APPENDIX A

CRYSTALLOGRAPHIC SUPPORTING INFORMATION

A.1 Ortep Plots

All thermal ellipsid plots in this appendix are generated with the program ORTEP-III [24] at 40% probability level. Cyan, red, and green ellipses represent CD carbon, oxygen, and water oxygen atoms; hydrogen atoms are omitted. Glucose residues of DIMEB and TRIMEG are sequentially numbered with 1–7 and 1–8, respectively. Dashed lines indicate O$\cdots$O hydrogen bonds within 3.5 Å distance. Atomic numbering see Figures 1.3 (page 6) and 1.11 (page 20); atomic coordinates and temperature factors see next section below.

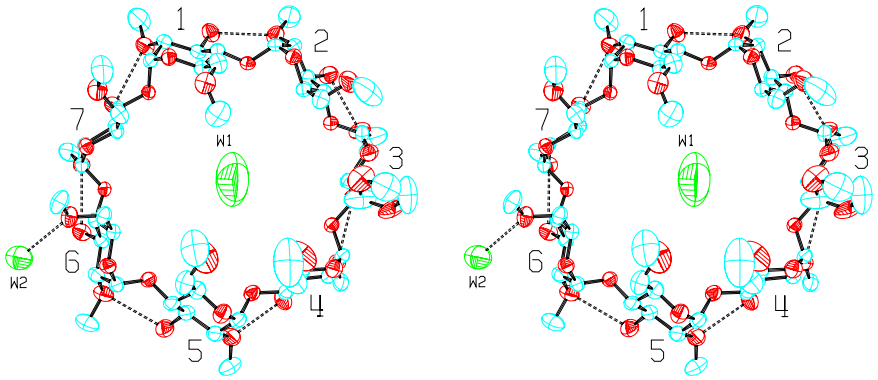


Figure A.1: ORTEP-III stereo plot of DIMEB·2H_2O

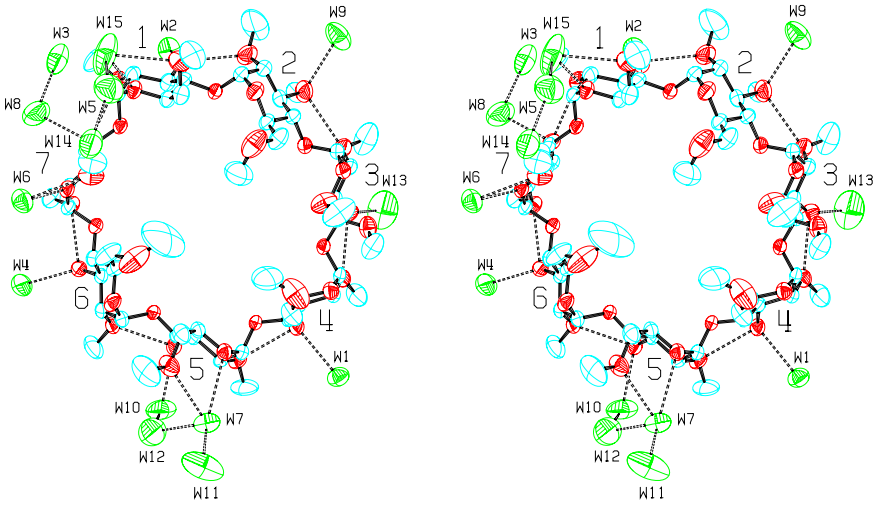


Figure A.2: ORTEP-III stereo plot of DIMEB·15H_2O

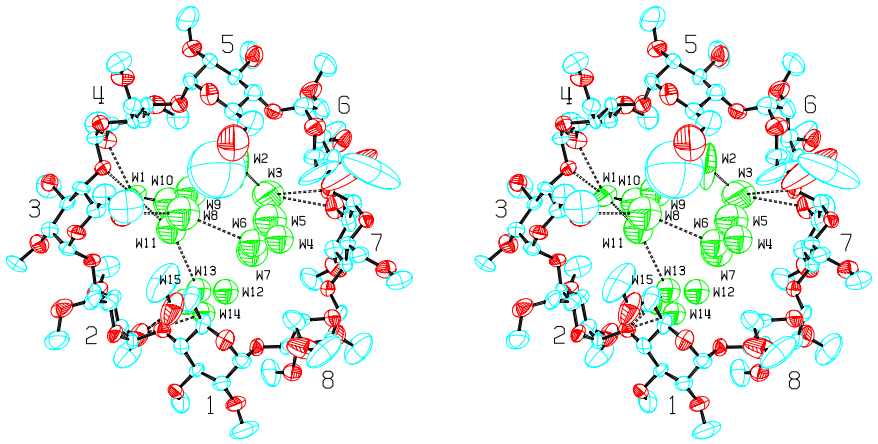
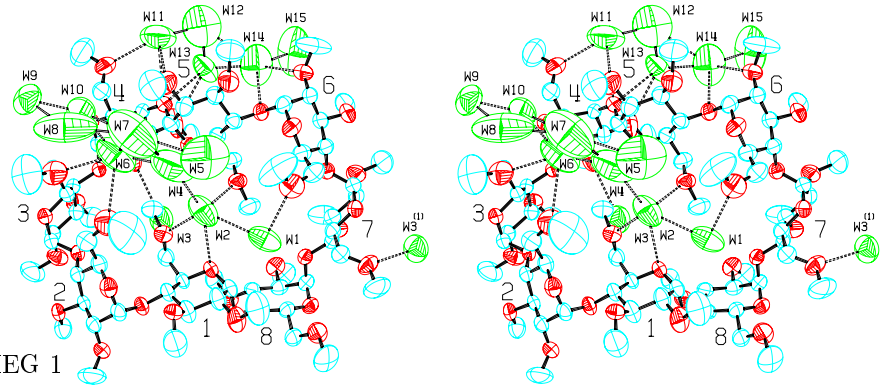
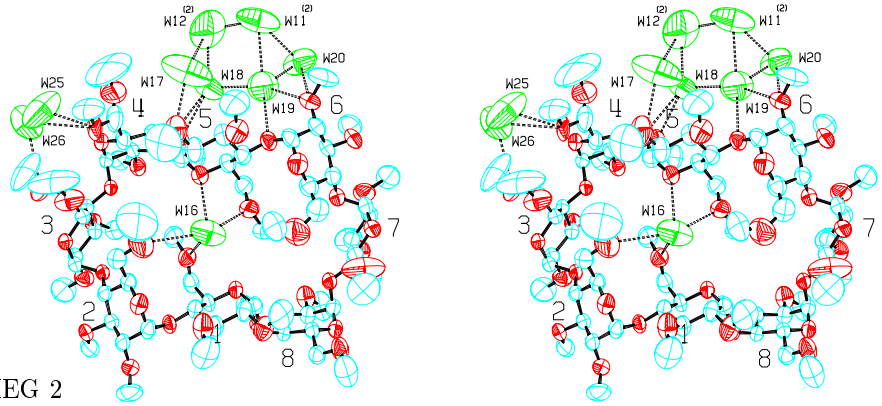


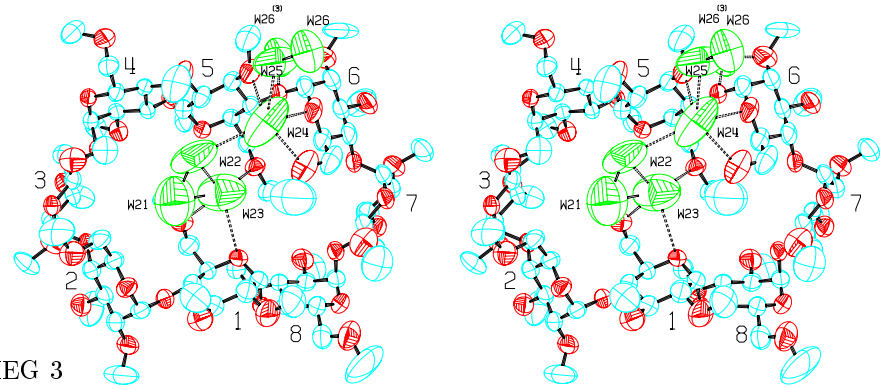
Figure A.3: ORTEP-III stereo plot of TRIMEG·4.5H_2O



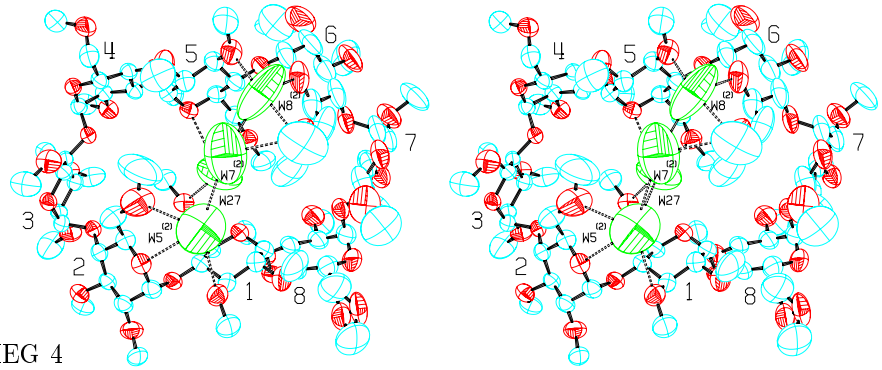
(a) TRIMEG 1



(b) TRIMEG 2



(c) TRIMEG 3



(d) TRIMEG 4

Figure A.4: ORTEP-III stereo plots of four TRIMEG in (4TRIMEG)·19.3H_2O

A.2 Tables of Atomic Coordinates & Temperature Factors

The crystallographic data listed below have been deposited with the Cambridge Crystallographic Data Center and can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: + 44-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk). Quoting numbers CCDC-116999 for DIMEB·2H_2O, CCDC-118694 for DIMEB·15 H_2O, CCDC-117544 for (4TRIMEG)·19.3H_2O, and CCDC-118818 for TRIMEG·4.5H_2O.

Table A.1: Fractional atomic coordinates and equivalent isotropic thermal displacement factors of DIMEB·2H_2O

