

## Supplemental Information

### Supramolecular Structure of 5-Hydroxyisophthalic Acid-Acetone 1:1 Solvate

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**Table 2S Hydrogen bond geometry**

D-H...A	D-H / Å	H...A / Å	D...A / Å	D-H...A / °
O(1)-H(1)...O(30)	0.96(3)	1.92(3)	2.656(3)	177(3)
O(7)-H(7)...O(24)	0.96(3)	1.88(4)	2.654(2)	172(3)
O(12)-H(12)...O(19) <sup>(i)</sup>	0.95(3)	1.72(4)	2.649(2)	174(2)
O(14)-H(14)...O(34)	0.87(3)	1.93(4)	2.779(3)	177(3)
O(20)-H(20)...O(11) <sup>(ii)</sup>	0.92(3)	1.89(4)	2.615(2)	174(2)
O(25)-H(25)...O(6)	0.91(3)	1.75(4)	2.609(2)	175(3)

Symmetry codes: (i)-1+x, y, 1+z; (ii)1+x, y, -1+z

**Table 3S Final atomic coordinates ( × 10<sup>4</sup>) and equivalent isotropic temperature factors**

(Å<sup>2</sup> × 10<sup>3</sup>).  $U_{eq}$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

Atom	x	y	z	$U_{eq}$
O(1)	-1871(3)	9382(1)	8149(1)	55(1)

C(2)	-1607(3)	8139(2)	8189(2)	35(1)
C(3)	-802(3)	7461(2)	7498(1)	32(1)
C(4)	-532(3)	6186(2)	7584(1)	29(1)
C(5)	368(3)	5491(2)	6842(1)	29(1)
O(6)	838(2)	6026(1)	6154(1)	38(1)
O(7)	609(3)	4294(1)	6971(1)	42(1)
C(8)	-1073(3)	5570(2)	8356(1)	31(1)
C(9)	-1895(3)	6254(2)	9038(1)	30(1)
C(10)	-2509(3)	5600(2)	9858(1)	32(1)
O(11)	-2300(3)	4447(1)	9897(1)	43(1)
O(12)	-3215(3)	6244(2)	10488(1)	44(1)
C(13)	-2166(3)	7528(2)	8959(1)	34(1)
O(14)	5907(3)	-72(2)	3721(1)	48(1)
C(15)	5493(3)	1181(2)	3604(2)	36(1)
C(16)	6011(3)	1835(2)	2842(1)	33(1)
C(17)	5540(3)	3118(2)	2765(1)	31(1)
C(18)	6045(3)	3810(2)	1941(1)	31(1)
O(19)	5746(2)	4971(2)	1906(1)	44(1)
O(20)	6772(2)	3176(2)	1308(1)	41(1)
C(21)	4571(3)	3773(2)	3441(1)	31(1)
C(22)	4050(3)	3111(2)	4200(1)	30(1)
C(23)	2993(3)	3783(2)	4933(1)	33(1)
O(24)	2562(3)	3233(1)	5620(1)	43(1)
O(25)	2581(3)	4987(2)	4795(1)	43(1)
C(26)	4491(3)	1831(2)	4282(1)	34(1)
C(27)	-3053(5)	12148(3)	6732(2)	78(1)
C(28)	-1617(4)	11241(3)	6238(2)	56(1)
C(29)	-938(6)	11668(3)	5350(2)	84(1)
O(30)	-1005(3)	10177(2)	6535(1)	64(1)
C(31)	10237(5)	-1856(3)	1145(2)	75(1)
C(32)	8396(5)	-1158(3)	1599(2)	62(1)
C(33A)	6590(20)	-550(20)	1119(9)	106(5)
C(33B)	7360(50)	-133(18)	982(10)	86(6)
O(34)	8245(3)	-1218(2)	2382(2)	73(1)

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**Table 4S Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ).**

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}$
H(1)	-1590(40)	9700(30)	7570(20)	66
H(3)	-437	7871	6967	39
H(7)	1420(40)	3900(20)	6508(18)	51
H(8)	-883	4697	8414	37
H(12)	-3520(40)	5740(20)	10984(18)	53
H(13)	-2734	7984	9431	41
H(14)	6600(40)	-420(30)	3289(19)	58
H(16)	6687	1401	2375	40
H(20)	7030(40)	3670(20)	822(18)	50
H(21)	4268	4650	3388	37
H(25)	1910(40)	5340(20)	5264(18)	51
H(26)	4112	1396	4799	41
H(27A)	-3357	11754	7302	117
H(27B)	-4272	12443	6424	117
H(27C)	-2480	12847	6799	117
H(29A)	14	10985	5099	126
H(29B)	-304	12353	5378	126
H(29C)	-2080	11947	4992	126
H(31A)	9875	-2354	736	113
H(31B)	11087	-2398	1569	113
H(31C)	10953	-1271	835	113
H(33A)	5546	-140	1520	159
H(33B)	6132	-1166	850	159
H(33C)	6921	72	673	159
H(33D)	6149	331	1270	129
H(33E)	7010	-479	484	129
H(33F)	8235	421	789	129

