# APPENDIXES

# APPENDIX 1A

**Symbol, Atomic Number, Outer electronic configuration and S, L and J values of Ln(III)**

| NAME | Symbol | Atomic Number | Electronic Configuration | S | L | J |
|---|---|---|---|---|---|---|
| **Praseodimium** | Pr | 59 | $[Xe]6s^2$ , $4f^2$ | 2/2 | 5 | 8/2 |
| **Neodymium** | Nd | 60 | $[Xe]6s^2$ , $4f^3$ | ¾ | 6 | 9/2 |
| **Samarium** | Sm | 62 | $[Xe]6s^2$ , $4f^3$ | 2 / 2 | 5 | 4 |
| **Europium** | Eu | 63 | $[Xe]6s^2$ , $4f^3$ | 6/2 | 3 | 0 |
| **Dysprosium** | Dy | 66 | $[Xe]6s^2$ , $4f^3$ | 5/2 | 5 | 15/2 |
| **Erbium** | Er | 68 | $[Xe]\ 6s^2$ , $4f^{11}$ | 3/2 | 6 | 15/2 |
| **Thulium** | Tm | 69 | $[Xe]6s^2$ , $4f^3$ . | 2/2 | 5 | 4 |

# APPENDIX 1B

Some properties of lanthanoids (atomic radius and ionic radius)

| Ln(III) | $4f^n$ | $R^{0}_{(1)}$ | $R^{3+}_{(2)}$ | $R^{3+}_{(3)}$ | $R^{4+}_{(4)}$ |
|---|---|---|---|---|---|
| Pr(III) | $4f^2$ | 1.16 | 1.013 | 1.126 | 0.901 |
| Nd(III) | $4f^3$ | 1.15 | 0.995 | 1.109 | 0.889 |
| Sm(III) | $4f^5$ | 1.13 | 0.964 | 1.079 | 0.867 |
| Eu(III) | $4f^6$ | 1.13 | 0.950 | 1.066 | 0.856 |
| Dy(III) | $4f^9$ | 1.07 | 0.908 | 1.027 | 0.833 |
| Er(III) | $4f^{11}$ | 1.04 | 0.881 | 1.004 | 0.820 |
| Tm(III) | $4f^{12}$ | 1.04 | 0.869 | 0.994 | 0.815 |

