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Table S1. Crystallographic Data and Details of the Structure Determination for [(1*R*,2*R*)-$C_6H_{10}(NH_3)_2$][$Ga(OH)(HPO_4)_2$]·H_2O (**1**) and [*trans*-1,2-$C_6H_{10}(NH_3)_2$][$Ga(OH)(HPO_4)_2$]·H_2O (**2**)

	1	**2**
Crystal Data		
empirical formula	$C_6GaH_{21}N_2O_{10}P_2$	$C_6GaH_{21}N_2O_{10}P_2$
fw	412.91	412.91
color, habit	colorless, plate	colorless, plate
size (mm)	0.38 × 0.06 × 0.02	0.22 × 0.09 × 0.02
crystal system	monoclinic	orthorhombic
space group	$P2_1$ (No. 4)	*Pbcm* (No. 57)
a, Å	8.7208(2)	8.6993(2)
b, Å	7.1276(2)	21.8612(1)
c, Å	11.1411(4)	7.1557(2)
β, °	96.129(1)	
V, Å^3	688.55(5)	1360.85(5)
Z	2	4
T, °C	23	23
μ(Mo Kα), cm^{-1}	22.8	23.1
ρ_{calcd}, g·cm^{-3}	1.992	2.015
F(000)	424	848
Data Collection		
diffractometer used	Siemens Smart CCD	Siemens Smart CCD
radiation	Mo Kα (λ = 0.71073 Å)	Mo Kα (λ = 0.71073 Å)
monochromator	graphite crystal	graphite crystal
maximum 2θ, °	56.2	56.2
scan speed	20 sec per frame	20 sec per frame
reflection collected	4090	7930
obsd unique reflns ($F_o > 4\ \sigma(F_o)$)	2118	1087
$T_{min/max}$	0.863/0.919	0.720/0.942
R_{int}	0.0342	0.0893

Solution and Refinement

system used	Siemens SHELXTL PC	Siemens SHELXTL PC
solution	direct methods	direct methods
secondary extinction coefficient	0.0085	0.0044
weighting scheme	a = 0.0807, b = 0.53	a = 0.0558, b = 6.90
number of parameters	190	132
Flack x parameter	0.06(4)	
R1[a]	0.0514	0.0591
wR2[b]	0.1317	0.1324
Goodness-of-fit	1.085	1.135
$(\Delta\rho)_{max}$, $(\Delta\rho)_{min}$	0.74, -0.57	0.82, -0.44

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$

[b] $wR2 = \{\Sigma\,[w(F_o^2 - F_c^2)^2]/[w(F_o^2)^2]\}^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (a*P)^2 + b*P]$ with $P = (MaxF_o^2 + 2*F_c^2)/3$.

Table S2. Atomic coordinates and thermal parameters (A**2) for [(1R,2R)-C6H10(NH3)2][Ga(OH)(HPO4)2].H2O