Atom	*x/a*	*y/b*	*z/c*	*Ueq* (Å^2)
C11	0.6833(3)	0.0128(6)	0.6308(2)	0.0572(12)
C21	0.6449(4)	0.1439(6)	0.6199(2)	0.0628(13)
C31	0.5458(3)	0.1429(5)	0.6213(2)	0.0559(12)
C41	0.4978(3)	0.0442(5)	0.5799(2)	0.0512(11)
C51	0.5425(3)	−0.0825(5)	0.5911(2)	0.0543(11)
C61	0.5049(4)	−0.1789(6)	0.5448(2)	0.0722(15)
C71	0.7151(7)	0.3424(9)	0.6429(5)	0.145(4)
C81	0.4982(7)	−0.3695(9)	0.5947(5)	0.127(3)
O21	0.6944(3)	0.2254(4)	0.66238(18)	0.005(12)
O31	0.5104(3)	0.2651(4)	0.60697(19)	0.774(11)
O41	0.4077(2)	0.0394(4)	0.58835(12)	0.0537(8)
O51	0.6360(2)	−0.0718(4)	0.58938(13)	0.0606(9)
O61	0.5407(3)	−0.3013(5)	0.5581(2)	0.0844(12)
C12	0.3364(3)	0.0581(6)	0.5398(2)	0.0582(13)
C22	0.2733(3)	0.1553(6)	0.5561(2)	0.0610(13)
C32	0.2254(3)	0.1064(6)	0.6021(2)	0.0614(13)
C42	0.1851(3)	−0.0199(6)	0.5858(2)	0.0567(12)
C52	0.2516(3)	−0.1129(6)	0.5680(2)	0.0583(12)
C62	0.2117(4)	−0.2358(7)	0.5454(3)	0.0776(16)
C72	0.2819(7)	0.3826(8)	0.5587(5)	0.124(3)
C82	0.0988(10)	−0.3330(10)	0.4767(6)	0.181(6)
O22	0.3238(3)	0.2653(4)	0.5747(2)	0.0828(12)
O32	0.1596(3)	0.1949(5)	0.6094(2)	0.0839(12)
O42	0.1558(2)	−0.0662(4)	0.63646(13)	0.0596(9)
O52	0.2900(2)	−0.0563(4)	0.52282(14)	0.0642(9)
O62	0.1405(3)	−0.2189(5)	0.4983(2)	0.1005(15)
C13	0.0635(3)	−0.0939(8)	0.6325(3)	0.0779(18)
C23	0.0345(4)	−0.0320(7)	0.6847(3)	0.0758(17)
C33	0.0818(3)	−0.0930(6)	0.7407(2)	0.0612(13)
C43	0.0693(3)	−0.2331(6)	0.7379(2)	0.0626(13)
C53	0.0949(5)	−0.2872(6)	0.6827(2)	0.0699(14)
C63	0.0751(8)	−0.4211(9)	0.6750(3)	0.142(4)
C73	−0.0029(7)	0.1797(9)	0.7106(5)	0.136(4)
C83A[a]	0.0232(12)	−0.5571(11)	0.5971(8)	0.158(7)
C83B[a]	−0.051(3)	−0.515(5)	0.6089(12)	0.29(4)
O23	0.0505(3)	0.0991(5)	0.6826(2)	0.0951(15)
O33	0.0498(3)	−0.0438(5)	0.78967(17)	0.0766(10)
O43	0.1255(2)	−0.2811(4)	0.79001(14)	0.0572(8)
O53	0.0488(3)	−0.2223(5)	0.63249(16)	0.0834(13)
O63A[a]	0.0834(7)	−0.4603(8)	0.6200(3)	0.137(3)
O63B[a]	−0.0080(9)	−0.4777(17)	0.6657(7)	0.111(6)
C14	0.0890(3)	−0.3691(6)	0.8241(2)	0.0609(13)
C24	0.1136(4)	−0.3301(6)	0.8880(2)	0.0599(12)
C34	0.2128(4)	−0.3429(5)	0.9125(2)	0.0567(11)
C44	0.2418(3)	−0.4745(6)	0.9003(2)	0.0610(12)
C54	0.2161(4)	−0.5034(6)	0.8359(3)	0.0711(14)
C64	0.2389(7)	−0.6339(8)	0.8201(4)	0.112(3)
C74	0.0569(4)	−0.1746(7)	0.9458(2)	0.0733(15)
C84	0.2752(13)	−0.748(3)	0.7451(9)	0.289(14)
O24	0.0810(2)	−0.2055(4)	0.89174(15)	0.0659(9)
O34	0.2315(3)	−0.3152(5)	0.97308(17)	0.0790(12)
O44	0.3374(2)	−0.4783(4)	0.92111(16)	0.0626(9)
O54	0.1206(3)	−0.4903(4)	0.81736(17)	0.0720(10)
O64	0.2352(7)	−0.6419(8)	0.7605(3)	0.168(3)
C15	0.3740(4)	−0.5829(6)	0.9545(3)	0.0676(14)
C25	0.4278(4)	−0.5385(7)	1.0124(3)	0.0709(14)
C35	0.5141(4)	−0.4721(6)	1.0046(2)	0.0656(13)
C45	0.5635(3)	−0.5477(5)	0.9666(2)	0.0644(13)
C55	0.5005(4)	−0.5867(6)	0.9095(3)	0.0687(14)
C65	0.5420(5)	−0.6722(8)	0.8717(4)	0.093(2)
C75	0.3682(6)	−0.4880(8)	1.0964(3)	0.103(2)
C85	0.5306(10)	−0.727(2)	0.7736(6)	0.210(8)
O25	0.3754(3)	−0.4563(6)	1.03941(18)	0.0940(14)
O35	0.5681(3)	−0.4504(5)	1.05989(17)	0.0840(12)
O45	0.6333(2)	−0.4675(4)	0.95395(16)	0.0612(8)
O55	0.4262(3)	−0.6545(4)	0.9240(2)	0.0781(11)
O65	0.4985(6)	−0.6555(10)	0.8128(3)	0.173(4)
C16	0.7232(3)	−0.5080(6)	0.9689(2)	0.0614(13)
C26	0.7784(4)	−0.3973(6)	0.9973(2)	0.0631(13)
C36	0.7724(4)	−0.2903(5)	0.9537(2)	0.0550(11)
C46	0.7986(3)	−0.3368(5)	0.8980(2)	0.0507(11)
C56	0.7480(3)	−0.4562(5)	0.8740(2)	0.0537(11)
C66	0.7816(3)	−0.5157(6)	0.8244(2)	0.0626(12)
C76	0.7903(6)	−0.4260(8)	1.1003(3)	0.099(2)
C86	0.9071(5)	−0.5959(7)	0.7943(3)	0.090(2)
O26	0.7507(3)	−0.3573(4)	1.04852(16)	0.0765(11)
O36	0.8276(3)	−0.1897(4)	0.97885(16)	0.0712(10)
O46	0.77881(18)	−0.2370(4)	0.85614(13)	0.0494(7)
O56	0.7548(2)	−0.5489(4)	0.91920(15)	0.0586(8)
O66	0.8745(2)	−0.5368(4)	0.83951(17)	0.0722(10)
C17	0.8486(3)	−0.1914(5)	0.83089(19)	0.0496(10)
C27	0.8444(3)	−0.0487(5)	0.82940(19)	0.0515(11)
C37	0.7625(3)	−0.0017(5)	0.78521(19)	0.0472(10)
C47	0.7601(3)	−0.0650(5)	0.72705(18)	0.0472(10)
C57	0.7622(3)	−0.2071(5)	0.7336(2)	0.0524(11)
C67	0.7615(4)	−0.2762(6)	0.6772(2)	0.0685(14)
C77	0.8840(5)	0.1120(7)	0.9040(3)	0.0847(18)
C87	0.8240(6)	−0.2799(13)	0.5945(3)	0.137(4)
O27	0.8452(2)	−0.0087(4)	0.88758(14)	0.0617(9)
O37	0.7675(3)	0.1308(4)	0.78111(16)	0.0686(9)
O47	0.67918(18)	−0.0235(4)	0.68846(12)	0.0508(7)
O57	0.8428(2)	−0.2404(4)	0.77409(13)	0.0549(8)
O67	0.8294(3)	−0.2308(6)	0.65121(16)	0.0905(14)
W1	0.406(2)	−0.222(5)	0.767(3)	0.72(5)
W2	1.0010(6)	−0.5535(11)	0.9500(4)	0.179(3)

[a] Occupancy factors of disordered O63–C83 are 0.7 and 0.3 for sites A and B, respectively.

Table A.2: Fractional atomic coordinates and equivalent isotropic thermal displacement factors of DIMEB·15H_2O

Atom	*x/a*	*y/b*	*z/c*	*Ueq* (Å^2)
C11	0.4306(5)	−0.1227(3)	−0.0618(2)	0.0608(16)
C21	0.4912(5)	−0.1057(4)	−0.1022(3)	0.0682(18)
C31	0.4693(5)	−0.0377(3)	−0.1190(2)	0.0640(16)
C41	0.3645(5)	−0.0306(3)	−0.1255(2)	0.0588(15)
C51	0.3086(5)	−0.0511(3)	−0.0840(2)	0.0611(15)
C61	0.2014(5)	−0.0523(4)	−0.0913(3)	0.0750(19)
C71	0.6325(7)	−0.1661(5)	−0.1033(5)	0.133(4)
C81	0.0836(7)	−0.0956(7)	−0.1372(5)	0.138(5)
O21	0.5901(3)	−0.1090(3)	−0.09111(18)	0.0808(14)
O31	0.5165(4)	−0.0253(3)	−0.1603(2)	0.0945(17)
O41	0.3511(3)	0.03628(19)	−0.13495(14)	0.0611(11)
O51	0.3359(3)	−0.11559(19)	−0.07206(16)	0.0635(11)
O61	0.1824(4)	−0.0931(3)	−0.1287(2)	0.0946(17)
C12	0.2886(6)	0.0533(4)	−0.1711(2)	0.074(2)
C22	0.3403(8)	0.1001(4)	−0.2017(3)	0.089(3)
C32	0.3530(6)	0.1647(3)	−0.1780(2)	0.076(2)
C42	0.2623(5)	0.1881(3)	−0.1578(2)	0.0622(16)
C52	0.2224(5)	0.1367(3)	−0.1266(3)	0.0633(17)
C62	0.1262(6)	0.1535(4)	−0.1065(4)	0.092(3)
C72	0.440(2)	0.0581(13)	−0.2594(5)	0.36(2)
C82	0.1227(15)	0.1165(8)	−0.0335(5)	0.188(8)
C92[a]	0.4822(15)	0.2185(16)	−0.2115(10)	0.070(8)
O22	0.4295(6)	0.0732(3)	−0.2138(2)	0.113(2)
O32	0.3881(5)	0.2109(3)	−0.2101(2)	0.106(2)
O42	0.2807(3)	0.2455(2)	−0.13272(15)	0.0671(12)
O52	0.2063(4)	0.0795(2)	−0.15374(18)	0.0801(14)
O62	0.0905(6)	0.1070(4)	−0.0785(4)	0.143(3)
C13	0.2343(5)	0.3016(3)	−0.1469(2)	0.0630(17)
C23	0.3013(6)	0.3585(3)	−0.1435(2)	0.0683(18)
C33	0.3257(5)	0.3707(3)	−0.0932(2)	0.0668(18)
C43	0.2344(5)	0.3795(3)	−0.0664(2)	0.0550(15)
C53	0.1687(5)	0.3232(3)	−0.0731(2)	0.0577(15)
C63	0.0772(5)	0.3296(3)	−0.0498(3)	0.081(2)
C73	0.4062(11)	0.3858(7)	−0.2025(5)	0.193(8)
C83A[b]	−0.0801(8)	0.2898(13)	−0.0469(12)	0.159(12)
C83B[b]	−0.0500(11)	0.3942(9)	−0.0341(7)	0.114(7)
O23	0.3842(4)	0.3452(3)	−0.16919(18)	0.0891(16)
O33	0.3838(4)	0.4266(2)	−0.09099(18)	0.0831(15)
O43	0.2628(3)	0.38462(18)	−0.01950(14)	0.0584(10)
O53	0.1526(3)	0.3129(2)	−0.12068(15)	0.0656(11)
O63A[b]	0.0158(7)	0.2774(5)	−0.0544(5)	0.107(4)
O63B[b]	0.0326(7)	0.3878(4)	−0.0600(4)	0.085(3)
C14	0.2292(6)	0.4377(3)	0.0063(3)	0.0612(18)
C24	0.3104(5)	0.4688(3)	0.0303(2)	0.0585(15)
C34	0.3495(5)	0.4249(3)	0.0667(2)	0.0562(15)
C44	0.2717(5)	0.3992(3)	0.0976(2)	0.0564(15)
C54	0.1902(5)	0.3719(3)	0.0696(2)	0.0643(17)
C64	0.1052(6)	0.3560(5)	0.0988(3)	0.097(3)
C74	0.4273(9)	0.5453(5)	0.0038(3)	0.120(4)
C84	0.0431(17)	0.2580(9)	0.0772(6)	0.198(8)
O24	0.3788(4)	0.4851(2)	−0.00305(16)	0.0735(13)
O34	0.4178(3)	0.4596(2)	0.09298(15)	0.0687(12)
O44	0.3130(3)	0.34954(18)	0.12523(13)	0.0568(10)
O54	0.1582(3)	0.4184(2)	0.03716(15)	0.0682(12)
O64	0.0336(6)	0.3232(6)	0.0754(3)	0.156(4)
C15	0.3034(5)	0.3526(3)	0.1731(2)	0.0554(15)
C25	0.3988(5)	0.3450(3)	0.1953(2)	0.0547(15)
C35	0.4393(5)	0.2789(3)	0.1842(2)	0.0557(15)
C45	0.3691(5)	0.2284(3)	0.1995(2)	0.0516(14)
C55	0.2719(5)	0.2394(3)	0.1798(2)	0.0585(15)
C65	0.1973(6)	0.1960(4)	0.2003(3)	0.083(2)
C75	0.4835(11)	0.4416(5)	0.2078(4)	0.137(5)
C85	0.1472(11)	0.1584(8)	0.2731(5)	0.174(7)
O25	0.4623(4)	0.3932(2)	0.17948(17)	0.0739(13)
O35	0.5265(3)	0.2711(2)	0.20748(16)	0.0665(12)
O45	0.4061(3)	0.16845(18)	0.18545(13)	0.0579(11)
O55	0.2403(3)	0.3042(2)	0.18888(14)	0.0624(11)
O65	0.1976(4)	0.2064(3)	0.24828(18)	0.0946(17)
C16	0.4110(6)	0.1176(3)	0.2173(2)	0.0705(19)
C26	0.5115(5)	0.0916(3)	0.2177(2)	0.0629(17)
C36	0.5341(5)	0.0587(3)	0.1735(2)	0.0556(15)
C46	0.4568(5)	0.0096(3)	0.1608(2)	0.0600(16)
C56	0.3614(6)	0.0418(3)	0.1610(3)	0.0691(18)
C66	0.2800(7)	−0.0027(4)	0.1529(5)	0.113(4)
C76	0.6249(10)	0.1404(6)	0.2666(3)	0.133(5)
C86	0.175(2)	0.059(2)	0.0996(9)	0.40(3)
O26	0.5762(4)	0.1422(2)	0.22573(15)	0.0753(14)
O36	0.6235(4)	0.0275(2)	0.17726(16)	0.0709(12)
O46	0.4805(3)	−0.01516(18)	0.11715(14)	0.0590(10)
O56	0.3459(4)	0.0692(2)	0.20595(17)	0.0744(13)
O66	0.1938(5)	0.0321(4)	0.1444(4)	0.148(4)
C17	0.5038(5)	−0.0809(3)	0.1135(2)	0.0562(15)
C27	0.5891(5)	−0.0884(3)	0.0827(2)	0.0625(16)
C37	0.5654(4)	−0.0714(3)	0.0342(2)	0.0535(14)
C47	0.4782(5)	−0.1069(3)	0.0186(2)	0.0557(15)
C57	0.3987(5)	−0.0979(3)	0.0516(2)	0.0577(15)
C67	0.3119(5)	−0.1373(4)	0.0399(3)	0.074(2)
C77	0.7567(5)	−0.0768(4)	0.1014(3)	0.086(2)
C87	0.1517(7)	−0.1495(6)	0.0602(4)	0.122(4)
O27	0.6634(3)	−0.0483(2)	0.10025(18)	0.0743(13)
O37	0.6433(3)	−0.0858(2)	0.00506(16)	0.0688(12)
O47	0.4564(3)	−0.08084(18)	−0.02538(14)	0.0586(10)
O57	0.4272(3)	−0.11648(19)	0.09610(14)	0.0601(11)
O67	0.2395(4)	−0.1221(3)	0.0720(2)	0.0946(17)
W1	0.3475(5)	0.5767(3)	0.1284(2)	0.1057(19)
W2	0.7091(5)	−0.0251(5)	−0.1829(3)	0.118(2)
W3	0.8770(7)	−0.1968(4)	−0.0923(5)	0.175(4)
W4	0.7544(6)	−0.0376(4)	0.2369(3)	0.134(3)
W5	0.0164(9)	−0.2196(6)	−0.0288(4)	0.187(4)
W6	0.3009(6)	−0.2063(4)	0.1504(3)	0.117(2)
W7	0.2010(5)	0.3360(4)	0.2911(2)	0.122(2)
W8	0.7608(10)	−0.1964(6)	0.0039(4)	0.208(5)
W9	0.3772(7)	0.2139(6)	−0.3071(3)	0.171(4)
W10	0.5360(8)	0.3173(6)	0.2983(3)	0.192(5)
W11	0.0427(7)	0.3332(9)	0.3508(3)	0.232(7)
W12	0.3579(9)	0.2822(6)	0.3375(4)	0.195(4)
W13	0.5017(11)	0.5225(9)	−0.1334(7)	0.279(9)
W14	−0.0689(8)	−0.2108(4)	0.0544(4)	0.158(3)
W15	0.2049(10)	−0.2268(4)	−0.0822(7)	0.245(8)

