STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 74 (2018)

Supporting information for article:

Charge density and electrostatic potential of hepatitis C anti-viral agent andrographolide: an experimental and theoretical study

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Supplementary Information

Table S1. Expansion/Contraction Multipole Model Parameters.

Atom	κ	κ'
O(1)	0.969	0.874
O(2)	0.969	0.874
O(3)	0.982	1.133
O(4)	0.969	0.874
O(5)	0.969	0.779
C(1)	0.993	0.793
C(2)	0.994	0.964
C(3)	0.993	0.793
C(4)	0.986	0.858
C(5)	0.986	0.858
C(6)	0.994	0.964
C(7)	0.986	0.858
C(8)	0.991	0.919
C(9)	0.986	0.858
C(10)	0.986	0.858
C(11)	0.994	0.94
C(12)	0.994	0.964
C(13)	0.991	0.919
C(14)	0.986	0.858
C(15)	0.986	0.858
C(16)	0.99	0.899
C(17)	0.99	0.899
C(18)	1.014	0.975
C(19)	0.986	0.858
C(20)	0.994	0.964

Table. S2. The geometrical parameters of Andrographolide.

Bond lengths (Å)

O(1)−H(1)	0.9673(13)	C(10)−C(11)	1.5065(6)
O(2)−H(22)	0.9667(13)	C(10)−H(10A)	1.092(2)
O(3)−C(18)	1.3438(5)	C(10)−H(10B)	1.0938(10)
O(4)−C(20)	1.4245(5)	C(11)−C(12)	1.5092(5)
O(4)−H(21)	0.9667(4)	C(11)−C(14)	1.3389(7)
O(5)−C(18)	1.2194(5)	C(12)−C(15)	1.5374(4)
C(2)−C(9)	1.5360(6)	C(12)−H(12)	1.0994(9)
C(2)−H(2)	1.0993(8)	C(13)−H(13A)	1.0583(12)
C(3)−C(13)	1.5341(5)	C(13)−H(13B)	1.061(2)
C(4)−C(5)	1.5280(5)	C(13)−H(13C)	1.0582(4)
C(4)−H(4A)	1.0932(6)	C(14)−H(14A)	1.0763(7)
C(4)−H(4B)	1.0915(8)	C(14)−H(14B)	1.076(2)
C(5)−C(6)	1.5170(6)	C(15)−C(16)	1.4960(5)
C(5)−H(5A)	1.0928(8)	C(15)−H(15A)	1.0922(8)
C(5)−H(5B)	1.091(2)	C(15)−H(15B)	1.092(2)
C(6)−H(6)	1.1005(8)	C(16)−C(17)	1.3390(4)
C(7)−H(7A)	1.0912(5)	C(16)−H(16)	1.0776(4)
C(7)−H(7B)	1.094(2)	C(17)−C(18)	1.4747(4)
C(8)−H(8A)	1.0585(14)	C(17)−C(20)	1.5065(5)
C(8)−H(8B)	1.0603(6)	C(19)−C(20)	1.5307(5)
C(8)−H(8C)	1.060(2)	C(19)−H(19A)	1.0913(12)
C(9)−C(10)	1.5372(6)	C(19)−H(19B)	1.094(2)
C(9)−H(9A)	1.0929(10)	C(20)−H(20)	1.0997(17)
C(9)−H(9B)	1.0921(6)		

Bond angles (°)

C(20)−O(4)−H(21)	106.64(12)	H(8A)−C(8)−H(8B)	110.50(13)
C(9)−C(2)−H(2)	106.09(11)	H(8A)−C(8)−H(8C)	107.87(7)
C(5)−C(4)−H(4A)	112.14(8)	H(8B)−C(8)−H(8C)	101.37(12)
C(5)−C(4)−H(4B)	106.76(8)	C(2)−C(9)−C(10)	110.87(3)
H(4A)−C(4)−H(4B)	111.74(8)	C(2)−C(9)−H(9A)	106.57(11)
C(4)−C(5)−C(6)	111.03(4)	C(2)−C(9)−H(9B)	110.92(12)
C(4)−C(5)−H(5A)	111.64(8)	C(10)−C(9)−H(9A)	111.97(8)
C(4)−C(5)−H(5B)	110.56(4)	C(10)−C(9)−H(9B)	110.67(7)
C(6)−C(5)−H(5A)	109.00(5)	H(9A)−C(9)−H(9B)	105.67(9)
C(6)−C(5)−H(5B)	112.25(4)	C(9)−C(10)−C(11)	110.59(4)
H(5A)−C(5)−H(5B)	102.05(11)	C(9)−C(10)−H(10A)	111.09(4)
C(5)−C(6)−H(6)	107.01(5)	C(9)−C(10)−H(10B)	108.82(8)
H(7A)−C(7)−H(7B)	104.92(13)	C(11)−C(10)−H(10A)	108.42(5)

C(11)−C(10)−H(10B)	105.78(5)	C(16)−C(15)−H(15A)	107.56(6)
H(10A)−C(10)−H(10 B)	112.03(11)	C(16)−C(15)−H(15B)	106.36(3)
C(10)−C(11)−C(12)	113.29(4)	H(15A)−C(15)−H(15 B)	106.65(11)
C(10)−C(11)−C(14)	122.57(4)	C(15)−C(16)−C(17)	125.95(3)
C(12)−C(11)−C(14)	124.06(4)	C(15)−C(16)−H(16)	116.61(5)
C(11)−C(12)−C(15)	113.71(3)	C(17)−C(16)−H(16)	116.93(4)
C(11)−C(12)−H(12)	107.52(11)	C(16)−C(17)−C(18)	122.04(3)
C(15)−C(12)−H(12)	108.88(5)	C(16)−C(17)−C(20)	130.30(3)
C(3)−C(13)−H(13A)	113.39(8)	C(18)−C(17)−C(20)	107.65(3)
C(3)−C(13)−H(13B)	112.09(4)	O(3)−C(18) O(5)	121.46(3)
C(3)−C(13)−H(13C)	108.18(5)	O(3)−C(18)−C(17)	109.49(3)
H(13A)−C(13)−H(13 B)	105.65(7)	O(5)−C(18)−C(17)	129.04(3)
H(13A)−C(13)−H(13 C)	108.56(10)	C(20)−C(19)−H(19A)	109.98(5)
H(13B)−C(13)−H(13C)	108.83(15)	C(20)−C(19)−H(19B)	113.51(5)
C(11)−C(14)−H(14A)	127.54(12)	H(19A)−C(19)−H(19 B)	109.92(8)
C(11)−C(14)−H(14B)	120.19(6)	O(4)−C(20)−C(17)	111.71(3)
H(14A)−C(14)−H(14 B)	112.18(15)	O(4)−C(20)−C(19)	109.20(3)
C(12)−C(15)−C(16)	112.54(3)	O(4)−C(20)−H(20)	110.59(8)
C(12)−C(15)−H(15A)	116.27(6)	C(17)−C(20)−C(19)	100.85(3)
C(12)−C(15)−H(15B)	106.87(3)	C(17)−C(20)−H(20)	115.95(5)
		C(19)−C(20)−H(20)	107.89(5)

Torsion angles (°)

H(21)−O(4)−C(20)−C(17)	95.14(14)	C(4)−C(5)−C(6)−H(6)	60.55(12)
H(21)−O(4)−C(20)−C(19)	-154.18(15)	H(5A)−C(5)−C(6)−H(6)	-176.06(15)
H(21)−O(4)−C(20)−H(20)	-35.59(11)	H(5B)−C(5)−C(6)−H(6)	-63.76(12)
H(2)−C(2)−C(9)−C(10)	-55.14(11)	C(2)−C(9)−C(10)−C(11)	-53.71(12)
H(2)−C(2)−C(9)−H(9A)	-177.23(14)	C(2)−C(9)−C(10)−H(10A)	-174.15(15)
H(2)−C(2)−C(9)−H(9B)	68.23(12)	C(2)−C(9)−C(10)−H(10B)	62.07(12)
H(4A)−C(4)−C(5)−C(6)	179.31(16)	H(9A)−C(9)−C(10)−C(11)	65.16(12)
H(4A)−C(4)−C(5)−H(5A)	57.45(12)	H(9A)−C(9)−C(10)−H(10A)	-55.28(12)
H(4A)−C(4)−C(5)−H(5B)	-55.42(12)	H(9A)−C(9)−C(10)−H(10B)	-179.06(16)
H(4B)−C(4)−C(5)−C(6)	-58.00(12)	H(9B)−C(9)−C(10)−C(11)	-177.24(15)
H(4B)−C(4)−C(5)−H(5A)	-179.86(15)	H(9B)−C(9)−C(10)−H(10A)	62.33(12)
H(4B)−C(4)−C(5)−H(5B)	67.27(12)	H(9B)−C(9)−C(10)−H(10B)	-61.46(12)

C(9)−C(10)−C(11)−C(12)	56.16(12)	H(15A)−C(15)−C(16)−H(16)	-160.14(16)
C(9)−C(10)−C(11)−C(14)	-120.59(17)	H(15B)−C(15)−C(16)−C(17)	-85.63(15)
H(10A)−C(10)−C(11)−C(12)	178.17(15)	H(15B)−C(15)−C(16)−H(16)	85.90(13)
H(10A)−C(10)−C(11)−C(14)	1.42(12)	C(15)−C(16)−C(17)−C(18)	175.5(2)
H(10B)−C(10)−C(11)−C(12)	-61.51(12)	C(15)−C(16)−C(17)−C(20)	-3.54(13)
H(10B)−C(10)−C(11)−C(14)	121.74(17)	H(16)−C(16)−C(17)−C(18)	3.97(11)
C(10)−C(11)−C(12)−C(15)	171.54(16)	H(16)−C(16)−C(17)−C(20)	-175.0(2)
C(10)−C(11)−C(12)−H(12)	50.92(11)	C(16)−C(17)−C(18)−O(3)	-169.51(18)
C(10)−C(11)−C(14)−H(14A)	176.1(2)	C(16)−C(17)−C(18)−O(5)	11.47(15)
C(10)−C(11)−C(14)−H(14B)	-0.17(12)	C(16)−C(17)−C(20)−O(4)	-84.69(17)
C(14)−C(11)−C(12)−C(15)	-11.76(13)	C(16)−C(17)−C(20)−C(19)	159.41(18)
C(14)−C(11)−C(12)−H(12)	-132.38(17)	C(16)−C(17)−C(20)−H(20)	43.24(14)
C(12)−C(11)−C(14)−H(14A)	-0.31(12)	C(20)−C(17)−C(18)−O(3)	9.70(11)
C(12)−C(11)−C(14)−H(14B)	-176.6(2)	C(18)−C(17)−C(20)−O(4)	96.19(13)
C(11)−C(12)−C(15)−C(16)	-62.33(12)	C(20)−C(17)−C(18)−O(5)	-169.3(2)
C(11)−C(12)−C(15)−H(15A)	62.35(13)	C(18)−C(17)−C(20)−C(19)	-19.71(10)
C(11)−C(12)−C(15)−H(15B)	-178.73(15)	C(18)−C(17)−C(20)−H(20)	-135.88(15)
H(12)−C(12)−C(15)−C(16)	57.52(12)	H(19A)−C(19)−C(20)−O(4)	24.38(11)
H(12)−C(12)−C(15)−H(15A)	-177.79(16)	H(19A)−C(19)−C(20)−C(17)	142.12(13)
H(12)−C(12)−C(15)−H(15B)	-58.88(11)	H(19A)−C(19)−C(20)−H(20)	-95.87(13)
C(12)−C(15)−C(16)−C(17)	157.67(18)	H(19B)−C(19)−C(20)−O(4)	147.99(15)
C(12)−C(15)−C(16)−H(16)	-30.80(11)	H(19B)−C(19)−C(20)−C(17)	-94.27(13)
H(15A)−C(15)−C(16)−C(17)	28.33(13)	H(19B)−C(19)−C(20)−H(20)	27.74(11)

