Supporting Information for: "Atomic Carbon as a Terminal Ligand: Studies of a Carbidomolybdenum Anion Featuring Solid-State ^{13}C NMR Data and Proton Transfer Self-Exchange Kinetics"

revision draft of a Full Paper to J. Am. Chem. Soc. *by*

Jane B. Greco,[†] Jonas C. Peters,[†] Thomas A. Baker,[†] William M. Davis,[†] Christopher C. Cummins,[†]* and Gang Wu[§]*

[†] *Department of Chemistry, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA 02139-4307*
[§] *Department of Chemistry, Queen's University, Kingston, Ontario, Canada K7L 3N6*

Contents

1 X-Ray Tables for 1-CH

Table 1: Bond Lengths (Å) for **1-CH**.

Mo(1)-C(1)	1.702(5)	Mo(1)-N(3)	1.964(4)	Mo(1)-N(1)	1.981(4)
Mo(1)-N(2)	1.991(4)	N(1)-C(11)	1.441(6)	N(1)-C(17)	1.505(6)
N(2)-C(21)	1.429(6)	N(2)-C(28)	1.516(6)	N(3)-C(31)	1.456(6)
N(3)-C(37)	1.515(6)	C(11)-C(12)	1.391(7)	C(11)-C(16)	1.391(7)
C(12)-C(13)	1.379(7)	C(13)-C(14)	1.388(8)	C(13)-C(131)	1.501(8)
C(14)-C(15)	1.378(8)	C(15)-C(16)	1.394(7)	C(15)-C(151)	1.516(8)
C(17)-C(19)	1.518(8)	C(17)-C(110)	1.524(8)	C(17)-C(18)	1.532(7)
C(21)-C(22)	1.393(7)	C(21)-C(26)	1.411(7)	C(22)-C(23)	1.382(8)
C(23)-C(24)	1.385(8)	C(23)-C(231)	1.511(8)	C(24)-C(25)	1.393(8)
C(25)-C(26)	1.373(8)	C(25)-C(251)	1.512(8)	C(27)-C(28)	1.504(9)
C(28)-C(210)	1.484(9)	C(28)-C(29)	1.561(9)	C(31)-C(36)	1.380(7)
C(31)-C(32)	1.404(7)	C(32)-C(33)	1.396(7)	C(33)-C(34)	1.378(8)
C(33)-C(331)	1.526(8)	C(34)-C(35)	1.375(7)	C(35)-C(36)	1.411(7)
C(35)-C(351)	1.509(8)	C(37)-C(39)	1.514(7)	C(37)-C(310)	1.530(8)
C(37)-C(38)	1.539(8)				

Table 2: Bond Angles (°) for **1-CH**.

C(1)-Mo(1)-N(3)	101.6(2)	C(1)-Mo(1)-N(1)	102.4(2)
N(3)-Mo(1)-N(1)	113.2(2)	C(1)-Mo(1)-N(2)	101.7(2)
N(3)-Mo(1)-N(2)	117.1(2)	N(1)-Mo(1)-N(2)	117.2(2)
C(11)-N(1)-C(17)	115.2(4)	C(11)-N(1)-Mo(1)	110.0(3)
C(17)-N(1)-Mo(1)	133.6(3)	C(21)-N(2)-C(28)	114.2(4)
C(21)-N(2)-Mo(1)	110.3(3)	C(28)-N(2)-Mo(1)	135.2(3)
C(31)-N(3)-C(37)	115.6(4)	C(31)-N(3)-Mo(1)	110.6(3)
C(37)-N(3)-Mo(1)	132.7(3)	C(12)-C(11)-C(16)	119.0(5)
C(12)-C(11)-N(1)	121.1(4)	C(16)-C(11)-N(1)	119.9(4)
C(13)-C(12)-C(11)	121.9(5)	C(12)-C(13)-C(14)	117.9(5)
C(12)-C(13)-C(131)	121.0(6)	C(14)-C(13)-C(131)	121.1(5)
C(15)-C(14)-C(13)	122.0(5)	C(14)-C(15)-C(16)	119.1(5)
C(14)-C(15)-C(151)	121.5(5)	C(16)-C(15)-C(151)	119.3(5)
C(11)-C(16)-C(15)	120.1(5)	N(1)-C(17)-C(19)	110.5(4)
N(1)-C(17)-C(110)	110.9(4)	C(19)-C(17)-C(110)	110.0(5)
N(1)-C(17)-C(18)	109.1(4)	C(19)-C(17)-C(18)	109.0(5)
C(110)-C(17)-C(18)	107.2(5)	C(22)-C(21)-C(26)	118.5(5)
C(22)-C(21)-N(2)	121.3(4)	C(26)-C(21)-N(2)	120.1(4)
C(23)-C(22)-C(21)	121.1(5)	C(22)-C(23)-C(24)	118.8(5)
C(22)-C(23)-C(231)	120.7(5)	C(24)-C(23)-C(231)	120.5(5)
C(23)-C(24)-C(25)	121.8(5)	C(26)-C(25)-C(24)	118.6(5)
C(26)-C(25)-C(251)	121.2(5)	C(24)-C(25)-C(251)	120.1(5)
C(25)-C(26)-C(21)	121.2(5)	C(210)-C(28)-C(27)	111.7(6)
C(210)-C(28)-N(2)	110.2(5)	C(27)-C(28)-N(2)	112.8(5)
C(210)-C(28)-C(29)	104.6(6)	C(27)-C(28)-C(29)	108.1(7)
N(2)-C(28)-C(29)	109.0(5)	C(36)-C(31)-C(32)	118.9(5)
C(36)-C(31)-N(3)	119.9(4)	C(32)-C(31)-N(3)	121.2(4)
C(33)-C(32)-C(31)	121.1(5)	C(34)-C(33)-C(32)	118.0(5)
C(34)-C(33)-C(331)	121.7(5)	C(32)-C(33)-C(331)	120.2(5)
C(35)-C(34)-C(33)	122.9(5)	C(34)-C(35)-C(36)	118.2(5)
C(34)-C(35)-C(351)	122.5(5)	C(36)-C(35)-C(351)	119.3(5)
C(31)-C(36)-C(35)	120.8(5)	C(39)-C(37)-N(3)	110.3(4)
C(39)-C(37)-C(310)	110.9(4)	N(3)-C(37)-C(310)	109.9(4)
C(39)-C(37)-C(38)	107.9(5)	N(3)-C(37)-C(38)	107.9(4)
C(310)-C(37)-C(38)	109.9(5)		

Table 3: Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1-CH**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [(ha*)^{2}U$_{11}$ + ··· + 2hka*b*U$_{12}$].

