Spectroscopy of Non-Heme Iron Thiolate Complexes: insight into the electronic structure of the low spin active site of Nitrile Hydratase

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Spectroscopy of Low-Spin Iron Thiolate Complexes

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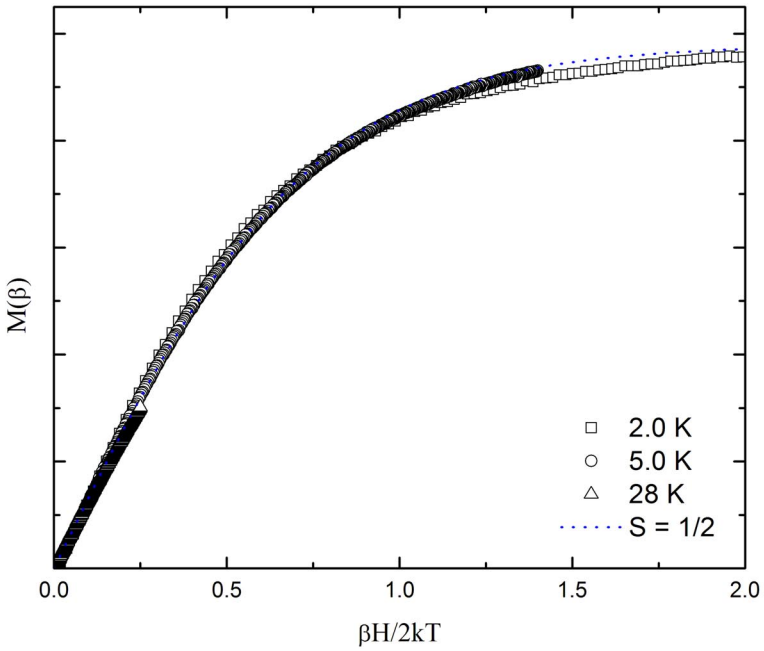
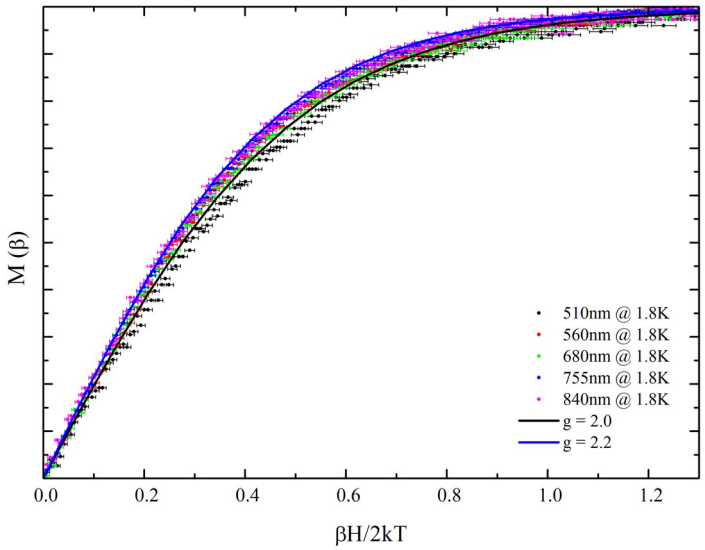
Supporting Information

The following information is available as supporting information to this manuscript: (S1) the saturation magnetization behavior for complex **1**; (S2) the computational details for DFT and ROHF-CISD calculations for complex **1**; (S3) the computational details for DFT and ROHF-CISD calculations

for complex **2**; (S4) LT-Abs mull spectra of **2**; and (S5) the computational details for DFT calculations on a truncated version of **1**.

(S1) Saturation Magnetization Behaviour of (**1**) at different temperatures at 450*nm* (top) and at different wavelengths (bottom).





(S2) Computational details for DFT and ROHF-CISD calculations for (**1**).

ADF Input File (crystallographic coordinates)

ROHF-CISD Input File for ORCA

```
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# *** ROHF + CI singles/doubles
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   Version = ZINDO_S;
   RunTyp  = Energy;
[End]
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   Metal4sp   = Gouterman;
[End]
[PARAS]
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   ZDOIPPar  = IP_Cache;
[End]
[REDEF]
   SOCFe3d= 430;
[End]
[SCF]
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   HFtyp     = ROHF;
   SCFtolE   = 5e-9;
   CNVRico   = yes;
   SCFTolErr = 5e-8;
   UHFNatOrb = yes;
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   MOInp     = "FES2N3+N3-ROHF.OUT";
[End]
[COORDS]
   ctyp   = Cartesian;
   charge = 0;
   mult   = 2;
   coords
      #
      # Molecular Fragments:
      #   (1) Fe(III) ion
      #   (2) S*CH2- group
      #   (3) S*CH2- group
      #   (4) -CH2N*=CH- group
      #   (5) -CH2CH2N*HCH2CH2- group
      #   (6) -CH2N*=CH- group
      #   (7) N3
      #
      #   Ligand structure is broken down as follows:
      #      *SCH2-CH=N*CH2-CH2CH2N*HCH2CH2-CH2N*H=CH-CH2S*
      #     |  2  |   4    |       5       |    6    |  3  |
      #
      #   Fragment-Fragment interactions of interest:
      #     1-2 & 1-3 = Fe-thiolate bonds
      #     1-4 & 1-6 = Fe-imine bonds
      #           1-5 = Fe-amine bond
      #           1-7 = Fe-azide bond
      #           2-4 = C-C bond
      #           4-5 = C-C bond
      #           5-6 = C-C bond
      #           6-3 = C-C bond
      #
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```

```
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      #27#    H(5)   0.00   -3.6331     .8407     .2164
      #28#    H(5)   0.00   -2.7836     .8541    1.5160
      #29#    H(5)   0.00   -1.9372    2.1612    -.8188
      #30#    H(5)   0.00   -2.7869    2.9020     .2439
      #31#    H(4)   0.00    -.9790    2.3781    1.7986
      #32#    H(4)   0.00    -.7014    3.5172     .7811
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      #34#    H(2)   0.00    3.5404    1.9198     .5684
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      #36#    N(7)  -1.00     .1060    -.5095    1.9121
      #37#    N(7)   0.00     .7189     .1532    2.6442
      #38#    N(7)   0.00    1.3457     .8309    3.3930
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[End]
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   NVecs     = 35;
   Reduce    = yes;
   MaxE      = 75000;
   MaxT      = 1000;
   NSelec    = -1;
   CIDiag    = Givens;
   RootE     = 75000;
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   NewRef=( o(46)22222221200, 0.5 );
   NewRef=( o(46)22222122200, 0.5 );
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   End;
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```