APPENDIX 2

DETAILS OF THE LIGANDS USED THE PRESENT WORK

**1. SARCOSINE ( N - Methylglycine )**

*Molecular formula* - $C_3H_7O_2N$

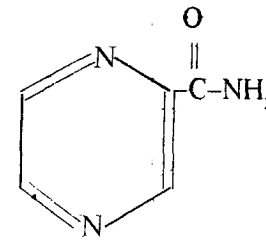
*Molecular weight* - 89.10

$$CH_3\text{-}NH\text{-}CH_2\text{-}COOH$$

**2. PYRAZINE CARBOXAMIDE (Pyrazinamide ) :**

*Molecular formula* - $C_5H_5N_3O$

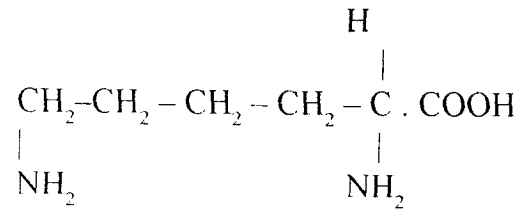
*Molecular weight* - 123.12




**3. LYCINE (L-2,6 diamino hexanoic acid ) :**

*Molecular formula* - $C_6H_{14}O_2N_2$

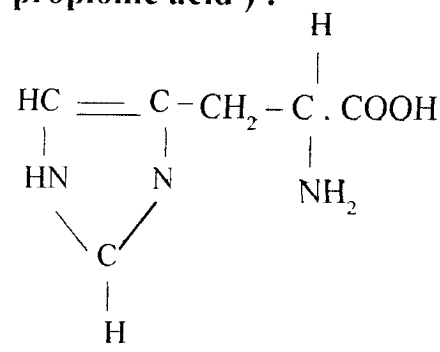
*Molecular weight* - 182.65




**4. HISTIDINE ( L-2,amino 3-(4 midizole) propionic acid ) :**

*Molecular formula* - $C_6H_9O_2N_3$

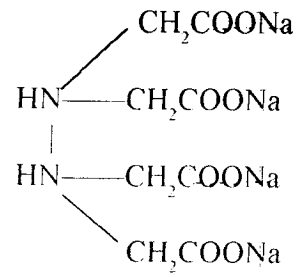
*Molecular weight* - 155.16




**EDTA (Ethylenediamine Tetra acetic Acid**

*Molecular formula* - $C_{10}H_{10}O_8N_2Na_4$

*Molecular weight* - 372.21



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## APPENDIX 3

Details of the formulae used for the calculations of Partial charge on Ligands Donor atoms

$$q = \frac{[\text{SR of the molecule} - \text{SR of the atom}]}{2.08 \times \sqrt{\text{SR of atom}}}$$

where SR of molecule = Stability Ratio of the molecule given by

$$SR_{Molecule} = [(SR \text{ of } \mathbf{C})^{n1} \times (SR \text{ of } \mathbf{H})^{n2} \times (SR \text{ of } \mathbf{N})^{n3} \times (SR \text{ of } \mathbf{O})^{n4}]^{1/(n1+n2+n3+n4)}$$

Where C,H,N and O represent the atoms involved in the formation of a molecule and n1,n2,n3 and n4 represent Their respective numbers in a molecule.

SR of C = $2.47^{R1}$; SR of H = $2.31^{R1}$;
SR of N = $2.93^{R1}$; SR of O = $3.46^{R1}$;

R1= J.E. Huheey, *Inorganic Chemistry, Principle, Structure and Reactivity,* III Edn., Harper International Education, Cambridge, 1983, p 146.

AM3 PM1
INPUT FORMATS
and Outputs
for some Representative
cases
MOPAC7 Programmes

APPENDIX 4

Input format for MOPAC7.BIG Ligand = Pyrazinamide

AM1 precise gnorm=0.01 vector

pyrazinamide

Jittu

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| N | 0.000000 | 0 | 0.000000 | 0 | 0.000000 | 0 | 0 | 0 | 0 |
| C | 2.417287 | 1 | 0.000000 | 0 | 0.000000 | 0 | 1 | 0 | 0 |
| N | 1.275114 | 1 | 90.325401 | 1 | 0.000000 | 0 | 2 | 1 | 0 |
| C | 1.280527 | 1 | 121.188522 | 1 | 1.336034 | 1 | 3 | 2 | 1 |
| C | 1.347439 | 1 | 122.619881 | 1 | -2.550982 | 1 | 4 | 3 | 2 |
| C | 1.502987 | 1 | 116.992798 | 1 | -180.000000 | 1 | 4 | 3 | 2 |
| N | 1.361150 | 1 | 163.426422 | 1 | -119.448753 | 1 | 6 | 4 | 3 |
| C | 1.360042 | 1 | 33.182922 | 1 | -179.387070 | 1 | 1 | 2 | 3 |
| H | 0.970400 | 1 | 154.385178 | 1 | 179.445740 | 1 | 1 | 2 | 3 |
| H | 1.103494 | 1 | 119.482712 | 1 | 179.340317 | 1 | 2 | 3 | 1 |
| H | 1.103624 | 1 | 120.803024 | 1 | -177.945190 | 1 | 5 | 4 | 3 |
| O | 1.260919 | 1 | 84.127907 | 1 | -114.815346 | 1 | 6 | 4 | 3 |
| H | 0.959518 | 1 | 118.638565 | 1 | -178.443542 | 1 | 7 | 6 | 4 |
| H | 0.963183 | 1 | 124.808350 | 1 | 2.763430 | 1 | 7 | 6 | 4 |
| H | 1.100935 | 1 | 121.161736 | 1 | -179.537750 | 1 | 8 | 1 | 2 |