[a] Occupancy factor of C92 is 0.25.

[b] Occupancy factors of disordered O63–C83 are 0.5 for both sites A and B.

Table A.3: Fractional atomic coordinates and equivalent isotropic thermal displacement factors of (4TRIMEG)·19.3H_2O

Atom	*x/a*	*y/b*	*z/c*	*Ueq* (Å^2)
		TRIMEG 1		
C11_1	0.1115(3)	0.5290(4)	0.4273(2)	0.0792(19)
C21_1	0.1309(3)	0.4767(4)	0.3999(3)	0.098(3)
C31_1	0.1698(3)	0.5094(4)	0.3815(3)	0.104(3)
C41_1	0.1580(3)	0.5833(4)	0.3640(3)	0.076(2)
C51_1	0.1352(2)	0.6318(4)	0.3923(2)	0.0726(19)
C61_1	0.1152(3)	0.6993(5)	0.3718(2)	0.085(2)
C71_1	0.1141(7)	0.3536(8)	0.4157(7)	0.204(8)
C81_1	0.2159(5)	0.4177(9)	0.3595(6)	0.200(8)
C91_1	0.0571(4)	0.7405(8)	0.3227(4)	0.130(4)
O21_1	0.1454(3)	0.4109(4)	0.4198(3)	0.120(2)
O31_1	0.1781(3)	0.4648(4)	0.3480(3)	0.143(3)
O41_1	0.19680(19)	0.6241(4)	0.35604(18)	0.0785(14)
O51_1	0.09924(18)	0.5944(4)	0.40736(18)	0.0797(14)
O61_1	0.0831(2)	0.6797(5)	0.3393(2)	0.1001(18)
C12_1	0.2180(2)	0.6039(5)	0.3224(2)	0.083(2)
C22_1	0.2548(2)	0.6600(5)	0.3199(2)	0.0811(19)
C32_1	0.2350(2)	0.7353(4)	0.3133(2)	0.0717(18)
C42_1	0.1980(2)	0.7364(4)	0.2783(2)	0.0700(17)
C52_1	0.1657(3)	0.6719(4)	0.2763(2)	0.0795(19)
C62_1	0.1404(3)	0.6603(6)	0.2346(3)	0.105(3)
C72_1	0.3274(4)	0.6263(14)	0.3529(4)	0.203(9)
C82_1	0.2909(4)	0.8237(7)	0.3392(3)	0.105(3)
C92_1	0.0987(10)	0.5513(8)	0.2437(10)	0.39(2)
O22_1	0.28707(19)	0.6592(5)	0.3550(2)	0.0975(18)
O32_1	0.26751(18)	0.7873(4)	0.30466(18)	0.0811(14)
O42_1	0.17058(18)	0.8007(3)	0.28132(16)	0.0704(12)
O52_1	0.1891(2)	0.6041(4)	0.28640(18)	0.0899(15)
O62_1	0.0995(4)	0.6246(6)	0.2341(3)	0.180(4)
C13_1	0.1727(3)	0.8568(4)	0.2529(2)	0.0781(19)
C23_1	0.1645(2)	0.9291(5)	0.2723(3)	0.083(2)
C33_1	0.1182(2)	0.9302(5)	0.2850(2)	0.0732(18)
C43_1	0.0822(2)	0.9107(5)	0.2505(2)	0.0709(17)
C53_1	0.0945(2)	0.8450(5)	0.2270(2)	0.0751(19)
C63_1	0.0666(3)	0.8406(7)	0.1859(3)	0.099(3)
C73_1	0.2367(4)	0.9773(10)	0.2959(6)	0.168(6)
C83_1	0.1196(4)	1.0141(9)	0.3398(3)	0.137(4)
C93_1	0.0882(10)	0.7711(14)	0.1325(6)	0.286(13)
O23_1	0.1973(2)	0.9440(4)	0.3055(2)	0.1058(19)
O33_1	0.1072(2)	1.0008(4)	0.2984(2)	0.0914(16)
O43_1	0.04034(16)	0.8958(3)	0.26545(16)	0.0698(12)
O53_1	0.14049(17)	0.8471(4)	0.21868(16)	0.0796(14)
O63_1	0.0699(4)	0.7734(6)	0.1682(3)	0.149(3)
C14_1	0.0055(2)	0.9470(5)	0.2571(2)	0.0779(19)
C24_1	−0.0224(3)	0.9508(5)	0.2914(2)	0.088(2)
C34_1	−0.0461(3)	0.8789(5)	0.2974(2)	0.0770(19)
C44_1	−0.0738(3)	0.8574(4)	0.2581(2)	0.0716(18)
C54_1	−0.0460(3)	0.8590(5)	0.2234(2)	0.078(2)
C64_1	−0.0742(3)	0.8508(7)	0.1828(3)	0.117(3)
C74_1	0.0103(4)	1.0476(7)	0.3321(6)	0.176(7)
C84_1	−0.0651(6)	0.8940(11)	0.3654(2)	0.185(7)
C94_1	−0.1153(8)	0.9551(10)	0.1547(7)	0.264(12)
O24_1	0.0042(3)	0.9709(5)	0.3281(2)	0.117(2)
O34_1	−0.0788(3)	0.8870(6)	0.3247(2)	0.152(3)
O44_1	−0.09927(18)	0.7924(4)	0.25969(18)	0.0794(14)
O54_1	−0.02294(19)	0.9280(4)	0.22149(17)	0.0859(15)
O64_1	−0.1120(3)	0.8933(7)	0.1784(3)	0.170(4)
C15_1	−0.0773(3)	0.7237(4)	0.2632(2)	0.082(2)
C25_1	−0.1106(3)	0.6654(5)	0.2463(2)	0.095(2)
C35_1	−0.1467(3)	0.6532(6)	0.2731(2)	0.092(2)
C45_1	−0.1239(2)	0.6353(5)	0.3158(2)	0.0776(19)
C55_1	−0.0922(2)	0.6990(5)	0.3297(2)	0.0724(18)
C65_1	−0.0671(3)	0.6893(5)	0.3708(2)	0.085(2)
C75_1	−0.1183(7)	0.6393(12)	0.1761(4)	0.205(8)
C85_1	−0.2181(5)	0.6137(14)	0.2401(6)	0.231(10)
C95_1	−0.0147(4)	0.6183(7)	0.4115(4)	0.119(4)
O25_1	−0.1310(3)	0.6844(6)	0.2072(2)	0.134(3)
O35_1	−0.1751(3)	0.5945(5)	0.2581(2)	0.123(2)
O45_1	−0.15548(19)	0.6336(3)	0.34453(17)	0.0782(14)
O55_1	−0.05908(18)	0.7076(4)	0.30278(17)	0.0819(14)
O65_1	−0.0424(2)	0.6236(4)	0.3732(2)	0.0929(17)
C16_1	−0.1813(3)	0.5688(5)	0.3455(3)	0.087(2)
C26_1	−0.2119(3)	0.5782(5)	0.3772(2)	0.093(2)
C36_1	−0.1851(3)	0.5874(5)	0.4189(2)	0.085(2)
C46_1	−0.1516(3)	0.5266(5)	0.4276(2)	0.0790(19)
C56_1	−0.1266(3)	0.5068(5)	0.3927(2)	0.088(2)
C66_1	−0.1080(4)	0.4292(6)	0.3977(3)	0.107(3)
C76_1	−0.2842(4)	0.6221(13)	0.3514(8)	0.240(10)
C86_1	−0.2263(4)	0.6535(7)	0.4633(4)	0.129(4)
C96_1	−0.0897(9)	0.3956(16)	0.3340(4)	0.299(15)
O26_1	−0.2402(2)	0.6392(5)	0.3687(3)	0.126(2)
O36_1	−0.2143(2)	0.5841(4)	0.4491(2)	0.1019(18)
O46_1	−0.11866(19)	0.5480(3)	0.46094(16)	0.0756(13)
O56_1	−0.1550(2)	0.5064(3)	0.35445(18)	0.0932(16)
O66_1	−0.0751(3)	0.4158(6)	0.3745(3)	0.149(3)
C17_1	−0.1165(3)	0.5083(5)	0.4967(2)	0.0793(19)
C27_1	−0.1031(2)	0.5593(5)	0.5319(2)	0.086(2)
C37_1	−0.0568(2)	0.5902(4)	0.5299(3)	0.0746(19)
C47_1	−0.0229(2)	0.5298(4)	0.5278(2)	0.0692(17)
C57_1	−0.0392(2)	0.4720(4)	0.4964(3)	0.0721(18)
C67_1	−0.0128(3)	0.4023(5)	0.5016(3)	0.087(2)
C77_1	−0.1694(5)	0.6043(12)	0.5559(5)	0.187(7)
C87_1	−0.0516(5)	0.7072(6)	0.5614(5)	0.159(6)
C97_1	0.0083(6)	0.3047(7)	0.5452(5)	0.180(6)
O27_1	−0.1347(2)	0.6163(5)	0.5329(2)	0.1052(19)
O37_1	−0.0415(2)	0.6315(4)	0.5652(2)	0.1010(18)
O47_1	0.01863(16)	0.5588(3)	0.51643(16)	0.0678(12)
O57_1	−0.08539(18)	0.4501(3)	0.49880(19)	0.0815(14)
O67_1	−0.0163(3)	0.3720(4)	0.5390(2)	0.112(2)
C18_1	0.0553(2)	0.5672(4)	0.5463(2)	0.0731(18)
C28_1	0.0822(3)	0.6340(4)	0.5385(2)	0.0778(19)
C38_1	0.1031(2)	0.6285(3)	0.4993(2)	0.0712(18)
C48_1	0.1278(3)	0.5569(4)	0.4991(2)	0.0732(18)
C58_1	0.1037(3)	0.4912(4)	0.5137(3)	0.080(2)
C68_1	0.1360(3)	0.4279(5)	0.5238(4)	0.098(3)
C78_1	0.0644(5)	0.7385(7)	0.5746(3)	0.127(4)
C88_1	0.1179(4)	0.7513(5)	0.4808(3)	0.101(3)
C98_1	0.1394(6)	0.3013(7)	0.5384(7)	0.201(8)
O28_1	0.0573(2)	0.6988(3)	0.5383(2)	0.0900(16)
O38_1	0.13399(19)	0.6829(3)	0.4959(2)	0.0932(17)
O48_1	0.14394(17)	0.5401(4)	0.46191(17)	0.0743(13)
O58_1	0.08362(19)	0.5055(3)	0.54978(18)	0.0800(14)
O68_1	0.1116(3)	0.3629(4)	0.5272(3)	0.128(3)
		TRIMEG 2		
C11_2	0.3884(3)	0.5411(5)	0.0460(2)	0.087(2)
C21_2	0.3755(3)	0.4868(4)	0.0763(3)	0.098(2)
C31_2	0.3365(4)	0.5150(4)	0.0962(3)	0.095(2)
C41_2	0.3476(3)	0.5903(4)	0.1138(3)	0.081(2)
C51_2	0.3634(3)	0.6413(4)	0.0820(3)	0.078(2)
C61_2	0.3811(3)	0.7127(5)	0.1001(3)	0.097(2)
C71_2	0.3948(6)	0.3635(8)	0.0645(7)	0.199(7)
C81_2	0.2954(8)	0.4180(10)	0.1212(6)	0.243(10)
C91_2	0.4383(5)	0.7640(8)	0.1461(5)	0.152(5)
O21_2	0.3630(3)	0.4188(4)	0.0579(3)	0.130(3)
O31_2	0.3297(4)	0.4679(5)	0.1293(3)	0.148(3)
O41_2	0.3096(2)	0.6274(4)	0.12557(17)	0.0832(15)
O51_2	0.3990(2)	0.6090(4)	0.06413(18)	0.0866(15)
O61_2	0.4164(3)	0.6992(5)	0.1310(2)	0.114(2)
C12_2	0.2911(3)	0.6042(5)	0.1594(2)	0.092(2)
C22_2	0.2553(2)	0.6597(5)	0.1665(3)	0.096(2)
C32_2	0.2763(2)	0.7344(5)	0.1754(2)	0.0808(19)
C42_2	0.3147(2)	0.7305(4)	0.2094(2)	0.0756(18)
C52_2	0.3463(3)	0.6661(4)	0.2055(3)	0.0805(19)
C62_2	0.3743(3)	0.6484(6)	0.2459(3)	0.108(3)
C72_2	0.1872(5)	0.6155(13)	0.1300(5)	0.225(10)
C82_2	0.2217(4)	0.8275(8)	0.1552(3)	0.118(3)
C92_2	0.4402(11)	0.582(3)	0.2691(9)	0.51(3)
O22_2	0.2222(2)	0.6671(5)	0.1325(2)	0.119(2)
O32_2	0.24397(19)	0.7843(4)	0.18698(19)	0.0911(16)
O42_2	0.34225(18)	0.7950(3)	0.20944(16)	0.0701(12)
O52_2	0.3227(2)	0.5998(4)	0.19426(18)	0.0958(16)
O62_2	0.4114(5)	0.6089(10)	0.2377(4)	0.232(6)
C13_2	0.3371(3)	0.8480(4)	0.2388(2)	0.0784(19)
C23_2	0.3479(2)	0.9217(5)	0.2226(3)	0.0807(19)
C33_2	0.3965(2)	0.9243(5)	0.2148(2)	0.0765(18)
C43_2	0.4285(2)	0.9029(5)	0.2519(2)	0.0731(18)
C53_2	0.4125(2)	0.8345(5)	0.2716(2)	0.078(2)
C63_2	0.4352(3)	0.8207(7)	0.3131(2)	0.114(3)