	U11	U22	U33	U23	U13	U12
Mo(1)	24(1)	18(1)	25(1)	2(1)	3(1)	0(1)
N(1)	29(2)	22(2)	29(2)	0(2)	3(2)	-1(2)
N(2)	29(2)	20(2)	31(2)	-2(2)	-1(2)	5(2)
N(3)	29(2)	17(2)	30(2)	3(2)	6(2)	1(2)
C(1)	37(3)	18(3)	32(3)	6(2)	5(2)	7(2)
C(11)	18(2)	27(3)	25(2)	0(2)	-1(2)	-3(2)
C(12)	30(3)	31(3)	33(3)	-2(2)	6(2)	-4(2)
C(13)	32(3)	48(4)	31(3)	0(3)	5(2)	-6(3)
C(14)	39(3)	50(4)	30(3)	1(3)	-2(2)	-15(3)
C(15)	29(3)	31(3)	38(3)	7(2)	-1(2)	-9(2)
C(16)	23(3)	28(3)	30(3)	2(2)	1(2)	-3(2)
C(17)	30(3)	27(3)	33(3)	0(2)	3(2)	-9(2)
C(18)	51(4)	61(4)	46(3)	-2(3)	1(3)	-30(3)
C(19)	53(4)	28(3)	74(4)	-16(3)	13(3)	-15(3)
C(21)	18(2)	28(3)	37(3)	0(2)	7(2)	-7(2)
C(22)	23(3)	39(3)	32(3)	-2(2)	2(2)	-3(2)
C(23)	29(3)	34(3)	44(3)	5(3)	4(2)	-8(3)
C(24)	27(3)	27(3)	58(4)	3(3)	7(3)	-5(2)
C(25)	22(3)	35(3)	43(3)	-4(3)	2(2)	-3(2)
C(26)	23(3)	31(3)	29(3)	2(2)	3(2)	2(2)
C(27)	78(6)	95(7)	113(7)	-49(5)	-48(5)	64(5)
C(28)	30(3)	35(3)	48(3)	-4(3)	0(3)	14(3)
C(29)	77(6)	85(6)	120(7)	12(5)	58(5)	32(5)
C(31)	26(3)	23(3)	29(3)	0(2)	7(2)	6(2)
C(32)	32(3)	28(3)	39(3)	4(2)	9(2)	1(2)
C(33)	26(3)	43(4)	42(3)	1(3)	3(2)	11(3)
C(34)	40(3)	23(3)	42(3)	6(2)	7(3)	15(3)
C(35)	34(3)	21(3)	37(3)	0(2)	3(2)	8(2)
C(36)	26(3)	22(3)	36(3)	-4(2)	5(2)	4(2)
C(37)	42(3)	30(3)	27(3)	-1(2)	8(2)	4(3)
C(38)	56(4)	50(4)	32(3)	9(3)	1(3)	18(3)
C(39)	52(4)	36(3)	30(3)	-2(2)	8(3)	6(3)
C(110)	32(3)	52(4)	58(4)	14(3)	-12(3)	-19(3)
C(131)	63(4)	79(5)	50(4)	2(4)	31(3)	-14(4)
C(151)	53(4)	37(4)	54(4)	17(3)	3(3)	-4(3)

C(210)	54(4)	35(4)	136(7)	-24(4)	31(4)	8(3)
C(231)	57(4)	50(4)	57(4)	15(3)	13(3)	-18(3)
C(251)	58(4)	38(4)	52(4)	-9(3)	0(3)	-4(3)
C(310)	64(4)	37(3)	40(3)	2(3)	17(3)	-1(3)
C(331)	31(3)	67(5)	87(5)	19(4)	6(3)	8(3)
C(351)	53(4)	26(3)	58(4)	14(3)	8(3)	4(3)

Table 4: Atomic Coordinates ($\times 10^4$) for the X-ray Structure of **1-CH** and equivalent isotropic displacement parameters ($Å^2 \times 10^3$).

	x	y	z	U(eq)
Mo(1)	9100(1)	3364(1)	797(1)	22(1)
N(1)	10336(4)	3496(2)	1688(2)	27(1)
N(2)	7395(4)	3236(2)	932(2)	27(1)
N(3)	9649(3)	2714(2)	54(2)	26(1)
C(1)	9063(4)	4256(3)	405(3)	29(1)
C(11)	10048(4)	3016(3)	2266(2)	24(1)
C(12)	9330(4)	3292(3)	2746(3)	31(1)
C(13)	9046(5)	2842(4)	3303(3)	37(1)
C(14)	9473(5)	2087(4)	3363(3)	40(1)
C(15)	10179(5)	1789(3)	2895(3)	34(1)
C(16)	10468(4)	2258(3)	2341(3)	28(1)
C(17)	11334(4)	4072(3)	1914(3)	30(1)
C(18)	11906(6)	4277(4)	1251(3)	53(2)
C(19)	10841(6)	4804(3)	2204(4)	51(2)
C(21)	7087(4)	2433(3)	931(3)	28(1)
C(22)	7233(4)	2008(3)	1576(3)	32(1)
C(23)	6968(5)	1226(3)	1570(3)	36(1)
C(24)	6591(5)	863(3)	906(3)	37(1)
C(25)	6455(4)	1265(3)	248(3)	34(1)
C(26)	6685(4)	2046(3)	266(3)	28(1)
C(27)	5349(7)	3695(5)	312(5)	103(4)
C(28)	6346(5)	3779(3)	961(3)	38(1)
C(29)	5813(8)	3602(5)	1662(5)	89(3)
C(31)	10328(4)	2052(3)	391(2)	26(1)
C(32)	11590(5)	2079(3)	588(3)	32(1)
C(33)	12239(5)	1449(3)	926(3)	37(1)

C(34)	11602(5)	802(3)	1067(3)	35(1)
C(35)	10366(5)	752(3)	887(3)	31(1)
C(36)	9727(4)	1392(3)	542(3)	28(1)
C(37)	9706(5)	2846(3)	-744(3)	33(1)
C(38)	8506(6)	3216(4)	-1107(3)	47(2)
C(39)	9835(5)	2082(3)	-1120(3)	40(1)
C(110)	12326(5)	3729(4)	2489(3)	50(2)
C(131)	8256(6)	3148(5)	3809(3)	62(2)
C(151)	10643(6)	964(3)	2966(3)	48(2)
C(210)	6781(6)	4590(4)	1057(5)	73(2)
C(231)	7108(6)	772(4)	2273(3)	54(2)
C(251)	6141(6)	835(4)	-467(3)	51(2)
C(310)	10756(6)	3388(4)	-811(3)	46(2)
C(331)	13607(5)	1500(4)	1158(4)	62(2)
C(351)	9679(6)	34(3)	1030(3)	46(2)

2 Experimental NMR spectra for proton transfer kinetic studies

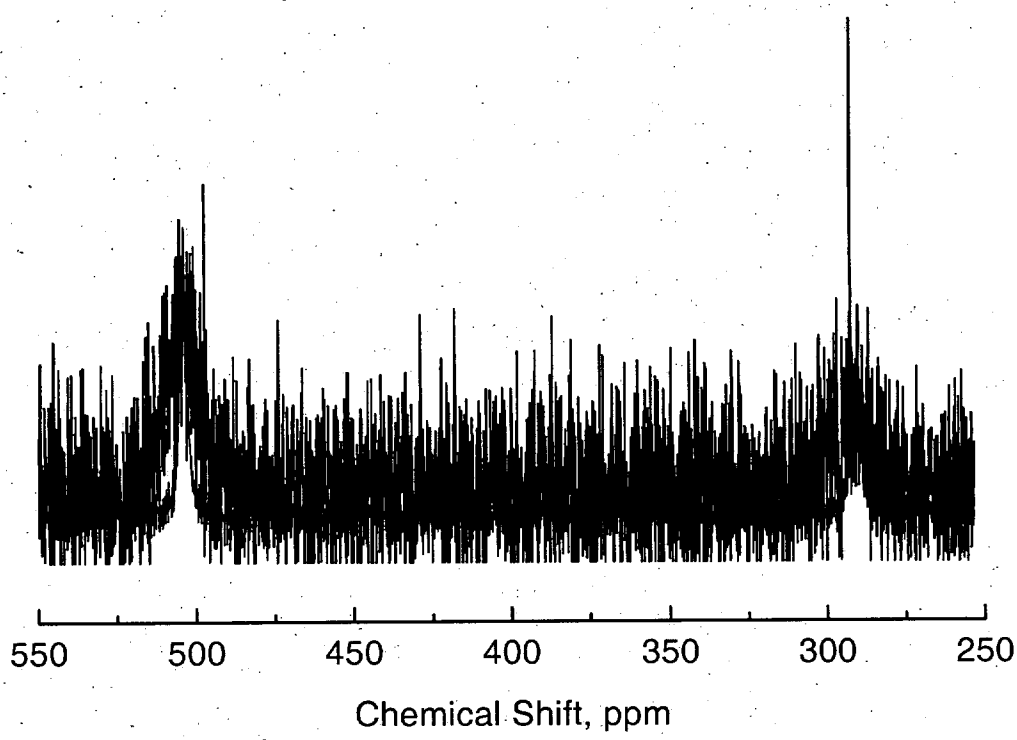

Figure 1: Observed ^{13}C NMR spectrum obtained at -60 °C for a sample that was 9 mM in **1-CH** and 18 mM in $[\mathbf{1\text{-}C}]^-$. The calculated spectrum is shown in the text.