APPENDIX 4C

Input format for MOPAC7.BIG Ligand = Lycine

lys01
Lycine
Jittu

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| H | 0.000000 | 0 | 0.000000 | 0 | 0.000000 | 0 | 0 | 0 | 0 |
| N | 1.015391 | 1 | 0.000000 | 0 | 0.000000 | 0 | 1 | 0 | 0 |
| C | 1.448717 | 1 | 111.201424 | 1 | 0.000000 | 0 | 2 | 1 | 0 |
| C | 1.520504 | 1 | 110.131256 | 1 | 64.764427 | 1 | 3 | 2 | 1 |
| C | 1.539529 | 1 | 109.485428 | 1 | -60.563427 | 1 | 3 | 2 | 1 |
| O | 1.339809 | 1 | 111.108559 | 1 | 77.673172 | 1 | 4 | 3 | 2 |
| C | 1.538049 | 1 | 113.091454 | 1 | -172.873520 | 1 | 5 | 3 | 2 |
| C | 1.537306 | 1 | 111.876709 | 1 | 178.334229 | 1 | 7 | 5 | 3 |
| C | 1.535666 | 1 | 111.854225 | 1 | 179.639008 | 1 | 8 | 7 | 5 |
| N | 1.445118 | 1 | 111.070526 | 1 | 179.392838 | 1 | 9 | 8 | 7 |
| H | 1.015536 | 1 | 111.117027 | 1 | -117.508965 | 1 | 2 | 3 | 1 |
| H | 1.100000 | 1 | 107.301682 | 1 | -178.813538 | 1 | 3 | 2 | 1 |
| O | 1.208672 | 1 | 127.079567 | 1 | -101.873886 | 1 | 4 | 3 | 2 |
| H | 1.110107 | 1 | 109.631378 | 1 | -50.258041 | 1 | 5 | 3 | 2 |
| H | 1.110107 | 1 | 109.631386 | 1 | 64.511032 | 1 | 5 | 3 | 2 |
| H | 1.110107 | 1 | 109.946510 | 1 | 55.896511 | 1 | 7 | 5 | 3 |
| H | 1.110107 | 1 | 109.946518 | 1 | -59.228184 | 1 | 7 | 5 | 3 |
| H | 1.110107 | 1 | 109.965797 | 1 | -57.934536 | 1 | 8 | 7 | 5 |
| H | 1.110108 | 1 | 109.965813 | 1 | 57.212200 | 1 | 8 | 7 | 5 |
| H | 1.110107 | 1 | 111.491150 | 1 | 57.891434 | 1 | 9 | 8 | 7 |
| H | 1.110108 | 1 | 111.491158 | 1 | -59.105518 | 1 | 9 | 8 | 7 |
| H | 1.015000 | 1 | 110.961998 | 1 | -176.385941 | 1 | 10 | 9 | 8 |
| H | 1.014913 | 1 | 111.047852 | 1 | -59.211697 | 1 | 10 | 9 | 8 |
| H | 0.971471 | 1 | 118.155312 | 1 | 179.210678 | 1 | 6 | 4 | 3 |

PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
SCF FIELD WAS ACHIEVED
Lycine