Atom	x/a	y/b	z/c	Ueq (Å^2)
C73_2	0.2872(6)	0.9919(10)	0.1903(6)	0.200(8)
C83_2	0.4093(4)	1.0051(7)	0.1619(3)	0.109(3)
C93A_2[a]	0.441(2)	0.844(3)	0.3826(5)	0.27(3)
C93B_2[a]	0.4452(18)	0.739(3)	0.3672(9)	0.39(4)
O23_2	0.3193(2)	0.9385(5)	0.1870(2)	0.1071(19)
O33_2	0.4081(2)	0.9954(4)	0.20366(19)	0.0863(15)
O43_2	0.47143(16)	0.8866(4)	0.23950(17)	0.0759(14)
O53_2	0.36502(18)	0.8349(4)	0.27507(16)	0.0854(15)
O63A_2[a]	0.4282(9)	0.8684(13)	0.3422(4)	0.173(9)
O63B_2[a]	0.4293(7)	0.7529(10)	0.3269(5)	0.174(7)
C14_2	0.5093(2)	0.9272(5)	0.2559(2)	0.080(2)
C24_2	0.5401(3)	0.9370(4)	0.2240(2)	0.0801(19)
C34_2	0.5557(3)	0.8633(4)	0.2102(2)	0.0740(18)
C44_2	0.5783(3)	0.8213(5)	0.2464(2)	0.084(2)
C54_2	0.5495(3)	0.8197(6)	0.2808(2)	0.103(3)
C64_2	0.5748(4)	0.7906(8)	0.3188(3)	0.158(5)
C74_2	0.5177(4)	1.0541(5)	0.1992(4)	0.112(3)
C84_2	0.5712(5)	0.8785(7)	0.1427(3)	0.118(4)
C94A_2[b]	0.6418(9)	0.802(3)	0.3630(7)	0.60(5)
C94B_2[b]	0.5706(16)	0.727(4)	0.3796(14)	0.19(3)
O24_2	0.5201(2)	0.9773(4)	0.1909(2)	0.0930(16)
O34_2	0.5884(2)	0.8705(4)	0.18377(19)	0.0938(17)
O44_2	0.5915(2)	0.7488(4)	0.23626(19)	0.0936(16)
O54_2	0.5334(2)	0.8915(4)	0.28924(17)	0.0981(18)
O64A_2[b]	0.6140(5)	0.8336(15)	0.3299(5)	0.266(11)
O64B_2[b]	0.5484(9)	0.764(2)	0.3458(6)	0.158(13)
C15_2	0.5590(3)	0.6957(5)	0.2224(3)	0.107(3)
C25_2	0.5773(4)	0.6208(6)	0.2344(3)	0.129(3)
C35_2	0.6163(4)	0.6029(6)	0.2112(2)	0.109(3)
C45_2	0.5996(3)	0.6069(5)	0.1669(2)	0.095(2)
C55_2	0.5793(3)	0.6828(5)	0.1565(2)	0.091(2)
C65_2	0.5575(3)	0.6857(6)	0.1134(3)	0.103(3)
C75_2	0.5675(10)	0.5700(18)	0.2979(6)	0.342(18)
C85_2	0.6664(6)	0.5178(11)	0.2483(6)	0.208(8)
C95_2	0.5044(5)	0.6296(10)	0.0650(4)	0.166(6)
O25_2	0.5926(4)	0.6180(7)	0.2765(3)	0.183(4)
O35_2	0.6279(3)	0.5259(5)	0.2200(3)	0.134(3)
O45_2	0.6361(2)	0.6022(4)	0.1425(2)	0.0971(17)
O55_2	0.5450(2)	0.6988(5)	0.18126(19)	0.1056(19)
O65_2	0.5260(3)	0.6275(5)	0.1057(2)	0.119(2)
C16_2	0.6522(3)	0.5309(6)	0.1368(3)	0.111(3)
C26_2	0.6856(3)	0.5370(6)	0.1067(3)	0.112(3)
C36_2	0.6627(2)	0.5599(6)	0.0660(2)	0.097(2)
C46_2	0.6244(3)	0.5078(6)	0.0523(2)	0.098(2)
C56_2	0.5942(3)	0.4937(7)	0.0839(3)	0.109(3)
C66_2	0.5651(4)	0.4267(8)	0.0756(4)	0.144(4)
C76_2	0.7613(4)	0.5569(15)	0.1324(8)	0.261(11)
C86_2	0.7121(5)	0.6244(9)	0.0285(5)	0.161(5)
C96_2	0.5150(7)	0.424(2)	0.1246(5)	0.314(17)
O26_2	0.7197(2)	0.5878(6)	0.1207(3)	0.149(3)
O36_2	0.6928(2)	0.5568(5)	0.0367(2)	0.119(2)
O46_2	0.5972(2)	0.5395(4)	0.01741(17)	0.0942(16)
O56_2	0.6191(3)	0.4806(4)	0.1229(2)	0.117(2)
O66_2	0.5213(4)	0.4337(9)	0.0851(5)	0.222(6)
C17_2	0.6016(3)	0.5056(5)	−0.0199(2)	0.102(2)
C27_2	0.5927(3)	0.5605(6)	−0.0535(3)	0.103(3)
C37_2	0.5450(3)	0.5883(5)	−0.0586(3)	0.096(2)
C47_2	0.5110(2)	0.5273(4)	−0.0595(3)	0.083(2)
C57_2	0.5250(3)	0.4657(5)	−0.0307(3)	0.091(2)
C67_2	0.5005(4)	0.3946(6)	−0.0424(4)	0.137(4)
C77_2	0.6612(5)	0.6131(13)	−0.0687(6)	0.222(10)
C87_2	0.5433(6)	0.7015(7)	−0.0953(5)	0.172(6)
C97_2	0.4797(7)	0.2891(9)	−0.0069(7)	0.233(9)
O27_2	0.6229(3)	0.6197(5)	−0.0485(3)	0.134(3)
O37_2	0.5341(3)	0.6263(4)	−0.0960(2)	0.111(2)
O47_2	0.46892(17)	0.5563(4)	−0.04895(17)	0.0801(14)
O57_2	0.5721(2)	0.4467(4)	−0.0279(2)	0.1008(18)
O67_2	0.5083(5)	0.3463(7)	−0.0110(5)	0.258(8)
C18_2	0.4316(3)	0.5609(5)	−0.0789(3)	0.084(2)
C28_2	0.4051(3)	0.6291(4)	−0.0716(3)	0.090(2)
C38_2	0.3898(3)	0.6267(4)	−0.0303(3)	0.0799(19)
C48_2	0.3645(3)	0.5570(4)	−0.0255(2)	0.0776(19)
C58_2	0.3868(3)	0.4893(4)	−0.0400(3)	0.082(2)
C68_2	0.3553(4)	0.4257(5)	−0.0444(4)	0.107(3)
C78_2	0.4258(6)	0.7168(8)	−0.1179(4)	0.164(6)
C88_2	0.3790(4)	0.7515(5)	−0.0117(4)	0.102(3)
C98_2	0.3513(7)	0.2985(8)	−0.0529(8)	0.253(12)
O28_2	0.4292(3)	0.6924(4)	−0.0769(2)	0.116(2)
O38_2	0.3594(2)	0.6848(4)	−0.0249(2)	0.0875(16)
O48_2	0.35310(18)	0.5458(4)	0.01391(16)	0.0802(14)
O58_2	0.4026(2)	0.4997(4)	−0.07799(18)	0.0867(15)
O68_2	0.3781(3)	0.3621(4)	−0.0498(3)	0.145(3)
		TRIMEG 3		
C11_3	0.4786(3)	0.2444(6)	0.2764(3)	0.111(3)
C21_3	0.5016(3)	0.2899(6)	0.2468(3)	0.122(3)
C31_3	0.5417(3)	0.2494(6)	0.2353(3)	0.104(2)
C41_3	0.5726(3)	0.2264(6)	0.2720(2)	0.095(2)
C51_3	0.5469(2)	0.1877(6)	0.3032(2)	0.095(3)
C61_3	0.5761(3)	0.1757(7)	0.3424(3)	0.120(3)
C71_3	0.4454(6)	0.3688(9)	0.2132(6)	0.193(7)
C81_3	0.5814(7)	0.3563(8)	0.2164(6)	0.183(6)
C91_3	0.6221(5)	0.2274(13)	0.3969(3)	0.193(8)
O21_3	0.4710(3)	0.3054(7)	0.2126(3)	0.170(4)
O31_3	0.5639(3)	0.2859(6)	0.2064(2)	0.136(2)
O41_3	0.60376(19)	0.1712(4)	0.26429(19)	0.0940(17)
O51_3	0.5090(2)	0.2312(5)	0.31140(19)	0.108(2)
O61_3	0.5963(3)	0.2386(6)	0.3581(2)	0.137(3)
C12_3	0.6390(3)	0.1868(5)	0.2420(2)	0.094(2)
C22_3	0.6663(3)	0.1165(5)	0.2429(3)	0.103(2)
C32_3	0.6843(3)	0.0975(5)	0.2861(3)	0.094(2)
C42_3	0.7124(3)	0.1606(5)	0.3050(2)	0.091(2)
C52_3	0.6881(3)	0.2338(5)	0.2989(2)	0.086(2)
C62_3	0.7173(3)	0.3001(6)	0.3090(3)	0.111(3)
C72_3	0.6429(7)	0.0429(13)	0.1862(4)	0.211(9)
C82_3	0.6903(6)	−0.0308(7)	0.3002(8)	0.213(9)
C92_3	0.7830(6)	0.3597(11)	0.3000(6)	0.218(9)
O22_3	0.6396(3)	0.0581(5)	0.2258(2)	0.128(3)
O32_3	0.7112(3)	0.0333(4)	0.2881(3)	0.125(2)
O42_3	0.72200(18)	0.1482(4)	0.34759(17)	0.0835(15)
O52_3	0.6672(2)	0.2435(4)	0.25825(19)	0.0991(17)
O62_3	0.7534(3)	0.2996(6)	0.2878(3)	0.145(3)
C13_3	0.7674(3)	0.1455(5)	0.3648(2)	0.088(2)
C23_3	0.7734(3)	0.0875(5)	0.3970(2)	0.091(2)
C33_3	0.7466(3)	0.1066(4)	0.4307(2)	0.0764(19)
C43_3	0.7592(3)	0.1819(4)	0.4469(2)	0.0738(18)
C53_3	0.7593(3)	0.2384(4)	0.4137(2)	0.0788(19)
C63_3	0.7823(3)	0.3079(5)	0.4290(3)	0.097(2)
C73_3	0.7931(5)	−0.0182(8)	0.3612(4)	0.151(5)
C83_3	0.7259(6)	−0.0030(7)	0.4616(4)	0.147(5)
C93_3	0.7321(5)	0.4022(8)	0.4086(5)	0.146(4)
O23_3	0.7616(3)	0.0165(4)	0.3826(3)	0.122(2)
O33_3	0.7565(2)	0.0563(4)	0.4630(2)	0.0961(17)
O43_3	0.72640(17)	0.2045(3)	0.47216(15)	0.0687(12)
O53_3	0.78273(19)	0.2130(4)	0.38151(18)	0.0885(16)
O63_3	0.7726(3)	0.3677(4)	0.4027(3)	0.126(2)
C14_3	0.7403(2)	0.2111(4)	0.5138(2)	0.0707(17)
C24_3	0.7024(2)	0.1891(4)	0.5365(3)	0.0716(18)
C34_3	0.6616(2)	0.2380(4)	0.5261(3)	0.0725(18)
C44_3	0.6765(2)	0.3163(4)	0.5352(3)	0.0708(18)
C54_3	0.7188(2)	0.3371(4)	0.5174(3)	0.0771(19)
C64_3	0.7397(3)	0.4082(5)	0.5327(3)	0.102(3)
C74_3	0.7209(4)	0.0665(6)	0.5526(4)	0.122(4)
C84_3	0.5976(3)	0.1658(7)	0.5370(4)	0.112(3)
C94_3	0.7951(4)	0.3895(11)	0.5881(4)	0.158(5)
O24_3	0.6897(2)	0.1155(4)	0.5307(2)	0.0904(16)
O34_3	0.62741(19)	0.2232(4)	0.5506(2)	0.0882(16)
O44_3	0.64109(18)	0.3676(3)	0.52417(17)	0.0779(13)
O54_3	0.75375(17)	0.2833(3)	0.52459(18)	0.0778(13)
O64_3	0.7503(3)	0.4116(5)	0.5736(3)	0.122(2)
C15_3	0.6231(2)	0.3776(5)	0.4840(3)	0.083(2)
C25_3	0.6074(3)	0.4561(4)	0.4782(3)	0.093(2)
C35_3	0.5668(2)	0.4699(4)	0.4997(3)	0.094(2)
C45_3	0.5302(2)	0.4167(4)	0.4827(3)	0.084(2)
C55_3	0.5480(2)	0.3379(4)	0.4885(3)	0.0753(19)
C65_3	0.5149(3)	0.2827(5)	0.4693(3)	0.086(2)
C75_3	0.6557(6)	0.5521(10)	0.4630(6)	0.206(8)
C85_3	0.5639(6)	0.5924(8)	0.5234(6)	0.204(8)
C95_3	0.4724(4)	0.2483(7)	0.4086(4)	0.121(4)
O25_3	0.6427(2)	0.5049(5)	0.4927(3)	0.134(3)
O35_3	0.5511(3)	0.5424(4)	0.4916(3)	0.134(3)
O45_3	0.49116(19)	0.4181(4)	0.5027(2)	0.1031(19)
O55_3	0.58819(18)	0.3291(4)	0.47076(19)	0.0837(15)
O65_3	0.5026(2)	0.3000(4)	0.4279(2)	0.0950(17)
C16_3	0.4612(3)	0.4772(6)	0.4956(3)	0.142(3)
C26_3	0.4198(3)	0.4591(8)	0.5150(3)	0.183(5)
C36_3	0.3943(3)	0.3963(7)	0.4924(3)	0.138(4)