ATOM	x	y	z	sof	U11	U22	U33	U23	U13	U12	Ueq
Ga	-0.00114	0.13960	-0.00339	1.00000	0.01257	0.00743	0.01764	-0.00058	0.00146	0.00020	0.01256
	0.00020	0.00000	0.00014	0.00000	0.00033	0.00034	0.00039	0.00030	0.00024	0.00027	0.00023
P1	-0.28242	-0.11183	-0.13794	1.00000	0.01106	0.01168	0.01694	0.00208	0.00084	-0.00072	0.01327
	0.00017	0.00066	0.00014	0.00000	0.00075	0.00077	0.00081	0.00169	0.00059	0.00180	0.00036
P2	0.12166	-0.11494	-0.21124	1.00000	0.01309	0.01344	0.01655	0.00143	0.00371	-0.00130	0.01420
	0.00018	0.00063	0.00014	0.00000	0.00075	0.00081	0.00080	0.00163	0.00061	0.00178	0.00036
O1	-0.27183	-0.12716	-0.27855	1.00000	0.02056	0.03498	0.01652	-0.00309	-0.00174	-0.00612	0.02429
	0.00061	0.00157	0.00043	0.00000	0.00252	0.00383	0.00235	0.00410	0.00195	0.00428	0.00136
O2	-0.20119	0.06899	-0.09230	1.00000	0.01643	0.00571	0.02570	0.00400	-0.00739	-0.00390	0.01664
	0.00097	0.00098	0.00070	0.00000	0.00498	0.00380	0.00432	0.00308	0.00366	0.00318	0.00203
O3	-0.45110	-0.10756	-0.12092	1.00000	0.01135	0.02511	0.02511	0.00275	-0.00053	0.00054	0.02070
	0.00049	0.00154	0.00043	0.00000	0.00219	0.00267	0.00239	0.00511	0.00181	0.00545	0.00101
O4	-0.20234	-0.28344	-0.07965	1.00000	0.01698	0.01489	0.03025	-0.00076	-0.00295	-0.00322	0.02110
	0.00104	0.00109	0.00081	0.00000	0.00498	0.00432	0.00436	0.00336	0.00362	0.00349	0.00201
O5	0.11182	0.05842	-0.13507	1.00000	0.03505	0.01778	0.02531	-0.00782	0.01672	-0.00768	0.02507
	0.00116	0.00120	0.00076	0.00000	0.00647	0.00492	0.00488	0.00355	0.00434	0.00392	0.00233
O6	0.28228	-0.11783	-0.26321	1.00000	0.01382	0.02113	0.02620	-0.00736	0.00904	-0.00390	0.01988
	0.00051	0.00147	0.00042	0.00000	0.00223	0.00271	0.00243	0.00534	0.00192	0.00490	0.00108
O7	0.11251	-0.28860	-0.13053	1.00000	0.02299	0.00900	0.02769	-0.00194	0.01006	-0.00408	0.01937
	0.00103	0.00106	0.00073	0.00000	0.00543	0.00445	0.00485	0.00327	0.00395	0.00329	0.00208
O8	0.00587	-0.12162	-0.32299	1.00000	0.01762	0.04543	0.01709	0.00088	0.00448	0.00578	0.02652
	0.00056	0.00163	0.00042	0.00000	0.00245	0.00362	0.00238	0.00514	0.00194	0.00543	0.00126
O9	-0.02349	0.38919	-0.07868	1.00000	0.01955	0.00842	0.01783	0.00030	0.00136	-0.00867	0.01531
	0.00050	0.00143	0.00037	0.00000	0.00221	0.00208	0.00218	0.00432	0.00176	0.00446	0.00091
N1	0.38556	-0.10462	0.07327	1.00000	0.01686	0.02242	0.01606	-0.00071	0.00233	-0.01053	0.01841
	0.00065	0.00191	0.00050	0.00000	0.00274	0.00349	0.00262	0.00524	0.00216	0.00578	0.00131
N2	0.23508	-0.06243	0.29676	1.00000	0.01516	0.03970	0.02617	0.00484	0.00164	0.00923	0.02705
	0.00081	0.00111	0.00064	0.00000	0.00347	0.00676	0.00374	0.00326	0.00294	0.00304	0.00230
C1	0.47712	-0.06433	0.19486	1.00000	0.01202	0.02475	0.01711	0.00233	-0.00210	0.00697	0.01822
	0.00090	0.00110	0.00071	0.00000	0.00358	0.00626	0.00376	0.00305	0.00302	0.00297	0.00217
C2	0.39533	-0.14611	0.29693	1.00000	0.01464	0.03527	0.02092	-0.00200	-0.00226	0.00392	0.02391
	0.00094	0.00157	0.00072	0.00000	0.00357	0.00825	0.00374	0.00395	0.00297	0.00378	0.00270
C3	0.48894	-0.10294	0.41791	1.00000	0.02387	0.03119	0.02389	0.00024	0.00419	0.00639	0.02620
	0.00088	0.00274	0.00067	0.00000	0.00369	0.00484	0.00357	0.00682	0.00291	0.00768	0.00179
C4	0.64943	-0.19943	0.41916	1.00000	0.02153	0.05290	0.02423	0.01263	-0.00030	0.00739	0.03308
	0.00110	0.00153	0.00083	0.00000	0.00480	0.00635	0.00490	0.00451	0.00398	0.00428	0.00238
C5	0.73426	-0.10719	0.31697	1.00000	0.01532	0.04099	0.02433	0.00650	-0.00322	-0.00020	0.02726
	0.00078	0.00273	0.00067	0.00000	0.00330	0.00474	0.00361	0.00852	0.00276	0.00845	0.00166
C6	0.63700	-0.14676	0.19303	1.00000	0.00872	0.02401	0.03298	0.00403	-0.00148	0.00503	0.02217
	0.00086	0.00134	0.00077	0.00000	0.00339	0.00759	0.00428	0.00382	0.00301	0.00331	0.00253
OW	-0.09586	0.22826	-0.46089	1.00000	0.04471	0.04046	0.03506	0.00086	0.01323	0.00374	0.03943
	0.00088	0.00109	0.00064	0.00000	0.00437	0.00451	0.00413	0.00344	0.00343	0.00355	0.00181