PM3 CALCULATION

VERSION 7.00
Thu Aug 10 08:35:31 2000

FINAL HEAT OF FORMATION = -108.94085 KCAL

TOTAL ENERGY = -1840.09988 EV
ELECTRONIC ENERGY = -9284.73778 EV
CORE-CORE REPULSION = 7444.63790 EV

IONIZATION POTENTIAL = 9.47326
NO. OF FILLED LEVELS = 30
MOLECULAR WEIGHT = 146.189

SCF CALCULATIONS = 79
COMPUTATION TIME = 24.940 SECONDS

| ATOM NUMBER (I) | CHEMICAL SYMBOL | BOND LENGTH (ANGSTROMS) NA:I | | BOND ANGLE (DEGREES) NB:NA:I | | TWIST ANGLE (DEGREES) NC:NB:NA:I | | NA | NB | NC |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | H | | | | | | | | | |
| 2 | N | .99844 | * | | | | | 1 | | |
| 3 | C | 1.48248 | * | 110.36686 | * | | | 2 | 1 | |
| 4 | C | 1.52728 | * | 112.02435 | * | 66.28002 | * | 3 | 2 | 1 |
| 5 | C | 1.53512 | * | 109.90585 | * | -56.05885 | * | 3 | 2 | 1 |
| 6 | O | 1.35129 | * | 115.72012 | * | 140.98844 | * | 4 | 3 | 2 |
| 7 | C | 1.52066 | * | 111.96670 | * | -161.26792 | * | 5 | 3 | 2 |
| 8 | C | 1.52077 | * | 110.96612 | * | -179.96564 | * | 7 | 5 | 3 |
| 9 | C | 1.52480 | * | 110.67595 | * | -179.73847 | * | 8 | 7 | 5 |
| 10 | N | 1.47946 | * | 110.76343 | * | -176.96992 | * | 9 | 8 | 7 |
| 11 | H | .99744 | * | 109.82349 | * | -120.97463 | * | 2 | 3 | 1 |
| 12 | H | 1.11973 | * | 106.19999 | * | -174.33633 | * | 3 | 2 | 1 |
| 13 | O | 1.21840 | * | 128.49619 | * | -37.91805 | * | 4 | 3 | 2 |
| 14 | H | 1.10994 | * | 109.34668 | * | -40.07596 | * | 5 | 3 | 2 |
| 15 | H | 1.10940 | * | 110.40081 | * | 75.64233 | * | 5 | 3 | 2 |
| 16 | H | 1.10910 | * | 110.02568 | * | 58.01188 | * | 7 | 5 | 3 |
| 17 | H | 1.10894 | * | 110.21802 | * | -57.95455 | * | 7 | 5 | 3 |
| 18 | H | 1.10947 | * | 109.78375 | * | -57.57253 | * | 8 | 7 | 5 |
| 19 | H | 1.10886 | * | 109.91091 | * | 58.12087 | * | 8 | 7 | 5 |
| 20 | H | 1.11250 | * | 109.71123 | * | 57.83921 | * | 9 | 8 | 7 |
| 21 | H | 1.10881 | * | 110.17473 | * | -58.50112 | * | 9 | 8 | 7 |
| 22 | H | .99800 | * | 109.24302 | * | -177.83832 | * | 10 | 9 | 8 |
| 23 | H | .99888 | * | 109.80198 | * | -58.30536 | * | 10 | 9 | 8 |
| 24 | H | .95253 | * | 110.12785 | * | 179.14625 | * | 6 | 4 | 3 |

## NET ATOMIC CHARGES AND DIPOLE CONTRIBUTIONS

| ATOM NO. | TYPE | CHARGE | ATOM ELECTRON DENSITY |
|---|---|---|---|
| 1 | H | .0413 | .9587 |
| 2 | N | -.0242 | 5.0242 |
| 3 | C | -.0727 | 4.0727 |
| 4 | C | .3435 | 3.6565 |
| 5 | C | -.1018 | 4.1018 |
| 6 | O | -.2991 | 6.2991 |
| 7 | C | -.1060 | 4.1060 |
| 8 | C | -.1030 | 4.1030 |
| 9 | C | -.1025 | 4.1025 |
| 10 | N | -.0347 | 5.0347 |
| 11 | H | .0342 | .9658 |
| 12 | H | .0964 | .9036 |
| 13 | O | -.3960 | 6.3960 |
| 14 | H | .0735 | .9265 |
| 15 | H | .0640 | .9360 |
| 16 | H | .0546 | .9454 |
| 17 | H | .0589 | .9411 |
| 18 | H | .0505 | .9495 |
| 19 | H | .0655 | .9345 |
| 20 | H | .0273 | .9727 |
| 21 | H | .0560 | .9440 |
| 22 | H | .0246 | .9754 |
| 23 | H | .0226 | .9774 |
| 24 | H | .2268 | .7732 |

| DIPOLE | X | Y | Z | TOTAL |
|---|---|---|---|---|
| POINT-CHG. | 1.382 | -.238 | -1.767 | 2.255 |
| HYBRID | .689 | .403 | 1.218 | 1.456 |
| SUM | 2.071 | .165 | -.549 | 2.148 |