Table S3. Hydrogen bonding interactions (Å, º)

D—H···A	D—H	H···A	D···A	∠D—H···A
O1−H1···O2	0.914(21)	1.825(23)	2.659(1)	150.4(2)
O4−H21···O5$^{(i)}$	0.827(16)	1.978(16)	2.802(1)	173.9(2)
O2−H22···O1$^{(ii)}$	0.865(19)	1.842(19)	2.695(1)	168.5(2)
C8−H8B···O2$^{(iii)}$	0.952(16)	2.762(16)	3.698(1)	167.7(1)
C13−H13C···O5$^{(i)}$	0.918(13)	2.996(19)	3.843(1)	154.2(2)
C15−H15A···O5$^{(i)}$	0.965(17)	2.699(17)	3.662(1)	175.2(1)

Symmetry code: (i) $x-1, y, z$. (ii) $-x+1, y+\frac{1}{2}, -z$. (iii) $x+1, y, z$.

Table S4. Differences of Mean-Squares Displacement Amplitudes (DMSDA)

BONDS	DMSDA $\times 10^{-4}$ Å^2
C1–C2	2
C2–C3	0
C3–C4	3
C4–C5	4
C5–C6	1
C1–C6	2
C1–C7	3
C1–C8	2
C2–C9	4
C3–C12	2
C3–C13	3
C9–C10	4
C10–C11	-4
C11–C12	5
C11–C14	8
C12–C15	5
C15–C16	-1
C16–C17	-3
C17–C18	-2
C17– C20	12
C19– C20	-4
C6–O1	1
C7–O2	6
C18–O3	4
C19–O3	11
C20–O4	9
C18–O5	0

Table S5. Topological properties of electron density of Andrographolide. (*First line*: experimental values; *Second line:* CRYSTAL09 calculations; *Third line:* single point energy DFT calculations)

Bond	$^{a}\rho_{bcp}(r)$	$^{b}\nabla^2\rho_{bcp}(r)$	$^{c}\lambda_1$	$^{c}\lambda_2$	$^{c}\lambda_3$	$^{d}R_{ij}$	$^{d}d_1$	$^{d}d_2$	$^{e}\varepsilon$
C1–C2	1.46(2)	-6.9(1)	-8.9	-8.3	10.3	1.571	0.793	0.779	0.07
	1.49	-7.4	-9.8	-9.2	11.6	1.57	0.792	0.778	0.06
	1.5	-10.7	-9.7	-9.6	8.6	1.578	0.789	0.789	0.014
C2–C3	1.54(2)	-7.9(1)	-9.8	-9	10.8	1.565	0.801	0.764	0.09
	1.51	-7.2	-9.7	-9.4	11.9	1.564	0.774	0.789	0.03
	1.52	-11	-9.9	-9.8	8.6	1.576	0.79	0.786	0.007
C3–C4	1.63(2)	-8.5(1)	-10.2	-9	10.7	1.54	0.756	0.784	0.12
	1.58	-8	-10.1	-9.9	12	1.539	0.769	0.77	0.02
	1.6	-12.4	-10.6	-10.5	8.7	1.547	0.77	0.777	0.005
C4–C5	1.54(2)	-9.3(1)	-9.7	-9.3	9.7	1.531	0.775	0.756	0.05
	1.6	-9	-10.5	-10.3	11.8	1.529	0.77	0.76	0.01
	1.62	-12.9	-10.7	-10.7	8.5	1.531	0.762	0.769	0.006
C5–C6	1.73(2)	-13.2(1)	-12.3	-11.1	10.3	1.519	0.754	0.764	0.11
	1.7	-10.6	-11.6	-11	12	1.517	0.745	0.772	0.05
	1.69	-14.1	-11.8	-11.3	8.9	1.524	0.753	0.771	0.043
C1–C6	1.60(2)	-9.5(1)	-10.8	-9.4	10.6	1.552	0.763	0.79	0.15
	1.58	-8.9	-10.5	-10.1	11.7	1.552	0.764	0.788	0.04
	1.63	-13	-11.1	-10.8	8.9	1.548	0.753	0.795	0.029
C1–C7	1.67(2)	-11.2(1)	-10.8	-10.3	9.9	1.543	0.765	0.778	0.05
	1.58	-8.9	-10.6	-10.1	11.8	1.543	0.776	0.767	0.05
	1.6	-12.3	-10.8	-10.4	8.9	1.555	0.777	0.778	0.038
C1–C8	1.60(2)	-9.5(1)	-10.1	-9.7	10.4	1.542	0.761	0.782	0.04
	1.56	-8.3	-10.2	-9.9	11.8	1.542	0.776	0.766	0.04
	1.58	-12.1	-10.4	-10.3	8.6	1.547	0.78	0.767	0.008
C2–C9	1.67(2)	-10.6(1)	-11	-10.4	10.8	1.536	0.785	0.75	0.06
	1.56	-8	-10.3	-9.6	11.9	1.536	0.771	0.765	0.08
	1.61	-12.6	-10.7	-10.5	8.6	1.539	0.766	0.773	0.013
C3–C12	1.46(2)	-6.4(1)	-8.7	-8.4	10.6	1.569	0.764	0.806	0.04
	1.48	-7.1	-9.5	-9.2	11.6	1.569	0.78	0.789	0.03
	1.49	-10.5	-9.6	-9.5	8.6	1.584	0.797	0.787	0.007
C3–C13	1.68(2)	-10.9(1)	-11	-10.5	10.5	1.535	0.737	0.798	0.05
	1.58	-8.9	-10.3	-10.2	11.6	1.535	0.789	0.746	0
	1.6	-12.4	-10.5	-10.5	8.6	1.542	0.769	0.773	0.002

C9–C10	1.55(2)	-8.4(4)	-9.7	-8.8	10.1	1.538	0.775	0.763	0.1
	1.56	-8.3	-10.2	-10	11.8	1.538	0.768	0.771	0.02
	1.6	-12.6	-10.6	-10.5	8.6	1.538	0.77	0.768	0.009
C10–C11	1.72(2)	-11.3 1)	-11.6	-10.4	10.8	1.508	0.739	0.769	0.11
	1.66	-9.8	-11.4	-10.3	11.9	1.508	0.739	0.769	0.11
	1.71	-14.5	-11.7	-11.4	8.6	1.509	0.764	0.745	0.034
C11–C12	1.81(3)	-12.6(1)	-12.3	-11.7	11.5	1.51	0.8	0.71	0.05
	1.69	-10.6	-11.4	-11.1	12	1.51	0.761	0.749	0.03
	1.67	-13.7	-11.5	-11	8.7	1.521	0.763	0.758	0.045
C11–C14	2.33(3)	-23.4(1)	-17.2	-14.3	8	1.338	0.72	0.618	0.21
	2.22	-18.6	-17.6	-12.2	11.1	1.337	0.694	0.643	0.44
	2.3	-23.9	-17.6	-13	6.7	1.334	0.654	0.68	0.353
C12–C15	1.55(2)	-8.3(1)	-10.2	-8.9	10.7	1.537	0.784	0.753	0.15
	1.56	-8.1	-10.3	-9.7	11.9	1.537	0.77	0.768	0.06
	1.59	-12.3	-10.5	-10.4	8.6	1.543	0.778	0.765	0.011
C15–C16	1.68(2)	-11.5(1)	-11.5	-10	9.9	1.497	0.728	0.77	0.14
	1.67	-9.5	-11	-10.6	12.1	1.497	0.735	0.763	0.04
	1.72	-14.8	-11.8	-11.4	8.5	1.5	0.772	0.728	0.031
C16–C17	2.30(3)	-23.6(1)	-18.4	-13.6	8.5	1.339	0.658	0.681	0.35
	2.29	-20.4	-17.6	-13.8	11	1.339	0.644	0.695	0.28
	2.3	-24.2	-17.7	-13.4	6.8	1.335	0.664	0.671	0.316
C17–C18	1.83(3)	-13.7(1)	-13.6	-11.2	11.1	1.476	0.707	0.77	0.21
	1.79	-12.1	-13.1	-10.9	11.9	1.476	0.69	0.786	0.2
	1.82	-16.2	-13.4	-11.8	9	1.485	0.762	0.723	0.137
C17– C20	1.78(2)	-11.8(1)	-12	-11.1	11.4	1.507	0.78	0.727	0.08
	1.69	-10.1	-11.4	-10.8	12.1	1.507	0.744	0.763	0.05
	1.76	-15.3	-12.2	-11.9	8.8	1.502	0.761	0.741	0.026
C19– C20	1.65(2)	-10.2(1)	-10.8	-9.9	10.6	1.532	0.78	0.752	0.1
	1.63	-9.5	-10.8	-10.6	11.9	1.531	0.788	0.743	0.02
	1.65	-13.3	-11.3	-11.2	9.2	1.549	0.781	0.768	0.016
C6–O1	1.62(3)	-6.4(1)	-10.9	-10.3	14.8	1.441	0.828	0.614	0.06
	1.588	-5.3	-10.9	-10.3	15.9	1.441	0.83	0.611	0.06
	1.632	-10.6	-10.3	-10.2	9.9	1.442	0.511	0.931	0.013
C7–O2	1.71(2)	-7.6(1)	-11.1	-10.5	14	1.441	0.855	0.586	0.06
	1.63	-4.9	-11.1	-10.7	16.8	1.44	0.823	0.617	0.04
	1.75	-12.9	-11.8	-11.5	10.3	1.421	0.508	0.913	0.025
C18–O3	2.25(4)	-19.5(2)	-19.2	-16.6	16.3	1.346	0.804	0.541	0.15
	2.05	-17.3	-16.3	-14.8	13.9	1.346	0.818	0.528	0.1
	1.94	-12.1	-14.3	-14.1	16.3	1.37	0.89	0.48	0.015
C19–O3	1.61(2)	-2.8(1)	-10.9	-8.6	16.8	1.462	0.858	0.604	0.27