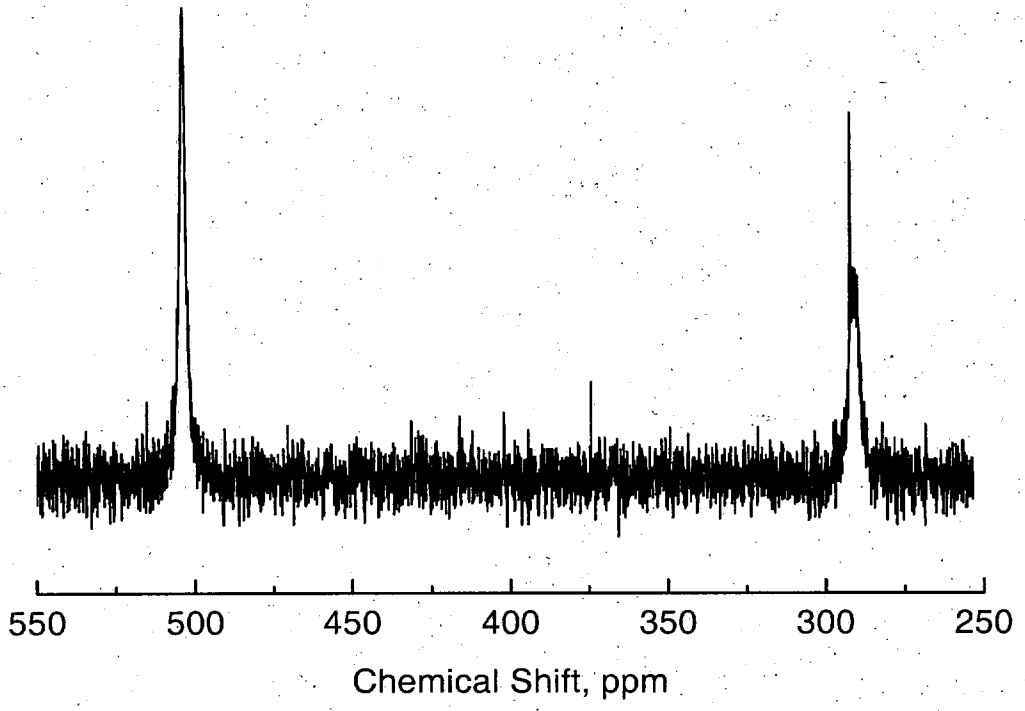

Figure 2: Observed ^{13}C NMR spectrum obtained at −90 °C for a sample that was 9 mM in **1-CH** and 18 mM in $[\mathbf{1\text{-}C}]^-$

3 Lineshape Equations for calculated spectrum

$$\upsilon \propto \frac{(1+\frac{\pi f_M}{T_{2C}}+\frac{\pi f_C}{T_{2M}})S+QR}{S^2+R^2}$$

$$Q = 2\pi\tau(\Delta\nu + f_M\delta\nu)$$

$$S = \frac{\tau}{T_{2C}T_{2M}} + \frac{f_M}{T_{2M}} + \frac{f_C}{T_{2C}} - 4\pi^2\tau\Delta\nu(\Delta\nu+\delta\nu)$$

$$R = 2\pi\tau(\frac{\Delta\nu+\delta\nu}{T_{2M}} + \frac{\Delta\nu}{T_{2C}}) + 2\pi(\tau + f_{2C}\delta\nu)$$

where T_{2C} is the T_2 relaxation time for [K(2,2,2-crypt)][**1-C**]
T_{2M} is the T_2 relaxation time for **1-CH**
f_C is the fraction of the sample that is [K(2,2,2-crypt)][**1-C**]
f_C is the fraction of the sample that is **1-CH**
τ is the lifetime of exchange
$\delta\nu$ is the difference (in Hz) between the two resonances in the absence of chemical exchange
$\Delta\nu$ is the difference (in Hz) between the chemical shift of the methylidyne and the frequency at which υ is being calculated.

4 Details of DFT calculations

4.1 $(H_2N)_3MoCH$

```
1(INPUT FILE)

title  HCMo(NH2)3 optimization


atoms  Zmatrix
1.  C   0 0 0
2.  Mo  1 0 0    rMoC
3.  N   2 1 0    rMoN   thetaA
4.  H   3 2 1    rNH1    thetaB1  phiA
5.  H   3 2 1    rNH2    thetaB2  phiB
6.  N   2 1 3    rMoN   thetaA  phiC
7.  H   6 2 1    rNH1    thetaB1  phiA
8.  H   6 2 1    rNH2    thetaB2  phiB
9.  N   2 1 3    rMoN   thetaA  -phiC
10. H   9 2 1    rNH1    thetaB1  phiA
11. H   9 2 1    rNH2    thetaB2  phiB
12. H   1 2 3    rCH    thetaC  phiD
end


geovar
rNH1=1.018131
rNH2=1.018131
rMoN=1.989808
rMoC=1.749913
rCH=1.091566
thetaA=102.013355
thetaB1=124.772175
thetaB2=124.772175
thetaC=180
phiA=0
phiB=180
phiC=120
phiD=180
end

relativistic scalar

corepotentials /disk3/usr/group/adf/ccc.relativ/t12r.MoNbSNUC ++
```

```
Mo 1
N  4
C  6
end

symmetry C(3V)

fragments
H   /disk3/usr/group/adf/ccc.atoms/t21.H
N   /disk3/usr/group/adf/ccc.relativ/t21r.N
C   /disk3/usr/group/adf/ccc.relativ/t21r.C
Mo  /disk3/usr/group/adf/ccc.relativ/t21r.Mo
end

xc
LDA VWN
GRADIENTS BECKE PERDEW
end

scf
ITERATIONS 99
MIXING 0.05
end

geometry
end

end input
1
*******************************************************************************
*                                                                             *
*  ------------------------------------                                       *
*   Amsterdam Density Functional  (ADF)        2.3.0     April 16, 1997      *
*  ------------------------------------                                       *
*                                                                             *
*   (c) Copyright 1993-1997, Theoretical Chemistry,                           *
*       Vrije Universiteit, Amsterdam, The Netherlands                        *
*   All rights reserved.                                                      *
*                                                                             *
*   Recommended citation:                                                     *
*     ADF 2.3.0, Theoretical Chemistry, Vrije Universiteit, Amsterdam         *
*     E.J.Baerends et.al., Chem.Phys. 2 (1973) 41                             *
*     G.te Velde, E.J.Baerends, J.Comp.Phys. 99 (1992) 84                     *
*     C.Fonseca Guerra et.al. METECC-95 (1995) 305                            *
*                                                                             *
```

```
*   Online information and documentation:                                *
*     http://tc.chem.vu.nl/SCM                                           *
*                                                                        *
*   E-mail: adf@chem.vu.nl                                               *
*                                                                        *
**************************************** sgi_irix ***********************

ADF 2.3.0  RunTime: Jan19-99 15:51:47
HCMo(NH2)3 optimization



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                                VWN
   Gradient Corrections:               Becke88 Perdew86                  == Not Defaul

SPIN  (restricted / unrestr.)
   Molecule:                           Restricted
   Fragments:                          Restricted

OTHER ASPECTS
   Relativistic Corrections:           scalar (Pauli,FrozenCore)         == Not Defaul
   Core Treatment:                     Frozen Orbital(s)

   Electric Field:                     ---

   Magnetic Field:                     ---



===========================
A T T A C H E D   F I L E S
===========================

Core Potentials :
             /disk3/usr/group/adf/ccc.relativ/t12r.MoNbSNUC


Fragment File(s)
----------------
C:
```

```
        file : /disk3/usr/group/adf/ccc.relativ/t21r.C
        jobid: ADF 2.3.0  RunTime: Jul08-98 14:49:18
        title: Carbon (IV, 1s frozen)
Mo:
        file : /disk3/usr/group/adf/ccc.relativ/t21r.Mo
        jobid: ADF 2.3.0  RunTime: Jun18-98 12:51:53
        title: Molybdenum (IV, 3d frozen)
N:
        file : /disk3/usr/group/adf/ccc.relativ/t21r.N
        jobid: ADF 2.3.0  RunTime: Jun18-98 13:51:02
        title: Nitrogen (III, 1s frozen)
H:
        file : /disk3/usr/group/adf/ccc.atoms/t21.H
        jobid: ADF 2.3.0  RunTime: Apr24-98 13:22:35
        title: Hydrogen (IV)
```

