Wavefunctions Derived from Experiment. III. Topological Analysis of Crystal Fragments: Supplementary Material

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1. Refinement of XD(low): Low Angle Data Set $\sin\theta/\lambda \leq 0.71$

Table 1. *Monopole and Dipole Populations*

atom	P_v	P_{11}	P_{1-1}	P_{10}
O(1)	5.90(8)	-0.06(2)	-0.10(2)	–
O(2)	6.15(6)	-0.09(2)	-0.01(1)	–
O(3)	5.91(9)	-0.12(3)	0.01(1)	–
C(1)	4.29(9)	0.06(3)	0.01(2)	–
H(1)	0.94(5)	–	–	0.17(5)
H(2)	0.91(4)	–	–	0.15(3)
H(3)	0.91(0)	–	–	0.15(0)

Table 2. *Quadrupole Populations*

atom	P_{20}	P_{22}	P_{2-2}
O(1)	0.01(1)	-0.05(1)	0.05(1)
O(2)	-0.08(1)	-0.03(2)	0.01(1)
O(3)	-0.05(1)	-0.06(1)	-0.01(1)
C(1)	-0.23(3)	0.09(2)	-0.04(2)
H(1)	0.16(5)	–	–
H(2)	0.12(3)	–	–
H(3)	0.12(0)	–	–

Table 3. *Octupole Populations*

atom	P_{31}	P_{3-1}	P_{33}	P_{3-3}
O(1)	-0.01(2)	-0.05(1)	0.10(2)	0.00(2)
O(2)	-0.02(2)	-0.01(1)	0.04(2)	0.00(2)
O(3)	0.10(2)	0.01(1)	0.00(1)	-0.05(1)
C(1)	0.00(2)	-0.06(2)	0.32(4)	0.09(3)

Table 4. *Hexadecapole Populations*

atom	P_{40}	P_{42}	P_{4-2}	P_{44}	P_{4-4}
O(1)	0.04(2)	0.06(2)	0.05(2)	0.00(2)	0.07(2)
O(2)	0.00(2)	0.02(2)	-0.02(2)	0.04(2)	0.02(2)
O(3)	-0.01(2)	0.03(2)	0.02(2)	-0.01(2)	-0.01(2)
C(1)	0.04(3)	0.09(3)	0.03(2)	-0.05(4)	-0.01(3)

2. Refinement of XD(low,re): Low Angle, Random-Error Data Set $\sin\theta/\lambda \leq 1.0$

Table 5. *Monopole and Dipole Populations*

atom	P_v	P_{11}	P_{1-1}	P_{10}
O(1)	5.90(9)	-0.08(2)	-0.10(3)	–
O(2)	6.09(7)	-0.10(3)	-0.01(2)	–
O(3)	5.89(9)	-0.11(2)	0.01(1)	–
C(1)	4.36(10)	0.07(3)	0.01(2)	–
H(1)	0.94(6)	–	–	0.16(5)
H(2)	0.91(4)	–	–	0.15(3)
H(3)	0.91(0)	–	–	0.15(0)

Table 6. *Quadrupole Populations*

atom	P_{20}	P_{22}	P_{2-2}
O(1)	0.02(2)	-0.06(2)	0.06(2)
O(2)	-0.07(2)	-0.04(2)	0.01(2)
O(3)	-0.04(1)	-0.06(1)	-0.02(1)
C(1)	-0.23(3)	0.12(3)	-0.04(2)
H(1)	0.13(5)	–	–
H(2)	0.13(3)	–	–
H(3)	0.13(0)	–	–

Table 7. *Octupole Populations*

atom	P_{31}	P_{3-1}	P_{33}	P_{3-3}
O(1)	-0.02(2)	-0.07(2)	0.10(2)	0.01(2)
O(2)	-0.02(2)	0.00(2)	0.03(2)	0.01(2)
O(3)	0.10(2)	0.01(1)	0.02(1)	-0.04(1)
C(1)	0.00(2)	-0.06(2)	0.35(5)	0.10(3)

Table 8. *Hexadecapole Populations*

atom	P_{40}	P_{42}	P_{4-2}	P_{44}	P_{4-4}
O(1)	0.06(2)	0.06(2)	0.05(2)	0.01(3)	0.07(2)
O(2)	-0.01(2)	0.03(2)	-0.02(2)	0.02(2)	0.02(2)
O(3)	-0.01(2)	0.01(2)	0.01(2)	-0.01(2)	-0.02(2)
C(1)	0.05(3)	0.07(3)	0.01(3)	-0.05(4)	-0.01(3)