## CARTESIAN COORDINATES

| NO. | ATOM | X | Y | Z |
|---|---|---|---|---|
| 1 | H | .0000 | .0000 | .0000 |
| 2 | N | .9984 | .0000 | .0000 |
| 3 | C | 1.5144 | 1.3898 | .0000 |
| 4 | C | 1.1798 | 2.1249 | 1.2962 |
| 5 | C | .9408 | 2.1603 | -1.1975 |
| 6 | O | 2.1480 | 2.9355 | 1.7774 |
| 7 | C | 1.7555 | 3.4039 | -1.5168 |
| 8 | C | 1.1675 | 4.1495 | -2.7047 |
| 9 | C | 1.9930 | 5.3913 | -3.0231 |
| 10 | N | 1.3821 | 6.1572 | -4.1318 |
| 11 | H | 1.3335 | -.4852 | .8045 |
| 12 | H | 2.6262 | 1.3103 | -.1061 |
| 13 | O | .1616 | 2.0624 | 1.9624 |
| 14 | H | .9227 | 1.4968 | -2.0871 |
| 15 | H | -.1175 | 2.4350 | -1.0095 |
| 16 | H | 2.8082 | 3.1248 | -1.7265 |
| 17 | H | 1.7962 | 4.0728 | -.6332 |
| 18 | H | 1.1238 | 3.4769 | -3.5860 |
| 19 | H | .1160 | 4.4296 | -2.4918 |
| 20 | H | 3.0463 | 5.0989 | -3.2299 |
| 21 | H | 2.0295 | 6.0627 | -2.1414 |
| 22 | H | 1.9579 | 6.9441 | -4.3444 |
| 23 | H | 1.3086 | 5.5785 | -4.9426 |
| 24 | H | | | |

**********060BY060

AM1 PRECISE GNORM=0.01
histidine
Jittu

| ATOM NUMBER (I) | CHEMICAL SYMBOL | BOND LENGTH (ANGSTROMS) NA:I | | BOND ANGLE (DEGREES) NB:NA:I | | TWIST ANGLE (DEGREES) NC:NB:NA:I | | NA | NB | NC |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | H | | | | | | | | | |
| 2 | N | 1.01599 | * | | | | | 1 | | |
| 3 | C | 1.44940 | * | 111.06342 | * | | | 2 | 1 | |
| 4 | C | 1.52013 | * | 110.61758 | * | -56.51305 | * | 3 | 2 | 1 |
| 5 | C | 1.53707 | * | 109.43315 | * | 178.71078 | * | 3 | 2 | 1 |
| 6 | O | 1.33954 | * | 110.79525 | * | 59.49612 | * | 4 | 3 | 2 |
| 7 | C | 1.49750 | * | 112.05994 | * | -173.96808 | * | 5 | 3 | 2 |
| 8 | C | 1.37432 | * | 130.41830 | * | 74.95516 | * | 7 | 5 | 3 |
| 9 | N | 1.39671 | * | 124.05028 | * | -105.52394 | * | 7 | 5 | 3 |
| 10 | N | 1.31972 | * | 109.06762 | * | 179.79253 | * | 8 | 7 | 5 |
| 11 | C | 1.39216 | * | 106.43097 | * | -179.86583 | * | 9 | 7 | 5 |
| 12 | H | 1.01526 | * | 111.47597 | * | 117.52164 | * | 2 | 3 | 1 |
| 13 | H | 1.11756 | * | 107.87356 | * | 60.43337 | * | 3 | 2 | 1 |
| 14 | O | 1.20887 | * | 127.13621 | * | -120.07666 | * | 4 | 3 | 2 |
| 15 | H | 1.11474 | * | 110.25812 | * | 63.59162 | * | 5 | 3 | 2 |
| 16 | H | 1.11558 | * | 109.96688 | * | -54.13857 | * | 5 | 3 | 2 |
| 17 | H | 1.09872 | * | 127.06572 | * | -.24228 | * | 8 | 7 | 5 |
| 18 | H | .95797 | * | 126.77873 | * | 1.00522 | * | 9 | 7 | 5 |
| 19 | H | 1.09841 | * | 127.66361 | * | -179.65114 | * | 11 | 9 | 7 |
| 20 | H | .97163 | * | 118.29936 | * | 178.82330 | * | 6 | 4 | 3 |