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         Popan("FeS2N3+N3_ROHF+2CISD_06.den" ,ZDO);
         Popan("FeS2N3+N3_ROHF+2CISD_07.den" ,ZDO);
         Popan("FeS2N3+N3_ROHF+2CISD_08.den" ,ZDO);
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   [End]
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      LOGFile   = yes;
      CACheFile = yes;
      PRINT[OrbCharge   ] = 1;
      PRINT[TransitionAn] = 1;
      PRINT[CIBasis]      = 100;
      PRINT[CIVecAn]      = 50;
   [End]
   [Properties]
      CalcGTensor = yes;
      CalcUVSpc   = yes;
      CalcCDSpc   = yes;
      UVB2        = 50;
[End]
```

(S3) Computational details for DFT and ROHF-CISD calculations for (**2**).

ADF input file (crystallographic coordinates):

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      realmemblock    1
      integermemblock 1/2
      logicalmemblock 1/32
      stringmemblock  3/2
      vectorlength    512
      scf
        converge    0.000001
        mixing      0.2
        iterations  200
      end
      xc
        lda scf    vwn
        gga energy becke perdew
      end
integration   3.50
 Symmetry  NOSYM  TOL=0.2
 charge    +1.00  1.00
 unrestricted
 restart ./adfwork/FeS2N3_LSccsp.t211
 Units
   Length  angstrom
   Angle   degrees
 End
 Atoms  cartesian
  Fe    0.000000    0.000000    0.000000
   S   -2.131989    0.000000   -0.059998
   S    1.107986   -1.849991    0.134995
   N   -0.056992    0.030000   -1.965988
   N    1.375992    1.512985    0.135986
   N    0.000000    0.000000    1.953995
   C   -2.436996   -0.306000   -1.831985
   C   -1.170990   -0.096985   -2.601990
   C    1.188995    0.186996   -2.753998
   C    2.358994    0.700989   -1.962997
   C    2.011993    1.911987   -1.137985
   C    0.799988    2.672989    0.849991
   C    0.502991    2.379990    2.293991
   C   -0.481995    1.262985    2.564987
   C    0.440994   -0.974991    2.638992
   C    1.008987   -2.181000    1.918000
   H    2.004990    1.157990    0.664993
   H   -3.237991    0.377000   -2.149994
   H   -2.757996   -1.352997   -1.941986
   H   -1.243988   -0.086990   -3.649994
   H    1.411987   -0.660995   -3.144989
   H    1.015000    0.801987   -3.469986
   H    2.668991    0.003998   -1.380997
   H    3.071991    0.923996   -2.564987
   H    1.405991    2.465988   -1.634995
   H    2.801987    2.423996   -0.954987
   H    1.408997    3.410995    0.791992
   H   -0.019989    2.928986    0.421997
   H    1.330994    2.120987    2.702988
   H    0.203995    3.179993    2.731995
   H   -1.323990    1.497986    2.170990
   H   -0.609985    1.140991    3.507996
   H    0.435989   -0.990997    3.687988
   H    2.018997   -2.415985    2.283997
   H    0.336000   -3.035995    2.078995
 End

 Fragments
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   S       ./atomic_frags/IV/S.1-.IV.2p.ebpvwn.t21
   C       ./atomic_frags/IV/C.00.IV.1s.ebpvwn.t21
   N       ./atomic_frags/IV/N.00.IV.1s.ebpvwn.t21
   H       ./atomic_frags/IV/H.00.IV.--.ebpvwn.t21
 End
 EPrint
   eigval 20 10
   orbpop 20 10
```

```
   subend
 End
 LocOrb
 End
 EndInput

(LOGFILE)
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 <Jan31-2000> <01:17:30>  Spin polar: 1 (Spin_A minus Spin_B electrons)
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 <Jan31-2000> <01:20:50>  Block Length= 512
 <Jan31-2000> <01:20:51>  >>>> PTCOR
 <Jan31-2000> <01:20:53>  >>>> PTBAS
 <Jan31-2000> <01:25:01>  >>>> CYCLE
 <Jan31-2000> <01:29:55>    1
 <Jan31-2000> <01:35:25>    2  ErrMat   0.00001057  MaxEl -0.00000173
 <Jan31-2000> <01:38:06>    3  ErrMat   0.00000426  MaxEl  0.00000087
 <Jan31-2000> <01:38:30>  SCF converged
 <Jan31-2000> <01:40:58>    4  ErrMat   0.00004083  MaxEl -0.00000924
 <Jan31-2000> <01:41:37>  >>>> COREPS
 <Jan31-2000> <01:42:40>  >>>> TOTEN
 <Jan31-2000> <02:07:16>  >>>> POPAN
 <Jan31-2000> <02:07:17>  >>>> DEBYE
 <Jan31-2000> <02:07:23>  >>>> AMETS
 <Jan31-2000> <02:07:59>   Bond Energy LDA      -9.45999314 a.u.
 <Jan31-2000> <02:07:59>   Bond Energy LDA    -257.41961605 eV
 <Jan31-2000> <02:07:59>           + GGA-X      -8.37358370 a.u.
 <Jan31-2000> <02:07:59>           + GGA-X    -227.85689884 eV
 <Jan31-2000> <02:07:59>          + GGA-XC      -8.83046523 a.u.
 <Jan31-2000> <02:07:59>          + GGA-XC    -240.28928312 eV
 <Jan31-2000> <02:07:59>  >>>> POPUL
 <Jan31-2000> <02:08:10>  >>>> LOCMO
 <Jan31-2000> <02:08:16>  NORMAL TERMINATION
 <Jan31-2000> <02:08:16>  END
 STOP NORMAL TERMINATION
 STOP
```

