Supplementary Material

Reply to "Comment on the paper 'On the calculation of the electrostatic potential, electric field and electric field gradient from the aspherical pseudoatom model', by Volkov, King, Coppens & Farrugia (2006)"

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Appendix A. Example of the XD2006 output of the ESP, EF and EFG at the nuclear positions (formamide, XD/PBE/6-31G** results).

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**************   ELECTROSTATIC PROPERTIES AT NUCLEAR POSITIONS   **************
**************                                                 **************
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Properties are in Atomic Units

   N  Atom        Potential     ------- Electric Field --------
                                   X          Y          Z

   1  O(1)        -22.41900     -0.27373   -0.17436    0.00360
   2  N(2)        -18.43584     -0.01908   -0.00865   -0.00031
   3  C(3)        -14.75993     -0.02568    0.00089   -0.00026
   4  H(4)         -1.00282      0.01296   -0.01044    0.00030
   5  H(5)         -1.02124      0.00096    0.01001   -0.00030
   6  H(6)         -1.08932      0.00285    0.02227   -0.00683

   N  Atom         ---------------- Electric Field Gradient Tensor ----------------
                      XX         XY         XZ         YY         YZ         ZZ

   1  O(1)       -1306.0221    -0.8057    -0.0258 -1305.0039     0.0474 -1306.4946
   2  N(2)        -863.4997    -0.0145    -0.0121  -863.5377    -0.0128  -862.6722
   3  C(3)        -534.2442     0.0477    -0.0020  -534.2304    -0.0118  -534.7550
   4  H(4)          -2.2857    -0.2958    -0.0124    -2.0905    -0.0092    -1.8194
   5  H(5)          -1.8692     0.0488    -0.0010    -2.4603     0.0017    -1.8163
   6  H(6)          -2.0037     0.0065    -0.0013    -2.4506    -0.0028    -1.9861

   N  Atom         ------- EFG Eigenvalues -------

   1  O(1)       -1306.4961 -1306.4661 -1304.5584
   2  N(2)        -863.5430  -863.4949  -862.6719
   3  C(3)        -534.7553  -534.2855  -534.1889
   4  H(4)          -2.4999    -1.8767    -1.8190
   5  H(5)          -2.4643    -1.8652    -1.8163
   6  H(6)          -2.4507    -2.0037    -1.9860

   N  Atom         ----------- Traceless Electric Field Gradient Tensor -----------
                      XX         XY         XZ         YY         YZ         ZZ

   1  O(1)          -0.2729    -1.2086    -0.0387     1.2545     0.0711    -0.9816
   2  N(2)          -0.3947    -0.0218    -0.0182    -0.4518    -0.0191     0.8465
   3  C(3)           0.2485     0.0716    -0.0030     0.2692    -0.0178    -0.5177
   4  H(4)          -0.3308    -0.4436    -0.0187    -0.0380    -0.0139     0.3687
   5  H(5)           0.2690     0.0732    -0.0014    -0.6175     0.0025     0.3485
   6  H(6)           0.2146     0.0097    -0.0020    -0.4557    -0.0041     0.2411

   N  Atom         -- Traceless EFG Eigenvalues --

   1  O(1)          -0.9838    -0.9389     1.9227
   2  N(2)          -0.4596    -0.3875     0.8471
   3  C(3)          -0.5181     0.1866     0.3315
   4  H(4)          -0.6521     0.2828     0.3693
   5  H(5)          -0.6235     0.2750     0.3485
   6  H(6)          -0.4559     0.2146     0.2413
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