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APPENDICES

APPENDIX A

Tolerance number

The Goldschmidt tolerance numbers were calculated based on equation A.1.

$$t = \frac{(r_A + r_O)}{\sqrt{2} \times (r_B + r_O)} \quad (\text{A.1})$$

where r_A , r_B and r_O represent the ionic crystal radii of A-site cation, B-site cation and oxygen ion, respectively. The example of the tolerance number calculation of La_2NiO_4 was showed as below.

$$\text{Tolerance number of } \text{La}_2\text{NiO}_4 = \frac{[(1.356 \times 2)/2 + 1.26]}{\sqrt{2} (0.83 + 1.26)} = 0.885$$

Table A.1 Ionic crystal radii of concerned metal ions [60]

Metal ion	Ionic charge	Coordination No.	Crystal radius (\AA)
La	3+	9	1.356
Sr	2+	9	1.45
Ca	2+	9	1.32
Ni	2+	6	0.83
	3+ (LS)		0.7
	3+ (HS)		0.74
	4+ (LS)		0.62
Co	2+ (LS)	6	0.79
	2+ (HS)		0.885
	3+ (LS)		0.685
	3+ (HS)		0.75
	4+ (HS)		0.67
Fe	2+ (LS)	6	0.75
	2+ (HS)		0.92
	3+ (LS)		0.69
	3+ (HS)		0.785
	4+		0.725
Zn	2+	6	0.88
O	2-	6	1.26

LS = Low spin configuration, HS = High spin configuration

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APPENDIX B

Activation energy (E_a)

Arrhenius equation (B.1) is shown below. The plot of $\ln(\sigma T)$ versus $\frac{1000}{T}$ (K) gives a straight line, whose slope can be used to determine the E_a of small polaron conduction.

$$\begin{aligned}\sigma &= \left(\frac{A}{T} \right) e^{\frac{-E_a}{RT}} \\ \ln(\sigma T) &= \ln A e^{\frac{-E_a}{RT}} \\ \ln(\sigma T) &= \ln e^{\frac{-E_a}{RT}} + \ln A \\ \ln(\sigma T) &= \left(\frac{-E_a}{R} \right) \left(\frac{1000}{T} \right) + \ln A \quad (B.1) \\ \downarrow & \quad \downarrow & \quad \downarrow & \quad \downarrow \\ y & \quad \text{slope} & x & \quad \text{intercept y axis}\end{aligned}$$

$$\begin{aligned}\left(\frac{-E_a}{R} \right) &= \text{slope of the linear} \\ E_a &= -\text{slope} \times R\end{aligned}$$

- Where A = material constant including the carrier concentration term
 σ = specific conductivity (S/cm)
 E_a = activation energy (kJ/mol)
 T = temperature (K)
 R = gas constant = 8.314472 J/K.mol