ADF input file (optimized coordinates):

```
title 'FeS2N3' Fe(III) with actual crystallographic coordinates

      maxmemoryusage  512
      realmemblock    1
      integermemblock 1/2
      logicalmemblock 1/32
      stringmemblock  3/2
      vectorlength    512
      scf
        converge    0.000001
        mixing      0.2
        iterations  200
      end
      xc
        lda scf    vwn
        gga energy becke perdew
      end
integration   3.25
Symmetry  NOSYM  TOL=0.2
charge    +1.00  1.00
unrestricted
Restart  FeS2N3_LSgo1.t21
Units
  Length  angstrom
  Angle   degrees
End
Geometry
   step rad=0.015
End
Atoms  cartesian
   1 Fe       0.007332    0.066699    0.002226
   2 S       -2.146927   -0.115329   -0.000105
   3 S        1.172320   -1.762886    0.075169
```

```
   4 N       -0.050007    0.052725   -1.902029
   5 N        1.395119    1.465221    0.135458
   6 N       -0.018926    0.035572    1.897491
   7 C       -2.435444   -0.249759   -1.852296
   8 C       -1.166185   -0.093195   -2.557075
   9 C        1.186640    0.086284   -2.713467
  10 C        2.375369    0.646765   -1.962454
  11 C        2.004267    1.866969   -1.154984
  12 C        0.782018    2.627814    0.836858
  13 C        0.534734    2.361138    2.305133
  14 C       -0.471153    1.256095    2.569777
  15 C        0.373009   -0.987496    2.591483
  16 C        0.888940   -2.177542    1.907803
  17 H        2.127952    1.038882    0.741333
  18 H       -3.181915    0.502634   -2.167081
  19 H       -2.868957   -1.249690   -2.055170
  20 H       -1.154346   -0.129994   -3.658002
  21 H        1.402472   -0.946806   -3.043208
  22 H        0.994967    0.705339   -3.611454
  23 H        2.809050   -0.119612   -1.292322
  24 H        3.158481    0.905608   -2.698258
  25 H        1.258134    2.481591   -1.692589
  26 H        2.891469    2.498964   -0.953104
  27 H        1.456097    3.501185    0.729800
  28 H       -0.163861    2.863104    0.312028
  29 H        1.492257    2.109798    2.804289
  30 H        0.168723    3.294045    2.772345
  31 H       -1.460066    1.524153    2.155503
  32 H       -0.581740    1.087278    3.658561
  33 H        0.307385   -0.969632    3.691784
  34 H        1.831740   -2.535173    2.358711
  35 H        0.155501   -3.005430    1.950051
End
Fragments
  Fe     ./atomic_frags/II/Fe.3+.II.3p.ebpvwn.t21
  S      ./atomic_frags/II/S.1-.II.2p.ebpvwn.t21
  C      ./atomic_frags/II/C.00.II.1s.ebpvwn.t21
  N      ./atomic_frags/II/N.00.II.1s.ebpvwn.t21
  H      ./atomic_frags/II/H.00.II.--.ebpvwn.t21
End
EndInput

<Jan28-2000> <09:12:31>  ADF 1999  RunTime: Jan28-2000 09:12:31
<Jan28-2000> <09:12:31>  'FeS2N3' Fe(III) with actual crystallographic coordinates
<Jan28-2000> <09:12:31>  RunType   : GEOMETRY OPTIMIZATION
<Jan28-2000> <09:12:31>  Net Charge: 1 (Nuclei minus Electrons)
<Jan28-2000> <09:12:31>  Spin polar: 1 (Spin_A minus Spin_B electrons)
<Jan28-2000> <09:12:31>  Symmetry  : NOSYM
<Jan28-2000> <09:12:31>  >>>> FRAGM
 Coordinates in Geometry Cycle 1
   Atom         X           Y           Z   (Angstrom)
   1.Fe        0.007332    0.066699    0.002226
   2.S        -2.146927   -0.115329   -0.000105
   3.S         1.172320   -1.762886    0.075169
   4.N        -0.050007    0.052725   -1.902029
   5.N         1.395119    1.465221    0.135458
   6.N        -0.018926    0.035572    1.897491
   7.C        -2.435444   -0.249759   -1.852296
   8.C        -1.166185   -0.093195   -2.557075
   9.C         1.186640    0.086284   -2.713467
  10.C         2.375369    0.646765   -1.962454
  11.C         2.004267    1.866969   -1.154984
  12.C         0.782018    2.627814    0.836858
  13.C         0.534734    2.361138    2.305133
  14.C        -0.471153    1.256095    2.569777
  15.C         0.373009   -0.987496    2.591483
  16.C         0.888940   -2.177542    1.907803
  17.H         2.127952    1.038882    0.741333
  18.H        -3.181915    0.502634   -2.167081
  19.H        -2.868957   -1.249690   -2.055170
  20.H        -1.154346   -0.129994   -3.658002
  21.H         1.402472   -0.946806   -3.043208
  22.H         0.994967    0.705339   -3.611454
  23.H         2.809050   -0.119612   -1.292322
  24.H         3.158481    0.905608   -2.698258
  25.H         1.258134    2.481591   -1.692589
  26.H         2.891469    2.498964   -0.953104
  27.H         1.456097    3.501185    0.729800
  28.H        -0.163861    2.863104    0.312028
  29.H         1.492257    2.109798    2.804289
  30.H         0.168723    3.294045    2.772345
  31.H        -1.460066    1.524153    2.155503
  32.H        -0.581740    1.087278    3.658561
  33.H         0.307385   -0.969632    3.691784
  34.H         1.831740   -2.535173    2.358711
  35.H         0.155501   -3.005430    1.950051
<Jan28-2000> <09:12:34>  >>>> CORORT
<Jan28-2000> <09:12:35>  >>>> FITINT
<Jan28-2000> <09:14:38>  >>>> ORTHON
```

```
<Jan28-2000> <09:14:40>  >>>> CRTP12
<Jan28-2000> <09:14:41>  >>>> GENPT
<Jan28-2000> <09:14:41>  Acc.Num.Int.=   3.250
<Jan28-2000> <09:15:00>  Block Length= 118
<Jan28-2000> <09:15:00>  >>>> PTCOR
<Jan28-2000> <09:15:03>  >>>> PTBAS
<Jan28-2000> <09:15:49>  >>>> CYCLE
<Jan28-2000> <09:17:20>    1
<Jan28-2000> <09:19:01>    2  ErrMat   0.01505071  MaxEl -0.00608868
<Jan28-2000> <09:20:30>    3  ErrMat   0.01597413  MaxEl -0.00722670
<Jan28-2000> <09:21:58>    4  ErrMat   0.00840834  MaxEl  0.00216529
<Jan28-2000> <09:23:30>    5  ErrMat   0.01342072  MaxEl -0.00379344
<Jan28-2000> <09:25:01>    6  ErrMat   0.00811880  MaxEl -0.00215636
<Jan28-2000> <09:26:31>    7  ErrMat   0.00358813  MaxEl -0.00060898
<Jan28-2000> <09:26:39>  SCF converged
<Jan28-2000> <09:27:59>    8  ErrMat   0.00210555  MaxEl -0.00041504
<Jan28-2000> <09:28:10>  >>>> TOTEN
<Jan28-2000> <09:35:07>  >>>> POPAN
<Jan28-2000> <09:35:08>  >>>> DEBYE
<Jan28-2000> <09:35:09>  >>>> AMETS
<Jan28-2000> <09:35:22>  >>>> FOCKC
<Jan28-2000> <09:36:18>  >>>> ENGRAD
<Jan28-2000> <09:58:16>  E-test:  old,new=   0.00000, -10.52964 hartree
<Jan28-2000> <09:58:16>  max gradient:      0.00336547 au/angstrom,radian
<Jan28-2000> <09:58:16>  max cart. step:    0.00617646 angstrom
<Jan28-2000> <09:58:16>  Geometry Converged
 Coordinates in Geometry Cycle 2
   Atom         X            Y            Z   (Angstrom)
   1.Fe        0.007442    0.067339    0.001445
   2.S        -2.147068   -0.115211    0.000670
   3.S         1.174175   -1.761985    0.075303
   4.N        -0.050377    0.052114   -1.902712
   5.N         1.397340    1.466026    0.135633
   6.N        -0.019705    0.035239    1.897786
   7.C        -2.435688   -0.250274   -1.851064
   8.C        -1.167093   -0.094377   -2.557280
   9.C         1.187172    0.084689   -2.712981
  10.C         2.375460    0.647414   -1.962856
  11.C         2.004024    1.868043   -1.156180
  12.C         0.782090    2.627739    0.837332
  13.C         0.535253    2.360365    2.305893
  14.C        -0.471354    1.255615    2.570245
  15.C         0.371045   -0.988683    2.591204
  16.C         0.886088   -2.178490    1.907455
  17.H         2.130038    1.039432    0.740548
  18.H        -3.181140    0.503854   -2.164742
  19.H        -2.870273   -1.248785   -2.053952
  20.H        -1.155618   -0.133499   -3.658244
  21.H         1.403359   -0.949062   -3.040029
  22.H         0.995661    0.701394   -3.612371
  23.H         2.809205   -0.118012   -1.292352
  24.H         3.158044    0.905266   -2.698823
  25.H         1.256491    2.481162   -1.693009
  26.H         2.890686    2.500866   -0.956052
  27.H         1.455075    3.501730    0.730229
  28.H        -0.164051    2.862881    0.313160
  29.H         1.492569    2.109468    2.805139
  30.H         0.169386    3.293245    2.772697
  31.H        -1.459917    1.523617    2.156359
  32.H        -0.581508    1.086265    3.658397
  33.H         0.305344   -0.971366    3.691222
  34.H         1.827136   -2.534399    2.361662
  35.H         0.149325   -3.003782    1.949100
<Jan28-2000> <09:58:18>  >>>> CORORT
<Jan28-2000> <09:58:18>  >>>> FITINT
<Jan28-2000> <10:00:23>  >>>> ORTHON
<Jan28-2000> <10:00:24>  >>>> GENPT
<Jan28-2000> <10:00:24>  Acc.Num.Int.=   3.250
<Jan28-2000> <10:00:41>  Block Length= 118
<Jan28-2000> <10:00:42>  >>>> PTCOR
<Jan28-2000> <10:00:45>  >>>> PTBAS
<Jan28-2000> <10:01:31>  >>>> CYCLE
<Jan28-2000> <10:03:01>    1
<Jan28-2000> <10:04:42>    2  ErrMat   0.01444798  MaxEl -0.00309507
<Jan28-2000> <10:06:13>    3  ErrMat   0.02466906  MaxEl  0.00538259
<Jan28-2000> <10:07:43>    4  ErrMat   0.00406720  MaxEl -0.00064074
<Jan28-2000> <10:09:10>    5  ErrMat   0.00083897  MaxEl  0.00014955
<Jan28-2000> <10:10:34>    6  ErrMat   0.00043398  MaxEl  0.00008929
<Jan28-2000> <10:11:55>    7  ErrMat   0.00016468  MaxEl  0.00003607
<Jan28-2000> <10:13:13>    8  ErrMat   0.00005311  MaxEl -0.00001203
<Jan28-2000> <10:14:27>    9  ErrMat   0.00002205  MaxEl -0.00000377
<Jan28-2000> <10:15:39>   10  ErrMat   0.00001138  MaxEl -0.00000222
<Jan28-2000> <10:16:48>   11  ErrMat   0.00000632  MaxEl  0.00000122
<Jan28-2000> <10:17:53>   12  ErrMat   0.00000340  MaxEl -0.00000062
<Jan28-2000> <10:18:02>  SCF converged
<Jan28-2000> <10:18:56>   13  ErrMat   0.00000183  MaxEl  0.00000029
<Jan28-2000> <10:19:07>  >>>> COREPS
<Jan28-2000> <10:19:55>  >>>> TOTEN
<Jan28-2000> <10:26:45>  >>>> POPAN
```

```
<Jan28-2000> <10:26:46>  >>>> DEBYE
<Jan28-2000> <10:26:47>  >>>> AMETS
<Jan28-2000> <10:27:01>  >>>> POPUL
<Jan28-2000> <10:27:02>   Bond Energy LDA     -10.52970482 a.u.
<Jan28-2000> <10:27:02>   Bond Energy LDA    -286.52796386 eV
<Jan28-2000> <10:27:02>            + GGA-X      -9.42523882 a.u.
<Jan28-2000> <10:27:02>            + GGA-X    -256.47390247 eV
<Jan28-2000> <10:27:02>           + GGA-XC      -9.87910600 a.u.
<Jan28-2000> <10:27:02>           + GGA-XC    -268.82426193 eV
<Jan28-2000> <10:27:02>  NORMAL TERMINATION
<Jan28-2000> <10:27:03>  END
```

