Status Alternate **QM:** Indexed (I) **Pressure/Temperature:** Ambient **Chemical Formula:** Na Cl
Empirical Formula: Cl Na **Weight %:** Cl60.66 Na39.34 **Atomic %:** Cl50.00 Na50.00
Compound Name: Sodium Chloride

Radiation: CuKá1 : 1.5406Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 4.71

SYS: Cubic **SPGR:** Fm-3m (225)
Author's Cell [AuthCell a: 5.6373(3)Å **AuthCell Vol:** 179.15Å³ **AuthCell Z:** 4.00 **AuthCell MolVol:** 44.79 **]**
Dcalc: 2.167g/cm³ **Dstruc:** 2.17g/cm³ **SS/FOM:** F(17) = 999.9(0.0003, 17)

Space Group: Fm-3m (225) **Molecular Weight:** 58.44
Crystal Data [XtlCell a: 5.637Å **XtlCell b:** 5.637Å **XtlCell c:** 5.637Å **XtlCell :** 90.00° **XtlCell :** 90.00°
XtlCell : 90.00° **XtlCell Vol:** 179.15Å³ **XtlCell Z:** 4.00 **]** **Crystal Data Axial Ratio [a/b:** 1.000 **c/b:** 1.000 **]**
Reduced Cell [RedCell a: 3.986Å **RedCell b:** 3.986Å **RedCell c:** 3.986Å **RedCell :** 60.00°
RedCell : 60.00° **RedCell :** 60.00° **RedCell Vol:** 44.79Å³ **]**

Crystal (Symmetry Allowed): Centrosymmetric

SG Symmetry Operators:

Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator
1	x,y,z	8	-x,-z,-y	15	z,-x,-y	22	-y,x,z	29	-y,z,-x	36	z,-y,x	43	-x,-z,y
2	-x,-y,-z	9	y,x,z	16	-z,x,y	23	z,-y,-x	30	y,-z,x	37	-x,-y,z	44	x,z,-y
3	z,x,y	10	-y,-x,-z	17	y,-z,-x	24	-z,y,x	31	-x,z,-y	38	x,y,-z	45	-y,-x,z
4	-z,-x,-y	11	z,y,x	18	-y,z,x	25	-x,y,-z	32	x,-z,y	39	-z,-x,y	46	y,x,-z
5	y,z,x	12	-z,-y,-x	19	x,-z,-y	26	x,-y,z	33	-y,x,-z	40	z,x,-y	47	-z,-y,x
6	-y,-z,-x	13	x,-y,-z	20	-x,z,y	27	-z,x,-y	34	y,-x,z	41	-y,-z,x	48	z,y,-x
7	x,z,y	14	-x,y,z	21	y,-x,-z	28	z,-x,y	35	-z,y,-x	42	y,z,-x		

Atomic Coordinates:

Atom	Num	Wyckoff	Symmetry	x	y	z	SOF	IDP	AET
Na	1	4a	m-3m	0.0	0.0	0.0	1.0		
Cl	2	4b	m-3m	0.5	0.5	0.5	1.0		

Pearson: cF8.00 **LPF Prototype Structure:** Na Cl,cF8,225 **LPF Prototype Structure (Alpha Order):** Cl Na
Subfile(s): LPF Pattern, Inorganic, Alternate Pattern **Entry Date:** 09/19/2011 **Last Modification Date:** 01/13/2012

Cross-Ref PDF #'s: 00-001-0993 (Deleted), 00-001-0994 (Deleted), 00-002-0818 (Deleted), 00-005-0628 (Primary), 01-070-2509 (Alternate), 01-071-3741 (Alternate), 01-071-3742 (Alternate), 01-071-4661 (Alternate), 01-071-4662 (Alternate), 01-075-0306 (Alternate), 01-076-3452 (Alternate), 01-076-3453 (Alternate), 01-076-3454 (Alternate), 01-076-3455 (Alternate), 01-076-3456 (Alternate), 01-076-3457 (Alternate), 01-076-3458 (Alternate), 01-077-2064 (Alternate), 01-077-3565 (Alternate), 01-077-8801 (Alternate), 01-078-0751 (Alternate), 01-083-1728 (Alternate), 01-088-2300 (Alternate), 01-089-3615 (Alternate), 04-002-1178 (Primary), 04-002-1266 (Alternate), 04-002-2489 (Alternate), 04-002-5016 (Alternate), 04-002-7174 (Alternate), 04-002-7263 (Alternate), 04-003-2501 (Alternate), 04-004-5108 (Alternate), 04-005-4267 (Alternate), 04-006-5357 (Alternate), 04-006-5374 (Alternate), 04-006-5937 (Alternate), 04-007-1261 (Alternate), 04-007-4193 (Alternate), 04-007-4474 (Alternate), 04-007-5248 (Alternate), 04-007-8795 (Alternate), 04-007-9714 (Alternate), 04-007-9715 (Alternate), 04-007-9723 (Alternate), 04-009-2091 (Alternate), 04-012-7883 (Alternate), 04-013-1689 (Alternate), 04-013-9769 (Alternate), 04-016-1668 (Alternate), 04-016-5475 (Alternate)

References:

Type	Reference
Primary Reference	Calculated from LPF using POWD-12++.
Structure	"Enhancement effect of LiAlH4 addition on reversible hydrogen storage property for the face-centered cubic hydride Mg7TiH16 prepared by a gigapascal hydrogen pressure method". Takasaki T., Mukai T., Kitamura N., Tanase S., Sakai T. J. Phys. Chem. C 112, 12540,12544 (2008).

Database Comments: LPF Collection Code: 1628045. Sample Preparation: STARTING MATERIAL: MgH2,TiH1.9,LiAlH4,NaBH4,Ca(OH)2. COMPOUND FORMATION: heated at 873 K and 8 GPa for 1 h three times.CRUCIBLE: NaCl capsule;carbon capsule;pyrophyllite cell. Minor Warning: LPF Editor Comment: editor deduced probable site occupation from nominal composition. Unit Cell Data Source: Powder Diffraction.

d-Spacings (17) - 04-016-2944 (Fixed Slit Intensity) - Cu K1 1.54056Å

2	d(Å)	I	h	k	l	*	2	d(Å)	I	h	k	l	*	2	d(Å)	I	h	k	l	*
27.3798	3.254700	91	1	1	1		56.5019	**1.627350**	169	2	2	2		84.0408	1.150710	107	4	2	2	
31.7191	**2.818650**	999	2	0	0		66.2623	1.409330	66	4	0	0		90.4700	1.084900	7	5	1	1	
45.4707	**1.993090**	586	2	2	0		73.1104	1.293290	7	3	3	1		101.2395	0.996543	30	4	4	0	
53.8962	1.699710	17	3	1	1		75.3340	1.260540	160	4	2	0		107.8744	0.952878	8	5	3	1	

2	d(Å)	I	h	k	l	*
110.1374	0.939550	62	6	0	0	
119.5800	0.891335	44	6	2	0	
127.2764	0.859680	4	5	3	3	
130.0159	0.849855	40	6	2	2	
142.4070	0.813674	12	4	4	4	