APPENDIX C

XRD Data

(La_{1.6}Sr_{0.4})NiO₄ PDF#89-8310

ចាន់អុល្សែ..... No: 2556
 លេខបោះពីំយន..... 7136
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PDF#89-8310: QM=Calculated(C); d=Calculated; I=Calculated										PDF Card				
Lanthanum Strontium Nickel Oxide						Lambda=1.54080								
(La _{1.6} Sr _{0.4}) Ni O ₄						2T=13 901-89 995								
Radiation=CuKα1						Filter=								
Calibration=						μfc(RIR)=6.58								
Ref. Calculated from ICSD using POWD-12++														
Tetragonal Powder Diffraction, I4/mmm (139)						Z=2	mp=							
CELL 3.819 * 3.819 * 12.73045 <90 0 * 90 0 * 90 0>						P S=I114 (?)								
Density(c)=6.796						Mwt=379.99	Vol=185.67							
Ref. Millburn, J.E., Green, M.A., Neumann, D.A., Rossinsky, M.J.						F(30)=243.9(0038 32/0)								
J Solid State Chem. v145 p401 (1999)														
FIZ=088633 TEM 298 RVP. No R value given. At least one TF missing. Evolution of the structure of the K ₂ NiF ₄ phases La _{2-x} Sr _x NiO _{4+d} with oxidation state, octahedral distortion and phase separation (0.2 < x < 1.0)														
Strong Lines: 2.84/X 2.70/7 1.91/3 2.06/3 3.66/3 1.58/3 2.12/2 3.18/1 1.64/1 1.42/1														
37 Lines. Wavelength to Compute Theta = 1.54056A(Cu). % Type = Peak Height														
#	d(nm)	I(f)	(h k l)	2-Theta	Theta	1/(2d)	#	d(nm)	I(f)	(h k l)	2-Theta	Theta	1/(2d)	
1	0.63652	5.5	(0 0 2)	13.901	6.951	0.00786	20	0.13710	5.2	(1 1 8)	68.367	34.184	0.03647	
2	0.36579	27.0	(1 0 1)	24.312	12.156	0.01367	21	0.13502	7.1	(2 2 0)	69.568	34.784	0.03703	
3	0.31826	14.8	(0 0 4)	28.013	14.006	0.01571	22	0.13764	0.1	(1 0 9)	71.002	35.501	0.03770	
4	0.28387	100.0	(1 0 3)	31.489	15.745	0.01761	23	0.13203	0.1	(2 2 2)	71.349	35.674	0.03785	
5	0.27004	71.8	(1 1 0)	33.147	16.573	0.01852	24	0.12730	0.3	(0 0 10)	74.468	37.234	0.03928	
6	0.24860	1.6	(1 1 2)	36.100	18.050	0.02011	25	0.12667	0.9	(3 0 1)	74.906	37.453	0.03947	
7	0.21184	23.5	(1 0 5)	42.644	21.322	0.02360	26	0.12450	6.1	(2 1 7)	76.444	38.222	0.04016	
8	0.21184	23.5	(0 0 6)	42.644	21.322	0.02360	27	0.12430	3.5	(2 2 4)	76.588	38.294	0.04023	
9	0.20591	30.4	(1 1 4)	43.936	21.968	0.02428	28	0.12225	5.0	(2 0 8)	78.116	39.058	0.04090	
10	0.19095	31.4	(2 0 0)	47.581	23.790	0.02618	29	0.12193	6.8	(3 0 3)	78.356	39.178	0.04101	
11	0.18290	0.3	(2 0 2)	49.815	24.906	0.02734	30	0.12077	6.4	(3 1 0)	79.259	39.630	0.04140	
12	0.16927	5.3	(2 1 1)	54.136	27.068	0.02954	31	0.11865	0.1	(3 1 2)	80.962	40.481	0.04214	
13	0.16084	8.2	(1 1 6)	54.993	27.497	0.02957	32	0.11515	1.5	(1 1 10)	83.969	41.995	0.04342	
14	0.16420	9.3	(1 0 7)	55.955	27.877	0.03045	33	0.11391	3.3	(3 0 5)	85.096	42.548	0.04389	
15	0.15374	11.4	(2 0 4)	56.124	28.062	0.03054	34	0.11391	3.3	(2 2 6)	85.096	42.548	0.04389	
16	0.15913	4.3	(0 0 8)	57.901	28.951	0.03142	35	0.11291	5.2	(3 1 4)	85.031	43.015	0.04428	
17	0.15844	26.6	(2 1 3)	58.178	29.089	0.03156	36	0.11076	4.9	(1 0 11)	88.129	44.065	0.04514	
18	0.14184	11.0	(2 0 6)	65.787	32.893	0.03525	37	0.10894	0.1	(2 1 9)	89.995	44.997	0.04590	
19	0.14184	11.0	(2 1 5)	65.787	32.893	0.03525								

Simulation Parameters: Fixed-Slit Intensities, Two-Theta Range = 11.9/01.96/0.02, FWHM = 0.1