**Table 4S Bond lengths (Å) and angles (°).**

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O(1)-C(2)	1.356(3)
C(2)-C(3)	1.393(3)
C(2)-C(13)	1.393(3)
C(3)-C(4)	1.388(3)
C(4)-C(5)	1.481(3)
C(4)-C(8)	1.395(3)
C(5)-O(6)	1.233(2)
C(5)-O(7)	1.307(2)
C(8)-C(9)	1.388(3)
C(9)-C(10)	1.490(3)
C(9)-C(13)	1.387(3)
C(10)-O(11)	1.259(2)
C(10)-O(12)	1.283(3)
O(14)-C(15)	1.359(3)
C(15)-C(16)	1.397(3)
C(15)-C(26)	1.397(3)
C(16)-C(17)	1.390(3)
C(17)-C(18)	1.490(3)
C(17)-C(21)	1.389(3)
C(18)-O(19)	1.262(3)
C(18)-O(20)	1.283(3)
C(21)-C(22)	1.399(3)
C(22)-C(23)	1.488(3)
C(22)-C(26)	1.387(3)
C(23)-O(24)	1.230(2)
C(23)-O(25)	1.308(3)
C(27)-C(28)	1.480(5)
C(28)-C(29)	1.495(4)
C(28)-O(30)	1.218(3)
C(31)-C(32)	1.500(4)
C(32)-C(33A)	1.496(7)
C(32)-C(33B)	1.498(9)
C(32)-O(34)	1.217(4)
O(1)-C(2)-C(3)	122.72(19)

O(1)-C(2)-C(13)	117.85(19)
C(2)-C(3)-C(4)	120.00(18)
C(2)-C(13)-C(9)	120.2(2)
C(3)-C(2)-C(13)	119.43(19)
C(3)-C(4)-C(5)	118.62(17)
C(3)-C(4)-C(8)	120.72(19)
C(4)-C(5)-O(6)	121.23(19)
C(4)-C(5)-O(7)	115.45(17)
C(4)-C(8)-C(9)	118.87(19)
C(5)-C(4)-C(8)	120.66(18)
O(6)-C(5)-O(7)	123.32(19)
C(8)-C(9)-C(10)	118.90(18)
C(8)-C(9)-C(13)	120.82(18)
C(9)-C(10)-O(11)	118.49(18)
C(9)-C(10)-O(12)	117.92(19)
C(10)-C(9)-C(13)	120.28(18)
O(11)-C(10)-O(12)	123.59(18)
O(14)-C(15)-C(26)	117.58(18)
O(14)-C(15)-C(16)	123.1(2)
C(15)-C(16)-C(17)	120.10(19)
C(15)-C(26)-C(22)	119.93(18)
C(16)-C(15)-C(26)	119.3(2)
C(16)-C(17)-C(18)	119.84(19)
C(16)-C(17)-C(21)	121.04(19)
C(17)-C(18)-O(19)	118.84(19)
C(17)-C(18)-O(20)	117.16(19)
C(17)-C(21)-C(22)	118.5(2)
C(18)-C(17)-C(21)	119.12(19)
O(19)-C(18)-O(20)	124.00(19)
C(21)-C(22)-C(23)	119.91(19)
C(21)-C(22)-C(26)	121.13(19)
C(22)-C(23)-O(24)	121.8(2)
C(22)-C(23)-O(25)	115.14(18)
C(23)-C(22)-C(26)	118.96(18)
O(24)-C(23)-O(25)	123.1(2)
C(27)-C(28)-C(29)	117.8(3)
C(27)-C(28)-O(30)	121.7(3)

C(29)-C(28)-O(30)	120.4(3)
C(31)-C(32)-O(34)	120.2(3)
C(31)-C(32)-C(33A)	121.1(6)
C(31)-C(32)-C(33B)	108.6(11)
C(33A)-C(32)-O(34)	117.9(7)
C(33B)-C(32)-O(34)	127.2(8)

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