

Appendix A. supplement

Note for Table 6,7, and 8: V_{tot} is defined by the interatomic boundaries in the crystal (zero flux surfaces) while V_{001} describes an atomic volume with a cutoff of $\rho=0.001$ au, which is commonly used in theory.

Table 6. *Experimental atomic properties for morphine*

Atom name	V_{tot}	V_{001}	N	N_{001}	Q
O(1)	18.16	16.27	9.21	9.21	-1.21
O(2)	17.84	16.25	9.23	9.22	-1.23
O(3)	14.86	13.90	9.03	9.03	-1.03
O(4)	20.81	17.03	9.24	9.23	-1.24
N(1)	9.58	9.56	8.26	8.26	-1.26
C(1)	13.53	12.00	6.06	6.06	-0.06
C(2)	15.48	12.99	6.09	6.08	-0.09
C(3)	9.98	8.62	5.48	5.48	0.52
C(4)	10.08	8.96	5.71	5.70	0.29
C(5)	7.58	7.47	5.89	5.89	0.11
C(6)	7.08	7.00	5.77	5.77	0.23
C(7)	14.28	12.31	6.21	6.21	-0.21
C(8)	15.47	12.31	6.18	6.17	-0.18
C(9)	6.99	6.98	5.93	5.93	0.07
C(10)	8.43	8.25	5.89	5.89	0.11
C(11)	10.88	10.16	6.07	6.07	-0.07
C(12)	10.61	9.32	6.29	6.29	-0.29
C(13)	6.71	6.68	6.20	6.20	-0.20
C(14)	7.52	7.38	6.12	6.12	-0.12
C(15)	9.54	9.27	6.19	6.19	-0.19
C(16)	9.50	9.14	6.14	6.14	-0.14
C(17)	14.43	12.47	6.29	6.28	-0.29
H(1)	7.69	4.83	0.86	0.85	0.14
H(2)	6.86	4.83	0.79	0.79	0.21
H(5)	6.55	5.93	0.78	0.78	0.22
H(6)	7.24	5.46	0.79	0.79	0.21
H(7)	5.57	4.46	0.66	0.66	0.34
H(8)	5.47	4.06	0.65	0.64	0.35
H(9)	5.94	5.15	0.79	0.79	0.21
H(10A)	7.48	5.85	0.91	0.91	0.09
H(10B)	6.40	5.47	0.86	0.86	0.14
H(11)	1.25	1.25	0.37	0.37	0.63
H(14)	7.09	5.41	0.84	0.83	0.16
H(15A)	7.59	6.24	0.84	0.83	0.16
H(15B)	9.26	6.47	0.84	0.83	0.16
H(16A)	7.39	6.52	0.83	0.83	0.17
H(16B)	7.54	6.13	0.83	0.83	0.17
H(17A)	5.66	4.44	0.68	0.68	0.32
H(17B)	5.35	4.36	0.67	0.67	0.33
H(17C)	6.16	4.28	0.66	0.65	0.34
H(21)	1.49	1.47	0.34	0.34	0.66
H(41)	0.90	0.88	0.26	0.26	0.74
H(42)	1.07	0.99	0.26	0.26	0.74
Sum	379.29	328.84	161.97	161.84	0.03

Values are given in Å³ and e. $V_{tot} \times 4 = 1517.16 \text{ Å}^3$ V(unit cell) = 1529.08 Å³

N × 4 = 647.88 e F(000) = 648.0 e

Table 7. Experimental volumes V_{001} , theoretical volumes of fragments 1-3 and from Matta*
(in \AA^3)