Table S3. Atomic coordinates and thermal parameters (A**2) for [trans-1,2-C6H10(NH3)2][Ga(OH)(HPO4)2].H2O

ATOM	x	y	z	sof	U11	U22	U33	U23	U13	U12	Ueq
Ga	0.00000	0.00000	0.00000	0.50000	0.01455	0.01599	0.01469	0.00155	0.00011	0.00092	0.01508
	0.00000	0.00000	0.00000	0.00000	0.00050	0.00051	0.00051	0.00049	0.00056	0.00051	0.00031
P1	0.15249	0.10611	0.75000	0.50000	0.01298	0.01391	0.02081	0.00000	0.00000	-0.00053	0.01590
	0.00030	0.00012	0.00000	0.00000	0.00130	0.00121	0.00146	0.00000	0.00000	0.00115	0.00060
P2	-0.26431	0.06981	0.75000	0.50000	0.01120	0.01472	0.01733	0.00000	0.00000	0.00110	0.01442
	0.00028	0.00012	0.00000	0.00000	0.00127	0.00125	0.00135	0.00000	0.00000	0.00111	0.00060
O1	0.13196	0.06687	0.92403	1.00000	0.02635	0.02462	0.01865	0.00037	0.00138	-0.01559	0.02320
	0.00055	0.00022	0.00069	0.00000	0.00283	0.00254	0.00258	0.00232	0.00232	0.00240	0.00118
O2	0.32243	0.13185	0.75000	0.50000	0.01542	0.02187	0.03150	0.00000	0.00000	-0.00209	0.02293
	0.00080	0.00032	0.00000	0.00000	0.00388	0.00375	0.00436	0.00000	0.00000	0.00330	0.00170
O3	0.05028	0.16183	0.75000	0.50000	0.01663	0.01675	0.04792	0.00000	0.00000	0.00241	0.02710
	0.00081	0.00031	0.00000	0.00000	0.00377	0.00372	0.00529	0.00000	0.00000	0.00318	0.00190
O4	-0.18942	0.04464	0.92565	1.00000	0.01682	0.03718	0.01590	-0.00034	0.00170	0.01305	0.02330
	0.00054	0.00023	0.00069	0.00000	0.00264	0.00288	0.00258	0.00236	0.00215	0.00244	0.00120
O5	-0.23718	0.14166	0.75000	0.50000	0.03018	0.01414	0.05523	0.00000	0.00000	0.00577	0.03318
	0.00092	0.00031	0.00000	0.00000	0.00487	0.00376	0.00578	0.00000	0.00000	0.00356	0.00211
O6	-0.43460	0.06070	0.75000	0.50000	0.01383	0.01786	0.03862	0.00000	0.00000	0.00148	0.02344
	0.00080	0.00031	0.00000	0.00000	0.00364	0.00391	0.00472	0.00000	0.00000	0.00322	0.00177
O7	-0.01131	0.04055	0.25000	0.50000	0.02742	0.01160	0.01709	0.00000	0.00000	0.00406	0.01870
	0.00085	0.00028	0.00000	0.00000	0.00398	0.00305	0.00359	0.00000	0.00000	0.00341	0.00152
C1	0.64376	0.15183	0.25000	0.50000	0.01534	0.00980	0.17996	0.00000	0.00000	0.00072	0.06837
	0.00145	0.00053	0.00000	0.00000	0.00657	0.00550	0.01893	0.00000	0.00000	0.00554	0.00585