Atom	x/a	y/b	z/c	Ueq (Å^2)
C46_3	0.3832(3)	0.4159(5)	0.4482(3)	0.128(3)
C56_3	0.4254(3)	0.4379(5)	0.4303(3)	0.115(3)
C66_3	0.4160(4)	0.4718(8)	0.3893(3)	0.154(4)
C76_3	0.4141(9)	0.481(2)	0.5845(6)	0.47(3)
C86_3	0.3520(6)	0.3186(12)	0.5299(5)	0.250(11)
C96_3	0.4639(10)	0.4438(18)	0.3406(9)	0.48(3)
O26_3	0.4315(4)	0.4388(10)	0.5558(3)	0.254(7)
O36_3	0.3530(3)	0.3833(7)	0.5077(3)	0.188(5)
O46_3	0.36432(19)	0.3521(4)	0.4269(2)	0.107(2)
O56_3	0.4496(2)	0.4937(4)	0.4552(3)	0.139(3)
O66_3	0.4558(4)	0.4850(8)	0.3732(4)	0.192(5)
C17_3	0.3197(3)	0.3582(5)	0.4071(3)	0.109(3)
C27_3	0.2948(3)	0.2872(5)	0.4104(3)	0.109(3)
C37_3	0.3198(3)	0.2254(5)	0.3918(3)	0.096(2)
C47_3	0.3258(3)	0.2455(4)	0.3495(3)	0.097(2)
C57_3	0.3403(3)	0.3240(5)	0.3432(3)	0.099(2)
C67_3	0.3274(4)	0.3476(6)	0.2999(3)	0.120(3)
C77_3	0.2536(4)	0.3075(9)	0.4648(4)	0.146(5)
C87_3	0.3009(5)	0.1125(7)	0.4224(4)	0.138(4)
C97_3	0.3378(7)	0.4372(12)	0.2524(6)	0.224(9)
O27_3	0.2892(3)	0.2699(5)	0.4497(2)	0.129(2)
O37_3	0.2936(2)	0.1599(4)	0.3890(2)	0.112(2)
O47_3	0.3614(2)	0.2022(4)	0.3362(2)	0.0963(17)
O57_3	0.3188(2)	0.3767(4)	0.3666(2)	0.1063(18)
O67_3	0.3537(4)	0.4071(6)	0.2912(3)	0.165(3)
C18_3	0.3491(3)	0.1411(5)	0.3121(3)	0.102(2)
C28_3	0.3855(3)	0.0845(5)	0.3216(3)	0.103(2)
C38_3	0.4304(3)	0.1135(5)	0.3112(3)	0.098(2)
C48_3	0.4248(2)	0.1423(5)	0.2686(3)	0.101(2)
C58_3	0.3832(3)	0.1882(7)	0.2573(3)	0.107(3)
C68_3	0.3736(4)	0.1931(9)	0.2120(3)	0.148(5)
C78_3	0.3623(5)	−0.0006(8)	0.3682(5)	0.164(5)
C88_3	0.4862(4)	0.0391(8)	0.3501(3)	0.127(4)
C98_3	0.3157(10)	0.2340(13)	0.1641(8)	0.42(2)
O28_3	0.3894(3)	0.0616(4)	0.3617(2)	0.119(2)
O38_3	0.4633(2)	0.0578(5)	0.3125(2)	0.120(2)
O48_3	0.4633(2)	0.1788(4)	0.2574(2)	0.1050(19)
O58_3	0.3437(2)	0.1570(5)	0.2710(2)	0.114(2)
O68_3	0.3423(4)	0.2464(7)	0.2009(3)	0.176(4)
		TRIMEG 4		
C11_4	1.0498(3)	0.2199(6)	0.2121(3)	0.107(3)
C21_4	1.0355(3)	0.2732(6)	0.2427(3)	0.108(3)
C31_4	0.9994(3)	0.2372(6)	0.2641(2)	0.095(2)
C41_4	0.9604(3)	0.2179(6)	0.2328(2)	0.085(2)
C51_4	0.9763(3)	0.1687(6)	0.2004(2)	0.090(2)
C61_4	0.9411(3)	0.1539(6)	0.1654(3)	0.098(2)
C71_4	1.0823(7)	0.3696(9)	0.2707(7)	0.229(10)
C81_4	1.0049(5)	0.2733(11)	0.3328(3)	0.151(5)
C91_4	0.8962(4)	0.2055(11)	0.1101(3)	0.159(6)
O21_4	1.0725(3)	0.2939(7)	0.2705(3)	0.153(3)
O31_4	0.9844(2)	0.2846(5)	0.2927(2)	0.110(2)
O41_4	0.92610(18)	0.1758(4)	0.24842(17)	0.0811(14)
O51_4	1.01319(19)	0.2022(5)	0.18378(18)	0.1001(18)
O61_4	0.9268(2)	0.2179(5)	0.1460(2)	0.115(2)
C12_4	0.8953(3)	0.2123(5)	0.2691(2)	0.085(2)
C22_4	0.8604(3)	0.1584(5)	0.2781(2)	0.085(2)
C32_4	0.8350(3)	0.1280(4)	0.2394(2)	0.0736(18)
C42_4	0.8156(3)	0.1899(4)	0.2127(2)	0.0720(17)
C52_4	0.8481(3)	0.2522(4)	0.2096(3)	0.086(2)
C62_4	0.8240(4)	0.3221(5)	0.1950(4)	0.127(4)
C72_4	0.8909(4)	0.1174(11)	0.3426(3)	0.149(6)
C82_4	0.8079(4)	0.0077(5)	0.2477(3)	0.102(3)
C92_4	0.8508(12)	0.397(2)	0.1460(7)	0.38(2)
O22_4	0.8791(3)	0.0997(5)	0.30212(19)	0.108(2)
O32_4	0.7986(2)	0.0836(4)	0.2472(2)	0.0878(15)
O42_4	0.80334(16)	0.1614(3)	0.17226(15)	0.0679(12)
O52_4	0.8734(2)	0.2712(4)	0.24724(19)	0.0867(15)
O62_4	0.8527(5)	0.3759(6)	0.1861(5)	0.228(6)
C13_4	0.7577(2)	0.1443(4)	0.1608(2)	0.0710(18)
C23_4	0.7533(3)	0.0847(4)	0.1300(2)	0.0716(18)
C33_4	0.7704(3)	0.1087(4)	0.0913(2)	0.0677(17)
C43_4	0.7501(3)	0.1812(4)	0.0762(2)	0.0646(16)
C53_4	0.7487(3)	0.2370(4)	0.1098(2)	0.0711(18)
C63_4	0.7178(3)	0.2998(5)	0.0979(3)	0.092(2)
C73_4	0.7509(6)	−0.0415(7)	0.1483(7)	0.197(8)
C83_4	0.7961(5)	0.0068(6)	0.0564(3)	0.128(4)
C93_4	0.6953(6)	0.3505(8)	0.1574(4)	0.156(5)
O23_4	0.7760(2)	0.0210(4)	0.1448(2)	0.0947(17)
O33_4	0.7604(2)	0.0566(4)	0.06061(19)	0.0902(16)
O43_4	0.77725(17)	0.2114(3)	0.04803(15)	0.0693(12)
O53_4	0.73306(18)	0.2057(3)	0.14498(17)	0.0767(13)
O63_4	0.7230(3)	0.3569(4)	0.1263(3)	0.121(2)
C14_4	0.7581(3)	0.2200(4)	0.0077(2)	0.0702(17)
C24_4	0.7924(2)	0.1988(4)	−0.0196(3)	0.0708(18)
C34_4	0.8345(2)	0.2460(4)	−0.0106(3)	0.0723(18)
C44_4	0.8199(2)	0.3247(4)	−0.0166(3)	0.0737(18)
C54_4	0.7797(2)	0.3462(4)	0.0036(3)	0.0761(19)
C64_4	0.7579(3)	0.4169(5)	−0.0113(3)	0.104(3)
C74_4	0.7704(4)	0.0771(5)	−0.0356(3)	0.109(3)
C84_4	0.8965(4)	0.1728(7)	−0.0280(4)	0.119(3)
C94_4	0.7048(4)	0.3914(9)	−0.0690(4)	0.139(4)
O24_4	0.8047(2)	0.1243(3)	−0.0157(2)	0.0877(15)
O34_4	0.8665(2)	0.2313(4)	−0.0375(2)	0.0934(17)
O44_4	0.85597(18)	0.3756(4)	−0.00885(17)	0.0793(14)
O54_4	0.74418(18)	0.2921(3)	−0.00114(18)	0.0760(13)
O64_4	0.7469(3)	0.4212(5)	−0.0533(3)	0.126(2)
C15_4	0.8780(2)	0.3840(5)	0.0304(3)	0.086(2)
C25_4	0.8955(3)	0.4618(4)	0.0346(3)	0.097(2)
C35_4	0.9325(3)	0.4726(4)	0.0079(3)	0.089(2)
C45_4	0.9695(3)	0.4178(4)	0.0211(3)	0.093(2)
C55_4	0.9497(3)	0.3401(5)	0.0180(3)	0.084(2)
C65_4	0.9835(3)	0.2841(5)	0.0337(3)	0.095(2)
C75_4	0.8520(8)	0.5602(11)	0.0549(6)	0.225(9)
C85_4	0.9348(5)	0.5963(7)	−0.0150(6)	0.174(6)
C95_4	1.0341(4)	0.2461(8)	0.0893(4)	0.129(4)
O25_4	0.8605(2)	0.5121(5)	0.0243(3)	0.123(2)
O35_4	0.9511(3)	0.5444(4)	0.0145(3)	0.125(2)
O45_4	1.0043(2)	0.4139(4)	−0.0043(2)	0.1092(19)
O55_4	0.91274(19)	0.3340(4)	0.04084(19)	0.0894(16)
O65_4	1.0036(2)	0.3003(4)	0.0727(2)	0.1038(19)
C16_4	1.0344(3)	0.4708(6)	−0.0055(4)	0.159(4)
C26_4	1.0702(3)	0.4498(7)	−0.0309(3)	0.202(5)
C36_4	1.0995(4)	0.3879(8)	−0.0104(3)	0.172(5)
C46_4	1.1182(3)	0.4105(6)	0.0323(3)	0.160(4)
C56_4	1.0810(4)	0.4358(6)	0.0556(3)	0.144(3)
C66_4	1.0972(5)	0.4695(10)	0.0958(4)	0.209(6)
C76A_4[c]	1.0262(12)	0.372(2)	−0.0796(6)	0.40(4)
C76B_4[c]	1.0237(12)	0.377(2)	−0.0811(8)	0.32(3)
C86_4	1.1367(7)	0.3072(13)	−0.0504(8)	0.276(12)
C96A_4[d]	1.0576(14)	0.432(2)	0.1490(10)	0.32(2)
C96B_4[d]	1.0644(13)	0.5432(18)	0.1415(9)	0.42(4)
O26_4	1.0538(4)	0.4335(10)	−0.0703(3)	0.295(9)
O36_4	1.1376(3)	0.3757(7)	−0.0310(4)	0.205(5)
O46_4	1.1405(2)	0.3479(4)	0.0529(3)	0.138(3)
O56_4	1.0544(3)	0.4920(4)	0.0328(3)	0.166(3)
O66_4	1.0620(5)	0.4819(9)	0.1179(4)	0.246(7)
C17_4	1.1862(3)	0.3551(6)	0.0687(3)	0.144(3)
C27_4	1.2113(3)	0.2850(5)	0.0634(3)	0.133(3)
C37_4	1.1912(4)	0.2228(5)	0.0856(3)	0.114(3)
C47_4	1.1891(4)	0.2420(5)	0.1286(3)	0.115(3)
C57_4	1.1739(5)	0.3201(5)	0.1354(4)	0.152(4)
C67_4	1.1938(6)	0.3427(8)	0.1784(4)	0.196(7)
C77_4	1.2441(6)	0.3051(11)	0.0041(6)	0.237(11)
C87_4	1.2043(5)	0.1091(8)	0.0536(5)	0.153(5)
C97_4	1.1946(10)	0.4324(15)	0.2271(7)	0.302(14)
O27_4	1.2125(3)	0.2663(6)	0.0234(3)	0.167(4)
O37_4	1.2179(3)	0.1584(5)	0.0856(3)	0.126(2)
O47_4	1.1581(2)	0.1961(4)	0.1459(2)	0.1054(19)
O57_4	1.1916(3)	0.3721(5)	0.1097(3)	0.146(3)
O67_4	1.1717(5)	0.4018(9)	0.1904(5)	0.240(6)
C18_4	1.1757(3)	0.1325(6)	0.1667(3)	0.119(3)
C28_4	1.1405(3)	0.0736(5)	0.1607(3)	0.117(3)
C38_4	1.0972(3)	0.0987(6)	0.1753(3)	0.111(3)
C48_4	1.1075(3)	0.1258(6)	0.2186(3)	0.133(3)
C58_4	1.1479(3)	0.1746(9)	0.2246(3)	0.146(4)
C68_4	1.1603(6)	0.2124(9)	0.2630(4)	0.297(10)
C78_4	1.1522(6)	−0.0151(7)	0.1126(5)	0.164(5)
C88_4	1.0348(4)	0.0299(9)	0.1413(4)	0.149(4)
C98_4	1.1923(8)	0.1922(19)	0.3308(4)	0.356(16)
O28_4	1.1318(3)	0.0521(5)	0.1201(2)	0.126(2)
O38_4	1.0661(3)	0.0407(5)	0.1761(3)	0.145(3)
O48_4	1.0698(2)	0.1583(5)	0.2331(2)	0.128(3)
O58_4	1.1858(2)	0.1491(6)	0.2081(2)	0.145(3)
O68A_4[e]	1.1954(4)	0.1877(17)	0.2903(4)	0.280(13)
O68B_4[e]	1.1753(5)	0.1644(11)	0.2936(4)	0.278(13)
W1[f]	0.0164(5)	0.4372(11)	0.3939(7)	0.201(6)