<img alt="XRD pattern showing intensity versus d-spacing (Å) for the sample. The pattern shows several sharp peaks, with the most intense peak at approximately 28 Å. Other labeled peaks include 18, 22, 24, 26, 28, 30, 32, 34, 36, 38, 40, 42, 44, 46, 48, 50, 52, 54, 56, 58, 60, 62, 64, 66, 68, 70, 72, 74, 76, 78, 80, 82, 84, 86, 88, 90, 92, 94, 96, 98, 100, 102, 104, 106, 108, 110, 112, 114, 116, 118, 120, 122, 124, 126, 128, 130, 132, 134, 136, 138, 140, 142, 144, 146, 148, 150, 152, 154, 156, 158, 160, 162, 164, 166, 168, 170, 172, 174, 176, 178, 180, 182, 184, 186, 188, 190, 192, 194, 196, 198, 200, 202, 204, 206, 208, 210, 212, 214, 216, 218, 220, 222, 224, 226, 228, 230, 232, 234, 236, 238, 240, 242, 244, 246, 248, 250, 252, 254, 256, 258, 260, 262, 264, 266, 268, 270, 272, 274, 276, 278, 280, 282, 284, 286, 288, 290, 292, 294, 296, 298, 300, 302, 304, 306, 308, 310, 312, 314, 316, 318, 320, 322, 324, 326, 328, 330, 332, 334, 336, 338, 340, 342, 344, 346, 348, 350, 352, 354, 356, 358, 360, 362, 364, 366, 368, 370, 372, 374, 376, 378, 380, 382, 384, 386, 388, 390, 392, 394, 396, 398, 400, 402, 404, 406, 408, 410, 412, 414, 416, 418, 420, 422, 424, 426, 428, 430, 432, 434, 436, 438, 440, 442, 444, 446, 448, 450, 452, 454, 456, 458, 460, 462, 464, 466, 468, 470, 472, 474, 476, 478, 480, 482, 484, 486, 488, 490, 492, 494, 496, 498, 500, 502, 504, 506, 508, 510, 512, 514, 516, 518, 520, 522, 524, 526, 528, 530, 532, 534, 536, 538, 540, 542, 544, 546, 548, 550, 552, 554, 556, 558, 560, 562, 564, 566, 568, 570, 572, 574, 576, 578, 580, 582, 584, 586, 588, 590, 592, 594, 596, 598, 600, 602, 604, 606, 608, 610, 612, 614, 616, 618, 620, 622, 624, 626, 628, 630, 632, 634, 636, 638, 640, 642, 644, 646, 648, 650, 652, 654, 656, 658, 660, 662, 664, 666, 668, 670, 672, 674, 676, 678, 680, 682, 684, 686, 688, 690, 692, 694, 696, 698, 700, 702, 704, 706, 708, 710, 712, 714, 716, 718, 720, 722, 724, 726, 728, 730, 732, 734, 736, 738, 740, 742, 744, 746, 748, 750, 752, 754, 756, 758, 760, 762, 764, 766, 768, 770, 772, 774, 776, 778, 780, 782, 784, 786, 788, 790, 792, 794, 796, 798, 800, 802, 804, 806, 808, 810, 812, 814, 816, 818, 820, 822, 824, 826, 828, 830, 832, 834, 836, 838, 840, 842, 844, 846, 848, 850, 852, 854, 856, 858, 860, 862, 864, 866, 868, 870, 872, 874, 876, 878, 880, 882, 884, 886, 888, 890, 892, 894, 896, 898, 900, 902, 904, 906, 908, 910, 912, 914, 916, 918, 920, 922, 924, 926, 928, 930, 932, 934, 936, 938, 940, 942, 944, 946, 948, 950, 952, 954, 956, 958, 960, 962, 964, 966, 968, 970, 972, 974, 976, 978, 980, 982, 984, 986, 988, 990, 992, 994, 996, 998, 1000, 1002, 1004, 1006, 1008, 1010, 1012, 1014, 1016, 1018, 1020, 1022, 1024, 1026, 1028, 1030, 1032, 1034, 1036, 1038, 1040, 1042, 1044, 1046, 1048, 1050, 1052, 1054, 1056, 1058, 1060, 1062, 1064, 1066, 1068, 1070, 1072, 1074, 1076, 1078, 1080, 1082, 1084, 1086, 1088, 1090, 1092, 1094, 1096, 1098, 1100, 1102, 1104, 