	1.54	-4.6	-10.4	-10	15.9	1.46	0.844	0.616	0.04
	1.66	-10.8	-10.5	-10.2	10	1.439	0.509	0.93	0.027
C20–O4	1.78(3)	-10.4(1)	-12.5	-11.6	13.6	1.427	0.851	0.576	0.07
	1.69	-6.6	-11.7	-11.6	16.6	1.426	0.812	0.614	0.01
	1.69	-12.4	-11.2	-11	9.9	1.433	0.917	0.516	0.017
C18–O5	2.91(5)	-30.1(3)	-29.9	-25.9	25.7	1.216	0.785	0.431	0.16
	2.89	-33	-27.7	-24.4	19	1.216	0.772	0.445	0.14
	2.86	-3.8	-27.4	-25.1	48.7	1.199	0.411	0.788	0.089
C2–H2	1.77(5)	-14.7(1)	-15.8	-15.2	16.3	1.099	0.705	0.395	0.04
	1.72	-11.5	-15	-14.4	17.9	1.099	0.703	0.396	0.04
	1.85	-21.6	-16.8	-16.7	11.9	1.088	0.695	0.393	0.006
C4–H4A	1.70(1)	-12.7(1)	-13.8	-11.4	12.5	1.094	0.628	0.466	0.22
	1.79	-14.4	-16.4	-15.4	17.4	1.092	0.704	0.388	0.07
	1.86	-22	-17	-16.9	11.9	1.08	0.691	0.389	0.004
C4–H4B	1.70(1)	-11.6(1)	-14	-12.9	15.3	1.094	0.674	0.419	0.09
	1.76	-13.1	-15.5	-14.7	17.1	1.092	0.689	0.404	0.06
	1.84	-21.5	-16.7	-16.6	11.8	1.085	0.694	0.391	0.007
C5–H5A	1.79(5)	-16.3(1)	-16.5	-14.9	15.1	1.093	0.702	0.39	0.11
	1.77	-14.2	-16	-15.9	17.6	1.092	0.712	0.381	0.01
	1.84	-21.5	-16.6	-16.5	11.6	1.084	0.691	0.393	0.002
C5–H5B	1.80(5)	-17.7(1)	-15.8	-15.4	13.5	1.092	0.686	0.407	0.03
	1.74	-13.6	-15.6	-15.4	17.5	1.092	0.711	0.382	0.01
	1.86	-22	-17.1	-17	12.1	1.08	0.386	0.694	0.003
C6–H6	1.84(5)	-16.4(1)	-17.2	-15.4	16.3	1.1	0.703	0.397	0.11
	1.78	-14.3	-16.1	-15.4	17.2	1.099	0.705	0.394	0.05
	1.89	-22.6	-17.9	-17.3	12.6	1.088	0.703	0.385	0.036
C7–H7A	1.87(5)	-18.6(1)	-16.7	-15.5	13.6	1.093	0.694	0.4	0.07
	1.82	-14.4	-16.7	-16.3	18.6	1.092	0.716	0.376	0.02
	1.92	-23.6	-18.5	-17.8	12.8	1.077	0.379	0.698	0.036
C7–H7B	1.97(6)	-20.1(1)	-17.5	-16.5	13.9	1.093	0.674	0.42	0.06
	1.82	-14.8	-16.9	-16.3	18.4	1.092	0.718	0.374	0.04
	1.89	-22.7	-17.9	-17.3	12.5	1.082	0.696	0.386	0.038
C8–H8A	1.85(6)	-15.5(2)	-16	-15.4	15.9	1.06	0.672	0.388	0.04
	1.92	-17.6	-17.8	-17.4	17.6	1.059	0.686	0.373	0.02
	1.86	-22	-17.1	-16.9	12	1.077	0.386	0.691	0.011
C8–H8B	1.86(6)	-17.2(1)	-16.6	-15.4	14.9	1.06	0.66	0.4	0.08
	1.91	-16.4	-17.9	-17	18.5	1.059	0.691	0.368	0.05
	1.84	-21.5	-16.7	-16.5	11.6	1.081	0.69	0.391	0.01
C8–H8C	1.84(6)	-15.7(1)	-16.4	-15.2	15.9	1.059	0.674	0.386	0.08
	1.88	-15.6	-16.9	-16.3	17.5	1.059	0.673	0.386	0.04
	1.88	-22.6	-17.6	-17.4	12.4	1.074	0.695	0.379	0.008

C9–H9A	1.87(6)	-16.0(1)	-16.3	-15.9	16.2	1.093	0.7	0.393	0.02
	1.77	-13.6	-15.8	-15.4	17.6	1.092	0.702	0.39	0.03
	1.86	-22	-17	-16.9	11.9	1.08	0.388	0.692	0.007
C9–H9B	1.69(5)	-13.1(1)	-13.4	-12.3	12.6	1.093	0.642	0.451	0.09
	1.89	-15.2	-16.1	-15.9	16.8	1.092	0.695	0.397	0.02
	1.87	-22.3	-17.2	-17.2	12.1	1.074	0.692	0.386	0.005
C10–H10A	1.84(6)	-15.7(1)	-15.6	-14.4	14.3	1.092	0.677	0.416	0.08
	1.81	-14.4	-16.4	-16.2	18.1	1.092	0.712	0.38	0.01
	1.87	-22.2	-17.2	-17.1	12.1	1.079	0.386	0.693	0.005
C10–H10B	1.74(5)	-14.4(1)	-14.1	-13.9	13.6	1.093	0.661	0.433	0.02
	1.74	-13.5	-15.5	-15.1	17.1	1.092	0.697	0.395	0.02
	1.83	-21.4	-16.6	-16.6	11.8	1.086	0.696	0.39	0.003
C12–H12	1.74(5)	-14.1(1)	-15.2	-14.9	16	1.099	0.707	0.393	0.02
	1.74	-12.3	-15.4	-15.1	18.1	1.099	0.712	0.387	0.02
	1.84	-21.5	-16.8	-16.6	11.9	1.088	0.697	0.391	0.008
C13–H13A	1.89(6)	-18.3(2)	-17.3	-16.3	15.3	1.059	0.676	0.384	0.06
	1.89	-16.1	-17	-16.9	17.8	1.059	0.681	0.378	0.01
	1.84	-21.6	-16.7	-16.6	11.7	1.08	0.39	0.69	0.01
C13–H13B	2.05(8)	-21.8(2)	-19.7	-18.6	16.5	1.06	0.697	0.363	0.06
	1.89	-16	-17.2	-16.8	18	1.059	0.681	0.378	0.02
	1.87	-22.1	-17.2	-17.1	12.2	1.076	0.383	0.693	0.009
C13–H13C	1.82(5)	-16.9(1)	-15.6	-14.2	12.8	1.059	0.641	0.418	0.09
	1.9	-16.9	-17.7	-17.5	18.3	1.059	0.695	0.364	0.01
	1.87	-22.1	-17.1	-17	12	1.075	0.689	0.386	0.009
C14–H14A	1.83(6)	-15.6(2)	-16.3	-15.7	16.3	1.079	0.698	0.382	0.04
	1.83	-15.4	-16.6	-16.2	17.5	1.077	0.693	0.384	0.03
	1.91	-23.4	-18.2	-17.9	12.7	1.068	0.371	0.697	0.017
C14–H14B	1.85(6)	-15.0(1)	-16.3	-13.9	15.2	1.078	0.665	0.413	0.18
	1.86	-15.6	-16.7	-16.6	17.7	1.077	0.692	0.385	0.01
	1.88	-22.7	-17.5	-17.3	12.1	1.071	0.381	0.69	0.017
C15–H15A	1.73(5)	-13.8(1)	-15.3	-13.3	14.8	1.094	0.689	0.404	0.15
	1.78	-13.6	-16.3	-15.9	18.6	1.092	0.721	0.371	0.02
	1.83	-21.4	-16.7	-16.6	11.9	1.083	0.696	0.387	0.006
C15–H15B	1.74(5)	-14.2(1)	-14.8	-13.6	14.2	1.093	0.676	0.418	0.09
	1.73	-13.6	-15.2	-14.8	16.4	1.092	0.695	0.398	0.02
	1.88	-22.5	-17.5	-17.4	12.4	1.077	0.38	0.697	0.009
C16–H16	1.85(5)	-18.8(2)	-18.1	-16.6	15.9	1.077	0.723	0.355	0.1
	1.85	-16	-17.1	-16.9	18	1.077	0.704	0.373	0.01
	1.9	-23.4	-18.3	-18.2	13.1	1.074	0.706	0.368	0.004
C19–H19A	1.81(5)	-14.7(1)	-15.3	-12.8	13.4	1.094	0.655	0.439	0.19
	1.85	-16	-17.4	-16.4	17.9	1.092	0.716	0.377	0.06

	1.92	-23.7	-18.7	-18.1	13.1	1.076	0.372	0.704	0.035
C19–H19B	1.84(5)	-15.3(1)	-15.5	-13.2	13.4	1.093	0.643	0.45	0.17
	1.8	-16	-17.1	-16.2	17.3	1.092	0.718	0.374	0.06
	1.91	-23.4	-18.5	-17.8	12.9	1.079	0.703	0.376	0.039
C20–H20	1.99(5)	-18.9(1)	-18	-17.3	16.4	1.099	0.69	0.409	0.04
	1.79	-14.1	-16.7	-15.9	18.5	1.099	0.726	0.374	0.05
	1.9	-22.9	-18.2	-17.6	12.8	1.083	0.703	0.38	0.034
O1–H1	2.22(6)	-34.9(5)	-36.3	-34.8	36.1	0.967	0.761	0.207	0.04
	2.2	-24.1	-32.4	-31.5	39.8	0.967	0.738	0.229	0.03
	2.48	-59.8	-42.7	-41.6	24.5	0.94	0.762	0.178	0.027
O2–H22	2.32(6)	-30.7(4)	-36	-34.6	39.8	0.967	0.751	0.216	0.04
	2.23	-23.8	-33	-32.4	41.7	0.967	0.74	0.227	0.02
	2.46	-60.8	-43.4	-42.3	24.8	0.943	0.772	0.171	0.026
O4–H21	2.23(5)	-29.7(3)	-34.1	-32.6	37.1	0.967	0.746	0.221	0.05
	2.2	-24.2	-32.7	-31.8	40.3	0.967	0.739	0.228	0.03
	2.48	-59.5	-42.5	-41.4	24.4	0.941	0.18	0.761	0.028

[a]electron density (eÅ^{-3}); [b]Laplacian of electron density (eÅ^{-5}) at *bcp*; [c]eigen values: $\lambda_1, \lambda_2, \lambda_3$.

[d]R_{ij}: total bond path length (Å), d_1, d_2: the distance between the *bcp* and each bonded atom (Å);

[e]bond ellipticty (ε).

*Further, the second derivative of electron density, that is Laplacian of electron density $\nabla^2\rho(r)$ at the *bcp* can be determined from the eigenvalues of Hessian matrix, viz $\lambda_1+\lambda_2+\lambda_3$ and the values are $\lambda_1, \lambda_2 < 0$ and $\lambda_3 > 0$.

Table S6. The topological bond order n_{topo} of C–H bonds present in AGH,calculated from experiment ($n_{topo, expt}$), CRYSTAL09 ($n_{topo, theor (cryst09)}$) and DFT ($n_{topo, theo (mol)}$).