Atom	x/a	y/b	z/c	Ueq (Å^2)
W2[f]	0.0203(5)	0.5546(12)	0.3278(5)	0.226(7)
W3[f]	0.0706(6)	0.8918(11)	0.3985(5)	0.192(5)
W4[g]	–0.0226(8)	0.548(2)	0.2431(12)	0.447(16)
W5[f]	–0.0567(17)	0.4177(17)	0.2335(16)	0.48(2)
W6[g]	0.0026(7)	0.6751(16)	0.2007(9)	0.362(12)
W7[f]	–0.0424(18)	0.520(4)	0.150(2)	0.58(4)
W8[f]	–0.0051(13)	0.597(2)	0.0859(13)	0.50(3)
W9[f]	–0.020(4)	0.733(6)	0.057(2)	0.24(3)
W10[f]	–0.035(2)	0.679(6)	0.118(2)	0.32(4)
W11[g]	–0.1888(6)	0.7999(13)	0.1937(9)	0.338(11)
W12[f]	–0.2340(13)	0.8232(18)	0.2509(11)	0.37(2)
W13[f]	–0.1781(5)	0.8475(10)	0.3027(7)	0.195(7)
W14[f]	–0.2196(10)	0.7840(10)	0.3480(9)	0.344(11)
W15[f]	–0.267(2)	0.833(2)	0.4063(16)	0.45(3)
W16[f]	0.4670(7)	0.5579(12)	0.1676(9)	0.235(9)
W17[f]	0.6898(8)	0.748(2)	0.2710(13)	0.47(2)
W18[g]	0.6801(5)	0.8168(16)	0.2046(7)	0.320(10)
W19[g]	0.7157(7)	0.7363(13)	0.1521(8)	0.347(11)
W20[f]	0.778(2)	0.754(6)	0.1126(14)	0.31(4)
W21[f]	0.6265(15)	0.400(4)	0.343(2)	0.46(3)
W22[f]	0.615(3)	0.488(6)	0.3782(15)	0.34(4)
W23[g]	0.5578(12)	0.3755(19)	0.3638(9)	0.410(14)
W24[g]	0.5274(8)	0.5736(16)	0.4078(8)	0.395(15)
W25[f]	0.542(3)	0.740(4)	0.439(2)	0.40(5)
W26[f]	0.5152(14)	0.853(2)	0.4181(15)	0.27(2)
W27[g]	0.9633(10)	0.3648(12)	0.1397(6)	0.320(10)

[a] Disordered O63–C93_2 with occupancy factors 0.45 and 0.55 for sites A and B, respectively.

[b] Disordered O64–C94_2 with occupancy factors 0.75 and 0.25 sites A and B, respectively.

[c] Disordered C76_4 with occupancy factors 0.45 and 0.55 for for A and B, respectively.

[d] Disordered C96_4 with occupancy factors 0.53 and 0.47 for sites A and B, respectively.

[e] Disordered O68_4 with occupancy factors 0.50 and 0.50 for sites A and B, respectively.

