Table 1. Monopole Populations, Radial Parameters and Net Atomic Charges.

| Atom | Pval | Kappa | P00 | Kappa' | Net charge |
|---|---|---|---|---|---|
| FE(1) | 5.865 | 0.994 | 0.000 | 0.979 | +0.13520 |
| NA(1) | 0.400 | 1.000 | 0.000 | 0.879 | +0.60000 |
| NA(2) | 0.400 | 1.000 | 0.000 | 0.879 | +0.60000 |
| O(1) | 6.004 | 1.002 | 0.000 | 0.934 | -0.00380 |
| O(1W) | 6.049 | 0.997 | 0.000 | 0.864 | -0.04910 |
| N(1) | 5.135 | 0.998 | 0.000 | 0.962 | -0.13480 |
| N(2) | 5.173 | 0.997 | 0.000 | 0.926 | -0.17340 |
| N(3) | 5.166 | 0.997 | 0.000 | 0.950 | -0.16620 |
| N(4) | 5.155 | 0.997 | 0.000 | 0.950 | -0.15540 |
| C(1) | 4.197 | 1.003 | 0.000 | 0.967 | -0.19740 |
| C(2) | 4.116 | 1.000 | 0.000 | 0.981 | -0.11640 |
| C(3) | 4.140 | 1.000 | 0.000 | 0.981 | -0.13970 |
| H(1WB) | 0.856 | 1.200 | 0.000 | 1.200 | +0.14430 |
| H(1WA) | 0.930 | 1.200 | 0.000 | 1.200 | +0.06970 |

Table 2. Dipole Population Parameters.

| Atom | D11+ | D11- | D10 | Kappa' |
|---|---|---|---|---|
| FE(1) | -0.001(5) | 0.010(5) | 0.000 | 0.979 |
| NA(1) | 0.000 | 0.000 | -0.212(84) | 0.879 |
| NA(2) | 0.000 | 0.000 | 0.277(60) | 0.879 |
| O(1) | -0.036(9) | -0.006(9) | 0.000 | 0.934 |
| O(1W) | -0.065(6) | -0.064(7) | -0.049(7) | 0.864 |
| N(1) | -0.107(10) | -0.002(9) | 0.000 | 0.962 |
| N(2) | 0.032(11) | -0.022(12) | 0.000 | 0.926 |
| N(3) | 0.002(8) | -0.005(8) | 0.023(7) | 0.950 |
| N(4) | 0.018(8) | 0.001(8) | 0.034(7) | 0.950 |
| C(1) | 0.017(13) | 0.019(13) | 0.000 | 0.967 |
| C(2) | -0.014(8) | -0.002(8) | 0.029(9) | 0.981 |
| C(3) | -0.015(9) | -0.005(8) | 0.031(9) | 0.981 |
| H(1WB) | 0.000 | 0.000 | 0.253(11) | 1.200 |
| H(1WA) | 0.000 | 0.000 | 0.291(13) | 1.200 |

Table 3. Quadrupole Population Parameters.

| Atom | Q20 | Q21+ | Q21- | Q22+ | Q22- | Kappa' |
|---|---|---|---|---|---|---|
| FE(1) | 0.025(6) | 0.000 | 0.000 | -0.088(6) | 0.010(6) | 0.979 |
| NA(1) | -0.064(64) | 0.000 | 0.000 | -0.112(58) | -0.113(60) | 0.879 |
| NA(2) | -0.109(70) | 0.000 | 0.000 | 0.155(62) | 0.335(62) | 0.879 |
| O(1) | -0.030(11) | 0.000 | 0.000 | 0.040(10) | -0.012(10) | 0.934 |
| O(1W) | -0.071(7) | -0.009(7) | 0.053(7) | 0.068(7) | -0.018(7) | 0.864 |
| N(1) | -0.137(10) | 0.000 | 0.000 | 0.220(9) | 0.050(10) | 0.962 |
| N(2) | -0.114(11) | 0.000 | 0.000 | 0.189(11) | 0.003(12) | 0.926 |
| N(3) | 0.226(8) | -0.009(8) | 0.010(8) | 0.013(8) | 0.006(8) | 0.950 |
| N(4) | 0.219(8) | -0.005(8) | -0.017(8) | -0.004(8) | 0.004(8) | 0.950 |
| C(1) | -0.170(12) | 0.000 | 0.000 | 0.268(13) | -0.033(13) | 0.967 |
| C(2) | 0.303(9) | 0.001(9) | -0.017(9) | -0.003(8) | 0.022(8) | 0.981 |
| C(3) | 0.321(9) | -0.006(9) | 0.013(9) | -0.007(8) | 0.014(8) | 0.981 |
| H(1WB) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 1.200 |
| H(1WA) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 1.200 |