Geometry optimization followd by single-point calculation using higher integration values

```
1(INPUT FILE)
 title 'FeS2N3' Fe(III) with optimized coordinates
      maxmemoryusage  96
      realmemblock    1
      integermemblock 1/2
      logicalmemblock 1/32
      stringmemblock  3/2
      vectorlength    512
      scf
        converge    0.000001
        mixing      0.2
        iterations  200
      end
      xc
        lda scf    vwn
        gga energy becke perdew
      end
integration   3.5
 Symmetry  NOSYM  TOL=0.2
 charge    +1.00  1.00
 unrestricted
 Restart  ./adfwork/FeS2N3_LSgosp.t211
 Units
   Length  angstrom
   Angle   degrees
 End
 Atoms  cartesian
    1 Fe     0.007442     0.067339    0.001445
    2 S     -2.147068    -0.115211    0.000670
    3 S      1.174175    -1.761985    0.075303
    4 N     -0.050377     0.052114   -1.902712
    5 N      1.397340     1.466026    0.135633
    6 N     -0.019705     0.035239    1.897786
    7 C     -2.435688    -0.250274   -1.851064
    8 C     -1.167093    -0.094377   -2.557280
    9 C      1.187172     0.084689   -2.712981
   10 C      2.375460     0.647414   -1.962856
   11 C      2.004024     1.868043   -1.156180
   12 C      0.782090     2.627739    0.837332
   13 C      0.535253     2.360365    2.305893
   14 C     -0.471354     1.255615    2.570245
   15 C      0.371045    -0.988683    2.591204
   16 C      0.886088    -2.178490    1.907455
   17 H      2.130038     1.039432    0.740548
   18 H     -3.181140     0.503854   -2.164742
   19 H     -2.870273    -1.248785   -2.053952
   20 H     -1.155618    -0.133499   -3.658244
   21 H      1.403359    -0.949062   -3.040029
   22 H      0.995661     0.701394   -3.612371
   23 H      2.809205    -0.118012   -1.292352
   24 H      3.158044     0.905266   -2.698823
   25 H      1.256491     2.481162   -1.693009
   26 H      2.890686     2.500866   -0.956052
   27 H      1.455075     3.501730    0.730229
   28 H     -0.164051     2.862881    0.313160
   29 H      1.492569     2.109468    2.805139
   30 H      0.169386     3.293245    2.772697
   31 H     -1.459917     1.523617    2.156359
   32 H     -0.581508     1.086265    3.658397
   33 H      0.305344    -0.971366    3.691222
   34 H      1.827136    -2.534399    2.361662
   35 H      0.149325    -3.003782    1.949100
 End
 Fragments
   Fe     ./atomic_frags/IV/Fe.3+.IV.3p.ebpvwn.t21
   S      ./atomic_frags/IV/S.1-.IV.2p.ebpvwn.t21
   C      ./atomic_frags/IV/C.00.IV.1s.ebpvwn.t21
   N      ./atomic_frags/IV/N.00.IV.1s.ebpvwn.t21
   H      ./atomic_frags/IV/H.00.IV.--.ebpvwn.t21
 End
 EPrint
   eigval 20 10
   orbpop 20 10
   subend
 End
```

```
 LocOrb
 End
 EndInput
```