* Final Geometry *

****

Coordinates (Internal)

==========

Atom	Connection Numbers R	Alpha	Beta	Coordinates Angstr	degree	degree	Pointers to Geomet (0:frozen, *:LT p
1 C	0	0	0	0.000000	0.000000	0.000000	0 0
2 Mo	1	0	0	1.744794	0.000000	0.000000	1 0
3 N	2	1	0	1.976513	102.019358	0.000000	2 3
4 H	3	2	1	1.015743	126.517824	0.000000	4 5
5 H	3	2	1	1.020387	123.192225	-180.000000	7 8
6 N	2	1	3	1.976513	102.019358	120.000000	2 3
7 H	6	2	1	1.015743	126.517824	0.000000	4 5
8 H	6	2	1	1.020387	123.192225	-180.000000	7 8
9 N	2	1	3	1.976513	102.019358	-120.000000	2 3
10 H	9	2	1	1.015743	126.517824	0.000000	4 5
11 H	9	2	1	1.020387	123.192225	-180.000000	7 8
12 H	1	2	3	1.091672	180.000000	180.000000	11 12

Coordinates (Cartesian)

Atom	bohr			angstrom		
	X	Y	Z	X	Y	Z
1 C	0.000000	0.000000	0.009010	0.000000	0.000000	0.004768
2 Mo	0.000000	0.000000	3.306194	0.000000	0.000000	1.749562
3 N	1.826593	3.163752	4.083993	0.966591	1.674185	2.161155
4 H	2.545807	4.409467	2.813042	1.347183	2.333389	1.488597
5 H	2.174819	3.766897	5.882078	1.150864	1.993355	3.112661
6 N	-3.653186	0.000000	4.083993	-1.933182	0.000000	2.161155
7 H	-5.091614	0.000000	2.813042	-2.694365	0.000000	1.488597
8 H	-4.349638	0.000000	5.882078	-2.301728	0.000000	3.112661
9 N	1.826593	-3.163752	4.083993	0.966591	-1.674185	2.161155
10 H	2.545807	-4.409467	2.813042	1.347183	-2.333389	1.488597
11 H	2.174819	-3.766897	5.882078	1.150864	-1.993355	3.112661
12 H	0.000000	0.000000	-2.053952	0.000000	0.000000	-1.086904

H I R S H F E L D C H A R G E A N A L Y S I S

For each fragment: the (numerical) integral of rho(scf) * rho(fragment)/rho(sum-of-fragment
(nuclear charges are included, electrons are counted negative)

-0.2379 0.5992 -0.3280 -0.3280 -0.3280 0.0984 0.0914 0.0984 0.0914
0.0914 0.0548

Sum of these charges (accuracy NumInt/Tails) = 0.00170830

Atom-Atom Population Matrix (off-diagonal elements not doubled)

1 :	3.3208								
2 :	0.4462	11.9441							
3 :	0.0381	0.0913	5.0551						
4 :	-0.0115	-0.0272	0.3524	0.5003					
5 :	0.0027	-0.0171	0.3323	-0.0598	0.5248				
6 :	0.0381	0.0913	0.0014	0.0007	-0.0013	5.0551			
7 :	-0.0115	-0.0272	0.0007	-0.0005	0.0001	0.3524	0.5003		
8 :	0.0027	-0.0171	-0.0013	0.0001	-0.0007	0.3323	-0.0598	0.5248	
9 :	0.0381	0.0913	0.0014	0.0007	-0.0013	0.0014	0.0007	-0.0013	5.0551
10 :	-0.0115	-0.0272	0.0007	-0.0005	0.0001	0.0007	-0.0005	0.0001	0.3524
11 :	0.0027	-0.0171	-0.0013	0.0001	-0.0007	-0.0013	0.0001	-0.0007	0.3323

```
          0.5248
 12 :     0.2913   -0.1998    0.0018   -0.0015    0.0001    0.0018   -0.0015    0.0001
          0.0001    1.2142
```

4.2 $(H_2N)_3MoC^-$

```
1(INPUT FILE)

 title -CMo(NH2)3 optimization


 atoms  Zmatrix
 1.  C   0 0 0
 2.  Mo  1 0 0    rMoC
 3.  N   2 1 0    rMoN   thetaA
 4.  H   3 2 1    rNH1    thetaB1  phiA
 5.  H   3 2 1    rNH2    thetaB2  phiB
 6.  N   2 1 3    rMoN   thetaA  phiC
 7.  H   6 2 1    rNH1    thetaB1  phiA
 8.  H   6 2 1    rNH2    thetaB2  phiB
 9.  N   2 1 3    rMoN   thetaA  -phiC
 10. H   9 2 1    rNH1    thetaB1  phiA
 11. H   9 2 1    rNH2    thetaB2  phiB
 end


 geovar
 rNH1=1.018131
 rNH2=1.018131
 rMoN=1.989808
 rMoC=1.749913
 thetaA=102.013355
 thetaB1=124.772175
 thetaB2=124.772175
 phiA=0
 phiB=180
 phiC=120
 end

 charge -1
```

```
relativistic scalar

corepotentials /disk3/usr/group/adf/ccc.relativ/t12r.MoNbSNUC ++
Mo 1
N  4
C  6
end

symmetry C(3V)

fragments
H   /disk3/usr/group/adf/ccc.atoms/t21.H
N   /disk3/usr/group/adf/ccc.relativ/t21r.N
C   /disk3/usr/group/adf/ccc.relativ/t21r.C
Mo  /disk3/usr/group/adf/ccc.relativ/t21r.Mo
end

xc
LDA VWN
GRADIENTS BECKE PERDEW
end

scf
ITERATIONS 99
MIXING 0.05
end

geometry
end

end input
1
*******************************************************************************
*                                                                             *
*  ------------------------------------                                       *
*   Amsterdam Density Functional  (ADF)        2.3.0     April 16, 1997      *
*  ------------------------------------                                       *
*                                                                             *
*   (c) Copyright 1993-1997, Theoretical Chemistry,                           *
*       Vrije Universiteit, Amsterdam, The Netherlands                        *
*   All rights reserved.                                                      *
*                                                                             *
*   Recommended citation:                                                     *
*     ADF 2.3.0, Theoretical Chemistry, Vrije Universiteit, Amsterdam         *
```

```
*     E.J.Baerends et.al., Chem.Phys. 2 (1973) 41                    *
*     G.te Velde, E.J.Baerends, J.Comp.Phys. 99 (1992) 84            *
*     C.Fonseca Guerra et.al. METECC-95 (1995) 305                   *
*                                                                    *
*   Online information and documentation:                            *
*     http://tc.chem.vu.nl/SCM                                       *
*                                                                    *
*   E-mail: adf@chem.vu.nl                                           *
*                                                                    *
********************************************  sgi_irix  ************************
*  Final Geometry  *
                                                 ********************
```