[f] Disordered water sites with occupancy factors less than 1.00: W1, 0.73; W2, 0.85; W3, 0.78; W5, 0.81; W7, 0.71; W8, 0.78; W9, 0.18; W10, 0.25; W12, 0.61; W13, 0.68; W14, 0.96; W15, 0.61; W16, 0.66; W17, 0.94; W20, 0.27; W21, 0.52; W22, 0.29; W25, 0.32; W26, 0.34.

[g] Fully occupied water sites: W4, W6, W11, W18, W19, W23, W24, W27.

Table A.4: Fractional atomic coordinates and equivalent isotropic thermal displacement factors of TRIMEG·4.5H_2O

Atom	*x/a*	*y/b*	*z/c*	*Ueq* (Å^2)
C11	0.2835(13)	0.1943(4)	0.8977(4)	0.079(4)
C21	0.1829(13)	0.2246(4)	0.8827(4)	0.078(4)
C31	0.0762(12)	0.1979(4)	0.8628(3)	0.063(3)
C41	0.1275(11)	0.1642(4)	0.8311(3)	0.065(3)
C51	0.2303(12)	0.1351(5)	0.8490(4)	0.081(4)
C61	0.2930(19)	0.1017(7)	0.8200(6)	0.143(7)
C71	0.1786(7)	0.2971(2)	0.9162(7)	0.194(11)
C81	−0.1170(14)	0.2367(6)	0.8681(5)	0.118(6)
C91	0.402(2)	0.0878(11)	0.7593(8)	0.282(16)
O21	0.1299(10)	0.2526(2)	0.9131(3)	0.109(4)
O31	−0.0112(10)	0.2274(3)	0.8437(2)	0.085(3)
O41	0.0326(8)	0.1325(2)	0.8182(2)	0.073(2)
O51	0.3253(8)	0.1656(3)	0.8652(3)	0.089(3)
O61	0.3332(13)	0.1223(7)	0.7840(5)	0.196(7)
C12	−0.0460(14)	0.1471(5)	0.7838(4)	0.090(5)
C22	−0.1657(14)	0.1201(5)	0.7836(5)	0.099(5)
C32	−0.1448(13)	0.0705(4)	0.7718(4)	0.076(4)
C42	−0.0708(11)	0.0679(4)	0.7333(4)	0.067(3)
C52	0.0479(13)	0.0949(4)	0.7354(4)	0.081(4)
C62	0.1258(14)	0.0990(4)	0.6969(4)	0.089(4)
C72	−0.3385(16)	0.1475(8)	0.8230(8)	0.199(11)
C82	−0.2778(16)	0.0088(6)	0.7834(6)	0.144(7)
C92	0.027(3)	0.1581(5)	0.6567(5)	0.178(11)
O22	−0.2207(10)	0.1236(4)	0.8232(3)	0.120(4)
O32	−0.2640(9)	0.0516(4)	0.7661(3)	0.108(3)
O42	−0.0461(7)	0.0204(2)	0.7248(2)	0.069(2)
O52	0.0186(10)	0.1423(3)	0.7467(2)	0.087(3)
O62	0.0544(12)	0.1093(3)	0.6612(3)	0.123(4)
C13	−0.0218(11)	0.0062(4)	0.6837(4)	0.068(3)
C23	−0.1127(11)	−0.0308(4)	0.6708(4)	0.066(3)
C33	−0.0915(11)	−0.0749(4)	0.6958(4)	0.065(3)
C43	0.0433(12)	−0.0874(4)	0.6971(4)	0.073(4)
C53	0.1248(10)	−0.0465(4)	0.7066(4)	0.075(4)
C63	0.2613(14)	−0.0590(5)	0.6977(6)	0.111(5)
C73	−0.2787(15)	0.0141(4)	0.6426(5)	0.116(6)
C83	−0.2786(14)	−0.1191(6)	0.6957(6)	0.142(7)
C93	0.448(2)	−0.0236(10)	0.7000(9)	0.236(13)
O23	−0.2390(8)	−0.0179(3)	0.6730(3)	0.099(3)
O33	−0.1573(8)	−0.1128(3)	0.6789(3)	0.084(3)
O43	0.0598(7)	−0.1222(2)	0.7286(2)	0.066(2)
O53	0.0975(8)	−0.0101(3)	0.6796(2)	0.077(2)
O63	0.3302(12)	−0.0245(5)	0.7152(4)	0.152(5)
C14	0.0703(11)	−0.1695(3)	0.7165(4)	0.063(3)
C24	0.0163(13)	−0.2004(4)	0.7487(4)	0.079(4)
C34	0.1044(12)	−0.2022(4)	0.7861(4)	0.070(3)
C44	0.2350(12)	−0.2139(4)	0.7721(3)	0.070(4)
C54	0.2755(10)	−0.1806(4)	0.7416(3)	0.061(3)
C64	0.4025(12)	−0.1897(4)	0.7215(4)	0.077(4)
C74	−0.1889(16)	−0.2225(6)	0.7620(6)	0.149(7)
C84	0.0320(18)	−0.2217(6)	0.8551(4)	0.133(6)
C94	0.5167(13)	−0.2440(5)	0.6850(5)	0.121(6)
O24	−0.1025(8)	−0.1870(3)	0.7606(3)	0.091(3)
O34	0.0554(9)	−0.2361(3)	0.8147(3)	0.099(3)
O44	0.3076(8)	−0.2123(3)	0.8100(2)	0.088(3)
O54	0.1926(7)	−0.1807(3)	0.7061(2)	0.069(2)
O64	0.4075(9)	−0.2346(3)	0.7074(3)	0.099(3)
C15	0.4191(12)	−0.2378(5)	0.8097(4)	0.078(4)
C25	0.4136(14)	−0.2758(4)	0.8429(4)	0.079(4)
C35	0.3973(13)	−0.2558(4)	0.8847(3)	0.072(4)
C45	0.4928(14)	−0.2215(5)	0.8955(4)	0.087(4)
C55	0.5039(12)	−0.1860(4)	0.8609(4)	0.078(4)
C65	0.614(2)	−0.1566(2)	0.8661(4)	0.174(9)
C75	0.3547(8)	−0.3496(2)	0.8204(7)	0.252(14)
C85	0.299(2)	−0.3082(7)	0.9295(6)	0.176(9)
C95	0.5365(4)	−0.0854(4)	0.8249(17)	0.89(9)
O25	0.3185(10)	−0.3051(3)	0.8318(3)	0.112(3)
O35	0.4103(11)	−0.2923(3)	0.9143(3)	0.106(3)
O45	0.4579(8)	−0.1980(3)	0.9327(3)	0.084(3)
O55	0.5193(9)	−0.2082(4)	0.8212(3)	0.103(3)
O65	0.6224(17)	−0.1215(5)	0.8366(5)	0.300(11)
C16	0.5403(13)	−0.2020(5)	0.9660(5)	0.098(5)
C26	0.4694(19)	−0.2091(6)	1.0074(5)	0.117(6)
C36	0.4038(16)	−0.1672(4)	1.0200(4)	0.100(5)
C46	0.4797(14)	−0.1248(5)	1.0203(4)	0.097(5)
C56	0.5513(4)	−0.1198(3)	0.9768(5)	0.107(5)
C66	0.6439(5)	−0.0837(4)	0.9646(2)	0.44(3)
C76	0.443(3)	−0.2872(6)	1.0241(7)	0.226(14)
C86	0.240(3)	−0.1892(8)	1.0652(7)	0.253(15)
C96	0.8297(3)	−0.0739(7)	1.0114(13)	0.62(6)
O26	0.3926(15)	−0.2464(4)	1.0075(3)	0.148(5)
O36	0.3617(14)	−0.1716(3)	1.0616(3)	0.131(5)
O46	0.4039(8)	−0.0829(3)	1.0257(2)	0.075(2)
O56	0.6138(9)	−0.1612(3)	0.9685(3)	0.111(3)
O66	0.7027(11)	−0.0869(6)	1.0024(3)	0.462(17)
C17	0.4176(12)	−0.0631(4)	1.0645(4)	0.071(4)
C27	0.2977(13)	−0.0438(5)	1.0788(4)	0.085(4)
C37	0.2646(12)	0.0014(5)	1.0579(4)	0.080(4)
C47	0.3687(11)	0.0348(4)	1.0561(4)	0.068(4)
C57	0.4796(12)	0.0100(4)	1.0382(4)	0.069(4)
C67	0.5959(14)	0.0381(4)	1.0331(4)	0.088(4)
C77	0.1264(17)	−0.0833(7)	1.1115(6)	0.168(9)
C87	0.0547(16)	0.0347(6)	1.0590(7)	0.158(8)
C97	0.7366(15)	0.0869(5)	1.0667(5)	0.119(6)
O27	0.1991(9)	−0.0759(4)	1.0761(3)	0.111(3)
O37	0.1618(9)	0.0205(4)	1.0808(3)	0.117(4)
O47	0.3312(8)	0.0727(3)	1.0319(2)	0.074(2)
O57	0.5100(7)	−0.0279(3)	1.0647(2)	0.070(2)
O67	0.6238(9)	0.0608(3)	1.0695(3)	0.093(3)
C18	0.3779(14)	0.1160(5)	1.0412(4)	0.082(4)
C28	0.2706(13)	0.1514(4)	1.0440(3)	0.075(4)
C38	0.2097(13)	0.1583(5)	1.0016(4)	0.082(4)
C48	0.3046(13)	0.1685(4)	0.9682(4)	0.076(4)
C58	0.4093(13)	0.1339(4)	0.9708(4)	0.076(4)
C68	0.5139(16)	0.1432(5)	0.9400(5)	0.119(6)
C78	0.1688(19)	0.1552(4)	1.1099(3)	0.236(14)
C88	0.0041(16)	0.1906(7)	0.9949(6)	0.151(8)
C98	0.6821(3)	0.2030(6)	0.9521(8)	0.248(14)
O28	0.1819(12)	0.1370(4)	1.0714(3)	0.122(4)
O38	0.1265(11)	0.1967(3)	1.0071(3)	0.112(3)
O48	0.2383(8)	0.1676(3)	0.9307(3)	0.075(2)
O58	0.4630(9)	0.1314(3)	1.0112(3)	0.093(3)
O68	0.5548(6)	0.1892(4)	0.9449(6)	0.186(7)
W1[a]	−0.148(6)	−0.1015(9)	0.8100(9)	0.28(3)
W2[a]	0.185(7)	−0.132(3)	0.9247(14)	0.38(4)
W3[a]	0.127(4)	−0.0945(14)	0.9805(17)	0.36(3)
W4[a]	0.545(7)	0.018(2)	0.916(2)	0.21(3)
W5[a]	0.442(11)	−0.020(4)	0.922(3)	0.30(4)
W6[a]	0.386(8)	0.013(3)	0.904(2)	0.21(3)
W7[a]	0.258(10)	0.014(3)	0.926(3)	0.27(4)
W8[a]	0.286(11)	−0.036(4)	0.813(3)	0.32(5)
W9[a]	0.214(9)	−0.080(3)	0.840(3)	0.26(4)
W10[a]	0.067(10)	−0.073(3)	0.830(3)	0.26(4)
W11[a]	0.051(8)	−0.032(3)	0.835(3)	0.24(3)
W12[a]	−0.072(6)	0.055(2)	0.9401(19)	0.18(2)
W13[a]	−0.056(6)	0.057(2)	0.8934(19)	0.17(2)
W14[a]	−0.112(5)	0.0902(18)	0.9103(16)	0.142(16)
W15[a]	−0.200(7)	0.065(2)	0.896(2)	0.20(3)

[a] Occupancy factors of water sites W1, W2, W3, and W4 to W15 are 0.50, 0.40, 0.60, and 0.25, respectively.

A.3 Tables of Hydrogen Bonds

Lists of O–H···O and C–H···O hydrogen bonds are given for O···O and C···O separation within 3.5 Å distance.