Bonds	$n_{topo, expt}$	$n_{topo, theor (cryst09)}$	$n_{topo, theo (mol)}$
C2–H2	0.975	0.978	0.930
C4–H4A	0.995	0.975	0.931
C4–H4B	0.989	0.984	0.926
C5–H5A	0.965	0.979	0.925
C5–H5B	0.953	0.959	0.929
C6–H6	0.989	0.960	0.930
C7–H7A	0.986	0.983	0.933
C7–H7B	1.028	0.980	0.933
C8–H8A	1.011	1.004	0.928
C8–H8B	1.005	1.011	0.973
C8–H8C	1.002	1.010	0.929
C9–H9A	0.973	0.975	0.932
C9–H9B	1.013	0.986	0.932
C10–H10A	1.014	0.978	0.914
C10–H10B	0.980	0.963	0.921
C12–H12	0.959	0.972	0.926
C13–H13A	0.991	1.008	0.926
C13–H13B	1.037	1.010	0.929
C13–H13C	0.988	1.001	0.932
C14–H14A	0.993	0.986	0.929
C14–H14B	1.029	0.997	0.926
C15–H15A	0.972	0.971	1.003
C15–H15B	0.973	0.961	0.929
C16–H16	0.947	0.980	0.923
C19–H19A	1.027	0.979	0.927
C19–H19B	1.034	0.955	0.929
C20–H20	0.983	0.967	0.928
O1–H1	0.529	0.451	0.955
O2–H22	0.516	0.423	0.924
O4–H21	0.529	0.440	0.960

Table S7. The atomic valence index V_{topo} of H-atoms present in AGH calculated from experiment ($V_{topo, expt}$), CRYSTAL09 ($V_{topo, theor (cryst09)}$) and quantum chemical calculations ($V_{topo, theo (mol)}$).

Atoms	$V_{topo, expt}$
H1	0.529
H2	0.975
H4A	0.995
H4B	0.989
H5A	0.965
H5B	0.953
H6	0.989
H7A	0.986
H7B	1.028
H8A	1.011
H8B	1.005
H8C	1.002
H9A	0.973
H9B	1.013
H10A	1.014
H10B	0.980
H12	0.959
H13A	0.991
H13B	1.037
H13C	0.988
H14A	0.993
H14B	1.029
H15A	0.972
H15B	0.973
H16	0.947
H19A	1.027
H19B	1.034
H20	0.983
H21	0.529
H22	0.516

Table S8. Atomic charges (e) and Volumes (Å^3) of present in AGH molecule.

	Experimental			CRYSTAL09	
Atoms	q(P_v)	q_{aim}	Volume	q_{aim}	Volume
C1	-0.08	0.08	5.90	-0.11	6.30
C2	-0.02	-0.14	7.02	0.03	6.61
C3	-0.06	0.09	5.64	-0.09	6.01
C4	-0.03	0.03	7.72	-0.04	7.66
C5	-0.01	0.22	7.95	-0.09	8.63
C6	0.14	0.31	6.51	0.31	6.34
C7	-0.04	0.37	7.30	0.31	7.42
C8	-0.18	-0.08	10.10	-0.15	9.77
C9	-0.10	0.11	8.23	-0.19	8.92
C10	-0.09	-0.01	9.83	-0.11	9.74
C11	-0.18	-0.28	10.71	-0.17	10.31
C12	-0.03	-0.06	6.93	-0.10	6.81
C13	-0.18	-0.09	9.89	-0.02	9.03
C14	-0.25	-0.08	14.70	-0.10	14.53
C15	-0.07	0.05	8.05	-0.07	8.17
C16	-0.09	-0.08	11.69	-0.04	10.78
C17	-0.21	-0.13	10.46	-0.10	10.49
C18	0.11	1.10	6.70	0.87	7.32
C19	-0.09	0.24	10.21	0.16	9.13
C20	0.06	0.37	6.48	0.23	6.92
O1	-0.33	-0.95	18.04	-0.86	17.78
O2	-0.46	-1.09	18.88	-0.92	18.34
O3	-0.33	-1.06	15.39	-0.84	15.17
O4	-0.36	-1.06	18.90	-0.87	18.20
O5	-0.43	-0.99	18.12	-0.75	17.00
H1	0.30	0.63	1.79	0.58	1.97
H2	0.09	0.08	6.11	0.07	6.22
H4A	0.01	0.00	5.76	0.13	5.51
H4B	0.02	-0.03	9.71	0.10	8.95
H5A	0.12	0.00	10.42	0.09	8.43
H5B	0.16	0.07	8.28	0.08	8.51
H6	0.09	0.08	7.38	0.04	7.81
H7A	0.19	0.16	5.61	0.10	6.74
H7B	0.06	-0.04	7.06	0.04	7.40
H8A	0.09	0.05	7.46	0.04	7.59
H8B	0.07	0.02	7.24	0.05	7.05
H8C	0.09	0.06	7.63	0.06	7.60
H9A	0.06	-0.04	8.25	0.09	6.77
H9B	0.05	0.00	6.50	0.07	6.77
H10A	0.09	0.04	8.61	0.05	9.72

H10B	0.09	0.05	8.65	0.10	9.16
H12	0.12	0.11	6.54	0.09	6.41
H13A	0.12	0.06	6.31	0.00	6.47
H13B	0.14	0.09	7.53	0.02	8.26
H13C	0.12	0.10	5.32	0.04	6.08
H14A	0.12	0.08	6.68	0.10	6.77
H14B	0.05	0.02	6.83	0.07	7.00
H15A	0.13	0.10	5.40	0.07	5.55
H15B	0.11	0.08	5.12	0.13	5.09
H16	0.24	0.23	5.64	0.09	6.46
H19A	0.09	0.09	6.86	0.10	8.36
H19B	0.02	-0.01	7.14	0.09	8.04
H20	0.01	-0.04	6.28	0.12	6.10
H21	0.26	0.60	1.95	0.57	2.14
H22	0.23	0.55	2.14	0.58	1.92
$\sum$	0.0	0.06	457.55	0.05	458.23

*The atomic volume is the space bounded by the isosurface of the electron density distribution of an atom. The isodensity envelope for the atomic volume calculation in the present study is 0.001 a.u.

MUTLIPOLE PROJECTION RESULTS

Table S9. Topological properties of electron density of AGH obtained from CRYSTAL09.
(*First line*: B3LYP/TZVP; *Second line:* B3PW/6-31G**; *Third line:* B3PW/TZVP)

Bond	[a] $\rho_{bcp}(r)$	[b] $\nabla^2\rho_{bcp}(r)$	[c] λ_1	[c] λ_2	[c] λ_3	[d] R_{ij}	[d] d_1	[d] d_2	[e] ε
C1–C2	1.506	-7.347	-9.43	-9.19	11.27	1.5707	0.7868	0.7839	0.03
	1.534	-8.39	-9.42	-9.18	10.21	1.5704	0.7913	0.7791	0.03
	1.502	-7.349	-9.25	-9.04	10.94	1.5706	0.7871	0.7836	0.02
C2–C3	1.512	-7.179	-9.43	-9.06	11.31	1.5641	0.7772	0.7869	0.04
	1.53	-7.852	-9.29	-8.94	10.38	1.5641	0.778	0.7861	0.04
	1.504	-7.112	-9.25	-8.86	10.99	1.5641	0.7762	0.7879	0.04
C3–C4	1.598	-8.45	-10.19	-9.9	11.64	1.5385	0.7585	0.78	0.03
	1.629	-9.461	-10.06	-9.91	10.51	1.5385	0.7653	0.7733	0.01
	1.596	-8.5	-10.04	-9.75	11.29	1.5385	0.7597	0.7789	0.03
C4–C5	1.63	-9.595	-10.93	-10.65	11.99	1.5294	0.7653	0.7641	0.03
	1.64	-10.581	-10.82	-10.46	10.71	1.5295	0.765	0.7644	0.03
	1.621	-9.602	-10.75	-10.46	11.61	1.5294	0.7653	0.7642	0.03
C5–C6	1.698	-10.697	-11.85	-10.83	11.99	1.5174	0.7499	0.7675	0.09
	1.716	-11.612	-11.68	-10.62	10.69	1.5174	0.7476	0.7698	0.1
	1.692	-10.749	-11.68	-10.66	11.59	1.5174	0.7496	0.7678	0.09
C1–C6	1.564	-8.729	-10.24	-9.72	11.23	1.5519	0.7605	0.7914	0.05
	1.574	-9.664	-10.14	-9.55	10.03	1.5519	0.7674	0.7845	0.06

	1.559	-8.802	-10.08	-9.58	10.86	1.5519	0.7607	0.7913	0.05
C1–C7	1.57	-8.541	-10.1	-9.78	11.34	1.5431	0.7698	0.7733	0.03
	1.594	-9.459	-10	-9.67	10.21	1.5433	0.7774	0.7659	0.04
	1.562	-8.505	-9.91	-9.59	10.99	1.5431	0.77	0.7731	0.03
C1–C8	1.565	-8.022	-10.02	-9.7	11.7	1.542	0.7632	0.7788	0.03
	1.588	-8.794	-9.91	-9.49	10.61	1.5421	0.7731	0.7691	0.04
	1.561	-8.014	-9.84	-9.53	11.36	1.542	0.7644	0.7777	0.03
C2–C9	1.571	-7.833	-10.26	-9.72	12.15	1.5359	0.7669	0.7689	0.06
	1.571	-8.368	-10.05	-9.34	11.02	1.5359	0.7664	0.7695	0.08
	1.562	-7.752	-10.09	-9.48	11.82	1.5359	0.7664	0.7695	0.06
C3–C12	1.481	-6.71	-9.28	-8.8	11.38	1.5698	0.7733	0.7965	0.05
	1.498	-7.589	-9.06	-8.86	10.33	1.5699	0.7758	0.7941	0.02
	1.475	-6.719	-9.09	-8.68	11.06	1.5698	0.7737	0.7961	0.05
C3–C13	1.563	-8.062	-9.96	-9.68	11.57	1.5348	0.7666	0.7682	0.03
	1.585	-8.989	-9.84	-9.55	10.4	1.5348	0.7829	0.7519	0.03
	1.554	-7.977	-9.73	-9.47	11.22	1.5348	0.7685	0.7663	0.03
C9–C10	1.569	-8.423	-10.31	-10.12	12.01	1.5382	0.7685	0.7697	0.02
	1.589	-9.384	-10.25	-10.02	10.89	1.5382	0.7683	0.7699	0.02
	1.567	-8.456	-10.15	-9.99	11.69	1.5382	0.7685	0.7697	0.02
Bond	[a] $\rho_{bcp}(r)$	[b] $\nabla^2\rho_{bcp}(r)$	[c] λ_1	[c] λ_2	[c] λ_3	[d] R_{ij}	[d] d_1	[d] d_2	[e] ε
C10–C11	1.678	-10.068	-11.37	-10.68	11.98	1.5079	0.7503	0.7577	0.06
	1.698	-11.281	-11.26	-10.57	10.55	1.508	0.7482	0.7598	0.07
	1.673	-10.084	-11.17	-10.55	11.64	1.5079	0.7498	0.7581	0.06
C11–C12	1.745	-11.519	-11.93	-11.45	11.86	1.5099	0.7631	0.7468	0.04
	1.772	-12.73	-11.71	-11.46	10.44	1.51	0.7733	0.7367	0.02
	1.738	-11.479	-11.71	-11.28	11.51	1.5099	0.7612	0.7487	0.04
C11–C14	2.271	-20.187	-18.06	-12.75	10.63	1.3371	0.7098	0.6273	0.42
	2.267	-22.02	-17.52	-12.53	8.03	1.3371	0.7281	0.6089	0.4
	2.26	-20.165	-17.72	-12.54	10.09	1.3371	0.7112	0.6258	0.41
C12–C15	1.563	-8.3	-10.21	-10.04	11.95	1.5376	0.7675	0.7701	0.02
	1.57	-8.927	-10.07	-9.73	10.87	1.5376	0.7655	0.7721	0.03
	1.557	-8.319	-10.05	-9.88	11.61	1.5377	0.7679	0.7698	0.02
C15–C16	1.697	-9.939	-11.39	-10.9	12.36	1.4972	0.7403	0.7569	0.04
	1.69	-10.662	-11.08	-10.48	10.9	1.4973	0.739	0.7583	0.06
	1.689	-9.94	-11.22	-10.68	11.95	1.4972	0.7416	0.7555	0.05
C16–C17	2.344	-21.254	-18.07	-14.4	11.22	1.339	0.6614	0.6776	0.26
	2.362	-22.833	-17.41	-14.23	8.81	1.339	0.6553	0.6836	0.22
	2.333	-21.222	-17.65	-14.15	10.57	1.339	0.6623	0.6767	0.25
C17–C18	1.791	-12.055	-12.85	-10.94	11.73	1.4761	0.6844	0.7917	0.17
	1.835	-13.874	-12.81	-10.81	9.75	1.4763	0.6805	0.7958	0.19
	1.785	-12.142	-12.51	-10.73	11.1	1.4761	0.6853	0.7909	0.17
C17– C20	1.675	-9.348	-11.03	-10.62	12.3	1.5069	0.7536	0.7533	0.04
	1.694	-10.342	-10.98	-10.3	10.94	1.5066	0.7495	0.7571	0.07