1106, 1108, 1110, 1112, 1114, 1116, 1118, 1120, 1122, 1124, 1126, 1128, 1130, 1132, 1134, 1136, 1138, 1140, 1142, 1144, 1146, 1148, 1150, 1152, 1154, 1156, 1158, 1160, 1162, 1164, 1166, 1168, 1170, 1172, 1174, 1176, 1178, 1180, 1182, 1184, 1186, 1188, 1190, 1192, 1194, 1196, 1198, 1200, 1202, 1204, 1206, 1208, 1210, 1212, 1214, 1216, 1218, 1220, 1222, 1224, 1226, 1228, 1230, 1232, 1234, 1236, 1238, 1240, 1242, 1244, 1246, 1248, 1250, 1252, 1254, 1256, 1258, 1260, 1262, 1264, 1266, 1268, 1270, 1272, 1274, 1276, 1278, 1280, 1282, 1284, 1286, 1288, 1290, 1292, 1294, 1296, 1298, 1300, 1302, 1304, 1306, 1308, 1310, 1312, 1314, 1316, 1318, 1320, 1322, 1324, 1326, 1328, 1330, 1332, 1334, 1336, 1338, 1340, 1342, 1344, 1346, 1348, 1350, 1352, 1354, 1356, 1358, 1360, 1362, 1364, 1366, 1368, 1370, 1372, 1374, 1376, 1378, 1380, 1382, 1384, 1386, 1388, 1390, 1392, 1394, 1396, 1398, 1400, 1402, 1404, 1406, 1408, 1410, 1412, 1414, 1416, 1418, 1420, 1422, 1424, 1426, 1428, 1430, 1432, 1434, 1436, 1438, 1440, 1442, 1444, 1446, 1448, 1450, 1452, 1454, 1456, 1458, 1460, 1462, 1464, 1466, 1468, 1470, 1472, 1474, 1476, 1478, 1480, 1482, 1484, 1486, 1488, 1490, 1492, 1494, 1496, 1498, 1500, 1502, 1504, 1506, 1508, 1510, 1512, 1514, 1516, 1518, 1520, 1522, 1524, 1526, 1528, 1530, 1532, 1534, 1536, 1538, 1540, 1542, 1544, 1546, 1548, 1550, 1552, 1554, 1556, 1558, 1560, 1562, 1564, 1566, 1568, 1570, 1572, 1574, 1576, 1578, 1580, 1582, 1584, 1586, 1588, 1590, 1592, 1594, 1596, 1598, 1600, 1602, 1604, 1606, 1608, 1610, 1612, 1614, 1616, 1618, 1620, 1622, 1624, 1626, 1628, 1630, 1632, 1634, 1636, 1638, 1640, 1642, 1644, 1646, 1648, 1650, 1652, 1654, 1656, 1658, 1660, 1662, 1664, 1666, 1668, 1670, 1672, 1674, 1676, 1678, 1680, 1682, 1684, 1686, 1688, 1690, 1692, 1694, 1696, 1698, 1700, 1702, 1704, 1706, 1708, 1710, 1712, 1714, 1716, 1718, 1720, 1722, 1724, 1726, 1728, 1730, 1732, 1734, 1736, 1738, 1740, 1742, 1744, 1746, 1748, 1750, 1752, 1754, 1756, 1758, 1760, 1762, 1764, 1766, 1768, 1770, 1772, 1774, 1776, 1778, 1780, 1782, 1784, 1786, 1788, 1790, 1792, 1794, 1796, 1798, 1800, 1802, 1804, 1806, 1808, 1810, 1812, 1814, 1816, 1818, 1820, 1822, 1824, 1826, 1828, 1830, 1832, 1834, 1836, 1838, 1840, 1842, 1844, 1846, 1848, 1850, 1852, 1854, 1856, 1858, 1860, 1862, 1864, 1866, 1868, 1870, 1872, 1874, 1876, 1878, 1880, 1882, 1884, 1886, 1888, 1890, 1892, 1894, 1896, 1898, 1900, 1902, 1904, 1906, 1908, 1910, 1912, 1914, 1916, 1918, 1920, 1922, 1924, 1926, 1928, 1930, 1932, 1934, 1936, 1938, 1940, 1942, 1944, 1946, 1948, 1950, 1952, 1954, 1956, 1958, 1960, 1962, 1964, 1966, 1968, 1970, 1972, 1974, 1976, 1978, 1980, 1982, 1984, 1986, 1988, 1990, 1992, 1994, 1996, 1998, 2000, 2002, 2004, 2006, 2008, 2010, 2012, 2014, 2016, 2018, 2020, 2022, 2024, 2026, 2028, 2030, 2032, 2034, 2036, 2038, 2040, 2042, 2044, 2046, 2048, 2050, 2052, 2054, 2056, 2058, 2060, 2062, 2064, 2066, 2068, 2070, 2072, 2074, 2076,