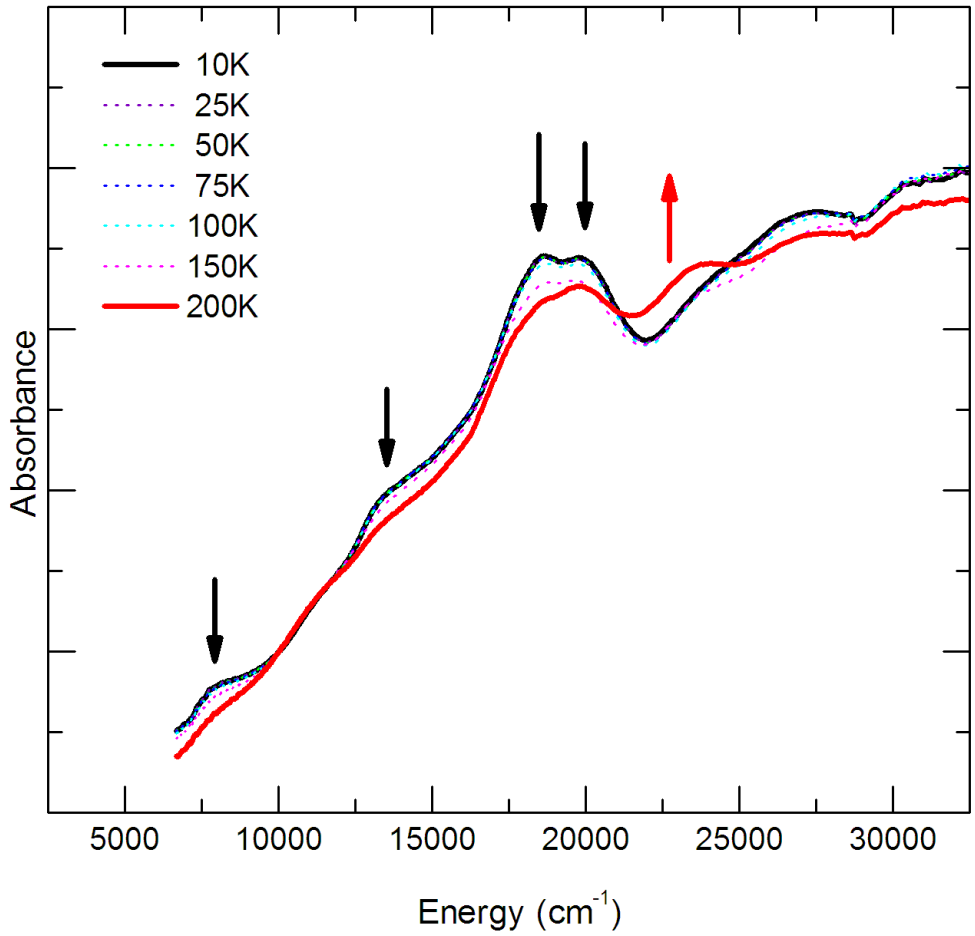
ROHF-CISD input file for ORCA (crystallographic coordinates)

```
# ***
# *** Model complexes for nitrile hydratase - 5C species
# *** initial geometry
[METHOD]
   Method  = INDO;
   Version = ZINDO_S;
   RunTyp  = Energy;
[END]
[BASIS]
   Metal3d    = Gouterman;
   Metal4sp   = Gouterman;
[END]
[PARAS]
   SOCPars   = Standard;
   ZDOIPPar  = IP_Cache;
[END]
[REDEF]
   SOCFe3d= 430;
[END]
[SCF]
   MaxIter   = 1000;
   HFtyp     = ROHF;
   SCFtolE   = 1e-8;
   CNVRico   = true;
   SCFTolErr = 1e-7;
   UHFNatOrb = true;
   Guess     = MORead;
   MOInp     = "FeS2N3open-LSINIT-ROHF.OUT";
[END]
[COORDS]
   ctyp   = cartesian;
   charge = 1;
   mult   = 2;
   coords
      #
      # Molecular Fragments:
      #   (1) Fe(III) ion
      #   (2) S*CH2- group
      #   (3) S*CH2- group
      #   (4) -CH2N*=CH- group
      #   (5) -CH2CH2N*HCH2CH2- group
      #   (6) -CH2N*=CH- group
      #
      #   Ligand structure is broken down as follows:
      #      *SCH2-CH=N*CH2-CH2CH2N*HCH2CH2-CH2N*H=CH-CH2S*
      #     |  2  |   4    |       5       |    6    |  3  |
      #
      #   Fragment-Fragment interactions of interest:
      #     1-2 & 1-3 = Fe-thiolate bonds
      #     1-4 & 1-6 = Fe-imine bonds
      #           1-5 = Fe-amine bond
      #           2-4 = C-C bond
      #           4-5 = C-C bond
      #           5-6 = C-C bond
      #           6-3 = C-C bond
      #
      #01# Fe(1)  +3.00     .0000     .0000     .0000
      #02#  S(2)  -1.00    2.1958     .0000     .0000
      #03#  S(3)  -1.00    -.2041    0.5208   -2.1368
      #04#  N(4)   0.00     .1784    1.9107    0.4788
      #05#  N(5)   0.00   -2.1390   -0.2212    0.1729
      #06#  N(6)   0.00    -.1284   -1.8584   -0.6396
      #07#  C(2)   0.00    2.5390    1.8074    0.0000
      #08#  C(4)   0.00    1.3043    2.5360    0.4731
      #09#  C(4)   0.00   -1.0059    2.6349    0.9697
      #10#  C(5)   0.00   -2.2884    2.2640    0.2215
      #11#  C(5)   0.00   -2.8849    0.9519    0.6608
      #12#  C(5)   0.00   -2.6330   -1.4337    0.8724
      #13#  C(5)   0.00   -2.1484   -2.7634    0.3375
      #14#  C(6)   0.00   -0.6167   -2.8679    0.3170
      #15#  C(6)   0.00     .0152   -2.1918   -1.8775
      #16#  C(3)   0.00     .2333   -1.0964   -2.9061
      #17#  H(3)   0.00    1.2829   -1.0816   -3.2354
      #18#  H(3)   0.00    -.4342   -1.2432   -3.7680
      #19#  H(6)   0.00    -.0369   -3.1763   -2.2389
      #20#  H(6)   0.00    -.3356   -3.7487    0.0585
      #21#  H(6)   0.00    -.2792   -2.6826    1.1964
      #22#  H(5)   0.00   -2.5214   -3.4843    0.8500
      #23#  H(5)   0.00   -2.4558   -2.8556   -0.5671
      #24#  H(5)   0.00   -2.3671   -1.3735    1.7927
```

```
      #25#  H(5)   0.00   -3.5927   -1.4336    0.8474
      #26#  H(5)   0.00   -2.4254   -0.3250   -0.6740
      #27#  H(5)   0.00   -3.7806    0.9016    0.3194
      #28#  H(5)   0.00   -2.9311    0.9149    1.6191
      #29#  H(5)   0.00   -2.0848    2.2220   -0.7158
      #30#  H(5)   0.00   -2.9345    2.9628    0.3469
      #31#  H(4)   0.00   -1.1265    2.4389    1.9016
      #32#  H(4)   0.00    -.8489    3.5780    0.8842
      #33#  H(4)   0.00    1.4267    3.5362    0.7683
      #34#  H(2)   0.00    3.3929    1.9806    0.6715
      #35#  H(2)   0.00    2.7950    2.1573   -1.0110
   end;
[END]
[CI]
   CITyp     = Rumer;
   UseSym    = no;
   NVecs     = 35;
   Reduce    = yes;
   MaxE      = 75000;
   MaxT      = 1000;
   NSelec    = -1;
   CIDiag    = Givens;
   RootE     = 75000;
   Flags     = 1,1,0,0,0,1;
   NewRef=( o(41)22222100, 0.5 );
   NewRef=( o(41)22222010, 0.5 );
   NewRef=( o(41)22212110, 0.5 );
   NewRef=( o(41)22122110, 0.5 );
   NewRef=( o(41)22212200, 0.5 );
   NewRef=( o(41)22122200, 0.5 );
   States
      CISD(10,76,26,48,0.5);
   End;
   Densities
      Create( 00,"FeS2N3open_ROHF+2CISD_00.den",true);
      Create( 01,"FeS2N3open_ROHF+2CISD_01.den",true);
      Create( 02,"FeS2N3open_ROHF+2CISD_02.den",true);
      Create( 03,"FeS2N3open_ROHF+2CISD_03.den",true);
      Create( 04,"FeS2N3open_ROHF+2CISD_04.den",true);
      Create( 05,"FeS2N3open_ROHF+2CISD_05.den",true);
      Create( 06,"FeS2N3open_ROHF+2CISD_06.den",true);
      Create( 07,"FeS2N3open_ROHF+2CISD_07.den",true);
      Create( 08,"FeS2N3open_ROHF+2CISD_08.den",true);
      Create( 09,"FeS2N3open_ROHF+2CISD_09.den",true);
      Create( 10,"FeS2N3open_ROHF+2CISD_10.den",true);
      Create( 11,"FeS2N3open_ROHF+2CISD_11.den",true);
      Create( 12,"FeS2N3open_ROHF+2CISD_12.den",true);
      Create( 13,"FeS2N3open_ROHF+2CISD_13.den",true);
      Create( 14,"FeS2N3open_ROHF+2CISD_14.den",true);
      Create( 15,"FeS2N3open_ROHF+2CISD_15.den",true);
      Create( 16,"FeS2N3open_ROHF+2CISD_16.den",true);
      Create( 17,"FeS2N3open_ROHF+2CISD_17.den",true);
      Create( 18,"FeS2N3open_ROHF+2CISD_18.den",true);
      Create( 19,"FeS2N3open_ROHF+2CISD_19.den",true);
      Create( 00,01,"FeS2N3open_ROHF+2CISD_TD01.den",true);
      Create( 00,02,"FeS2N3open_ROHF+2CISD_TD02.den",true);
      Create( 00,03,"FeS2N3open_ROHF+2CISD_TD03.den",true);
      Create( 00,04,"FeS2N3open_ROHF+2CISD_TD04.den",true);
      Create( 00,05,"FeS2N3open_ROHF+2CISD_TD05.den",true);
      Create( 00,06,"FeS2N3open_ROHF+2CISD_TD06.den",true);
      Create( 00,07,"FeS2N3open_ROHF+2CISD_TD07.den",true);