	1.666	-9.289	-10.82	-10.39	11.92	1.5069	0.7521	0.7548	0.04
C19– C20	1.621	-8.89	-10.72	-10.39	12.22	1.5313	0.7963	0.7349	0.03
	1.635	-9.683	-10.54	-10.22	11.07	1.5312	0.804	0.7272	0.03
	1.616	-8.892	-10.56	-10.22	11.88	1.5313	0.7969	0.7344	0.03
C6–O1	1.64	-4.722	-11.41	-11.03	17.72	1.4408	0.8102	0.6306	0.03
	1.69	-7.278	-11.61	-11.36	15.69	1.4408	0.8281	0.6127	0.02
	1.643	-5.077	-11.32	-10.96	17.21	1.4408	0.8123	0.6285	0.03
C7–O2	1.716	-3.612	-12.02	-11.45	19.86	1.4397	0.7937	0.646	0.05
	1.759	-5.814	-12.11	-11.45	17.75	1.4397	0.8108	0.6289	0.06
	1.719	-3.764	-11.87	-11.33	19.43	1.4397	0.7952	0.6445	0.05
C18–O3	2.07	-16.161	-16.07	-14.69	14.6	1.3454	0.8111	0.5343	0.09
	2.078	-19.282	-15.61	-14.38	10.71	1.3454	0.8475	0.498	0.09
	2.053	-15.987	-15.34	-14.23	13.58	1.3454	0.8187	0.5267	0.08
C19–O3	1.558	-4.323	-10.64	-10.25	16.57	1.4601	0.8369	0.6232	0.04
	1.584	-5.856	-10.67	-10.28	15.09	1.4601	0.8519	0.6081	0.04
	1.559	-4.332	-10.49	-10.12	16.28	1.4601	0.8385	0.6217	0.04

Bond	[a] $\rho_{bcp}(r)$	[b] $\nabla^2\rho_{bcp}(r)$	[c] λ_1	[c] λ_2	[c] λ_3	[d] R_{ij}	[d] d_1	[d] d_2	[e] ε
C20–O4	1.701	-4.065	-11.5	-11.27	18.7	1.4259	0.8001	0.6259	0.02
	1.738	-6.831	-11.62	-11.43	16.22	1.426	0.8203	0.6057	0.02
	1.706	-4.319	-11.4	-11.16	18.24	1.4259	0.8016	0.6243	0.02
C18–O5	2.837	-28.716	-26.41	-23.49	21.19	1.2162	0.7781	0.4381	0.12
	2.833	-17.362	-26.56	-24.29	33.49	1.2161	0.8029	0.4132	0.09
	2.815	-24.99	-25.32	-23.1	23.43	1.2162	0.7854	0.4308	0.1
C2–H2	1.748	-12.38	-15.28	-15.06	17.96	1.099	0.7092	0.3898	0.01
	1.751	-12.76	-14.98	-14.73	16.95	1.099	0.7103	0.3888	0.02
	1.74	-12.387	-15.14	-14.89	17.64	1.099	0.711	0.388	0.02
C4–H4A	1.795	-14.406	-16.45	-15.77	17.81	1.0921	0.7054	0.3867	0.04
	1.8	-15.074	-16.29	-15.49	16.71	1.0921	0.707	0.3851	0.05
	1.786	-14.417	-16.26	-15.56	17.39	1.0921	0.7053	0.3868	0.05
C4–H4B	1.768	-13.704	-16.03	-15.37	17.69	1.0922	0.7029	0.3893	0.04
	1.765	-14.11	-15.76	-14.98	16.64	1.0922	0.7042	0.388	0.05
	1.76	-13.739	-15.85	-15.19	17.3	1.0923	0.7029	0.3893	0.04
C5–H5A	1.737	-13.474	-15.85	-15.24	17.62	1.0922	0.7089	0.3833	0.04
	1.747	-14.283	-15.71	-15	16.43	1.0922	0.7102	0.3821	0.05
	1.739	-13.681	-15.75	-15.13	17.2	1.0922	0.7077	0.3845	0.04
C5–H5B	1.762	-14.136	-16.27	-15.6	17.74	1.0921	0.7115	0.3806	0.04
	1.78	-15.246	-16.26	-15.47	16.49	1.0921	0.7129	0.3792	0.05
	1.763	-14.313	-16.15	-15.45	17.29	1.0921	0.7101	0.382	0.05
C6–H6	1.79	-14.824	-16.17	-15.44	16.78	1.099	0.6998	0.3993	0.05
	1.804	-15.789	-16.2	-15.33	15.74	1.099	0.7059	0.3931	0.06
	1.791	-15.107	-16.11	-15.38	16.38	1.099	0.7004	0.3986	0.05

C7–H7A	1.824	-14.637	-16.53	-16.34	18.24	1.0923	0.7068	0.3855	0.01
	1.814	-15.162	-16.09	-15.91	16.84	1.0924	0.7082	0.3842	0.01
	1.819	-14.693	-16.34	-16.17	17.82	1.0923	0.7064	0.3859	0.01
C7–H7B	1.801	-14.069	-16.2	-15.94	18.07	1.0922	0.704	0.3882	0.02
	1.79	-14.639	-15.87	-15.47	16.71	1.0922	0.7054	0.3868	0.03
	1.795	-14.14	-16.01	-15.76	17.63	1.0921	0.7034	0.3887	0.02
C8–H8A	1.936	-17.201	-17.96	-17.72	18.48	1.0592	0.6856	0.3735	0.01
	1.932	-17.419	-17.35	-16.93	16.86	1.0592	0.6798	0.3793	0.03
	1.931	-17.266	-17.75	-17.51	17.99	1.0591	0.6847	0.3745	0.01
C8–H8B	1.961	-17.837	-18.33	-18.17	18.67	1.0592	0.6886	0.3706	0.01
	1.951	-17.963	-17.62	-17.34	17	1.0594	0.6823	0.377	0.02
	1.956	-17.89	-18.13	-17.96	18.2	1.0592	0.6878	0.3714	0.01
C8–H8C	1.834	-15.664	-16.42	-16.2	16.96	1.0592	0.669	0.3902	0.01
	1.825	-15.81	-15.78	-15.66	15.63	1.0591	0.6637	0.3954	0.01
	1.834	-15.769	-16.29	-16.06	16.58	1.0591	0.6687	0.3904	0.01
Bond	[a] $\rho_{bcp}(r)$	[b] $\nabla^2\rho_{bcp}(r)$	[c] λ_1	[c] λ_2	[c] λ_3	[d] R_{ij}	[d] d_1	[d] d_2	[e] ε
C9–H9A	1.758	-13.936	-15.95	-15.49	17.5	1.0922	0.7042	0.3879	0.03
	1.758	-14.715	-15.8	-15.31	16.39	1.0922	0.7087	0.3835	0.03
	1.756	-14.063	-15.84	-15.34	17.12	1.0922	0.7041	0.3881	0.03
C9–H9B	1.799	-14.311	-16.42	-16.05	18.16	1.092	0.7112	0.3809	0.02
	1.798	-15.011	-16.21	-15.83	17.03	1.0921	0.7158	0.3763	0.02
	1.796	-14.442	-16.3	-15.9	17.75	1.092	0.711	0.3811	0.03
C10–H10A	1.794	-14.243	-16.42	-16.02	18.19	1.092	0.7122	0.3799	0.02
	1.793	-14.843	-16.18	-15.79	17.14	1.0921	0.7165	0.3756	0.02
	1.793	-14.363	-16.3	-15.88	17.81	1.0921	0.7114	0.3807	0.03
C10–H10B	1.754	-13.885	-15.93	-15.48	17.52	1.0921	0.7051	0.387	0.03
	1.753	-14.548	-15.72	-15.31	16.48	1.0922	0.7092	0.383	0.03
	1.754	-14.006	-15.81	-15.37	17.17	1.0921	0.7044	0.3877	0.03
C12–H12	1.753	-13.082	-15.49	-15.42	17.83	1.0991	0.714	0.3851	0.02
	1.749	-13.781	-15.26	-15	16.48	1.0992	0.7165	0.3827	0.02
	1.746	-13.172	-15.35	-15.3	17.48	1.0991	0.7159	0.3832	0
C13–H13A	1.921	-16.538	-17.8	-17.49	18.75	1.0592	0.6853	0.3739	0.02
	1.909	-16.65	-17.1	-16.84	17.3	1.0591	0.6845	0.3746	0.02
	1.916	-16.502	-17.59	-17.29	18.37	1.0592	0.6853	0.3739	0.02
C13–H13B	1.882	-16.209	-17.35	-16.97	18.11	1.059	0.6787	0.3803	0.02
	1.858	-16.203	-16.65	-16.2	16.64	1.059	0.6765	0.3825	0.03
	1.871	-16.04	-17.07	-16.67	17.69	1.059	0.6779	0.3811	0.02
C13–H13C	1.904	-16.044	-17.41	-17.37	18.73	1.0591	0.6839	0.3751	0
	1.899	-16.423	-16.92	-16.85	17.35	1.059	0.6842	0.3748	0
	1.898	-16.016	-17.21	-17.16	18.36	1.059	0.6839	0.3752	0
C14–H14A	1.836	-15.336	-16.85	-16.37	17.88	1.077	0.6956	0.3814	0.03
	1.847	-16.355	-16.6	-16.25	16.49	1.0771	0.6967	0.3803	0.02
	1.839	-15.631	-16.78	-16.37	17.53	1.077	0.6968	0.3802	0.03