CaO PDF#48-1467

PDF#48-1467: Q=M=Calculated(C); d=Calculated; I=Calculated										PDF Card (pEXC)			
Calcium Oxide													
Ca O													
Radiation=CuKa1 Lambda=1.5405981 Filter=													
Calibration= 2T=32 199-147.782 I/Ic(RIR)=4.45													
Ref: Reardon, B., Hubbard, C., TM-11948 Oak Ridge Natl. Lab. Rep. ORNL (U.S.) (1992); Cubic - (Unknown), Fm: 3m (225) CELL: 4.81059 x 4.81059 x 4.81059 <90 0 x 90 0 x 90 0> Density(c)=3.345 Density(m)=2.59A Mw=56.08 Vol=111.33 F(13)=411.2(0.0024,13/0)													
Ref: McMurdie, H. Powder Diffraction, v1 p265 (1986)													
NOTE: See also 37-1497.													
Strong Lines: 2.41/X 1.70/5 2.78/4 0.80/2 1.45/2 0.81/2 1.39/1 1.08/1 0.98/1 1.10/1													
13 Lines, Wavelength to Compute Theta = 1.54056Å(Cu), 1%-Type = Peak Area													
#	d(nm)	I(f)	(h k l)	2-Theta	Theta	1/(2d)	#	d(nm)	I(f)	(h k l)	2-Theta	Theta	1/(2d)
1	0.27777	40.0	(1 1 1)	32.199	16.100	0.01800	8	0.10757	14.0	(4 2 0)	91.467	45.733	0.04648
2	0.24051	100.0	(2 0 0)	37.359	18.680	0.02079	9	0.09820	11.0	(4 2 2)	103.336	51.668	0.05092
3	0.17008	51.0	(2 2 0)	53.859	26.929	0.02940	10	0.09258	7.0	(5 1 1)	112.616	56.308	0.05401
4	0.14504	17.0	(3 1 1)	64.158	32.079	0.03447	11	0.08504	5.0	(4 4 0)	129.853	64.926	0.05879
5	0.13887	14.0	(2 2 2)	67.378	33.689	0.03601	12	0.08131	15.0	(5 3 1)	142.633	71.316	0.06149
6	0.12026	5.0	(4 0 0)	79.658	39.820	0.04158	13	0.08018	19.0	(4 4 2)	147.782	73.891	0.06236
7	0.11036	7.0	(3 3 1)	88.527	44.263	0.04531							
Simulation Parameters: Fixed-Slit Intensities, Two-Theta Range =30.2/149.78/0.02, FWHM = 0.1													