C2	0.55325	0.10063	0.29648	0.50000	0.01227	0.02176	0.03254	-0.00602	0.00438	0.00328	0.02219
	0.00156	0.00062	0.00199	0.00000	0.00591	0.00668	0.01515	0.00637	0.00589	0.00554	0.00506
C3	0.38704	0.10032	0.25000	0.50000	0.00706	0.01996	0.08463	0.00000	0.00000	-0.00306	0.03722
	0.00123	0.00050	0.00000	0.00000	0.00543	0.00588	0.01064	0.00000	0.00000	0.00498	0.00342
C4	0.31061	0.16343	0.25000	0.50000	0.02139	0.02590	0.04449	0.00000	0.00000	0.01451	0.03059
	0.00130	0.00051	0.00000	0.00000	0.00638	0.00608	0.00744	0.00000	0.00000	0.00539	0.00286
C5	0.40388	0.21400	0.16675	0.50000	0.02512	0.01284	0.06557	0.00672	-0.00486	0.00590	0.03451
	0.00176	0.00061	0.00252	0.00000	0.00861	0.00707	0.01316	0.00724	0.00806	0.00661	0.00465
C6	0.57087	0.21441	0.25000	0.50000	0.02273	0.01823	0.04275	0.00000	0.00000	0.00151	0.02790
	0.00130	0.00048	0.00000	0.00000	0.00602	0.00567	0.00775	0.00000	0.00000	0.00491	0.00278
N1	0.81053	0.15396	0.21340	0.50000	0.01672	0.02454	0.03147	0.00552	-0.00316	-0.00250	0.02424
	0.00128	0.00050	0.00308	0.00000	0.00548	0.00544	0.01980	0.00605	0.00622	0.00465	0.00637
N2	0.62341	0.03903	0.25000	0.50000	0.02447	0.01245	0.03011	0.00000	0.00000	-0.00205	0.02234
	0.00101	0.00037	0.00000	0.00000	0.00522	0.00417	0.00526	0.00000	0.00000	0.00387	0.00210
OW	-0.05526	0.25868	0.53336	0.25000	0.02861						
	0.00315	0.00201	0.00531	0.00000	0.00353						
OW'	-0.03331	0.23613	0.43737	0.25000	0.02861						
	0.00336	0.00167	0.00526	0.00000	0.00353						

Table S4. Bond lengths (A) and angles (deg) for [(1R,2R)-C6H10(NH3)2][Ga(OH)(HPO4)2].H2O

Ga -	Distance	Angles				
O7_$2	1.934 (0.009)					
O5	1.941 (0.009)	177.87 (0.44)				
O9	1.968 (0.009)	93.13 (0.27)	89.00 (0.31)			
O2	1.977 (0.008)	87.99 (0.35)	92.14 (0.38)	88.55 (0.25)		
O4_$2	1.989 (0.009)	93.71 (0.39)	86.22 (0.39)	89.53 (0.27)	177.50 (0.44)	
O9_$1	2.006 (0.009)	85.52 (0.27)	92.35 (0.30)	178.10 (0.28)	92.74 (0.26)	89.23 (0.29)
	Ga -	O7_$2	O5	O9	O2	O4_$2

P1 -	Distance	Angles		
O3	1.503 (0.005)			
O4	1.519 (0.008)	111.94 (0.51)		
O2	1.531 (0.007)	111.43 (0.52)	111.13 (0.27)	
O1	1.583 (0.005)	106.71 (0.28)	107.14 (0.56)	108.23 (0.50)
	P1 -	O3	O4	O2