      Create( 00,08,"FeS2N3open_ROHF+2CISD_TD08.den",true);
      Create( 00,09,"FeS2N3open_ROHF+2CISD_TD09.den",true);
      Create( 00,10,"FeS2N3open_ROHF+2CISD_TD10.den",true);
      Create( 00,11,"FeS2N3open_ROHF+2CISD_TD11.den",true);
      Create( 00,12,"FeS2N3open_ROHF+2CISD_TD12.den",true);
      Create( 00,13,"FeS2N3open_ROHF+2CISD_TD13.den",true);
      Create( 00,14,"FeS2N3open_ROHF+2CISD_TD14.den",true);
      Create( 00,15,"FeS2N3open_ROHF+2CISD_TD15.den",true);
      Create( 00,16,"FeS2N3open_ROHF+2CISD_TD16.den",true);
      Create( 00,17,"FeS2N3open_ROHF+2CISD_TD17.den",true);
      Create( 00,18,"FeS2N3open_ROHF+2CISD_TD18.den",true);
      Create( 00,19,"FeS2N3open_ROHF+2CISD_TD19.den",true);
      NatOrb("FeS2N3open_ROHF+2CISD_00.den","FeS2N3open_NatOrb00.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_01.den","FeS2N3open_NatOrb01.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_02.den","FeS2N3open_NatOrb02.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_03.den","FeS2N3open_NatOrb03.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_04.den","FeS2N3open_NatOrb04.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_05.den","FeS2N3open_NatOrb05.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_06.den","FeS2N3open_NatOrb06.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_07.den","FeS2N3open_NatOrb07.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_08.den","FeS2N3open_NatOrb08.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_09.den","FeS2N3open_NatOrb09.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_10.den","FeS2N3open_NatOrb10.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_11.den","FeS2N3open_NatOrb11.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_12.den","FeS2N3open_NatOrb12.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_13.den","FeS2N3open_NatOrb13.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_14.den","FeS2N3open_NatOrb14.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_15.den","FeS2N3open_NatOrb15.vec");
```

```
      NatOrb("FeS2N3open_ROHF+2CISD_16.den","FeS2N3open_NatOrb16.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_17.den","FeS2N3open_NatOrb17.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_18.den","FeS2N3open_NatOrb18.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_19.den","FeS2N3open_NatOrb19.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD01.den","FeS2N3open_TD01.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD02.den","FeS2N3open_TD02.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD03.den","FeS2N3open_TD03.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD04.den","FeS2N3open_TD04.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD05.den","FeS2N3open_TD05.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD06.den","FeS2N3open_TD06.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD07.den","FeS2N3open_TD07.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD08.den","FeS2N3open_TD08.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD09.den","FeS2N3open_TD09.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD10.den","FeS2N3open_TD10.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD11.den","FeS2N3open_TD11.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD12.den","FeS2N3open_TD12.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD13.den","FeS2N3open_TD13.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD14.den","FeS2N3open_TD14.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD15.den","FeS2N3open_TD15.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD16.den","FeS2N3open_TD16.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD17.den","FeS2N3open_TD17.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD18.den","FeS2N3open_TD18.vec");
      NatOrb("FeS2N3open_ROHF+2CISD_TD19.den","FeS2N3open_TD19.vec");
      Popan("FeS2N3open_ROHF+2CISD_00.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_01.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_02.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_03.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_04.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_05.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_06.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_07.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_08.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_09.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_10.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_11.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_12.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_13.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_14.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_15.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_16.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_17.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_18.den" ,ZDO);
      Popan("FeS2N3open_ROHF+2CISD_19.den" ,ZDO);
   End;
[End]
[Output]
   PDBFile   = yes;
   LOGFile   = yes;
   CACheFile = yes;
   PRINT[OrbCharge   ] = 1;
   PRINT[TransitionAn] = 1;
   PRINT[CIBasis]      = 100;
   PRINT[CIVecAn]      = 50;
[End]
[Properties]
   CalcGTensor = yes;
   CalcUVSpc   = yes;
   CalcCDSpc   = yes;
   UVB2        = 50;
[End]
```

