crystals

MDPI

Supplementary materials

Table S1. Intermolecular and intramolecular hydrogen bonds for **Estetrol.H$_2$O** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1A)-H(1AA)...O(8S)#1	0.84	2.03	2.783(7)	149
O(2A)-H(2AA)...O(3A)	0.84	2.16	2.659(7)	117.6
O(2A)-H(2AA)...O(5S)#2	0.84	2.32	2.958(8)	133.4
O(3A)-H(3AA)...O(1C)	0.84	2.29	2.750(7)	114.5
O(4A)-H(4AA)...O(12S)	0.85	2.15	2.772(7)	129.8
O(1B)-H(1B)...O(11S)	0.84	1.96	2.721(7)	149.5
O(2B)-H(2BB)...O(1A)	0.84	2.08	2.884(7)	161.3
O(3B)-H(3BB)...O(1D)#3	0.84	2.14	2.949(7)	161.3
O(4B)-H(4BB)...O(7S)#3	0.84	2.02	2.838(6)	166.1
O(1C)-H(1CC)...O(6S)#2	0.84	1.9	2.670(9)	151.5
O(2C)-H(2CC)...O(1D)#2	0.84	2.13	2.910(7)	153.8
O(3C)-H(3CC)...O(1A)#4	0.84	2.12	2.923(7)	160.9
O(1D)-H(1DD)...O(9S)	0.84	2.03	2.821(7)	156.5
O(2D)-H(2DD)...O(12S)	0.85	2.43	3.032(5)	128
O(3D)-H(3DD)...O(1B)	0.84	2.12	2.757(7)	132.8
O(4D)-H(4DD)...O(5S)	0.84	2.32	2.825(8)	119.5
O(1E)-H(1EE)...O(2S)	0.84	1.96	2.693(7)	144.6
O(3E)-H(3EE)...O(2E)	0.84	2.16	2.631(6)	115.6
O(4E)-H(4EE)...O(6S)#2	0.84	2.53	3.314(8)	155.3
O(1F)-H(1FF)...O(5S)	0.84	1.97	2.781(10)	161.6
O(2F)-H(2FF)...O(4B)	0.84	2.6	3.292(6)	140.3
O(2F)-H(2FF)...O(3F)	0.84	2.21	2.650(7)	112.6
O(3F)-H(3FF)...O(1G)#3	0.84	2.13	2.733(7)	128.4
O(4F)-H(4FF)...O(4M)#3	0.84	2.03	2.776(6)	148.2
O(1G)-H(1GG)...O(7S)	0.84	2	2.643(7)	133.1
O(2G)-H(2GG)...O(3G)	0.84	2.29	2.724(7)	112.6
O(3G)-H(3GG)...O(1F)	0.85	2.22	2.756(6)	121.6
O(4G)-H(4GG)...O(4I)	0.84	1.97	2.726(9)	149.8
O(1H)-H(1HH)...O(3E)	0.85	2.12	2.827(6)	139.9
O(2H)-H(2HH)...O(3H)	0.84	2.18	2.640(6)	114
O(2H)-H(2HH)...O(1S)#8	0.84	2.35	3.047(6)	140.6
O(3H)-H(3HH)...O(1E)#4	0.84	2.11	2.750(7)	133
O(4H)-H(4HH)...O(4B)#4	0.83	1.97	2.723(5)	149.4
O(1I)-H(1II)...O(12S)#9	0.84	1.87	2.695(7)	165.4
O(2I)-H(2II)...O(3I)	0.84	2.13	2.636(7)	118.1
O(3I)-H(3II)...O(1M)	0.84	2.08	2.717(7)	131.7