CARTESIAN COORDINATES

| NO. | ATOM | X | Y | Z |
|---|---|---|---|---|
| 1 | H | .0000 | .0000 | .0000 |
| 2 | N | 1.0160 | .0000 | .0000 |
| 3 | C | 1.5369 | 1.3526 | .0000 |
| 4 | C | .9967 | 2.1342 | -1.1866 |
| 5 | C | 3.0730 | 1.3090 | .0326 |
| 6 | O | -.3411 | 2.1914 | -1.1492 |
| 7 | C | 3.6714 | 2.6738 | .1800 |
| 8 | C | 3.7544 | 3.4965 | 1.2777 |
| 9 | N | 4.2944 | 3.3708 | -.8577 |
| 10 | N | 4.3749 | 4.6100 | .9360 |
| 11 | C | 4.7142 | 4.5845 | -.3204 |
| 12 | H | 1.2898 | -.5038 | -.8379 |
| 13 | H | 1.1704 | 1.8613 | .9251 |
| 14 | O | 1.6365 | 2.6476 | -2.0746 |
| 15 | H | 3.4652 | .8255 | -.8921 |
| 16 | H | 3.4184 | .6910 | .8948 |
| 17 | H | 3.3762 | 3.2919 | 2.2888 |
| 18 | H | 4.3996 | 3.0774 | -1.7636 |
| 19 | H | 5.2390 | 5.4007 | -.8352 |
| 20 | H | -.8009 | 2.6824 | -1.8502 |

Histidine

NET ATOMIC CHARGES AND DIPOLE CONTRIBUTIONS

| ATOM NO. | TYPE | CHARGE | ATOM ELECTRON DENSITY |
|---|---|---|---|
| 1 | H | .1705 | .8295 |
| 2 | N | -.3265 | 5.3265 |
| 3 | C | -.0084 | 4.0084 |
| 4 | C | .2642 | 3.7358 |
| 5 | C | -.0817 | 4.0817 |
| 6 | O | -.3230 | 6.3230 |
| 7 | C | -.1453 | 4.1453 |
| 8 | C | -.1580 | 4.1580 |
| 9 | N | -.1879 | 5.1879 |
| 10 | N | -.1472 | 5.1472 |
| 11 | C | -.1004 | 4.1004 |
| 12 | H | .1544 | .8456 |
| 13 | H | .1448 | .8552 |
| 14 | O | -.3846 | 6.3846 |
| 15 | H | .0998 | .9002 |
| 16 | H | .1277 | .8723 |
| 17 | H | .1787 | .8213 |
| 18 | H | .2750 | .7250 |
| 19 | H | .1978 | .8022 |
| 20 | H | .2500 | .7500 |

| DIPOLE | X | Y | Z | TOTAL |
|---|---|---|---|---|
| POINT-CHG. | -1.208 | -1.534 | -.686 | 2.070 |
| HYBRID | -1.391 | .689 | -2.649 | 3.071 |
| SUM | -2.599 | -.845 | -3.335 | 4.312 |