3. Refinement of XD(full): Full Data Set $\sin\theta/\lambda \leq 1.0$

Table 9. *Monopole and Dipole Populations*

atom	P_v	P_{11}	P_{1-1}	P_{10}
O(1)	5.88(7)	-0.07(1)	-0.10(2)	–
O(2)	6.08(5)	-0.11(2)	-0.01(1)	–
O(3)	5.98(7)	-0.12(2)	0.00(1)	–
C(1)	4.38(8)	0.08(3)	0.01(2)	–
H(1)	0.91(4)	–	–	0.15(4)
H(2)	0.88(3)	–	–	0.12(2)
H(3)	0.88(0)	–	–	0.12(0)

Table 10. *Quadrupole Populations*

atom	P_{20}	P_{22}	P_{2-2}
O(1)	0.01(1)	-0.05(1)	0.05(1)
O(2)	-0.08(1)	-0.03(2)	0.01(1)
O(3)	-0.05(1)	-0.06(1)	-0.01(1)
C(1)	-0.24(2)	0.11(2)	-0.05(2)
H(1)	0.11(4)	–	–
H(2)	0.09(2)	–	–
H(3)	0.09(0)	–	–

Table 11. *Octupole Populations*

atom	P_{31}	P_{3-1}	P_{33}	P_{3-3}
O(1)	-0.02(1)	-0.05(1)	0.11(2)	0.00(1)
O(2)	-0.03(1)	-0.01(1)	0.05(2)	0.01(1)
O(3)	0.10(1)	0.02(1)	0.01(1)	-0.04(1)
C(1)	0.00(2)	-0.05(2)	0.35(4)	0.08(2)

Table 12. *Hexadecapole Populations*

atom	P_{40}	P_{42}	P_{4-2}	P_{44}	P_{4-4}
O(1)	0.05(2)	0.05(2)	0.06(2)	0.01(2)	0.07(2)
O(2)	0.01(2)	0.01(2)	-0.02(2)	0.05(2)	0.02(2)
O(3)	-0.01(1)	0.03(1)	0.02(1)	-0.01(1)	-0.01(1)
C(1)	0.05(2)	0.09(2)	0.03(2)	-0.06(3)	-0.02(2)

4. Atomic Graph Data

Table 13. *Values of (3,-3) critical points in L and their distances from the relevant nuclei d(3,-3) for $H_2C_2O_4.4H_2O$ wavefunctions obtained from DZP calculations using the low-angle data set. All values are given in atomic units. An approximate description of the atomic graph is given for each atom, along with a description of the relative position of the (3,-3) critical points with respect to the other nuclei.*

	CHF	CHF(re)	HF	BLYP	Description
C1 trigonal planar					
L	1.01	1.06	1.20	0.97	bonding
d(3,-3)	0.966	0.967	0.960	0.960	along C1-C1′
L	1.09	1.08	1.02	0.75	bonding
d(3,-3)	0.949	0.954	0.990	0.997	along C1-O1
L	0.95	0.97	1.13	0.88	bonding
d(3,-3)	0.976	0.971	0.963	0.988	along C1-O2
O1 trigonal planar					
L	2.88	2.76	2.17	2.26	bonding
d(3,-3)	0.714	0.72	0.752	0.728	along O1-C1
L	3.90	3.82	3.34	3.27	bonding
d(3,-3)	0.686	0.686	0.707	0.701	along O1-H1
L	4.77	4.57	4.81	4.65	non-bonding
d(3,-3)	0.641	0.643	0.638	0.638	
O2 trigonal planar					
L	2.98	2.86	2.05	2.17	bonding
d(3,-3)	0.712	0.718	0.771	0.751	along O2-C1
L	4.31	4.15	4.88	4.52	bonding
d(3,-3)	0.642	0.645	0.640	0.643	along O2$\cdots$H4
L	4.238	4.36	5.054	4.748	non-bonding
d(3,-3)	0.646	0.644	0.636	0.639	
O3 tetrahedral					
L	3.04	3.04	3.22	3.14	bonding
d(3,-3)	0.708	0.705	0.750	0.777	along O3-H2
L	2.93	3.03	2.58	2.52	bonding
d(3,-3)	0.715	0.714	0.746	0.739	along O3-H3
L	4.78	5.06	4.67	4.42	bonding
d(3,-3)	0.636	0.634	0.644	0.646	along O3$\cdots$H1
L	3.91	3.80	4.85	4.71	non-bonding
d(3,-3)	0.655	0.656	0.638	0.638	
O4 tetrahedral					
L	3.24	3.22	2.71	2.65	bonding
d(3,-3)	0.704	0.702	0.739	0.732	along O4-H4
L	2.66	2.78	3.05	2.95	bonding
d(3,-3)	0.726	0.725	0.759	0.752	along O4-H5
L	4.03	3.90	4.65	4.47	non-bonding
d(3,-3)	0.651	0.655	0.642	0.643	
L	4.39	4.64	4.65	4.49	non-bonding
d(3,-3)	0.64	0.641	0.64	0.64	