Table 4. Octupole Population Parameters.

| Atom | O30 | O31+ | O31- | O32+ | O32- | O33+ | O33- | Kappa' |
|---|---|---|---|---|---|---|---|---|
| FE(1) | 0.000 | 0.000(8) | -0.001(7) | 0.000 | 0.000 | 0.011(7) | 0.007(8) | 0.979 |
| NA(1) | -0.019(73) | 0.000 | 0.000 | -0.173(64) | -0.012(62) | 0.000 | 0.000 | 0.879 |
| NA(2) | 0.154(61) | 0.000 | 0.000 | -0.056(59) | 0.070(59) | 0.000 | 0.000 | 0.879 |
| O(1) | 0.000 | 0.012(13) | -0.004(14) | 0.000 | 0.000 | -0.006(12) | -0.021(13) | 0.934 |
| O(1W) | 0.050(10) | -0.006(9) | -0.029(9) | 0.035(9) | 0.024(9) | 0.024(9) | -0.030(9) | 0.864 |
| N(1) | 0.000 | -0.086(13) | 0.001(12) | 0.000 | 0.000 | 0.078(12) | 0.008(13) | 0.962 |
| N(2) | 0.000 | -0.032(14) | -0.009(14) | 0.000 | 0.000 | 0.043(14) | 0.004(15) | 0.926 |
| N(3) | 0.065(10) | -0.021(11) | 0.009(11) | -0.011(10) | -0.002(10) | -0.003(10) | 0.012(10) | 0.950 |
| N(4) | 0.078(10) | -0.021(11) | -0.001(10) | 0.004(10) | -0.012(10) | 0.014(10) | 0.011(10) | 0.950 |
| C(1) | 0.000 | 0.032(16) | -0.001(15) | 0.000 | 0.000 | -0.033(15) | 0.021(17) | 0.967 |
| C(2) | -0.039(11) | -0.011(12) | -0.031(12) | -0.003(11) | 0.006(11) | 0.004(10) | -0.001(10) | 0.981 |
| C(3) | -0.051(12) | -0.018(12) | 0.004(12) | -0.003(11) | -0.011(11) | 0.016(10) | -0.014(10) | 0.981 |
| H(1WB) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 1.200 |
| H(1WA) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 1.200 |

Table 5. Hexadecapole Population Parameters.

| Atom | H40 | H41+ | H41- | H42+ | H42- | H43+ | H43- | H44+ | H44- | Kappa' |
|---|---|---|---|---|---|---|---|---|---|---|
| FE(1) | 0.086(9) | 0.000 | 0.000 | 0.307(12) | -0.070(9) | 0.000 | 0.000 | -0.159(10) | -0.085(10) | 0.979 |
| NA(1) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.879 |
| NA(2) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.879 |
| O(1) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.934 |
| O(1W) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.864 |
| N(1) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.962 |
| N(2) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.926 |
| N(3) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.950 |
| N(4) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.950 |
| C(1) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.967 |
| C(2) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.981 |
| C(3) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.981 |
| H(1WB) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 1.200 |
| H(1WA) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 1.200 |