Coordinates (Internal)

Atom	Connection Numbers R	Alpha	Beta	Coordinates Angstr	degree	degree	Pointers to Geomet (0:frozen, *:LT p	
1 C	0	0	0	0.000000	0.000000	0.000000	0	0
2 Mo	1	0	0	1.741849	0.000000	0.000000	1	0
3 N	2	1	0	2.022419	101.313402	0.000000	2	3
4 H	3	2	1	1.016493	124.976336	0.000000	4	5
5 H	3	2	1	1.019903	125.260776	-180.000000	7	8
6 N	2	1	3	2.022419	101.313402	120.000000	2	3
7 H	6	2	1	1.016493	124.976336	0.000000	4	5
8 H	6	2	1	1.019903	125.260776	-180.000000	7	8
9 N	2	1	3	2.022419	101.313402	-120.000000	2	3
10 H	9	2	1	1.016493	124.976336	0.000000	4	5
11 H	9	2	1	1.019903	125.260776	-180.000000	7	8

Coordinates (Cartesian)

Atom	bohr X	Y	Z	angstrom X	Y	Z
1 C	0.000000	0.000000	0.024523	0.000000	0.000000	0.012977
2 Mo	0.000000	0.000000	3.316143	0.000000	0.000000	1.754827
3 N	1.873778	3.245479	4.065890	0.991560	1.717433	2.151576
4 H	2.568031	4.447960	2.738529	1.358943	2.353758	1.449167

```
  5 H        2.264929    3.922971    5.827320     1.198548    2.075947    3.083684
  6 N       -3.747556    0.000000    4.065890    -1.983121    0.000000    2.151576
  7 H       -5.136062    0.000000    2.738529    -2.717886    0.000000    1.449167
  8 H       -4.529857    0.000000    5.827320    -2.397097    0.000000    3.083684
  9 N        1.873778   -3.245479    4.065890     0.991560   -1.717433    2.151576
 10 H        2.568031   -4.447960    2.738529     1.358943   -2.353758    1.449167
 11 H        2.264929   -3.922971    5.827320     1.198548   -2.075947    3.083684
 ------------------------------------------------------------------------------

H I R S H F E L D   C H A R G E   A N A L Y S I S
 ================================================

 For each fragment: the (numerical) integral of rho(scf) * rho(fragment)/rho(sum-of-fragment
 (nuclear charges are included, electrons are counted negative)

    -0.5334    0.3628   -0.3788   -0.3788   -0.3788    0.0578    0.0447    0.0578    0.0447
     0.0447

 Sum of these charges (accuracy NumInt/Tails) =          -0.99970942

 Atom-Atom Population Matrix (off-diagonal elements not doubled)
 ===============================================================

     1 :     4.0064
     2 :     0.5795   12.1144
     3 :     0.0276    0.1250    5.0497
     4 :    -0.0132   -0.0374    0.3432    0.5725
     5 :     0.0022   -0.0246    0.3267   -0.0757    0.6073
     6 :     0.0276    0.1250    0.0002    0.0006   -0.0011    5.0497
     7 :    -0.0132   -0.0374    0.0006   -0.0007    0.0004    0.3432    0.5725
     8 :     0.0022   -0.0246   -0.0011    0.0004   -0.0012    0.3267   -0.0757    0.6073
     9 :     0.0276    0.1250    0.0002    0.0006   -0.0011    0.0002    0.0006   -0.0011
    10 :    -0.0132   -0.0374    0.0006   -0.0007    0.0004    0.0006   -0.0007    0.0004
    11 :     0.0022   -0.0246   -0.0011    0.0004   -0.0012   -0.0011    0.0004   -0.0012
             0.6073
```

4.3 $CH_3Mo(NH_2)_3$

```
1(INPUT FILE)

 title  H3CMo(NH2)3 optimization
```

```
atoms  Zmatrix
1.  C   0 0 0
2.  Mo  1 0 0    rMoC
3.  N   2 1 0    rMoN   thetaA
4.  H   3 2 1    rNH1    thetaB1  phiA
5.  H   3 2 1    rNH2    thetaB2  phiB
6.  N   2 1 3    rMoN   thetaA  phiC
7.  H   6 2 1    rNH1    thetaB1  phiA
8.  H   6 2 1    rNH2    thetaB2  phiB
9.  N   2 1 3    rMoN   thetaA  -phiC
10. H   9 2 1    rNH1    thetaB1  phiA
11. H   9 2 1    rNH2    thetaB2  phiB
12. H   1 2 3    rCH1    thetaC  phiD
13. H   1 2 3    rCH1    thetaC  phiD2
14. H   1 2 3    rCH1    thetaC  phiD3
end


geovar
rNH1=1.018131
rNH2=1.018131
rMoN=1.989808
rMoC=1.749913
rCH1=1.091566
thetaA=102.013355
thetaB1=124.772175
thetaB2=124.772175
thetaC=109.5
phiA=0
phiB=180
phiC=120
phiD=180
phiD2=60
phiD3=-60
end

relativistic scalar

unrestricted
charge 0 2

occupations aufbau=3

corepotentials /disk3/usr/group/adf/ccc.relativ/t12r.MoNbSNUC ++
```

```
Mo 1
N  4
C  6
end

symmetry C(3V)

fragments
H   /disk3/usr/group/adf/ccc.atoms/t21.H
N   /disk3/usr/group/adf/ccc.relativ/t21r.N
C   /disk3/usr/group/adf/ccc.relativ/t21r.C
Mo  /disk3/usr/group/adf/ccc.relativ/t21r.Mo
end

xc
LDA VWN
GRADIENTS BECKE PERDEW
end

scf
ITERATIONS 99
MIXING 0.05
end

geometry
end

end input
1
*******************************************************************************
*                                                                             *
*  ------------------------------------                                       *
*   Amsterdam Density Functional  (ADF)        2.3.0     April 16, 1997      *
*  ------------------------------------                                       *
*                                                                             *
*   (c) Copyright 1993-1997, Theoretical Chemistry,                           *
*       Vrije Universiteit, Amsterdam, The Netherlands                        *
*   All rights reserved.                                                      *
*                                                                             *
*   Recommended citation:                                                     *
*     ADF 2.3.0, Theoretical Chemistry, Vrije Universiteit, Amsterdam         *
*     E.J.Baerends et.al., Chem.Phys. 2 (1973) 41                             *
*     G.te Velde, E.J.Baerends, J.Comp.Phys. 99 (1992) 84                     *
*     C.Fonseca Guerra et.al. METECC-95 (1995) 305                            *
*                                                                             *
```

```
*   Online information and documentation:                              *
*     http://tc.chem.vu.nl/SCM                                         *
*                                                                      *
*   E-mail: adf@chem.vu.nl                                             *
*                                                                      *
****************************************** sgi_irix ********************

ADF 2.3.0  RunTime: Feb02-99 14:22:49
H3CMo(NH2)3 optimization



================================
M O D E L   P A R A M E T E R S
================================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                 == Not Defaul

SPIN  (restricted / unrestr.)
   Molecule:                         UNrestricted                     == Not Defaul
   Fragments:                        Restricted

OTHER ASPECTS
   Relativistic Corrections:         scalar (Pauli,FrozenCore)        == Not Defaul
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Magnetic Field:                   ---

<LeftMouse Coordinates (Internal)
 ========================
```

