.00003	-0.000011
WH	-0.000454	-0.000612	-0.000002	-0.000005
SAH	0.000098	0.000041	0.000002	0
Total	-0.000689	-0.000892	-0.00003	-0.000016

t-butyl substituted

	NC- <i>Re</i>
S43	-0.000495
WH	-0.00106
SAH	0.000209
total	-0.001346

Activation energies, enthalpies, and Gibbs energies (kcal/mol) of the reaction between **1** and **2** in vacuum and PCM (in parentheses) using UB3LYP/6-31G(d).

TS	ΔE_0^\ddagger	ΔE_{298}^\ddagger	ΔH_{298}^\ddagger	ΔG_{298}^\ddagger
NC	15.3 (15.9)	15.1 (15.7)	14.5 (15.1)	28.4 (30.0)
NT	21.4 (19.5)	21.2 (19.4)	20.6 (18.8)	34.8 (32.8)
XC	16.0 (16.1)	15.4 (15.9)	14.8 (15.4)	28.8 (29.4)
XT	20.5 (30.7)	20.3 (20.2)	19.7 (19.6)	33.9 (33.6)