39149909009

La_2NiO_4 PDF#34-0314

PDF#34-0314: QM=Indexed(I); d=Guinier; I= Densitometer										PDF Card			
Nickel Lanthanum Oxide													
La ₂ NiO ₄													
Radiation=CuKa1										Lambda=1.5405			
Calibration=Internal(Si)										Filter=Ge			
Ref: Wustenberg, H., Hahn, Inst. fur Kristallogr., Technische Hochschule, Aachen, Germany.										I/Ic(RIR)=			
ICDD Grant-in-Aid (1981)													
Tetragonal - (Unknown), I4/mmm (139)										Z=2			
CELL: 3.8617 x 3.8617 x 12.683 <90.0 x 90.0 x 90.0>										mp=			
Density(c)=7.030										P.S=tI4 (K2 Ni F4)			
Density(m)=7.27A										Ic(30)=65.0(0132,35/0)			
Mw.=400.51										Vol=189.14			
Ref: Ibid													
NOTE: Sample is a decomposition product of La Ni O ₃ heated to 1500 C in air. To replace 33-712													
Strong Lines: 2.85/X 2.73/9 3.69/7 1.93/7 2.07/6 1.60/6 3.17/4 2.12/4 1.64/3 2.11/3													
37 Lines, Wavelength to Compute Theta = 1.54056A(Cu), I% Type = (Unknown)													
#	d(nm)	I(f)	(h k l)	2-Theta	Theta	I/(2d)	#	d(nm)	I(f)	(h k l)	2-Theta	Theta	I/(2d)
1	0.63390	10.0	(0 0 2)	13.959	6.980	0.00789	20	0.13241	3.0	(1 0 9)	71.146	35.573	0.03776
2	0.36940	65.0	(1 0 1)	24.071	12.036	0.01354	21	0.12805	4.0	(3 0 1)	73.961	36.981	0.03905
3	0.31700	35.0	(0 0 4)	28.126	14.063	0.01577	22	0.12684	1.0	(0 0 10)	74.787	37.393	0.03942
4	0.28510	100.0	(1 0 3)	31.350	15.675	0.01754	23	0.12539	8.0	(2 2 4)	75.803	37.902	0.03988
5	0.27320	90.0	(1 1 0)	32.753	16.376	0.01830	24	0.12499	18.0	(2 1 7)	76.089	38.044	0.04000
6	0.25090	5.0	(1 1 2)	35.758	17.879	0.01993	25	0.12312	18.0	(3 0 3)	77.457	38.729	0.04061
7	0.21240	35.0	(1 0 5)	42.527	21.263	0.02354	26	0.12252	14.0	(2 0 8)	77.908	38.954	0.04081
8	0.21140	25.0	(0 0 6)	42.738	21.369	0.02365	27	0.12211	19.0	(3 1 0)	78.220	39.110	0.04095
9	0.20697	60.0	(1 1 4)	43.699	21.850	0.02416	28	0.11502	5.0	(1 1 10)	84.087	42.043	0.04347
10	0.19312	65.0	(2 0 0)	47.014	23.507	0.02589	29	0.11471	8.0	(2 2 6)	84.366	42.183	0.04359
11	0.17118	16.0	(2 1 1)	53.485	26.743	0.02921	30	0.11395	20.0	(3 1 4)	85.061	42.530	0.04388
12	0.16721	20.0	(1 1 6)	54.860	27.430	0.02990	31	0.11047	15.0	(1 0 11)	88.418	44.209	0.04526
13	0.16496	20.0	(2 0 4)	55.673	27.836	0.03031	32	0.10674	3.0	(3 2 1)	92.380	46.190	0.04684
14	0.16405	30.0	(1 0 7)	56.009	28.004	0.03048	33	0.10599	3.0	(2 0 10)	93.229	46.614	0.04717
15	0.15990	60.0	(2 1 3)	57.596	28.798	0.03127	34	0.10573	7.0	(3 1 6)	93.527	46.764	0.04729
16	0.15856	11.0	(0 0 8)	58.129	29.065	0.03153	35	0.10493	7.0	(3 0 7)	94.461	47.230	0.04765
17	0.14262	20.0	(2 0 6)	65.380	32.690	0.03506	36	0.10381	13.0	(3 2 3)	95.806	47.903	0.04816
18	0.13709	14.0	(1 1 8)	69.372	34.186	0.03647	37	0.10346	7.0	(2 2 8)	96.236	48.118	0.04633
19	0.13653	17.0	(2 2 0)	58.691	34.346	0.03662							
Simulation Parameters: Fixed-Slit Intensities, Two-Theta Range =11.96/98.24/0.02, FWHM = 0.1													