Atom	Connection Numbers R	Alpha	Beta	Coordinates Angstr	degree	degree	Pointers to Geomet (0:frozen, *:LT p	
1 C	0	0	0	0.000000	0.000000	0.000000	0	0
2 Mo	1	0	0	2.132105	0.000000	0.000000	1	0
3 N	2	1	0	1.978678	97.565661	0.000000	2	3
4 H	3	2	1	1.020458	125.174775	0.000000	4	5
5 H	3	2	1	1.020807	125.177658	-180.000000	7	8
6 N	2	1	3	1.978678	97.565661	120.000000	2	3
7 H	6	2	1	1.020458	125.174775	0.000000	4	5

8 H	6	2	1	1.020807	125.177658	-180.000000	7	8
9 N	2	1	3	1.978678	97.565661	-120.000000	2	3
10 H	9	2	1	1.020458	125.174775	0.000000	4	5
11 H	9	2	1	1.020807	125.177658	-180.000000	7	8
12 H	1	2	3	1.101441	110.289274	-180.000000	11	12
13 H	1	2	3	1.101441	110.289274	60.000000	11	12
14 H	1	2	3	1.101441	110.289274	-60.000000	11	12

Coordinates (Cartesian)

Atom	bohr			angstrom		
	X	Y	Z	X	Y	Z
1 C	0.000000	0.000000	-0.564470	0.000000	0.000000	-0.298704
2 Mo	0.000000	0.000000	3.464626	0.000000	0.000000	1.833401
3 N	1.853305	3.210019	3.956933	0.980727	1.698668	2.093918
4 H	2.507683	4.343434	2.540656	1.327008	2.298445	1.344457
5 H	2.300344	3.984312	5.666273	1.217289	2.108407	2.998461
6 N	-3.706611	0.000000	3.956933	-1.961453	0.000000	2.093918
7 H	-5.015365	0.000000	2.540656	-2.654016	0.000000	1.344457
8 H	-4.600688	0.000000	5.666273	-2.434578	0.000000	2.998461
9 N	1.853305	-3.210019	3.956933	0.980727	-1.698668	2.093918
10 H	2.507683	-4.343434	2.540656	1.327008	-2.298445	1.344457
11 H	2.300344	-3.984312	5.666273	1.217289	-2.108407	2.998461
12 H	-0.976139	-1.690723	-1.286224	-0.516551	-0.894692	-0.680640
13 H	1.952279	0.000000	-1.286224	1.033101	0.000000	-0.680640
14 H	-0.976139	1.690723	-1.286224	-0.516551	0.894692	-0.680640

Atom-Atom Population Matrix (off-diagonal elements not doubled)

1 :	4.0530							
2 :	0.5395	12.1203						
3 :	0.0302	0.1534	5.3564					
4 :	-0.0138	-0.0302	0.3253	2.1079				
5 :	-0.0036	-0.0184	0.3316	-0.0461	2.1010			
6 :	0.0302	0.1534	0.0001	-0.0016	-0.0022	5.3564		
7 :	-0.0138	-0.0302	-0.0016	0.0002	0.0001	0.3253	2.1079	
8 :	-0.0036	-0.0184	-0.0022	0.0001	0.0000	0.3316	-0.0461	2.1010
9 :	0.0302	0.1534	0.0001	-0.0016	-0.0022	0.0001	-0.0016	-0.0022
10 :	-0.0138	-0.0302	-0.0016	0.0002	0.0001	-0.0016	0.0002	0.0001

11 :	-0.0036	-0.0184	-0.0022	0.0001	0.0000	-0.0022	0.0001	0.0000
	2.1010							
12 :	0.0035	-0.0108	-0.0598	0.3354	-0.0185	0.0016	0.0008	0.0008
	-0.0002	1.1376						
13 :	0.0035	-0.0108	-0.0002	0.0001	-0.0002	-0.0598	0.3354	-0.0185
	0.0008	0.0003	1.1376					
14 :	0.0035	-0.0108	0.0016	0.0008	0.0008	-0.0002	0.0001	-0.0002
	-0.0185	0.0003	0.0003	1.1376				
15 :	0.0035	-0.0108	-0.0598	0.3354	-0.0185	-0.0002	0.0001	-0.0002
	0.0008	-0.1760	0.0000	-0.0015	1.1376			
16 :	0.0035	-0.0108	0.0016	0.0008	0.0008	-0.0598	0.3354	-0.0185
	-0.0002	-0.0015	-0.1760	0.0000	0.0003	1.1376		
17 :	0.0035	-0.0108	-0.0002	0.0001	-0.0002	0.0016	0.0008	0.0008
	-0.0185	0.0000	-0.0015	-0.1760	0.0003	0.0003	1.1376	
18 :	0.0032	-0.0108	-0.0527	0.3986	0.0027	-0.0014	-0.0004	0.0003
	0.0003	-0.0665	-0.0001	0.0005	-0.0665	0.0005	-0.0001	0.9089
19 :	0.0032	-0.0108	-0.0014	-0.0004	0.0003	-0.0527	0.3986	0.0027
	0.0003	0.0005	-0.0665	-0.0001	-0.0001	-0.0665	0.0005	0.0006
20 :	0.0032	-0.0108	-0.0014	-0.0004	0.0003	-0.0014	-0.0004	0.0003
	0.0027	-0.0001	0.0005	-0.0665	0.0005	-0.0001	-0.0665	0.0006
21 :	0.0009	-0.0116	-0.0654	-0.0157	0.3364	0.0003	0.0001	-0.0006
	0.0018	-0.0331	-0.0001	-0.0012	0.0552	0.0004	0.0004	0.0019
	1.1463							
22 :	0.0009	-0.0116	0.0010	0.0005	0.0018	-0.0654	-0.0157	0.3364
	-0.0006	-0.0012	-0.0331	-0.0001	0.0004	0.0552	0.0004	0.0000
	0.0010	1.1463						
23 :	0.0009	-0.0116	0.0003	0.0001	-0.0006	0.0010	0.0005	0.0018
	0.3364	-0.0001	-0.0012	-0.0331	0.0004	0.0004	0.0552	-0.0001
	0.0010	0.0010	1.1463					
24 :	0.0009	-0.0116	-0.0654	-0.0157	0.3364	0.0010	0.0005	0.0018
	-0.0006	0.0552	0.0004	0.0004	-0.0331	-0.0012	-0.0001	0.0019
	-0.1783	-0.0054	-0.0002	1.1463				
25 :	0.0009	-0.0116	0.0003	0.0001	-0.0006	-0.0654	-0.0157	0.3364
	0.0018	0.0004	0.0552	0.0004	-0.0001	-0.0331	-0.0012	-0.0001
	-0.0002	-0.1783	-0.0054	0.0010	1.1463			
26 :	0.0009	-0.0116	0.0010	0.0005	0.0018	0.0003	0.0001	-0.0006
	0.3364	0.0004	0.0004	0.0552	-0.0012	-0.0001	-0.0331	0.0000
	-0.0054	-0.0002	-0.1783	0.0010	0.0010	1.1463		
27 :	-0.0001	0.0013	-0.0602	0.0028	0.3655	-0.0016	-0.0001	0.0001
	0.0001	0.0004	-0.0003	0.0007	0.0004	0.0007	-0.0003	-0.0097
	-0.0797	0.0049	-0.0008	-0.0797	-0.0008	0.0049	1.0298	
28 :	-0.0001	0.0013	-0.0016	-0.0001	0.0001	-0.0602	0.0028	0.3655
	0.0001	0.0007	0.0004	-0.0003	-0.0003	0.0004	0.0007	0.0002
	-0.0008	-0.0797	0.0049	0.0049	-0.0797	-0.0008	-0.0082	1.0298
29 :	-0.0001	0.0013	-0.0016	-0.0001	0.0001	-0.0016	-0.0001	0.0001

```
0.3655   -0.0003   0.0007   0.0004   0.0007   -0.0003   0.0004   0.0002
0.0049   -0.0008   -0.0797  -0.0008  0.0049   -0.0797   -0.0082  -0.0082
```