P2 -	Distance	Angles		
O5	1.507 (0.009)			
O8	1.518 (0.005)	114.51 (0.58)		
O7	1.537 (0.008)	108.75 (0.26)	112.53 (0.52)	
O6	1.572 (0.005)	108.96 (0.55)	103.79 (0.26)	107.99 (0.54)
	P2 -	O5	O8	O7

O1 -	Distance	Angles
P1	1.583 (0.005)	
	O1 -	

O2 -	Distance	Angles
P1	1.531 (0.007)	
Ga	1.977 (0.008)	137.12 (0.47)
	O2 -	P1

O3 -	Distance	Angles
P1	1.503 (0.005)	
	O3 -	

O4 -	Distance	Angles
P1	1.519 (0.008)	
Ga_$1	1.989 (0.009)	140.12 (0.51)
	O4 -	P1

O5 -	Distance	Angles
P2	1.507 (0.009)	
Ga	1.941 (0.009)	137.25 (0.57)
	O5 -	P2

O6 -	Distance	Angles
P2	1.572 (0.005)	
	O6 -	

O7 -	Distance	Angles
P2	1.537 (0.008)	
Ga_$1	1.934 (0.009)	136.56 (0.54)
	O7 -	P2

O8 -	Distance	Angles
P2	1.518 (0.005)	
	O8 -	

O9 -	Distance	Angles
Ga	1.968 (0.009)	
Ga_$2	2.006 (0.009)	127.52 (0.22)
	O9 -	Ga

N1 -	Distance	Angles
C1	1.525 (0.010)	
	N1 -	

N2 -	Distance	Angles
C2	1.519 (0.011)	
	N2 -	

C1 -	Distance	Angles	
C6	1.515 (0.011)		
C2	1.521 (0.012)	111.53 (0.68)	
N1	1.525 (0.010)	108.08 (0.67)	110.43 (0.65)
	C1 -	C6	C2

C2 -	Distance	Angles	
N2	1.519 (0.011)		
C1	1.521 (0.012)	110.68 (0.71)	
C3	1.531 (0.011)	109.04 (0.75)	109.43 (0.75)
	C2 -	N2	C1

C3 -	Distance	Angles
C2	1.531 (0.011)	
C4	1.558 (0.014)	108.25 (0.88)
	C3 -	C2

C4 -	Distance	Angles
C3	1.558 (0.014)	
C5	1.567 (0.013)	107.56 (0.88)
	C4 -	C3

C5 -	Distance	Angles
C6	1.567 (0.011)	
C4	1.567 (0.013)	108.16 (0.83)
	C5 -	C6

C6 -	Distance	Angles
C1	1.515 (0.011)	
C5	1.567 (0.011)	109.31 (0.77)
	C6 -	C1

Table S5. Bond lengths (A) and angles (deg) for [trans-1,2-C6H10(NH3)2][Ga(OH)(HPO4)2].H2O

Ga -	Distance	Angles				
O1_$3	1.937 (0.005)					
O1_$4	1.937 (0.005)	180.00				
O4_$4	1.988 (0.005)	87.38 (0.21)	92.62 (0.21)			
O4_$3	1.988 (0.005)	92.62 (0.21)	87.38 (0.21)	180.00		
O7_$6	1.999 (0.003)	93.12 (0.23)	86.88 (0.23)	88.91 (0.24)	91.09 (0.24)	
O7	1.999 (0.003)	86.88 (0.23)	93.12 (0.23)	91.09 (0.24)	88.91 (0.24)	180.00
	Ga -	O1_$3	O1_$4	O4_$4	O4_$3	O7_$6

P1 -	Distance	Angles		
O3	1.508 (0.007)			
O1_$5	1.523 (0.005)	112.70 (0.25)		
O1	1.523 (0.005)	112.70 (0.25)	109.74 (0.39)	
O2	1.582 (0.007)	105.29 (0.40)	108.06 (0.25)	108.06 (0.25)
	P1 -	O3	O1_$5	O1