Atomname	V_{001}	exp.	Part1	Part2	Part3	Matta	a_{vt} -exp
O(1)	16.27	17.13		17.20	17.41	0.98	
O(2)	16.25		17.15			0.90	
O(3)	13.90	14.73	14.42	14.83	14.48	0.72	
N(1)	9.56		12.09			2.53	
C(1)	12.00	11.91		12.06	11.65	-0.13	
C(2)	12.99	12.06		12.08	11.64	-1.06	
C(3)	8.62	8.68		8.76	8.50	0.03	
C(4)	8.96	8.55		8.49	8.61	-0.41	
C(5)	7.47	7.66	6.40	6.52	5.89	-0.85	
C(6)	7.00		6.00		5.20	-1.40	
C(7)	12.31		11.67		10.82	-1.07	
C(8)	12.31		11.69		10.58	-1.18	
C(9)	6.98			6.84	6.45	-0.34	
C(10)	8.25			8.49	7.80	-0.11	
C(11)	10.16	10.22		10.03	9.88	-0.12	
C(12)	9.32	9.84			8.64	-0.08	
C(13)	6.68	7.40			5.93	-0.02	
C(14)	7.38		6.68			-0.70	
C(15)	9.27		7.78		7.53	-1.62	
C(16)	9.14		7.04		7.38	-1.93	
C(17)	12.47		8.22		8.62	-4.05	
H(1)	4.83	6.89		6.98	7.12	2.17	
H(2)	4.83	7.00		7.00	6.81	2.11	
H(5)	5.93	6.83	6.95	6.61	6.52	0.80	
H(6)	5.46		7.04			1.58	
H(7)	4.46		7.18		6.77	2.52	
H(8)	4.06		7.45		7.02	3.18	
H(9)	5.15		7.29	6.59	6.77	1.73	
H(10A)	5.85			7.00	6.88	1.09	
H(10B)	5.47			6.67	6.69	1.21	
H(11)	1.25	2.90		2.90	2.54	1.53	
H(14)	5.41		6.95	6.89		1.51	
H(15A)	6.24		7.45		6.91	0.94	
H(15B)	6.47		7.52		6.94	0.76	
H(16A)	6.52		7.27		6.07	0.15	
H(16B)	6.13		7.57		6.82	1.07	
H(17A)	4.44		7.34		6.38	2.42	
H(17B)	4.36		7.34		6.79	2.71	
H(17C)	4.28		7.98		6.75	3.09	
H(21)	1.47		2.51			1.04	

a_{vt} is the average of the theoretical values

$$R_V = \sum |a_{vt} - \text{exp}| / \sum \text{exp}$$

$$R_V=0.163 \text{ (all atoms); } R_V=0.089 \text{ (hydrogens excluded)}$$

*Matta (2001)

Table 8. *Experimental electronic populations N₀₀₁, corresponding theoretical values for fragments 1-3 and from Matta (in e)*

Atomname	N ₀₀₁ exp.	Part1	Part2	Part3	Matta	a _{vt} -exp
O(1)	9.21	9.24		9.24	9.28	0.04
O(2)	9.22		9.23			0.01
O(3)	9.03	9.26	9.24	9.25	9.26	0.22
N(1)	8.26		8.30		8.30	0.04
C(1)	6.06	6.00		6.00	5.93	-0.08
C(2)	6.08	6.00		6.00	5.90	-0.11
C(3)	5.48	5.40		5.40	5.34	-0.11
C(4)	5.70	5.43		5.42	5.47	-0.29
C(5)	5.89	5.52	5.49	5.48	5.43	-0.41
C(6)	5.77		5.34		5.33	-0.44
C(7)	6.21		6.01		5.95	-0.23
C(8)	6.17		6.02		6.00	-0.16
C(9)	5.93			5.54		-0.39
C(10)	5.89			5.92	5.82	-0.02
C(11)	6.07	6.00		6.01	6.03	-0.06
C(12)	6.29	6.03			6.02	-0.27
C(13)	6.20	5.95			5.95	-0.25
C(14)	6.12		5.90			-0.22
C(15)	6.19		5.87		5.81	-0.35
C(16)	6.14		5.47		5.55	-0.63
C(17)	6.28		5.42		5.45	-0.85
H(1)	0.85	0.99		0.99	1.03	0.15
H(2)	0.79	1.00		1.00	0.99	0.21
H(5)	0.78	1.01	1.01	1.00	1.02	0.22
H(6)	0.79		1.02			0.23
H(7)	0.66		0.99		0.99	0.33
H(8)	0.64		1.02		1.02	0.38
H(9)	0.79		1.04	1.02		0.24
H(10A)	0.91			1.01	1.02	0.11
H(10B)	0.86			1.02	1.06	0.18
H(11)	0.37	0.40		0.40	0.35	0.01
H(14)	0.83		1.04	1.03		0.21
H(15A)	0.83		1.05		1.01	0.20
H(15B)	0.83		1.05		1.06	0.23
H(16A)	0.83		1.04		1.01	0.20
H(16B)	0.83		1.08		0.99	0.21
H(17A)	0.68		1.04		0.98	0.34
H(17B)	0.67		1.04		0.98	0.35
H(17C)	0.65		1.07		0.98	0.38
H(21)	0.34		0.37			0.03

a_{vt} is the average of the theoretical values

$$R_N = \sum |a_{vt} - \text{exp}| / \sum \text{exp}$$

$$R_N = 0.059 \text{ (all atoms)}; R_N = 0.035 \text{ (hydrogens excluded)}$$

*Matta (2001)