(S4) Comparison of the LT-Abs spectra of **1** and **2** in the solid state and in acetonitrile.



(S5) Computational details for DFT calculations on a truncated version of (**1**).

ADF Input File

```
title  FeS2N3+N3 6-coordinate model with optimized ligand
symmetry  nosym
charge  0.00  1.00
unrestricted
restart ./adfwork/FeS2N3+N3_geomopt.t13
units
  length  angstrom
  angle  degrees
end
geometry
end
geovar
  r2       2.19580627
  r3       1.83968984
  a3     100.75014167
  r4       1.50967087
  a4     108.75909006
  t4      19.32897022
  r5       1.97780001
  a5      84.82388415
  t5     -14.06854596
  r6       1.47239184
  a6     118.90084043
  t6    -174.93767783
  r7       1.53042673
  a7     113.07234189
  t7     -39.94960690
  r8       1.50676531
  a8     113.59162337
  t8      78.39859890
  r9       2.15737769
  a9      99.73515681
  t9     174.01986324
  r10      1.48439419
  a10    116.83804838
  t10   -131.37986027
  r11      1.51295269
  a11    116.40453904
  t11    -55.15687830
  r12      1.53537132
  a12    112.58608206
  t12     56.74796912
  r13      1.96954003
  a13     93.73924800
  t13    175.07699013
  r14      1.29011391
  a14    123.24680041
  t14    170.29889405
  r15      1.51834984
  a15    118.65452998
  t15     -2.79827098
  r16      2.20878114
  a16     95.30124231
  t16     90.37115880
  r17      1.10010430
  a17    109.84257841
  t17   -120.79320982
  r18      1.10002481
  a18    107.46196218
  t18    119.25057548
  r19      1.04995593
  a19    124.54594521
  t19   -178.01769866
  r20         .96000990
  a20    110.89243523
  t20    121.17113446
  r21         .95995073
  a21    110.23880549
  t21   -118.38329903
  r22         .95998246
  a22    110.28702003
  t22    123.41048136
  r23         .95985759
  a23    108.36110958
  t23   -118.74786847
  r24         .95988198
  a24    107.95935458
  t24    121.29252928
  r25         .96006692
  a25    108.68144325
  t25   -122.31627107
  r26         .90008396
  a26    104.58636931
```

```
  t26    114.20256829
  r27       .95988808
  a27    108.23232034
  t27    119.95763070
  r28       .96010380
  a28    108.91874901
  t28   -122.93315238
  r29       .96002791
  a29    108.06668270
  t29   -121.45413400
  r30       .95995375
  a30    108.88715460
  t30    121.96006674
  r31       .95998151
  a31    108.92532819
  t31    120.89757765
  r32       .95992637
  a32    108.78845500
  t32   -121.70979660
  r33      1.05006127
  a33    124.27957418
  t33    179.26185041
  r34      1.10002168
  a34    107.42599448
  t34    120.89665329
  r35      1.10001056
  a35    110.85106964
  t35   -119.76640896
  r36      2.06067192
  a36     91.28254656
  t36   -179.02332923
  r37      1.18861126
  a37    118.52112884
  t37     52.33819984
  r38      1.16219438
  a38    140.09790437
  t38    179.61021209
end
atoms  z-matrix
  1  Fe   0  0  0   0.0  0.0  0.0
  2  S    1  0  0   r2   0.0  0.0
  3  C    2  1  0   r3   a3   0.0
  4  C    3  2  1   r4   a4   t4
  5  N    1  2  3   r5   a5   t5
  6  C    5  1  4   r6   a6   t6
  7  C    6  5  1   r7   a7   t7
  8  C    7  6  5   r8   a8   t8
  9  N    1  5  2   r9   a9   t9
  10 C    9  1  8   r10  a10  t10
  11 C    10 9  1   r11  a11  t11
  12 C    11 10 9   r12  a12  t12
  13 N    1  2  5   r13  a13  t13
  14 C    13 1  12  r14  a14  t14
  15 C    14 13 1   r15  a15  t15
  16 S    1  2  5   r16  a16  t16
  17 H    15 16 14  r17  a17  t17
  18 H    15 16 14  r18  a18  t18
  19 H    14 13 15  r19  a19  t19
  20 H    12 13 11  r20  a20  t20
  21 H    12 13 11  r21  a21  t21
  22 H    11 10 12  r22  a22  t22
  23 H    11 10 12  r23  a23  t23
  24 H    10 9  11  r24  a24  t24
  25 H    10 9  11  r25  a25  t25
  26 H    9  1  8   r26  a26  t26
  27 H    8  9  7   r27  a27  t27
  28 H    8  9  7   r28  a28  t28
  29 H    7  6  8   r29  a29  t29
  30 H    7  6  8   r30  a30  t30
  31 H    6  5  7   r31  a31  t31
  32 H    6  5  7   r32  a32  t32
  33 H    4  5  3   r33  a33  t33
  34 H    3  2  4   r34  a34  t34
  35 H    3  2  4   r35  a35  t35
  36 N    1  2  16  r36  a36  t36
  37 N    36 1  2   r37  a37  t37
  38 N    37 1  36  r38  a38  t38
End
fragments
   Fe  ./atomic_frags/IV/Fe.3+.IV.2p.ebpvwn.t21
   S   ./atomic_frags/IV/S.1-.IV.2p.ebpvwn.t21
   N   ./atomic_frags/IV/N.00.IV.1s.ebpvwn.t21
   C   ./atomic_frags/IV/C.00.IV.1s.ebpvwn.t21
   H   ./atomic_frags/IV/H.00.IV.--.ebpvwn.t21
end
end input

<Apr18-2000> <20:00:40>  ADF 1999  RunTime: Apr18-2000 20:00:40
<Apr18-2000> <20:00:40>  FeS2N3+N3 6-coordinate model with optimized ligand
```

```
<Apr18-2000> <20:00:40>  RunType   : GEOMETRY OPTIMIZATION
<Apr18-2000> <20:00:41>  Net Charge: 0 (Nuclei minus Electrons)
<Apr18-2000> <20:00:41>  Spin polar: 1 (Spin_A minus Spin_B electrons)
<Apr18-2000> <20:00:41>  Symmetry  : NOSYM
<Apr18-2000> <20:00:42>  >>>> FRAGM
 Coordinates in Geometry Cycle 1
   Atom         X           Y           Z   (Angstrom)
   1.Fe        0.005095   -0.019561    0.017335
   2.S         2.212439   -0.041697   -0.075062
   3.C         2.488080    1.769650   -0.205971
   4.C         1.293484    2.497044    0.288391
   5.N         0.166431    1.886967    0.458340
   6.C        -0.958099    2.682573    0.976442
   7.C        -2.293570    2.340992    0.313866
   8.C        -2.867622    1.000737    0.762685
   9.N        -2.156258   -0.176643    0.214004
  10.C        -2.622142   -1.401376    0.921539
  11.C        -2.142291   -2.724560    0.322318
  12.C        -0.616507   -2.899388    0.258661
  13.N        -0.076670   -1.854373   -0.613498
  14.C         0.150810   -2.135835   -1.855816
  15.C         0.456161   -1.039712   -2.813860
  16.S        -0.266025    0.533644   -2.162975
  17.H         1.549211   -0.894214   -2.878164
  18.H         0.079878   -1.278083   -3.819121
  19.H         0.074493   -3.176794   -2.201492
  20.H        -0.364909   -3.897509   -0.133607
  21.H        -0.176112   -2.769979    1.254284
  22.H        -2.560627   -3.533642    0.941609
  23.H        -2.553543   -2.853278   -0.693631
  24.H        -2.250109   -1.309415    1.950737
  25.H        -3.727280   -1.404707    0.947664
  26.H        -2.358945   -0.241528   -0.794142
  27.H        -3.939041    0.940514    0.498225
  28.H        -2.802208    0.929524    1.859219
  29.H        -2.197345    2.378347   -0.782800
  30.H        -3.012735    3.125897    0.595943
  31.H        -1.022714    2.482390    2.058194
  32.H        -0.736617    3.753814    0.848359
  33.H         1.365401    3.573779    0.500244
  34.H         3.383379    2.073097    0.357539
  35.H         2.650339    2.040426   -1.264964
  36.N        -0.037765   -0.533909    1.994463
  37.N         0.485317    0.180213    2.822087
  38.N         0.973507    0.869503    3.628612
 Z-matrix coordinates
   Atom        i    j    k     R (Ang)    BondAngle    Dihedral
   1.Fe        0    0    0    0.000000    0.000000    0.000000
   2.S         1    0    0    2.209387    0.000000    0.000000
   3.C         2    1    0    1.836871   98.222740    0.000000
   4.C         4    2    1    1.483427  109.812354   20.551466
   5.N         1    2    4    1.963508   86.389697  -16.958126
   6.C        14    1    5    1.471730  122.764640  179.538754
   7.C         6   14    1    1.529433  113.200097  -39.182715
   8.C         7    6   14    1.525536  113.411538   73.442433
   9.N         1   14    2    2.175959   97.551139  176.169106
  10.C        15    1    8    1.489169  114.397367 -129.350156
  11.C         9   15    1    1.529752  115.285411  -55.958136
  12.C        10    9   15    1.537087  115.212477   59.220337
  13.N         1    2   14    1.941951   91.089478  174.147399
  14.C        16    1   11    1.293956  120.663778  169.632662
  15.C        12   16    1    1.487472  119.614964   -0.999325
  16.S         1    2   14    2.265678   94.689449   89.063380
  17.H        13    3   12    1.104564  107.147763 -118.507580
  18.H        13    3   12    1.099527  111.872832  122.940808
  19.H        12   16   13    1.099505  119.708094 -177.403726
  20.H        11   16   10    1.101553  110.508612  120.567988
  21.H        11   16   10    1.096339  107.973093 -119.339380
  22.H        10    9   11    1.101426  107.217515  120.826332
  23.H        10    9   11    1.103562  110.157737 -123.221376
  24.H         9   15   10    1.098232  105.688650  121.031584
  25.H         9   15   10    1.105451  109.054480 -122.538206
  26.H        15    1    8    1.030365   96.402123  114.588813
  27.H         8   15    7    1.105217  109.491922  123.801455
  28.H         8   15    7    1.100790  106.802731 -120.671337