P2 -	Distance	Angles		
O6	1.495 (0.007)			
O4	1.519 (0.005)	112.14 (0.24)		
O4_$5	1.519 (0.005)	112.14 (0.24)	111.69 (0.37)	
O5	1.588 (0.007)	106.20 (0.42)	107.13 (0.26)	107.13 (0.26)
	P2 -	O6	O4	O4_$5

O1 -	Distance	Angles
P1	1.523 (0.005)	
Ga_$1	1.937 (0.005)	136.42 (0.31)
	O1 -	P1

O2 -	Distance	Angles
P1	1.582 (0.007)	
	O2 -	

O3 -	Distance	Angles
P1	1.508 (0.007)	
	O3 -	

O4 -	Distance	Angles
P2	1.519 (0.005)	
Ga_$1	1.988 (0.005)	139.02 (0.30)
	O4 -	P2

O5 -	Distance	Angles
P2	1.588 (0.007)	
	O5 -	

O6 -	Distance	Angles
P2	1.495 (0.007)	
	O6 -	

O7 -	Distance	Angles
Ga	1.999 (0.003)	
Ga_$2	1.999 (0.003)	127.00 (0.32)
	O7 -	Ga

C1 -	Distance	Angles				
C2_$7	1.408 (0.018)					
C2	1.408 (0.018)	27.32 (1.18)				
N1_$7	1.475 (0.016)	128.09 (1.14)	122.21 (1.11)			
N1	1.475 (0.016)	122.21 (1.11)	128.09 (1.14)	20.46 (1.70)		
C6	1.508 (0.016)	119.08 (1.07)	119.08 (1.07)	112.64 (1.01)	112.64 (1.01)	
	C1 -	C2_$7	C2	N1_$7	N1	

C2 -	Distance	Angles		
C2_$7	0.665 (0.029)			
C1	1.408 (0.018)	76.34 (0.59)		
C3	1.484 (0.017)	77.05 (0.56)	119.70 (1.15)	
N2	1.515 (0.015)	77.32 (0.55)	115.42 (1.06)	109.83 (1.01)
	C2 -	C2_$7	C1	C3

C3 -	Distance	Angles	
C2_$7	1.484 (0.017)		
C2	1.484 (0.017)	25.91 (1.11)	
C4	1.531 (0.015)	114.77 (0.97)	114.77 (0.97)
	C3 -	C2_$7	C2

C4 -	Distance	Angles	
C5_$7	1.495 (0.018)		
C5	1.495 (0.018)	46.96 (1.40)	
C3	1.531 (0.015)	115.50 (0.92)	115.50 (0.92)
	C4 -	C5_$7	C5

C5 -	Distance	Angles	
C5_$7	1.191 (0.036)		
C4	1.495 (0.018)	66.52 (0.70)	
C6	1.570 (0.018)	67.70 (0.67)	110.80 (1.08)
	C5 -	C5_$7	C4

C6 -	Distance	Angles	
C1	1.508 (0.016)		
C5	1.570 (0.018)	112.58 (0.95)	
C5_$7	1.570 (0.018)	112.58 (0.95)	44.59 (1.33)
	C6 -	C1	C5

N1 -	Distance	Angles	
N1_$7	0.524 (0.044)		
C1	1.475 (0.016)	79.77 (0.85)	
	N1 -	N1_$7	

N2 -	Distance	Angles	
C2	1.515 (0.015)		
C2_$7	1.515 (0.015)	25.36 (1.09)	
	N2 -	C2	

OW -	Distance	Angles	
OW' $8	0.305 (0.050)		
OW_$8	0.610 (0.062)	140.20 (9.99)	
OW	0.867 (0.023)	128.11 (9.99)	13.03 (3.73)
	OW -	OW'_$8	OW_$8

OW' -	Distance	Angles	
OW_$8	0.305 (0.049)		
OW	0.867 (0.023)	26.77 (9.91)	
OW'_$8	1.082 (0.069)	39.06 (9.99)	12.83 (3.45)
	OW' -	OW_$8	OW