Table 9. *Modification of Table 3, containing additional bond topological descriptors*

T	V	H	Rho	Lap	Bond
0.298996	-0.829745	-0.530749	0.330449	-0.927009	O(1) -C(3)
0.258773	-0.627633	-0.368861	0.274139	-0.44035	O(2) -C(6)
0.322896	-0.800519	-0.477623	0.318298	-0.618905	O(3) -C(4)
0.234482	-0.53986	-0.305377	0.248355	-0.28358	O(3) -C(5)
0.252111	-0.616695	-0.364584	0.27162	-0.449894	N(1) -C(9)
0.267323	-0.632357	-0.365034	0.274287	-0.390846	N(1) -C(16)
0.241749	-0.588099	-0.346349	0.263766	-0.418399	N(1) -C(17)
0.309593	-0.787928	-0.478335	0.316519	-0.674966	C(1) -C(2)
0.325759	-0.829959	-0.5042	0.326596	-0.713764	C(1) -C(11)
0.288878	-0.764288	-0.47541	0.312519	-0.746131	C(2) -C(3)
0.311557	-0.842137	-0.53058	0.332227	-0.876094	C(3) -C(4)
0.32754	-0.865504	-0.537964	0.336672	-0.841695	C(4) -C(12)
0.204681	-0.512011	-0.30733	0.243761	-0.410598	C(5) -C(6)
0.20605	-0.513111	-0.307061	0.24391	-0.404042	C(5) -C(13)
0.236164	-0.610507	-0.374344	0.272213	-0.55272	C(6) -C(7)
0.376746	-1.01246	-0.635709	0.370755	-1.03585	C(7) -C(8)
0.224988	-0.564939	-0.339951	0.258728	-0.459853	C(8) -C(14)
0.197816	-0.475914	-0.278099	0.231907	-0.321134	C(9) -C(10)
0.213006	-0.541379	-0.328374	0.252652	-0.461471	C(9) -C(14)
0.216049	-0.53401	-0.317962	0.249541	-0.407652	C(10) -C(11)
0.315171	-0.819126	-0.503955	0.324966	-0.755135	C(11) -C(12)
0.229726	-0.556562	-0.326836	0.255023	-0.388439	C(12) -C(13)
0.206619	-0.510493	-0.303874	0.242872	-0.38902	C(13) -C(14)
0.209625	-0.529534	-0.319909	0.249096	-0.441139	C(13) -C(15)
0.219921	-0.561973	-0.342053	0.25858	-0.488526	C(15) -C(16)

all values in au

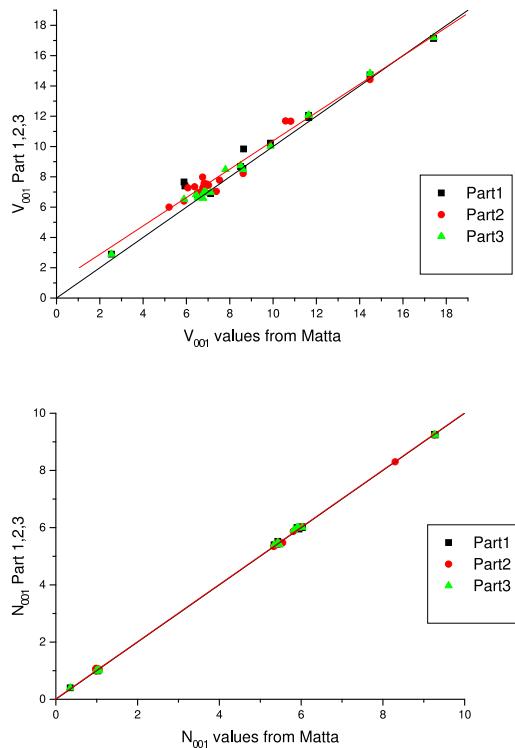


Fig. 6. Representation of the theoretical atomic properties . Above: Volumes V_{001} (in \AA^3), below: Electron populations (in e). Least squares line (red) and bisecting line (black) are also shown.

Synopsis

The electron density distribution of morphine hydrate has been derived from high resolution X-ray data set measurement at 25 K and was compared to the theoretical calculated fragment molecules from which the morphine molecule can be reconstructed.