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FE(1)       N(1)        X           FE(1)       DUM0        Y
NA(1)       DUM2        Z           NA(1)       N(2)        Y
NA(2)       DUM1        Z           NA(2)       H(1WA)      Y
O(1)        N(1)        X           O(1)        DUM0        Y
O(1W)       H(1WB)      Z           O(1W)       H(1WA)      Y
N(1)        O(1)        X           N(1)        DUM0        Y
N(2)        C(1)        X           N(2)        DUM0        Y
N(3)        C(2)        Z           N(3)        H(1WB)      Y
N(4)        C(3)        Z           N(4)        C(2)        Y
C(1)        N(2)        X           C(1)        DUM0        Y
C(2)        N(3)        Z           C(2)        C(3)        Y
C(3)        N(4)        Z           C(3)        C(2)        Y
H(1WB)      O(1W)       Z           H(1WB)      H(1WA)      Y
H(1WA)      O(1W)       Z           H(1WA)      H(1WB)      Y
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_atom_site_U_iso_or_equiv
FE(1)  -0.000514       0.780223       0.5            1    4    0.006
NA(1)   0.5            0.5            0.378004       1    4    0.012
NA(2)   0              0.5            0.24584        1    4    0.011
O(1)   -0.386145       0.905413       0.5            1    4    0.019
O(1W)   0.328268       0.622571       0.268678       1    8    0.016
N(1)   -0.226464       0.858044       0.5            1    4    0.009
N(2)    0.400366       0.623611       0.5            1    4    0.015
N(3)    0.250246       0.905396       0.355696       1    8    0.017
N(4)   -0.167061       0.619541       0.641946       1    8    0.015
C(1)    0.249771       0.682792       0.5            1    4    0.010
C(2)    0.154339       0.861798       0.410993       1    8    0.010
C(3)   -0.107172       0.679628       0.587871       1    8    0.010
H(1WB)  0.316899       0.701047       0.288081       1    8    0.038
H(1WA)  0.446693       0.623447       0.226425       1    8    0.053
DUM0    0.15445        0.86185        0.5            0    1    0
DUM1    0              0.5            0.26871        0    1    0
DUM2    0.5            0.5            0.26871        0    1    0
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_atom_site_aniso_U_23
FE(1) 0.00612 0.006687 0.005824 0.000229 0 0
NA(1) 0.011695 0.014053 0.011733 -0.000712 0 0
NA(2) 0.01095 0.012339 0.008954 0.002171 0 0
O(1) 0.011036 0.017258 0.02943 0.007061 0 0
O(1W) 0.015728 0.016723 0.016696 -0.001508 0.001895 0.002321
N(1) 0.007791 0.008745 0.011619 0.001909 0 0
N(2) 0.01224 0.01496 0.017194 0.006433 0 0
N(3) 0.015876 0.022325 0.01153 -0.004547 0.002296 0.00575
N(4) 0.014737 0.016543 0.012969 -0.002246 0.000708 0.006839
C(1) 0.009278 0.010476 0.01023 0.002729 0 0
C(2) 0.010118 0.012384 0.008208 -0.001341 0.000684 0.002075
C(3) 0.009898 0.010968 0.009041 -0.000946 0.000314 0.002474
```

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Differences of Mean-Squares Displacement Amplitudes (DMSDA)
(1.E4 A**2) along interatomic vectors (*bonds)

| ATOM--> | ATOM | / | DIST | DMSDA | ATOM | / | DIST | DMSDA | ATOM | / | DIST | DMSDA |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Fe(1) | N(1) | * | 1.6659 | 2 | C(1) | * | 1.9222 | 10 | C(2) | * | 1.9372 | 9 |
| | C(3) | * | 1.9276 | 9 | | | | | | | | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Na(1) | O(1W) | | 2.4718 | 36 | N(2) | 2.4731 | 15 |
| Na(2) | O(1W) | | 2.5097 | 21 | | | |
| O(1) | N(1) | * | 1.1298 | -1 | | | |
| N(1) | C(3) | | 2.6213 | 2 | | | |
| N(2) | C(1) | * | 1.1606 | 0 | | | |
| N(3) | C(2) | * | 1.1630 | -2 | | | |
| N(4) | C(3) | * | 1.1614 | -1 | | | |
| C(1) | C(2) | | 2.5993 | 6 | C(3) | 2.5830 | -3 |

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data_FFT
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_refine_diff_density_rms     0.041
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