C14–H14B	1.856	-15.57	-17.14	-16.54	18.11	1.077	0.6985	0.3786	0.04
	1.872	-16.938	-16.97	-16.58	16.61	1.0771	0.6994	0.3777	0.02
	1.854	-15.792	-17.03	-16.48	17.71	1.077	0.6992	0.3779	0.03
C15–H15A	1.765	-14.096	-16.19	-16.03	18.13	1.092	0.7178	0.3742	0.01
	1.772	-14.896	-16.01	-15.73	16.84	1.092	0.7179	0.3741	0.02
	1.764	-14.325	-16.1	-15.9	17.68	1.092	0.7176	0.3744	0.01
C15–H15B	1.743	-13.498	-15.86	-15.5	17.86	1.0922	0.7146	0.3776	0.02
	1.75	-14.194	-15.66	-15.24	16.7	1.0922	0.7155	0.3767	0.03
	1.74	-13.647	-15.72	-15.38	17.46	1.0922	0.7145	0.3777	0.02
C16–H16	1.872	-16.408	-17.59	-17.21	18.4	1.0771	0.7074	0.3696	0.02
	1.869	-17.314	-17.2	-16.9	16.78	1.0771	0.7101	0.367	0.02
	1.868	-16.582	-17.46	-17.09	17.96	1.0771	0.7085	0.3686	0.02

Bond	[a] $\rho_{bcp}(r)$	[b] $\nabla^2\rho_{bcp}(r)$	[c] λ_1	[c] λ_2	[c] λ_3	[d] R_{ij}	[d] d_1	[d] d_2	[e] ε
C19–H19A	1.865	-16.66	-17.86	-17.1	18.3	1.092	0.7231	0.3689	0.04
	1.874	-17.547	-17.68	-16.68	16.81	1.092	0.7215	0.3705	0.06
	1.866	-16.889	-17.75	-16.99	17.86	1.092	0.7223	0.3698	0.04
C19–H19B	1.808	-16.101	-17.1	-16.49	17.48	1.0922	0.7138	0.3783	0.04
	1.822	-16.873	-16.94	-16.18	16.25	1.0922	0.7139	0.3784	0.05
	1.809	-16.292	-16.98	-16.39	17.08	1.0922	0.7131	0.3791	0.04
C20–H20	1.777	-13.8	-16.21	-15.68	18.09	1.0992	0.7194	0.3797	0.03
	1.795	-14.947	-16.22	-15.43	16.7	1.0992	0.7207	0.3785	0.05
	1.776	-14.006	-16.07	-15.55	17.61	1.0992	0.7184	0.3807	0.03
O1–H1	2.192	-23.465	-32.57	-31.51	40.61	0.967	0.7373	0.2297	0.03
	2.216	-27.302	-33.76	-32.9	39.35	0.967	0.7454	0.2216	0.03
	2.189	-24.063	-32.65	-31.63	40.21	0.967	0.7387	0.2283	0.03
O2–H22	2.252	-23.036	-32.91	-31.83	41.7	0.967	0.7318	0.2352	0.03
	2.251	-26.714	-33.86	-32.99	40.13	0.967	0.7417	0.2254	0.03
	2.251	-23.543	-32.98	-31.94	41.38	0.967	0.7329	0.2341	0.03
O4–H21	2.222	-22.139	-32.53	-31.44	41.83	0.967	0.7331	0.2339	0.03
	2.22	-24.176	-33.13	-32.23	41.18	0.967	0.7409	0.2261	0.03
	2.229	-22.497	-32.63	-31.57	41.7	0.967	0.7334	0.2336	0.03

[a] electron density (eÅ^{-3}); [b] Laplacian of electron density (eÅ^{-5}) at *bcp*; [c] eigen values: $\lambda_1, \lambda_2, \lambda_3$.

[d] R_{ij}: total bond path length (Å), d_1, d_2: the distance between the *bcp* and each bonded atom (Å);

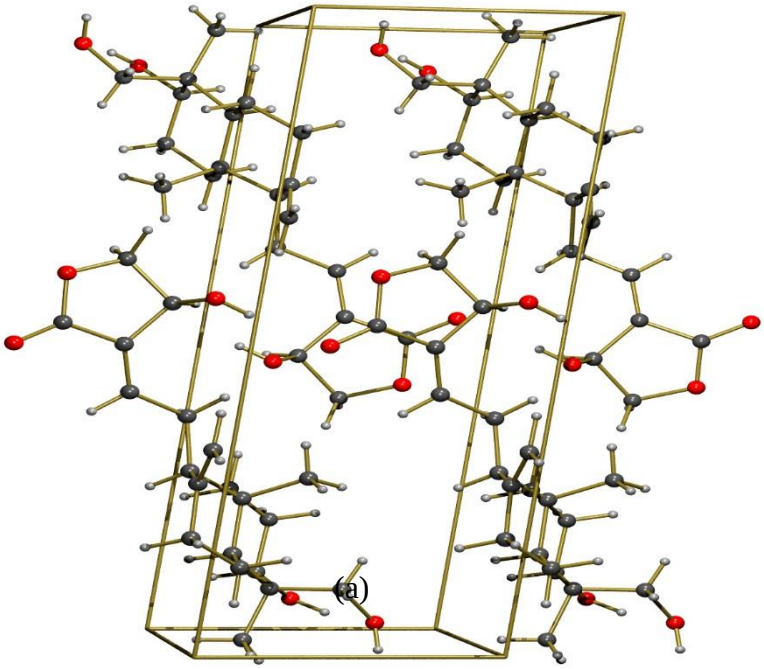
[e] bond ellipticty (ε).

Table S10. Dipole moment (D) of the AGH obtained from CRYSTAL09.

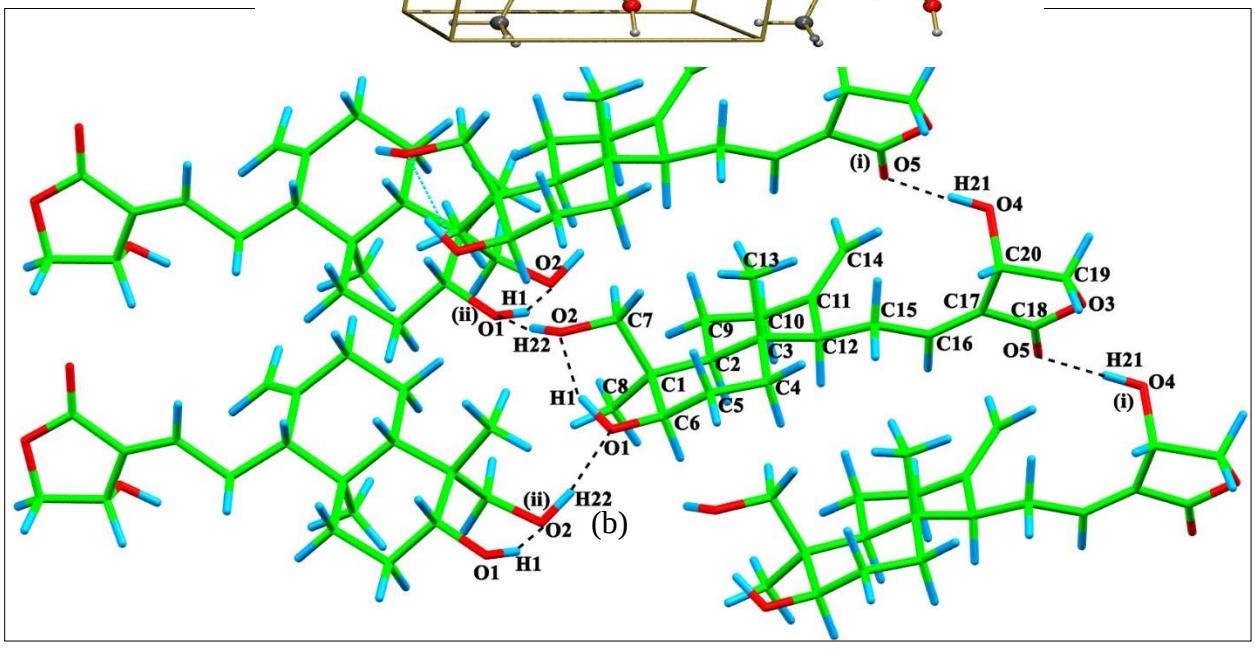
(*First line*: B3LYP/TZVP; *Second line:* B3PW/6-311G*; *Third line:* B3PW/TZVP)

	μ_{tot}
B3LYP/TZVP	11.3876
B3PW/6-31G**	12.5192
B3PW/TZVP	11.9708

Supplementary Figures



(a)



(b)

Fig. S1. (a) Unit cell packing of the AGH molecule along b-axis, (b) Displaying the hydrogen bonding interactions of andrographolide molecule.

Symmetry code: (i) $x-1, y, z$. (ii) $-x+1, y+\frac{1}{2}, -z$.