35149606

La_2O_3 PDF#05-0602

PDF#05-0602: QM=Star(S); d=(Unknown); i=Diffractometer										PDF Card (cSCR)			
Lanthanum Oxide													
La_2O_3													
Radiation=CuKa1										Lambda=1.5405			
Calibration=										2T=26.110-148.312			
Ref: Swanson, Fuyat. Natl. Bur. Stand. (U.S.), Circ. 539, viii p33 (1954)										Filter=Ni			
Hexagonal - Powder Diffraction P-2m1 (164)										Z=1			
CELL: 3.9373 x 3.9373 x 6.1299 <90.0 x 90.0 x 120.0>										mp=			
Density(c)=6.573										P S=hPS (La_2O_3)			
Density(n)=6.22A										F(30)=46.8 { 0160.40/0}			
Mwt=325.81										Vol=82.30			
Ref: Ibid.													
NOTE: Sample from Fairmount Chemical Company. Spectroscopic analysis: <0.01% Ca, Mg, Si; <0.001% Al, Cu, Fe, Pb. Pattern taken at 26 C. Sample was annealed at 1200 C for one hour and mounted in petrolatum to prevent reabsorption of $\text{O}_2 + \text{H}_2\text{O}$. Merck Index, 8th Ed., p. 608. Opaque mineral optical data on specimen from Nansenke, Uganda. R3R% = 14.2, Disp = Std. VHN100 = 782-813. Pattern reviewed by Holzer, J., McCarthy, G., North Dakota State Univ., Fargo, North Dakota, USA, ICDD Grant-in-Aid (1990). Validated by calculated pattern except for the following: 2.278 23 102; 1.968 28 110, 1.753 23 103. Calculated pattern indicates that the following reflections might be observable: 6.130 <1 001; 2.043 <1 003; 1.8744 <1 111; 1.4177 <1 113; 1.2260 <1 005.													
Color: Colorless													
Strong Lines: 2.98/X 1.97/6 2.28/6 1.75/5 3.41/3 3.05/3 1.66/2 1.64/2 1.26/1 1.31/1													
39 Lines, Wavelength to Compute Theta = 1.54056 Å(Cu), 1% Type = (Unknown)													
#	d(nm)	I(f)	(h k l)	2-Theta	Theta	I/(2d)	#	d(nm)	I(f)	(h k l)	2-Theta	Theta	I/(2d)
1	0.34100	34.0	(1 0 0)	26.110	13.055	0.01466	21	0.10901	7.0	(2 1 3)	89.920	44.960	0.04587
2	0.30630	31.0	(0 0 2)	29.130	14.565	0.01632	22	0.10658	4.0	(3 0 2)	92.560	46.280	0.04691
3	0.29800	100.0	(1 0 1)	29.960	14.980	0.01678	23	0.10220	0.0	(0 0 6)	97.824	48.912	0.04892
4	0.22780	58.0	(1 0 2)	39.527	19.764	0.02195	24	0.09952	3.0	(2 0 5)	101.428	50.714	0.05024
5	0.19680	63.0	(1 1 0)	46.084	23.042	0.02541	25	0.09840	3.0	(2 2 0)	103.036	51.518	0.05081
6	0.17530	52.0	(1 0 3)	52.132	26.066	0.02852	26	0.09787	1.0	(1 0 6)	103.820	51.910	0.05109
7	0.17050	4.0	(2 0 0)	53.716	26.858	0.02933	27	0.09459	0.0	(3 1 0)	109.043	54.522	0.05286
8	0.16560	24.0	(1 1 2)	55.439	27.720	0.03019	28	0.09372	3.0	(2 2 2)	110.550	55.275	0.05335
9	0.16420	17.0	(2 0 1)	55.953	27.977	0.03045	29	0.09345	5.0	(3 1 1)	111.029	55.515	0.05350
10	0.15320	3.0	(0 0 4)	60.370	30.185	0.03264	30	0.09131	2.0	(3 0 4)	115.042	57.521	0.05476
11	0.14900	5.0	(2 0 2)	62.258	31.125	0.03356	31	0.09070	2.0	(1 1 6)	116.263	58.131	0.05513
12	0.13980	2.0	(1 0 4)	66.870	33.435	0.03577	32	0.08883	5.0	(2 1 5)	120.256	60.128	0.05629
13	0.13090	7.0	(2 0 3)	72.094	36.047	0.03820	33	0.08766	1.0	(2 0 6)	122.975	61.488	0.05704
14	0.12890	2.0	(2 1 0)	73.393	36.697	0.03879	34	0.08583	4.0	(3 1 3)	127.649	63.825	0.05825
15	0.12610	12.0	(2 1 1)	75.302	37.651	0.03965	35	0.08480	2.0	(1 0 7)	130.556	65.278	0.05996
16	0.12090	6.0	(1 1 4)	79.155	39.578	0.04136	36	0.08443	1.0	(4 0 1)	131.659	65.829	0.05922
17	0.11879	4.0	(2 1 2)	80.848	40.424	0.04209	37	0.08283	2.0	(2 2 4)	136.855	68.427	0.06036
18	0.11538	4.0	(1 0 5)	83.765	41.882	0.04334	38	0.08050	1.0	(3 1 4)	146.222	73.111	0.06211
19	0.11396	2.0	(2 0 4)	85.051	42.526	0.04388	39	0.08007	2.0	(2 1 6)	148.312	74.156	0.06245
20	0.11367	4.0	(3 0 0)	85.320	42.660	0.04399							

