

Table S1 Results of $\text{Mg}(\text{ClO}_4)_2(\text{H}_2\text{O})_4$ structure refinement in $C2$ space groupFractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Mg	0.00000	0.00000	0.00000	0.0288
Cl	0.2976 (2)	0.002 (4)	0.3937 (5)	0.0405
O1	0.1635 (4)	-0.010 (3)	0.3194 (7)	0.0475
O2	0.3305 (11)	0.144 (3)	0.305 (4)	0.1259
O21	0.3358 (12)	-0.148 (3)	0.311 (4)	0.0997
O3	0.3512 (5)	0.004 (5)	0.6544 (12)	0.0812
O4	0.00000	0.251 (5)	0.00000	0.0619
O41	0.00000	-0.253 (4)	0.00000	0.0576
O5	-0.1013 (14)	0.009 (6)	0.221 (4)	0.0563
H1	0.070 (8)	0.258 (9)	0.11 (2)	0.01 (2)*
H11	0.034 (5)	-0.344 (8)	0.148 (11)	0.01 (2)*
H2	-0.100 (11)	-0.12 (2)	0.285 (17)	0.01 (2)*
H21	-0.141 (5)	0.115 (19)	0.17 (2)	0.01 (2)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg	0.028 (3)	0.038 (6)	0.023 (4)	0.0000	0.013 (3)	0.0000
Cl	0.027 (4)	0.045 (3)	0.049 (6)	-0.002 (5)	0.014 (3)	-0.009 (6)
O1	0.022 (6)	0.102 (10)	0.018 (6)	-0.046 (14)	0.006 (5)	-0.033 (12)
O2	0.063 (11)	0.135 (15)	0.15 (2)	-0.057 (9)	0.003 (11)	0.102 (10)
O21	0.164 (15)	0.060 (10)	0.138 (15)	0.020 (11)	0.130 (11)	0.019 (12)
O3	0.057 (8)	0.108 (10)	0.042 (8)	0.005 (17)	-0.023 (6)	-0.069 (13)
O4	0.06 (2)	0.10 (2)	0.03 (4)	0.0000	0.03 (3)	0.0000
O41	0.07 (2)	-0.010 (11)	0.07 (3)	0.0000	-0.03 (2)	0.0000
O5	0.069 (5)	0.073 (7)	0.047 (5)	0.074 (15)	0.044 (3)	0.012 (15)

Geometric parameters (\AA , $^\circ$)

Cl—O1	1.435 (6)	Mg—O41	2.02 (4)
Cl—O2	1.36 (4)	Mg—O5	2.06 (2)
Cl—O21	1.43 (4)	O4—H1	0.81 (8)
Cl—O3	1.432 (7)	O41—H11	1.10 (7)
Mg—O1	2.103 (4)	O5—H2	1.07 (18)
Mg—O4	2.01 (4)	O5—H21	0.95 (15)
O1—Cl—O2	111.2 (17)	O4—Mg—O5	88.0 (14)
O1—Cl—O21	105.6 (18)	O41—Mg—O5	92.0 (14)
O1—Cl—O3	107.7 (4)	O5—Mg—O5 ⁱ	176 (3)
O2—Cl—O21	113.6 (13)	Mg—O4—H1	94 (6)
O2—Cl—O3	110 (2)	H1—O4—H1 ⁱ	173 (12)
O21—Cl—O3	109 (2)	Mg—O41—H11	132 (4)
O1—Mg—O1 ⁱ	175.4 (12)	H11—O41—H11 ⁱ	96 (7)
O1—Mg—O4	92.3 (6)	Mg—O5—H2	105 (8)
O1—Mg—O41	87.7 (6)	Mg—O5—H21	98 (8)
O1—Mg—O5	87.3 (4)	H2—O5—H21	152 (9)
O1—Mg—O5 ⁱ	92.8 (4)		

Symmetry code: (i) $-x, y, -z$.

Table S2 Comparison of atomic coordinates and their estimated standard uncertainties (e.s.u.) for $\text{Mg}(\text{ClO}_4)_2(\text{H}_2\text{O})_4$ structure models refined in space groups $C2/m$ and $C2$.