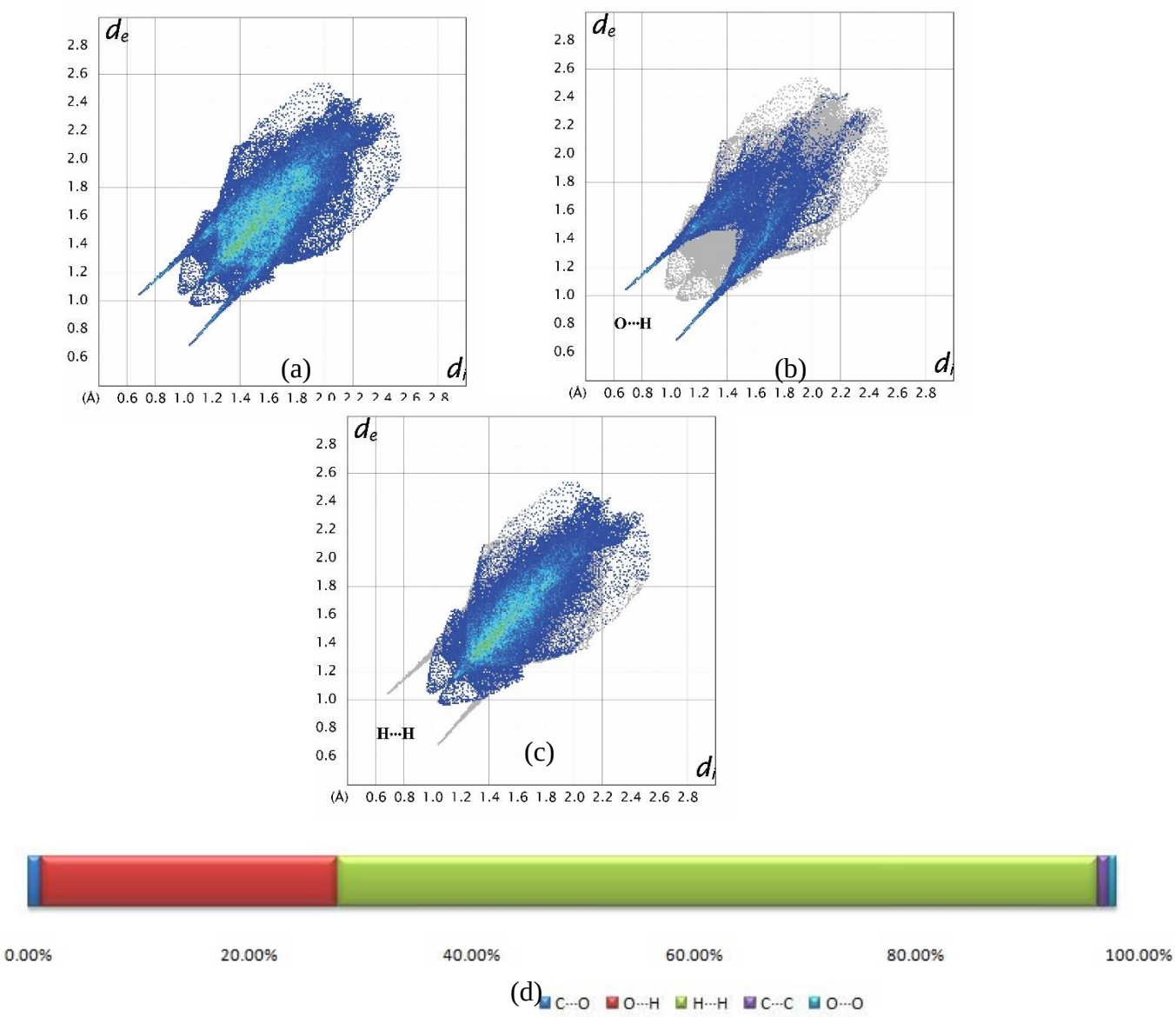


Fig S2. Fingerprint plots: (a) full (b) resolved into O···H/H···O and (c) H···H and (d) showing the percentage of contact contributing to the total Hirshfeld surface area of the andrographolide molecule in the crystal.

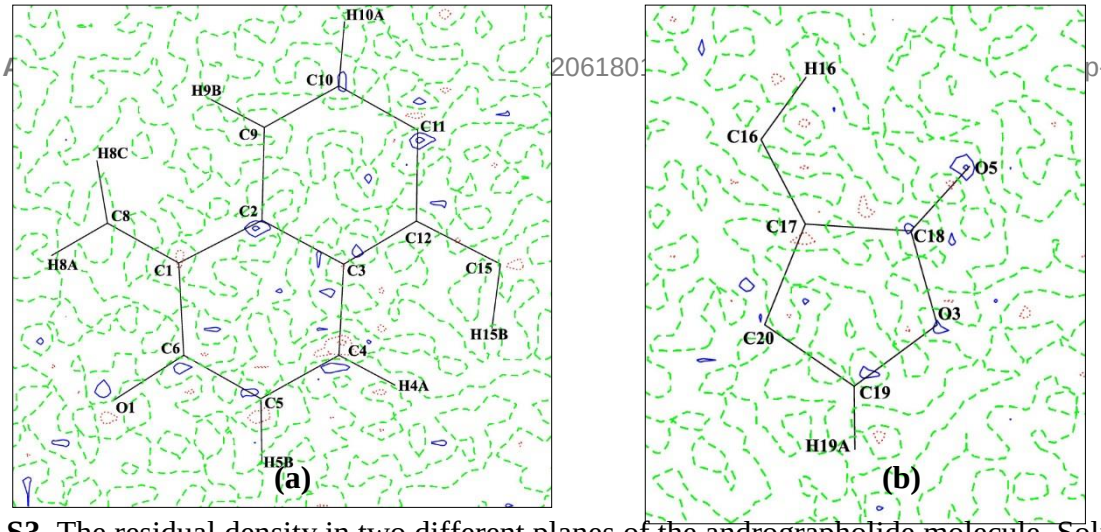


Fig. S3. The residual density in two different planes of the andrographolide molecule. Solid lines indicate the positive contours (blue), negative contours (red) are dotted and the zero contours (green) are dashed lines. The contour interval is 0.05 eÅ^{-3}

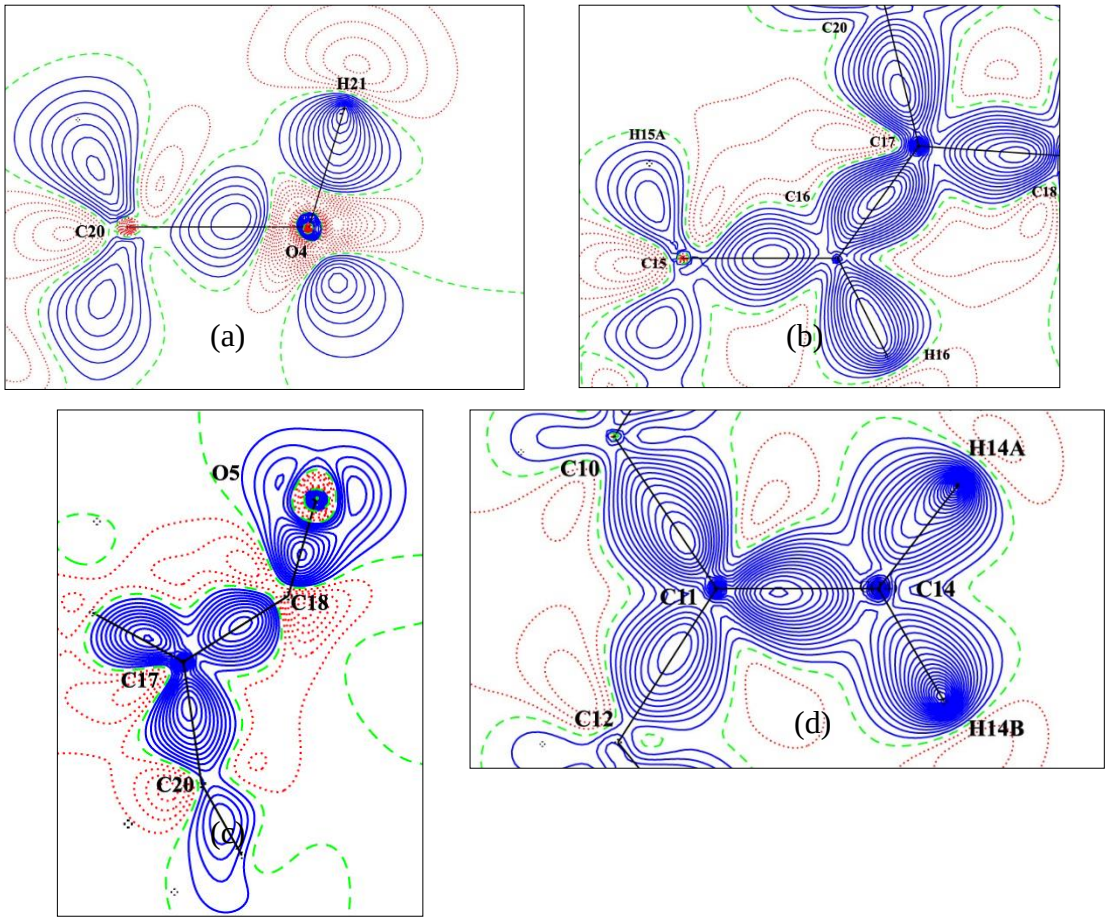


Fig. S4 The experimental deformation density maps of selected planes of AGH molecule. Contour intervals are 0.05 eÅ^{-3}. The solid lines(blue) represents positive contours, dotted (red) lines are negative contours and dashed (green) lines are zero contours.

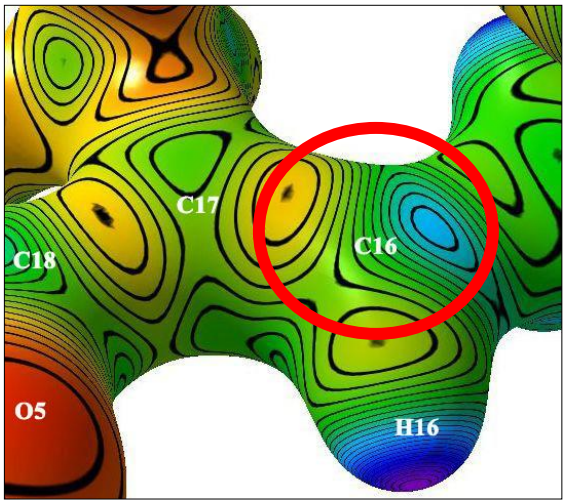


Fig S5. MOLISO representation of ESP surface contour line map. The isosurface of electron density is 0.5 eÅ^{-3}. (Red circle indicates the maxima at the vicinity of C16)