  29.H         7    6    8    1.101513  110.331936 -125.005644
  30.H         7    6    8    1.101291  107.461623  118.992454
  31.H         6   14    7    1.102014  106.987580  120.684616
  32.H         6   14    7    1.101370  109.342170 -123.045488
  33.H         5   14    4    1.099733  119.585580  179.174174
  34.H         4    2    5    1.100539  110.945508  122.372374
  35.H         4    2    5    1.105040  109.388025 -118.980155
  36.N         1    2    3    2.043386   93.376557  179.492632
  37.N        17    1    2    1.211837  120.226479   60.370671
  38.N        18    1   17    1.167875  142.252963 -178.781694
<Apr18-2000> <20:00:44>  >>>> CORORT
<Apr18-2000> <20:00:45>  >>>> FITINT
<Apr18-2000> <20:04:17>  >>>> ORTHON
<Apr18-2000> <20:04:38>  >>>> CRTP12
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<Apr18-2000> <20:05:02>  Block Length=  87
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<Apr18-2000> <20:10:17>  >>>> CYCLE
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<Apr18-2000> <20:30:33>    2  ErrMat   0.00090022  MaxEl -0.00017457
<Apr18-2000> <20:30:59>  SCF converged
<Apr18-2000> <20:38:34>    3  ErrMat   0.00154990  MaxEl  0.00027585
<Apr18-2000> <20:39:17>  >>>> TOTEN
<Apr18-2000> <21:09:56>  >>>> POPAN
<Apr18-2000> <21:09:58>  >>>> DEBYE
<Apr18-2000> <21:10:05>  >>>> AMETS
<Apr18-2000> <21:10:46>  >>>> FOCKC
<Apr18-2000> <21:15:46>  >>>> ENGRAD
<Apr18-2000> <22:16:44>  E-test:  old,new=   0.00000, -10.10434 hartree
<Apr18-2000> <22:16:44>  max gradient:      0.00841027 au/angstrom,radian
<Apr18-2000> <22:16:44>  max bond step:     0.00377056 angstrom
<Apr18-2000> <22:16:44>  max angular step:  0.47747550 degree
<Apr18-2000> <22:16:44>  Geometry Converged
 Coordinates in Geometry Cycle 2
   Atom         X           Y           Z   (Angstrom)
   1.Fe        0.006023   -0.019714    0.018986
   2.S         2.214077   -0.040580   -0.076845
   3.C         2.483910    1.770833   -0.219474
   4.C         1.292172    2.498139    0.280418
   5.N         0.167989    1.887464    0.458388
   6.C        -0.955170    2.681603    0.981675
   7.C        -2.292852    2.342638    0.322648
   8.C        -2.868691    1.001665    0.768242
   9.N        -2.155876   -0.174238    0.215293
  10.C        -2.623853   -1.399726    0.920044
  11.C        -2.145860   -2.722729    0.319563
  12.C        -0.620043   -2.899074    0.260251
  13.N        -0.075861   -1.855222   -0.612592
  14.C         0.155484   -2.135487   -1.854771
  15.C         0.466963   -1.040467   -2.810672
  16.S        -0.266592    0.531836   -2.165475
  17.H         1.560361   -0.894455   -2.865167
  18.H         0.099101   -1.279259   -3.818972
  19.H         0.079447   -3.175634   -2.203060
  20.H        -0.370927   -3.898120   -0.131330
  21.H        -0.179836   -2.769720    1.256087
  22.H        -2.568212   -3.531436    0.936632
  23.H        -2.555621   -2.850029   -0.697340
  24.H        -2.253652   -1.310779    1.950360
  25.H        -3.729151   -1.401899    0.945248
  26.H        -2.356636   -0.237729   -0.793420
  27.H        -3.940188    0.942518    0.503273
  28.H        -2.803216    0.928090    1.864676
  29.H        -2.199874    2.383908   -0.774317
  30.H        -3.011194    3.126403    0.610171
  31.H        -1.017390    2.480716    2.063629
  32.H        -0.732944    3.752902    0.854213
  33.H         1.365086    3.575159    0.489587
  34.H         3.384514    2.079334    0.332670
  35.H         2.635694    2.036124   -1.281405
  36.N        -0.034948   -0.538237    1.992233
  37.N         0.481012    0.178059    2.822593
  38.N         0.962527    0.868632    3.631747
 Z-matrix coordinates
   Atom        i    j    k     R (Ang)   BondAngle    Dihedral
   1.Fe        0    0    0    0.000000    0.000000    0.000000
   2.S         1    0    0    2.210231    0.000000    0.000000
   3.C         2    1    0    1.836946   98.094383    0.000000
   4.C         4    2    1    1.482937  109.841018   20.919949
   5.N         1    2    4    1.963832   86.357902  -17.278397
   6.C        14    1    5    1.471724  122.727556  179.418641
   7.C         6   14    1    1.529250  113.248913  -39.405077
   8.C         7    6   14    1.525894  113.518814   73.456454
   9.N         1   14    2    2.176286   97.510185  176.292456
  10.C        15    1    8    1.489126  114.412839 -129.277484
  11.C         9   15    1    1.529508  115.330098  -55.913418
  12.C        10    9   15    1.537118  115.125389   59.327420
  13.N         1    2   14    1.942855   91.093868  174.088131
  14.C        16    1   11    1.294248  120.600410  169.651806
  15.C        12   16    1    1.486552  119.676623   -0.905455
  16.S         1    2   14    2.269448   94.621070   89.086236
  17.H        13    3   12    1.104449  107.290908 -118.453157
  18.H        13    3   12    1.099551  111.808760  122.891706
  19.H        12   16   13    1.099542  119.768918 -177.485040
  20.H        11   16   10    1.101584  110.505603  120.411092
  21.H        11   16   10    1.096450  107.928526 -119.491806
  22.H        10    9   11    1.101437  107.176302  120.838021
  23.H        10    9   11    1.103722  110.209809 -123.296127
  24.H         9   15   10    1.098413  105.745589  121.078559
  25.H         9   15   10    1.105587  109.061759 -122.531313
  26.H        15    1    8    1.030455   96.293036  114.731049
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  27.H         8   15    7    1.105357  109.531763  123.792490
  28.H         8   15    7    1.100848  106.855392 -120.604368
  29.H         7    6    8    1.101672  110.302594 -125.061226
  30.H         7    6    8    1.101350  107.474961  118.912510
  31.H         6   14    7    1.102203  107.083360  120.762187
  32.H         6   14    7    1.101505  109.250003 -122.991001
  33.H         5   14    4    1.099564  119.642890  179.201566
  34.H         4    2    5    1.100511  110.957928  122.536791
  35.H         4    2    5    1.105041  109.361559 -118.916626
  36.N         1    2    3    2.040649   93.415964  179.287001
  37.N        17    1    2    1.211937  120.251267   60.848146
  38.N        18    1   17    1.167681  142.309565 -178.820303
<Apr18-2000> <22:16:46>  >>>> CORORT
<Apr18-2000> <22:16:47>  >>>> FITINT
<Apr18-2000> <22:19:37>  >>>> ORTHON
<Apr18-2000> <22:19:53>  >>>> GENPT
<Apr18-2000> <22:19:53>  Acc.Num.Int.=   4.000
<Apr18-2000> <22:20:10>  Block Length=  87
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<Apr18-2000> <22:48:35>    3  ErrMat   0.00463745  MaxEl  0.00066362
<Apr18-2000> <22:56:34>    4  ErrMat   0.01806760  MaxEl -0.00306233
<Apr18-2000> <23:04:35>    5  ErrMat   0.00532028  MaxEl -0.00100432
<Apr18-2000> <23:12:10>    6  ErrMat   0.00124088  MaxEl  0.00017099
<Apr18-2000> <23:19:27>    7  ErrMat   0.00044399  MaxEl  0.00004329
<Apr18-2000> <23:26:23>    8  ErrMat   0.00012404  MaxEl  0.00002407
<Apr18-2000> <23:32:51>    9  ErrMat   0.00006107  MaxEl  0.00000683
<Apr18-2000> <23:39:06>   10  ErrMat   0.00227477  MaxEl -0.00062612
<Apr18-2000> <23:44:00>   11  ErrMat   0.00006071  MaxEl -0.00000796
<Apr18-2000> <23:50:06>   12  ErrMat   0.00003052  MaxEl  0.00000660
<Apr18-2000> <23:55:49>   13  ErrMat   0.00000693  MaxEl  0.00000089
<Apr19-2000> <00:01:14>   14  ErrMat   0.00000678  MaxEl  0.00000105
<Apr19-2000> <00:06:31>   15  ErrMat   0.00000384  MaxEl -0.00000045
<Apr19-2000> <00:11:40>   16  ErrMat   0.00000577  MaxEl -0.00000095
<Apr19-2000> <00:16:38>   17  ErrMat   0.00000235  MaxEl -0.00000044
<Apr19-2000> <00:21:48>   18  ErrMat   0.00000280  MaxEl -0.00000043
<Apr19-2000> <00:26:58>   19  ErrMat   0.00000173  MaxEl -0.00000043
<Apr19-2000> <00:31:52>   20  ErrMat   0.00000183  MaxEl -0.00000043
<Apr19-2000> <00:36:50>   21  ErrMat   0.00000065  MaxEl  0.00000009
<Apr19-2000> <00:37:14>  SCF converged
<Apr19-2000> <00:41:33>   22  ErrMat   0.00000068  MaxEl -0.00000017
<Apr19-2000> <00:42:12>  >>>> COREPS
<Apr19-2000> <00:45:53>  >>>> TOTEN
<Apr19-2000> <01:11:32>  >>>> POPAN
<Apr19-2000> <01:11:34>  >>>> DEBYE
<Apr19-2000> <01:11:40>  >>>> AMETS
<Apr19-2000> <01:12:16>  >>>> POPUL
<Apr19-2000> <01:12:28>   Bond Energy LDA     -10.81449156 a.u.
<Apr19-2000> <01:12:28>   Bond Energy LDA    -294.27740829 eV
<Apr19-2000> <01:12:28>            + GGA-X      -9.57975200 a.u.
<Apr19-2000> <01:12:28>            + GGA-X    -260.67842184 eV
<Apr19-2000> <01:12:28>           + GGA-XC     -10.10440790 a.u.
<Apr19-2000> <01:12:28>           + GGA-XC    -274.95504099 eV
<Apr19-2000> <01:12:28>  NORMAL TERMINATION
<Apr19-2000> <01:12:29>  END
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