Atom, coordinate	$C2/m$		$C2$		Δ	$ \Delta / \text{e.s.u.}$
	value	e.s.u.	value	e.s.u.		
Cl, x	0.2974	0.0002	0.2976	0.0002	-0.0002	0.71
O1, x	0.1627	0.0003	0.1635	0.0004	-0.0008	1.60
O2, x	0.3321	0.0002	0.3305	0.0011	0.0016	1.43
O2, x	0.3321	0.0002	0.3358	0.0012	-0.0037	3.04
O3, x	0.3507	0.0003	0.3512	0.0005	-0.0005	0.86
O5, x	-0.1013	0.0004	-0.1013	0.0014	0.0000	0.00
Cl, y	0.0000	0.0000	0.0022	0.0040	-0.0022	0.55
O1, y	0.0000	0.0000	-0.0104	0.0028	0.0104	3.71
O2, y	0.1458	0.0003	0.1438	0.0030	0.0020	0.66
O2, y	-0.1458	0.0003	-0.1480	0.0028	0.0022	0.78
O3, y	0.0000	0.0000	0.0044	0.0045	-0.0044	0.98
O4, y	0.2513	0.0005	0.2513	0.0048	0.0000	0.00
O4, y	-0.2513	0.0005	-0.2528	0.0044	0.0015	0.34
O5, y	0.0000	0.0000	0.0092	0.0061	-0.0092	1.51
Cl, z	0.3935	0.0005	0.3937	0.0005	-0.0002	0.28
O1, z	0.3207	0.0006	0.3194	0.0007	0.0013	1.41
O2, z	0.3056	0.0006	0.3046	0.0037	0.0010	0.27
O2, z	0.3056	0.0006	0.3111	0.0038	-0.0055	1.43
O3, z	0.6526	0.0008	0.6544	0.0012	-0.0018	1.25
O5, z	0.2218	0.0009	0.2213	0.0036	0.0005	0.13
H1, x	0.0362	0.0046	0.0696	0.0075	-0.0334	3.80
H1, x	0.0362	0.0046	0.0342	0.0052	0.0020	0.29
H2, x	-0.1237	0.0024	-0.1004	0.0113	-0.0233	2.02
H2, x	-0.1237	0.0024	-0.1413	0.0048	0.0176	3.28
H1, y	0.3117	0.0037	0.2578	0.0095	0.0539	5.29
H1, y	-0.3117	0.0037	-0.3443	0.0083	0.0326	3.59
H2, y	-0.0988	0.0038	-0.1156	0.0224	0.0168	0.74
H2, y	0.0988	0.0038	0.1145	0.0192	-0.0157	0.80
H1, z	0.1209	0.0060	0.1079	0.0243	0.0130	0.52
H1, z	0.1209	0.0060	0.1482	0.0105	-0.0273	2.26
H2, z	0.2218	0.0056	0.2851	0.0165	-0.0633	3.63
H2, z	0.2218	0.0056	0.1680	0.0216	0.0538	2.41
$< \text{e.s.u.} > = 0.0019$		$< \text{e.s.u.} > = 0.0066$				

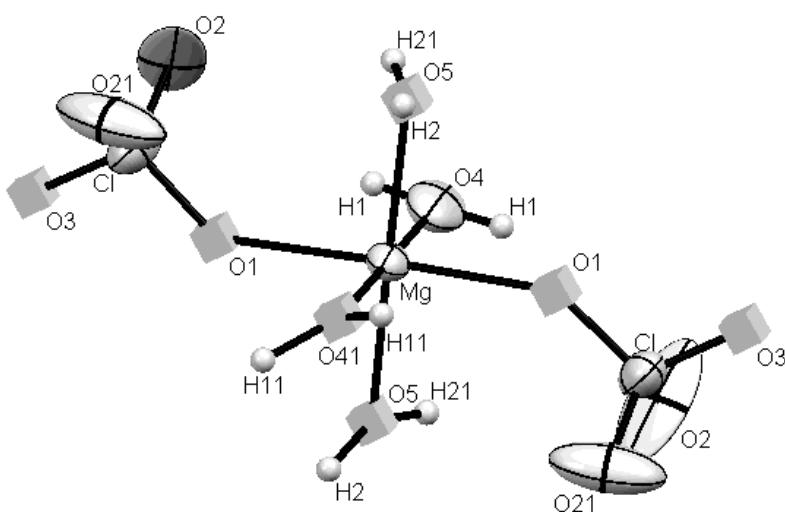


Figure S1 Ellipsoid plot of $\text{Mg}(\text{ClO}_4)_2(\text{H}_2\text{O})_4$ crystal structure refined in $C2$ space group. Invalid displacement ellipsoids are shown by cubes.