4.4 HCC^-

```
alkyne anion
1(INPUT FILE)

 title C2H2 optimization

 atoms Zmatrix
 1.  C  0 0 0
 2.  C  1 0 0 CC
 3.  XX 2 1 0 CX CCX
 4.  H  1 2 3 CH HCC HCCH1
 end

 geovar
 CC=1.6
 CH=1.1
 CX=1.5
 CCX=90.0
 HCC=180
 XCCX=180
 HCCH1=90
 end

 charge -1 0

 unrestricted

 relativistic scalar

 corepotentials /disk3/usr/group/adf/ccc.relativ/t12r.MoNbSNUC ++
 C 6
 end

 symmetry C(LIN)

 fragments
 H   /disk3/usr/group/adf/ccc.atoms/t21.H
 C   /disk3/usr/group/adf/ccc.relativ/t21r.C
```

```
end

xc
LDA VWN
GRADIENTS BECKE PERDEW
end

scf
ITERATIONS 99
MIXING 0.05
end

geometry
end

end input
1
*******************************************************************************
*                                                                             *
*  ------------------------------------                                       *
*   Amsterdam Density Functional  (ADF)        2.3.0     April 16, 1997      *
*  ------------------------------------                                       *
*                                                                             *
*   (c) Copyright 1993-1997, Theoretical Chemistry,                           *
*       Vrije Universiteit, Amsterdam, The Netherlands                        *
*   All rights reserved.                                                      *
*                                                                             *
*   Recommended citation:                                                     *
*     ADF 2.3.0, Theoretical Chemistry, Vrije Universiteit, Amsterdam         *
*     E.J.Baerends et.al., Chem.Phys. 2 (1973) 41                             *
*     G.te Velde, E.J.Baerends, J.Comp.Phys. 99 (1992) 84                     *
*     C.Fonseca Guerra et.al. METECC-95 (1995) 305                            *
*                                                                             *
*   Online information and documentation:                                     *
*     http://tc.chem.vu.nl/SCM                                                *
*                                                                             *
*   E-mail: adf@chem.vu.nl                                                    *
*                                                                             *
*******************************************  sgi_irix  **********************

ADF 2.3.0  RunTime: Feb05-99 22:36:37
C2H2 optimization
```

```
================================
M O D E L   P A R A M E T E R S
================================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                                VWN
   Gradient Corrections:               Becke88 Perdew86                    == Not Defaul

SPIN  (restricted / unrestr.)
   Molecule:                           UNrestricted                        == Not Defaul
   Fragments:                          Restricted

OTHER ASPECTS
   Relativistic Corrections:           scalar (Pauli,FrozenCore)           == Not Defaul
   Core Treatment:                     Frozen Orbital(s)

   Electric Field:                     ---

   Magnetic Field:                     ---
```

Coordinates (Internal)

Atom	Connection Numbers R	Alpha	Beta	Coordinates Angstr	degree	degree	Pointers to Geomet (0:frozen, *:LT p	
1 C	0	0	0	0.000000	0.000000	0.000000	0	0
2 C	1	0	0	1.252027	0.000000	0.000000	1	0
3 XX	2	1	0	1.510976	96.910347	0.000000	2	3
4 H	1	2	3	1.080236	180.000000	90.000000	4	5

Coordinates (Cartesian)

Atom	bohr X	Y	Z	angstrom X	Y	Z
1 C	0.000000	0.000000	0.314032	0.000000	0.000000	0.166178
2 C	0.000000	0.000000	2.680020	0.000000	0.000000	1.418205
3 XX	0.000000	2.834590	3.023563	0.000000	1.500000	1.600000
4 H	0.000000	0.000000	-1.727320	0.000000	0.000000	-0.914058

```
 -------------------------
-Atom-Atom Population Matrix (off-diagonal elements not doubled)
 ================================================================

                                    ***** SPIN 1 *****

    1 :     1.5290
    2 :     0.6105    1.6376
    3 :     0.0000    0.0000    0.0000
    4 :     0.0886   -0.0604    0.0000    0.5561

                                    ***** SPIN 2 *****

    1 :     1.5290
    2 :     0.6105    1.6376
    3 :     0.0000    0.0000    0.0000
    4 :     0.0886   -0.0604    0.0000    0.5561
```

4.5 HCCH

```
1(INPUT FILE)

 title C2H2 optimization

 atoms Zmatrix
 1.  C  0 0 0
 2.  C  1 0 0 CC
 3.  XX 2 1 0 CX CCX
 4.  XX 1 2 3 CX CCX XCCX
 5.  H  1 2 3 CH HCC HCCH1
 6.  H  2 1 4 CH HCC HCCH1
 end

 geovar
 CC=1.6
 CH=1.1
 CX=1.5
 CCX=90.0
 HCC=180
 XCCX=180
 HCCH1=90
 end
```

unrestricted

relativistic scalar

****
* R E S U L T S *
****

Coordinates (Internal)
==========

Atom	Connection Numbers R	Alpha	Beta	Coordinates Angstr	degree	degree	Pointers to Geomet (0:frozen, *:LT p	
1 C	0	0	0	0.000000	0.000000	0.000000	0	0
2 C	1	0	0	1.207011	0.000000	0.000000	1	0
3 XX	2	1	0	1.512815	97.463045	0.000000	2	3
4 XX	1	2	3	1.512815	97.463045	-180.000000	2	3
5 H	1	2	3	1.071131	180.000000	90.000000	5	6
6 H	2	1	4	1.071131	180.000000	90.000000	5	6

Coordinates (Cartesian)
==========

Atom	bohr X	Y	Z	angstrom X	Y	Z
1 C	0.000000	0.000000	-1.140460	0.000000	0.000000	-0.603505
2 C	0.000000	0.000000	1.140460	0.000000	0.000000	0.603505
3 XX	0.000000	2.834590	1.511781	0.000000	1.500000	0.800000
4 XX	0.000000	-2.834590	-1.511781	0.000000	-1.500000	-0.800000
5 H	0.000000	0.000000	-3.164605	0.000000	0.000000	-1.674636
6 H	0.000000	0.000000	3.164605	0.000000	0.000000	1.674636