O(4I)-H(4II)...O(4S)	0.84	2.18	2.917(12)	146.5
O(1L)-H(1LL)...O(3N)	0.84	2.01	2.774(6)	150.5
O(2L)-H(2LL)...O(3L)	0.84	2.12	2.655(7)	121.5
O(3L)-H(3LL)...O(1N)#3	0.84	1.89	2.728(6)	172.9
O(4L)-H(4LL)...O(4A)#10	0.85	1.94	2.743(5)	156.4
O(1M)-H(1MM)...O(10S)#9	0.84	1.84	2.623(7)	153.7
O(2M)-H(2MM)...O(3M)	0.84	2.13	2.647(7)	119.2
O(3M)-H(3MM)...O(2S)#4	0.84	1.99	2.827(7)	172.3
O(4M)-H(4MM)...O(2H)	0.84	2.23	2.854(6)	131.7
O(1N)-H(1NN)...O(1S)#4	0.84	1.85	2.675(7)	168
O(2N)-H(2NN)...O(4G)	0.85	2.65	3.279(7)	131.4
O(4N)-H(4NN)...O(9S)#9	0.84	2.15	2.754(8)	129.2
O(1A)-H(1AA)...O(8S)#1	0.84	2.03	2.782(7)	149
O(2A)-H(2AA)...O(3A)	0.84	2.16	2.659(7)	117.6
O(2A)-H(2AA)...O(5S)#2	0.84	2.32	2.958(8)	133.4
O(3A)-H(3AA)...O(1C)	0.84	2.29	2.750(7)	114.5
O(4A)-H(4AA)...O(12S)	0.85	2.15	2.772(7)	129.8
O(1B)-H(1B)...O(11S)	0.84	1.96	2.721(7)	149.5
O(2B)-H(2BB)...O(1A)	0.84	2.08	2.884(7)	161.3
O(3B)-H(3BB)...O(1D)#3	0.84	2.14	2.949(7)	161.3
O(4B)-H(4BB)...O(7S)#3	0.84	2.02	2.838(6)	166.1
O(1C)-H(1CC)...O(6S)#2	0.84	1.9	2.670(9)	151.5
O(2C)-H(2CC)...O(1D)#2	0.84	2.13	2.910(7)	153.8
O(3C)-H(3CC)...O(1A)#4	0.84	2.12	2.923(7)	160.9
O(1D)-H(1DD)...O(9S)	0.84	2.03	2.821(7)	156.5
O(2D)-H(2DD)...O(12S)	0.85	2.43	3.032(5)	128
O(3D)-H(3DD)...O(1B)	0.84	2.12	2.757(7)	132.8
O(4D)-H(4DD)...O(5S)	0.84	2.32	2.825(8)	119.5
O(1E)-H(1EE)...O(2S)	0.84	1.96	2.693(7)	144.6
O(2E)-H(2EE)...O(3S)#2	0.84	2.05	2.706(6)	134.9
O(3E)-H(3EE)...O(2E)	0.84	2.16	2.631(6)	115.6
O(4E)-H(4EE)...O(6S)#2	0.84	2.53	3.314(8)	155.3
O(1F)-H(1FF)...O(5S)	0.84	1.97	2.781(10)	161.6
O(2F)-H(2FF)...O(4B)	0.84	2.6	3.292(6)	140.3
O(2F)-H(2FF)...O(3F)	0.84	2.21	2.650(7)	112.6
O(3F)-H(3FF)...O(1G)#3	0.84	2.13	2.733(7)	128.4
O(4F)-H(4FF)...O(4M)#3	0.84	2.03	2.776(6)	148.2
O(1G)-H(1GG)...O(7S)	0.84	2	2.643(7)	133.1
O(3G)-H(3GG)...O(1F)	0.85	2.22	2.756(6)	121.6
O(4G)-H(4GG)...O(4I)	0.84	1.97	2.726(9)	149.8
O(1H)-H(1HH)...O(3E)	0.85	2.12	2.827(6)	139.9

O(2H)-H(2HH)...O(3H)	0.84	2.18	2.640(6)	114
O(2H)-H(2HH)...O(1S)#8	0.84	2.35	3.047(6)	140.6
O(3H)-H(3HH)...O(1E)#4	0.84	2.11	2.750(7)	133
O(4H)-H(4HH)...O(4B)#4	0.83	1.97	2.723(5)	149.4
O(1I)-H(1II)...O(12S)#9	0.84	1.87	2.695(7)	165.4
O(2I)-H(2II)...O(3I)	0.84	2.13	2.636(7)	118.1
O(3I)-H(3II)...O(1M)	0.84	2.08	2.717(7)	131.7
O(4I)-H(4II)...O(4S)	0.84	2.18	2.917(12)	146.5
O(1L)-H(1LL)...O(3N)	0.84	2.01	2.774(6)	150.5
O(2L)-H(2LL)...O(3L)	0.84	2.12	2.655(7)	121.5
O(3L)-H(3LL)...O(1N)#3	0.84	1.89	2.728(6)	172.9
O(4L)-H(4LL)...O(4A)#10	0.85	1.94	2.743(5)	156.4
O(1M)-H(1MM)...O(10S)#9	0.84	1.84	2.623(7)	153.7
O(2M)-H(2MM)...O(3M)	0.84	2.13	2.647(7)	119.2
O(3M)-H(3MM)...O(2S)#4	0.84	1.99	2.827(7)	172.3
O(4M)-H(4MM)...O(2H)	0.84	2.23	2.854(6)	131.7
O(1N)-H(1NN)...O(1S)#4	0.84	1.85	2.675(7)	168
O(2N)-H(2NN)...O(4G)	0.85	2.65	3.279(7)	131.4
O(4N)-H(4NN)...O(9S)#9	0.84	2.15	2.754(8)	129.2

Symmetry transformations used to generate equivalent atoms: #1

#1 x+1,y,z-1 #2 x+1,y,z #3 x,y,z-1 #4 x,y,z+1

#5 x+1,y+1,z #6 x-1,y,z #7 x-1,y,z-1 #8 x+1,y,z+1

#9 x,y-1,z #10 x-1,y-1,z

Table S2. Intermolecular hydrogen bonds for **Estetrol.0.5CH$_3$OH** [Å and °].

D-H...A d(D-H)		d(H...A)	d(D...A)	<(DHA)
O(4)-H(4O)...O(1)#2	0.84	1.90	2.732(2)	172.6
O(3)-H(3O)...O(4)#3	0.84	1.96	2.764(2)	159.6
O(2)-H(2O)...O(4)#4	0.84	2.42	3.038(3)	131.5
O(1)-H(1O)...O(1S^a)	0.84	1.87	2.645(4)	153.0
O(1)-H(1O)...O(1S^a)#1	0.84	1.97	2.797(4)	167.6
C(1S)-H(1SC^a)...O(2)#5	0.98	2.59	3.527(3)	160.6
O(1S^a)-(H1S^a)...O(2)#6	0.84	1.99	2.834(4)	177.0

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z #2 x+1/2,y-1/2,z+1 #3 -x+3/2,y+1/2,-z+2

#4 x,y+1,z #5 -x+1/2,y-1/2,-z+1 #6 x-1/2,y-1/2,z-1