CARTESIAN COORDINATES

| NO. | ATOM | X | Y | Z |
|---|---|---|---|---|
| 1 | H | .0000 | .0000 | .0000 |
| 2 | N | 1.0013 | .0000 | .0000 |
| 3 | C | 1.5143 | 1.3477 | .0000 |
| 4 | C | .9994 | 2.2474 | -1.1238 |
| 5 | C | 3.0592 | 1.3824 | -.0075 |
| 6 | O | -.2069 | 1.8858 | -1.6423 |
| 7 | C | 3.5878 | 2.5204 | .7644 |
| 8 | C | 4.2535 | 2.5208 | 2.0124 |
| 9 | N | 3.5485 | 3.8582 | .3538 |
| 10 | N | 4.6104 | 3.8163 | 2.3632 |
| 11 | C | 4.1738 | 4.6047 | 1.3517 |
| 12 | H | 1.3368 | -.5208 | -.7852 |
| 13 | H | 1.1459 | 1.8409 | .9540 |
| 14 | O | 1.5088 | 3.2659 | -1.6045 |
| 15 | H | 3.4245 | 1.4210 | -1.0688 |
| 16 | H | 3.4572 | .4398 | .4601 |
| 17 | H | 4.4838 | 1.6683 | 2.6497 |
| 18 | H | 3.1245 | 4.1883 | -.4782 |
| 19 | H | 4.2865 | 5.6920 | 1.2957 |
| 20 | H | -.4761 | 2.5191 | -2.3290 |

| ATOM NUMBER (I) | CHEMICAL SYMBOL | BOND LENGTH (ANGSTROMS) NA:I | | BOND ANGLE (DEGREES) NB:NA:I | | TWIST ANGLE (DEGREES) NC:NB:NA:I | | NA | NB | NC |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | H | | | | | | | | | |
| 2 | N | 1.00132 | * | | | | | 1 | | |
| 3 | C | 1.44202 | * | 110.83987 | * | | | 2 | 1 | |
| 4 | C | 1.52890 | * | 115.47892 | * | -54.50790 | * | 3 | 2 | 1 |
| 5 | C | 1.54526 | * | 112.12775 | * | -179.69794 | * | 3 | 2 | 1 |
| 6 | O | 1.36192 | * | 114.95584 | * | 24.50127 | * | 4 | 3 | 2 |
| 7 | C | 1.47322 | * | 111.93284 | * | -145.58368 | * | 5 | 3 | 2 |
| 8 | C | 1.41449 | * | 129.15135 | * | 108.67875 | * | 7 | 5 | 3 |
| 9 | N | 1.39995 | * | 125.05754 | * | -73.18172 | * | 7 | 5 | 3 |
| 10 | N | 1.38885 | * | 110.12231 | * | 178.57930 | * | 8 | 7 | 5 |
| 11 | C | 1.39435 | * | 106.80207 | * | -178.77402 | * | 9 | 7 | 5 |
| 12 | H | 1.00021 | * | 111.55267 | * | 122.42442 | * | 2 | 3 | 1 |
| 13 | H | 1.13535 | * | 106.89195 | * | 61.41680 | * | 3 | 2 | 1 |
| 14 | O | 1.23612 | * | 129.19550 | * | -157.16763 | * | 4 | 3 | 2 |
| 15 | H | 1.12298 | * | 109.30439 | * | 91.52825 | * | 5 | 3 | 2 |
| 16 | H | 1.12501 | * | 109.43848 | * | -26.37898 | * | 5 | 3 | 2 |
| 17 | H | 1.08897 | * | 128.00529 | * | -1.29505 | * | 8 | 7 | 5 |
| 18 | H | .99034 | * | 125.23448 | * | 3.02343 | * | 9 | 7 | 5 |
| 19 | H | 1.09459 | * | 122.77410 | * | -179.90161 | * | 11 | 9 | 7 |
| 20 | H | .97209 | * | 109.95519 | * | 178.29813 | * | 6 | 4 | 3 |

VERSION 7.00
Thu Aug 10 09:00:11 2000

FINAL HEAT OF FORMATION = -51.83804 KCAL

TOTAL ENERGY = -2153.79412 EV
ELECTRONIC ENERGY = -10084.71691 EV
CORE-CORE REPULSION = 7930.92279 EV

IONIZATION POTENTIAL = 8.97801
NO. OF FILLED LEVELS = 30
MOLECULAR WEIGHT = 155.156

SCF CALCULATIONS = 139
COMPUTATION TIME = 42.350 SECONDS