Table A.5: O–H···O and C–H···O hydrogen bonds in DIMEB·2H_2O

Interaction	Distance
W2···O36$^{(1)a}$	3.15(1)
W2···O66	2.89(1)
C24···W2$^{(2)}$	3.42(1)
C74···W2$^{(3)}$	3.04(1)
C11···O67	3.39(1)
C84···O32$^{(4)}$	3.35(2)
O35···O55$^{(5)}$	3.17(1)
C15···O26$^{(6)}$	3.48(1)
C75···O27$^{(6)}$	3.36(1)
C76···O33$^{(6)}$	3.40(1)
C86···O54$^{(7)}$	3.38(1)
C27···O33$^{(7)}$	3.44(1)
C87···O53$^{(7)}$	3.43(1)
C87···O63B$^{(7)}$	3.45(2)

[a] Superscripts in parentheses describe equivalent positions: (1) $-x+2$, $y-0.5$, $-z+2$; (2) $x-1$, y, z; (3) $-x+1$, $y+0.5$, $-z+2$; (4) x, $y-1$, z; (5) $-x+1$, $y+0.5$, $-z+2$; (6) $-x+1$, $y-0.5$, $-z+2$; (7) $x+1$, y, z.

Table A.6: O–H···O and C–H···O hydrogen bonds in DIMEB·15H_2O

Interaction	Distance
W1···W2$^{(1)a}$	2.75(1)
W1···W3$^{(1)}$	2.75(1)
W1···O34	2.83(1)
W2···W4$^{(2)}$	2.74(1)
W2···O31	2.81(1)
W3···W5$^{(3)}$	2.75(2)
W3···W6$^{(4)}$	2.85(1)
W3···W8	3.26(2)
W4···W7$^{(5)}$	2.83(1)
W4···O36	2.89(1)
W5···W14	2.72(2)
W5···W15	3.10(2)
W6···W9$^{(6)}$	2.82(1)
W6···W10$^{(5)}$	2.80(1)
W6···O57	3.04(1)
W6···O67	3.02(1)
W7···W11	2.84(1)
W7···W12	2.84(2)
W7···O55	3.11(1)
W7···O65	2.98(1)
W8···W14$^{(3)}$	2.84(2)
W8···W15$^{(4)}$	2.90(2)
W8···O37	2.84(1)
W9···W11$^{(7)}$	2.84(2)
W9···O32	2.84(1)
W10···W12	2.86(2)
W10···O35	2.83(1)
W10···O57$^{(8)}$	3.42(1)
W11···W13$^{(9)}$	3.11(3)
W11···W14$^{(10)}$	2.94(2)
W12···W15$^{(6)}$	2.76(2)
W13···O33	2.88(2)
W13···O66$^{(7)}$	2.97(2)
W15···O51	2.98(1)
W15···O61	3.12(1)
O62···O34$^{(1)}$	2.84(1)
O62···O25$^{(1)}$	3.47(1)
O53···O26$^{(1)}$	3.39(1)
O63B···O46$^{(1)}$	3.22(1)
C11···W14$^{(4)}$	3.48(1)
C81···W1$^{(1)}$	3.38(1)
C62···O25$^{(1)}$	3.30(1)
C72···W13$^{(11)}$	3.33(3)
C92···W9	3.17(3)
C13···O26$^{(1)}$	3.42(1)
C14···O37$^{(1)}$	3.33(1)
C34···O62$^{(7)}$	3.49(1)
C36···O63B$^{(7)}$	3.50(1)
C76···W1$^{(5)}$	3.37(1)
C86···W13$^{(1)}$	3.14(4)
C17···W10$^{(5)}$	3.39(1)
C87···W14	3.38(2)

[a] Superscripts in parentheses describe equivalent positions: (1) $x-0.5$, $-y+0.5$, $-z$; (2) $-x+1.5$, $-y$, $z-0.5$; (3) $x+1$, y, z; (4) $x+0.5$, $-y-0.5$, $-z$; (5) $-x+1$, $y-0.5$, $-z+0.5$; (6) $-x+0.5$, $-y$, $z+0.5$; (7) $x+0.5$, $-y+0.5$, $-z$; (8) $-x+1$, $y+0.5$, $-z+0.5$; (9) $-x+0.5$, $-y+1$, $z+0.5$; (10) $-x$, $y+0.5$, $-z+0.5$; (11) $-x+1$, $y-0.5$, $-z-0.5$.

Table A.7: O–H···O and C–H···O hydrogen bonds in (4TRIMEG)·19.3H_2O

Interaction	Distance
W1···W2	3.063
W1···O66_1	2.744
W2···W4	2.919
W2···O51_1	3.360
W2···O61_1	2.923
W2···O65_1	2.849
W3···O24_1	3.179
W3···O67_1$^{(1)a}$	2.830
W4···W5	2.562
W4···W6	2.843
W4···W7	3.092
W5···W7	3.388
W5···W27$^{(2)}$	3.381
W5···O31_4$^{(2)}$	3.231
W5···O52_4$^{(2)}$	3.438
W5···O62_4$^{(2)}$	3.027
W6···W7	3.437
W6···W10	2.806
W6···O62_1	3.088
W6···O63_1	2.993
W7···W8	2.910
W7···W10	3.074
W7···W27$^{(2)}$	2.820
W8···W9	2.648
W8···W10	2.096
W8···O35_4$^{(2)}$	2.711
W8···O56_4$^{(2)}$	3.279
W8···O66_4$^{(2)}$	2.982
W9···W10	2.366
W11···W12	2.510
W11···W19$^{(2)}$	3.201
W11···W20$^{(2)}$	2.854
W11···O44_1	3.210
W11···O64_1	2.946
W11···O25_1	2.707
W12···W13	2.258
W12···W14	3.267
W12···W17$^{(2)}$	2.817
W12···W18$^{(2)}$	2.801
W13···W14	2.372
W13···O34	3.039
W13···O44	3.084
W14···W15	2.702
W14···O45_1	3.329
W14···O26_1	2.790
W16···O61_2	3.115
W16···O62_2	3.180
W16···O55_2	3.431
W16···O65_2	3.145
W17···W18	2.510
W17···O44_2	2.997
W18···W19	2.606
W18···O34_2	2.896
W18···O44_2	3.226
W19···W20	2.436
W19···O45_2	3.373
W19···O26_2	2.880
W20···O26_2	3.490
W21···W22	2.027
W21···W23	2.297
W21···O61_3	3.090
W22···W23	2.656
W22···W24	3.326
W23···O51_3	3.343
W23···O61_3	2.738
W23···O65_3	3.178
W24···W25	3.186
W24···O35_3	2.827
W24···O56_3	3.316
W24···O66_3	2.785
W25···W26	2.261
W25···O64B_2^{b}	3.131
W26···O63A_2^{c}	3.366
W26···O64B_2^{b}	3.155
W26···O45_3$^{(3)}$	2.914
W26···O26_3$^{(3)}$	2.298
W27···O61_4	2.881
W27···O55_4	3.455
W27···O65_4	2.918
C11_1···W1	3.339
C21_1···W1	3.473
C71_1···W1	3.270
C81_1···O57_3	3.138

Interaction	Distance
C91_1···O43_1	3.377
C91_1···O55_1	3.493
C82_1···O53_2	3.285
C83_1···W3	3.408
C94_1···O23_4$^{(4)}$	3.427
C15_1···W6	3.488
C25_1···W4	3.386
C75_1···W7	3.329
C75_1···W10	3.416
C95_1···W1	3.464
C95_1···W2	3.309
C95_1···O51_1	3.453
C96_1···O31_4$^{(2)}$	3.411
C88_1···O51_1	3.096
C81_2···O57_4$^{(2)}$	3.176
C91_2···O55_2	3.443
C82_2···O53_1	3.448
C13_2···O32_1	3.403
C93B_2^{d}···W25	3.495
C93A_2^{c}···W26	2.359
C93B_2^{d}···W26	3.232
C74_2···O48_3$^{(5)}$	3.500
C84_2···O58_2$^{(6)}$	3.234
C94A_2^{e}···W15$^{(7)}$	2.945
C94B_2^{b}···W24	3.238
C94B_2^{b}···W25	2.243
C94B_2^{b}···W26	3.187
C75_2···W22	3.214
C95_2···O51_2	3.167
C26_2···O63_4	3.463
C96_2···W16	3.235
C78_2···O31_3$^{(6)}$	3.242
C81_3···O35_2	3.352
C91_3···W23	3.379
C91_3···O55_3	3.329
C72_3···O34_2$^{(8)}$	3.500
C73_3···W13$^{(9)}$	3.292
C83_3···W15$^{(9)}$	3.500
C83_3···O36_3$^{(10)}$	3.388
C25_3···W22	3.405
C75_3···W22	3.117
C95_3···O51_3	3.561
C26_3···W26	3.337

Interaction	Distance
C76_3···W26	3.138
C86_3···W25	3.458
C96_3···W23	3.062
C97_3···O52_2	3.500
C78_3···O63_2$^{(8)c}$	3.269
C91_4···O55_4	3.349
C82_4···W13$^{(9)}$	3.409
C82_4···O32_3	3.384
C92_4···W27	3.434
C83_4···O36_4$^{(11)}$	3.267
C93_4···O56_2	3.354
C65_4···W9$^{(7)}$	3.462
C95_4···O51_4	3.374
C76A_4^{f}···W9$^{(7)}$	2.625
C76B_4^{g}···W9$^{(7)}$	2.714
C96A_4^{h}···W27	3.042
C96B_4^{i}···W7$^{(7)}$	3.271
C96B_4^{i}···W8$^{(7)}$	2.753
C87_4···O25_4$^{(11)}$	3.474
C98_4···O37_3$^{(7)}$	3.403

[a] Superscripts in parentheses describe equivalent positions: (1) $-x$, 0.5 + y, 1 − z; (2) –1 + x, y, z; (3) 1 − x, 0.5 + y, 1 − z; (4) –1 + x, 1 + y, z; (5) x, 1 + y, z; (6) 1 − x, 0.5 + y, $-z$; (7) 1 + x, y, z; (8) x, –1 + y, z; (9) 1 + x, –1 + y, z; (10) 1 − x, –0.5 + y, 1 − z; (11) 2 − x, –0.5 + y, $-z$.

[b] Disordered O64–C94_2 with occupancy factor 0.25 for site B.

[c] Disordered O63–C93_2 with occupancy factor 0.45 for site A.

[d] Disordered C93_2 with occupancy factor 0.55 for site B.

[e] Disordered C94_2 with occupancy factor 0.75 for site A.

[f,g] Disordered C76_4 with occupancy factors 0.45 and 0.55 for sites A and B, respectively.

[h,i] Disordered C96_4 with occupancy factors 0.53 and 0.47 for sites A and B, respectively.

Table A.8: O–H···O and C–H···O hydrogen bonds in TRIMEG·4.5H_2O

Interaction	Distance
W1···W10	2.54(11)
W1···W11	3.06(10)
W1···O43	3.50(4)
W1···O24	2.99(3)
W1···O65$^{(1)a}$	2.69(6)
W2···W3	2.19(8)
W2···W9	3.12(11)
W3···O46	3.34(4)
W3···O27	3.23(5)
W4···W15$^{(2)}$	3.13(11)
W6···W8	3.43(13)
W8···O63	3.20(10)
W11···W13	3.40(11)
W13···O41	3.40(6)
W13···O22	3.47(6)
W14···O22	3.20(5)
W15···O22	2.92(7)
C65···W1$^{(2)}$	3.50(5)
C95···W1$^{(2)}$	3.47(6)
C96···W3$^{(2)}$	3.41(4)
C11···O68	3.30(2)
C12···O31	3.05(2)
C13···O62	3.19(2)
C14···O33	3.20(1)
C15···O64	3.31(2)
C16···O35	3.41(2)
C17···O36	3.21(2)
C18···O67	3.23(2)
C81···O54$^{(3)}$	3.49(2)
C92···O34$^{(3)}$	3.33(2)
C92···O36$^{(4)}$	3.32(2)
C23···O67$^{(4)}$	3.39(2)
C93···O23$^{(2)}$	3.49(3)
C17···O62$^{(5)}$	3.41(2)
C98···O38$^{(6)}$	3.25(2)

[a] Superscripts in parentheses describe equivalent positions: (1) $x-1$, y, z; (2) $x+1$, y, z; (3) $-x$, $y+0.5$, $-z+1.5$; (4) $-x+0.5$, $-y$, $z-0.5$; (5) $-x+0.5$, $-y$, $z+0.5$; (6) $x+0.5$, $-y+0.5$, $-z+2$.