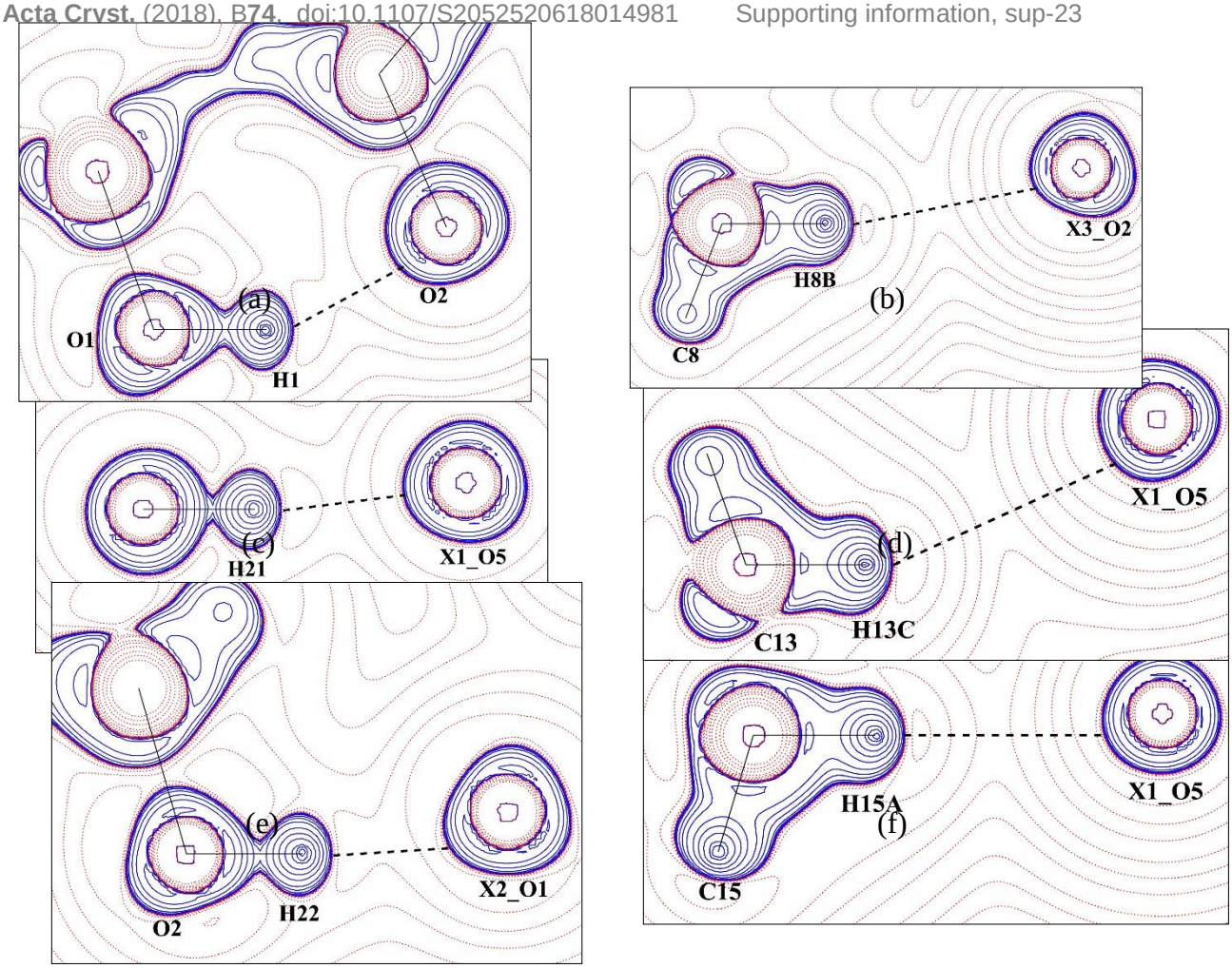


Fig. S6 The contour maps of negative Laplacian electron density of O(1)—H(1)···O(2) ,O(4)—H(21)···O(5)$^{(i)}$, O(2)—H(22)···O(1)$^{(ii)}$, C(8)—H(8B)···O(2)$^{(iii)}$,C(13)—H(13)···O(5)$^{(i)}$ and C(15) —H(15A)···O(5)$^{(i)}$ hydrogen bonding interactions. Contours are in a logarithmic scale, 3×2^{N} eÅ$^{\pm5}$, where N=2,4 and 8×10^{n}, n= -2, -1, 0, 1, 2. Solid blue lines and dotted red lines represent positive and negative contours, respectively. X1, X2 and X3 represent the symmetry codes: (i) $x-1,y,z$. (ii) $-x+1,y+\frac{1}{2},-z$. (iii) $x+1,y,z$.

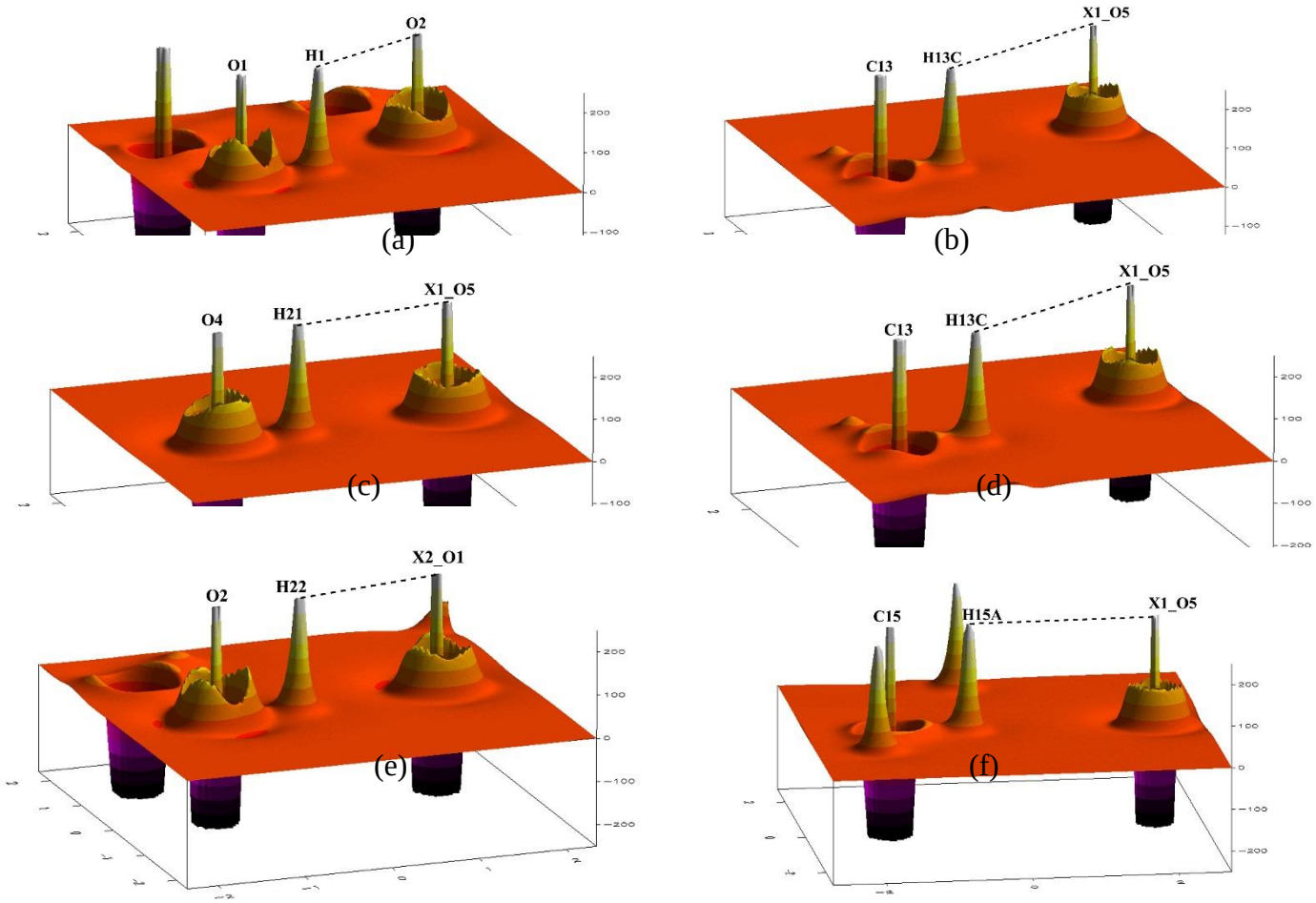


Fig. S7 The maps (a-f) show the 3D representation of relief maps of O(1)—H(1)···O(2) ,O(4)—H(21)···O(5)[(i)], O(2)—H(22)···O(1)[(ii)], C(8)—H(8B)···O(2)[(iii)],C(13)—H(13)···O(5)[(i)] and C(15) —H(15A)···O(5)[(i)] hydrogen bonding interactions. The 3D relief map plotted values range from -250 to 250 eÅ^{-5}. X1, X2 and X3 represent the symmetry codes: (i) $x-1, y, z$. (ii) $-x+1, y+\frac{1}{2}, -z$. (iii) $x+1, y, z$.

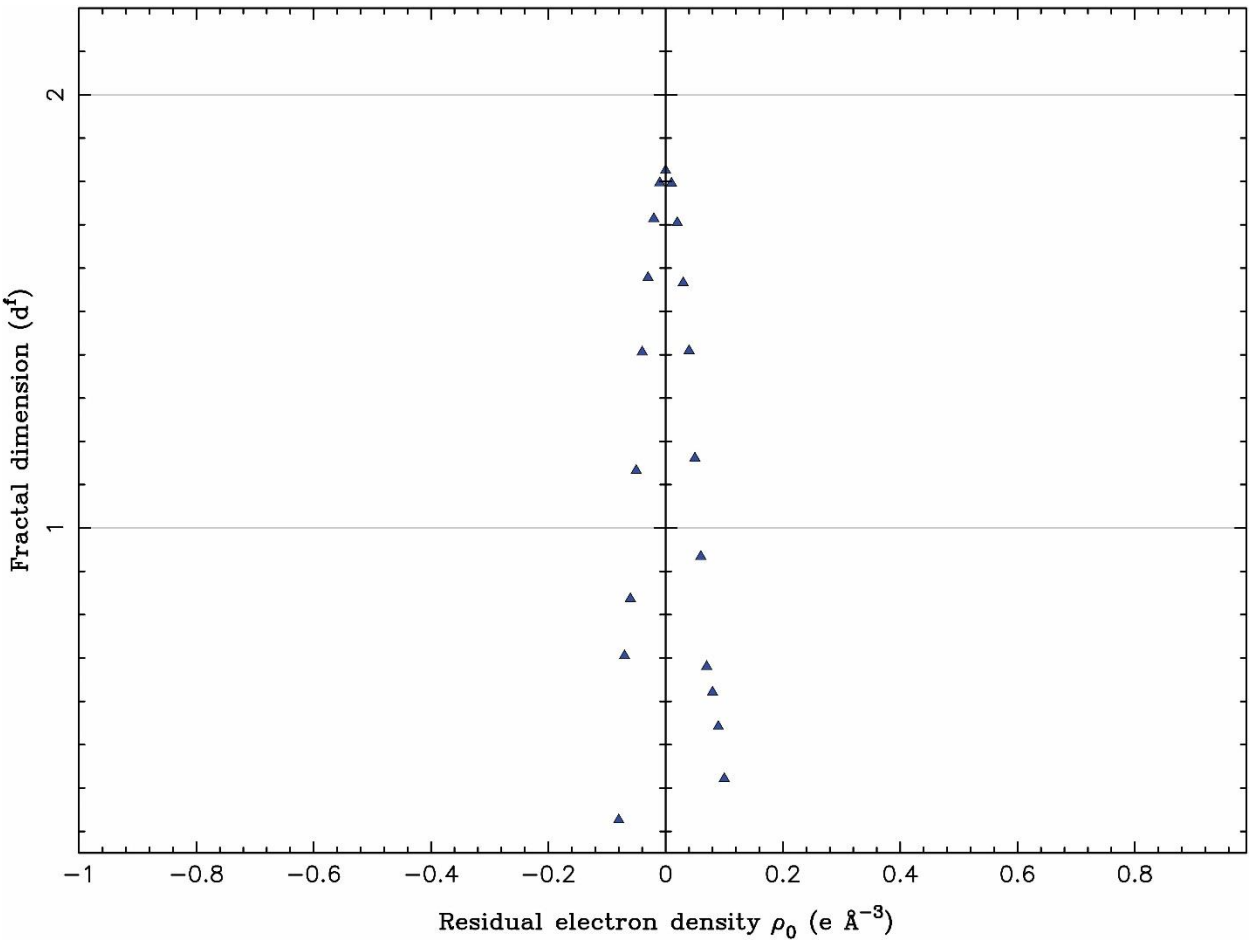


Fig S8. Fractal dimension plot of the experimental multipole refinement.