Atom-Atom Population Matrix (off-diagonal elements not doubled)
==========

***** SPIN 1 *****

```
 1 :    1.3705
 2 :    0.4148    1.3705
 3 :    0.0000    0.0000    0.0000
 4 :    0.0000    0.0000    0.0000    0.0000
 5 :    0.2347   -0.0581    0.0000    0.0000    0.3714
 6 :   -0.0581    0.2347    0.0000    0.0000   -0.0100    0.3714

                              ***** SPIN 2 *****

 1 :    1.3705
 2 :    0.4148    1.3705
 3 :    0.0000    0.0000    0.0000
 4 :    0.0000    0.0000    0.0000    0.0000
 5 :    0.2347   -0.0581    0.0000    0.0000    0.3714
 6 :   -0.0581    0.2347    0.0000    0.0000   -0.0100    0.3714
```

4.6 H_2CCH_2

```
1(INPUT FILE)

 title C2H4 optimization

 atoms Zmatrix
 1.  C  0 0 0
 2.  C  1 0 0 CC
 3.  H  1 2 0 CH HCC
 4.  H  1 2 3 CH HCC HCCH1
 5.  H  2 1 3 CH HCC HCCH2
 6.  H  2 1 5 CH HCC HCCH1
 end

 geovar
 CC=1.6
 CH=1.1
 HCC=120
 HCCH1=180
 HCCH2=0
 end

 unrestricted

 relativistic scalar
```

```
corepotentials /disk3/usr/group/adf/ccc.relativ/t12r.MoNbSNUC ++
C 6
end

symmetry D(2H)

Coordinates (Internal)
======================
```

Atom	Connection Numbers R	Alpha	Beta	Coordinates Angstr	degree	degree	Pointers to Geomet (0:frozen, *:LT p	
1 C	0	0	0	0.000000	0.000000	0.000000	0	0
2 C	1	0	0	1.333950	0.000000	0.000000	1	0
3 H	1	2	0	1.091994	121.615141	0.000000	2	3
4 H	1	2	3	1.091994	121.615141	-180.000000	2	3
5 H	2	1	3	1.091994	121.615141	0.000000	2	3
6 H	2	1	5	1.091994	121.615141	-180.000000	2	3

```
Coordinates (Cartesian)
=======================
```

Atom	bohr X	Y	Z	angstrom X	Y	Z
1 C	-1.260400	0.000000	0.000000	-0.666975	0.000000	0.000000
2 C	1.260400	0.000000	0.000000	0.666975	0.000000	0.000000
3 H	-2.342147	1.757313	0.000000	-1.239410	0.929930	0.000000
4 H	-2.342147	-1.757313	0.000000	-1.239410	-0.929930	0.000000
5 H	2.342147	1.757313	0.000000	1.239410	0.929930	0.000000
6 H	2.342147	-1.757313	0.000000	1.239410	-0.929930	0.000000

```
Atom-Atom Population Matrix (off-diagonal elements not doubled)
================================================================

                                ***** SPIN 1 *****

    1 :     1.2135
    2 :     0.2950    1.2135
    3 :     0.2058   -0.0225    0.4628
    4 :     0.2058   -0.0225   -0.0604    0.4628
    5 :    -0.0225    0.2058   -0.0329    0.0095    0.4628
```

```
    6 :    -0.0225    0.2058    0.0095   -0.0329   -0.0604    0.4628

                                ***** SPIN 2 *****

    1 :     1.2135
    2 :     0.2950    1.2135
    3 :     0.2058   -0.0225    0.4628
    4 :     0.2058   -0.0225   -0.0604    0.4628
    5 :    -0.0225    0.2058   -0.0329    0.0095    0.4628
    6 :    -0.0225    0.2058    0.0095   -0.0329   -0.0604    0.4628
```

4.7 H_3CCH_3

```
1(INPUT FILE)

 title C2H6 optimization

 atoms Zmatrix
 1.  C  0 0 0
 2.  C  1 0 0 CC
 3.  H  1 2 0 CH HCC
 4.  H  1 2 3 CH HCC HCCH1
 5.  H  1 2 3 CH HCC HCCH2
 6.  H  2 1 3 CH HCC HCCH3
 7.  H  2 1 6 CH HCC HCCH1
 8.  H  2 1 6 CH HCC HCCH2
 end

 geovar
 CC=1.6
 CH=1.1
 HCC=109.5
 HCCH1=120
 HCCH2=-120
 HCCH3=180
 end

 unrestricted

 relativistic scalar
                                        * R E S U L T S *
                                          ******************
```

Coordinates (Internal)
==========

Atom	Connection Numbers R	Alpha	Beta	Coordinates Angstr	degree	degree	Pointers to Geomet (0:frozen, *:LT p	
1 C	0	0	0	0.000000	0.000000	0.000000	0	0
2 C	1	0	0	1.533546	0.000000	0.000000	1	0
3 H	1	2	0	1.099676	111.333929	0.000000	2	3
4 H	1	2	3	1.099676	111.333929	120.000000	2	3
5 H	1	2	3	1.099676	111.333929	-120.000000	2	3
6 H	2	1	3	1.099676	111.333929	-180.000000	2	3
7 H	2	1	6	1.099676	111.333929	120.000000	2	3
8 H	2	1	6	1.099676	111.333929	-120.000000	2	3

Coordinates (Cartesian)
==========

Atom	bohr X	Y	Z	angstrom X	Y	Z
1 C	0.000000	0.000000	-1.448992	0.000000	0.000000	-0.766773
2 C	0.000000	0.000000	1.448992	0.000000	0.000000	0.766773
3 H	0.000000	1.935688	-2.205006	0.000000	1.024322	-1.166838
4 H	1.676355	-0.967844	-2.205006	0.887089	-0.512161	-1.166838
5 H	-1.676355	-0.967844	-2.205006	-0.887089	-0.512161	-1.166838
6 H	0.000000	-1.935688	2.205006	0.000000	-1.024322	1.166838
7 H	1.676355	0.967844	2.205006	0.887089	0.512161	1.166838
8 H	-1.676355	0.967844	2.205006	-0.887089	0.512161	1.166838

Atom-Atom Population Matrix (off-diagonal elements not doubled)
==========

***** SPIN 1 *****

1 :	1.1268			
2 :	0.1752	1.1268		
3 :	0.2021	-0.0206	0.4255	
4 :	0.2021	-0.0206	-0.0200	0.4255

5 :	0.2021	-0.0206	-0.0200	-0.0200	0.4255			
6 :	-0.0206	0.2021	0.0055	-0.0106	-0.0106	0.4255		
7 :	-0.0206	0.2021	-0.0106	-0.0106	0.0055	-0.0200	0.4255	
8 :	-0.0206	0.2021	-0.0106	0.0055	-0.0106	-0.0200	-0.0200	0.4255

***** SPIN 2 *****

1 :	1.1268							
2 :	0.1752	1.1268						
3 :	0.2021	-0.0206	0.4255					
4 :	0.2021	-0.0206	-0.0200	0.4255				
5 :	0.2021	-0.0206	-0.0200	-0.0200	0.4255			
6 :	-0.0206	0.2021	0.0055	-0.0106	-0.0106	0.4255		
7 :	-0.0206	0.2021	-0.0106	-0.0106	0.0055	-0.0200	0.4255	
8 :	-0.0206	0.2021	-0.0106	0.0055	-0.0106	-0.0200	-0.0200	0.4255