Simulation Parameters: Fixed-Slit Intensities, Two-Theta Range = 24.11/150.31/0.02, FWHM = 0.1

391699506

(La_{0.9}Sr_{0.1}) ((Ga_{0.8}Mg_{0.2}) O_{2.87}) PDF#89-6965

PDF#89-6965: QM=Calculated(C), d=Calculated; I=Calculated										PDF Card			
Lanthanum Strontium Gallium Magnesium Oxide													
(La _{0.9} Sr _{0.1}) ((Ga _{0.8} Mg _{0.2}) O _{2.87})													
Radiation=CuK _{α1}													
Calibration=													
Ref: Calculated from ICSD using POWD-12++													
Monoclinic - Powder Diffraction, I2/a (15)													
CELL: 7.81603 x 5.5883 x 5.51467 <90.0 x 90.06 x 90.0>													
Density(c)=6.685 Density(n)=6.44A Mw=240.33 Vol=238.76 F(30)= 28.51/0140,75/0													
Ref: Slater, P.R., Irvine, J.T.S., Ishihara, T., Takita, Y. J. Solid State Chem., v139 p135 (1998)													
FIZ-051040: ICSD SG: I12/A1 IT is: 15 SG short form: I2/a ATF TEM 298. RVP. ITF TF are of mixed type. TF are converted prior to pattern calculation ITF High-temperature powder neutron diffraction study of the oxide ion conductor Li _{0.9} Sr _{0.1} Ga _{0.8} Mg _{0.2} O _{2.85}													
Strong Lines: 2.76/X 1.95/3 1.59/2 1.60/2 3.91/2 2.25/1 2.26/1 1.38/1 1.24/1 1.23/1													
64 Lines, Wavelength to Compute Theta = 1.54056A(Cu), I%-Type = Peak Height													
#	d(nm)	I(f)	(h k l)	2-Theta	Theta	I/(2d)	#	d(nm)	I(f)	(h k l)	2-Theta	Theta	I/(2d)
1	0.45194	0.1	(1 1 0)	19.627	9.813	0.01106	33	0.13237	0.1	(-1 4 1)	71.172	35.586	0.03777
2	0.39081	16.1	(2 0 0)	22.734	11.367	0.01279	34	0.13237	0.1	(1 4 1)	71.172	35.586	0.03777
3	0.39081	16.1	(0 1 1)	22.734	11.367	0.01279	35	0.13217	0.1	(-5 1 2)	71.295	35.648	0.03783
4	0.27645	100.0	(2 1 1)	32.358	16.179	0.01809	36	0.13217	0.1	(3 3 2)	71.295	35.648	0.03783
5	0.27645	100.0	(-2 1 1)	32.358	16.179	0.01809	37	0.13201	0.1	(3 2 3)	71.394	35.697	0.03788
6	0.27573	78.9	(0 0 2)	32.444	16.222	0.01813	38	0.13201	0.1	(5 1 2)	71.394	35.697	0.03788
7	0.23576	0.6	(3 1 0)	38.140	19.070	0.02121	39	0.13184	0.1	(1 1 4)	71.497	35.749	0.03792
8	0.23576	0.6	(1 2 1)	38.140	19.070	0.02121	40	0.13042	0.8	(4 3 1)	72.401	36.201	0.03834
9	0.23532	0.5	(-1 1 2)	38.214	19.107	0.02125	41	0.13042	0.8	(-4 3 1)	72.401	36.201	0.03834
10	0.23532	0.5	(1 1 2)	38.214	19.107	0.02125	42	0.13027	0.9	(0 3 3)	72.497	36.249	0.03838
11	0.22597	0.7	(2 2 0)	39.861	19.930	0.02213	43	0.13027	0.9	(-1 1 3)	72.497	36.249	0.03838
12	0.22519	10.7	(2 0 2)	40.005	20.002	0.02220	44	0.13008	0.9	(2 0 4)	72.623	36.312	0.03844
13	0.22519	10.7	(2 0 2)	40.005	20.002	0.02220	45	0.13008	0.9	(4 1 3)	72.623	36.312	0.03844
14	0.19541	33.7	(4 0 0)	46.431	23.216	0.02559	46	0.12361	8.0	(6 1 1)	77.091	38.546	0.04045
15	0.19541	33.7	(0 2 2)	46.431	23.216	0.02559	47	0.12361	8.0	(-2 3 3)	77.091	38.546	0.04045
16	0.17970	0.1	(1 3 0)	50.764	25.382	0.02782	48	0.12342	4.7	(0 2 4)	77.233	38.617	0.04051
17	0.17910	0.1	(3 2 1)	50.944	25.472	0.02792	49	0.11931	0.1	(3 4 1)	80.426	40.213	0.04191
18	0.17910	0.1	(3 1 2)	50.944	25.472	0.02792	50	0.11931	0.1	(5 3 0)	80.426	40.213	0.04191
19	0.17472	3.5	(4 1 1)	52.318	26.159	0.02862	51	0.11896	0.1	(3 1 4)	80.707	40.353	0.04203
20	0.17472	3.5	(2 2 2)	52.318	26.159	0.02862	52	0.11896	0.1	(-1 1 4)	80.707	40.353	0.04203
21	0.17447	2.4	(0 1 3)	52.400	26.200	0.02866	53	0.11796	0.8	(2 4 2)	81.535	40.767	0.04239
22	0.15977	17.8	(4 2 0)	57.649	28.825	0.03130	54	0.11796	0.8	(-2 4 2)	81.535	40.767	0.04239
23	0.15977	17.8	(2 3 1)	57.649	28.825	0.03130	55	0.11788	0.7	(-6 0 2)	81.604	40.802	0.04242
24	0.15925	23.3	(2 1 0)	57.852	28.926	0.03140	56	0.11788	0.7	(6 2 0)	81.604	40.802	0.04242
25	0.15925	23.3	(4 0 2)	57.852	28.926	0.03140	57	0.11766	1.1	(-2 2 4)	81.789	40.894	0.04250
26	0.15044	0.1	(5 1 0)	61.594	30.797	0.03323	58	0.11766	1.1	(2 2 4)	81.789	40.894	0.04250
27	0.15044	0.1	(-1 2 3)	61.594	30.797	0.03323	59	0.11299	1.9	(4 4 0)	85.962	42.981	0.04425
28	0.15028	0.1	(1 2 3)	61.672	30.836	0.03327	60	0.11271	2.0	(-4 0 4)	86.227	43.114	0.04436
29	0.13848	3.0	(0 4 0)	67.591	33.796	0.03611	61	0.11259	1.3	(4 0 4)	86.333	43.167	0.04441
30	0.13812	8.6	(4 2 2)	67.792	33.896	0.03620	62	0.10969	0.1	(1 5 0)	89.213	44.606	0.04558
31	0.13812	8.6	(-4 2 2)	67.792	33.896	0.03620	63	0.10946	0.1	(1 3 4)	89.455	44.727	0.04568
32	0.13787	6.4	(0 0 4)	67.934	33.967	0.03627	64	0.10946	0.1	(7 1 0)	89.455	44.727	0.04568

Simulation Parameters: Fixed-Slit Intensities, Two Theta Range = 17.63/91.45/0.02, FWHM = 0.1

39749606

SrLaGa₃O₇ PDF#45-0637

PDF#45-0637: QM=Star(S); d=Diffractometer; I=Diffractometer										PDF Card					
Sr Lanthanum Gallium Oxide															
Sr La Ga3 O7															
Radiation=CuKa1															
Lambda=1.54056															
Calibration=External(Al2O3)															
2T=15.540-110.206															
Filter=Ni															
I/Ic(RIR)=7.21															
Ref: Ivanov, S., Zhurov, V., Karpov Inst. of Physical Chemistry, Moscow, Russia.															
ICDD Grant-in-Aid (1994);															
Tetragonal - Powder Diffraction, P-421m (113)															
CELL: 8.0541 x 8.0541 x 5.3325 <90 0 >90 0 >90 0 >															
P S=P24 (?)															
Density(c)=5.290															
Density(m)=5.240															
Mwt=547.68															
Vol=345.91															
F(30)=298.9(.0030,33/0)															
Ref: Toropov, N., Ismatov, A.															
Dokl. Akad. Nauk SSSR, v183 p609 (1968)															
NOTE: EDS analysis (LINK system) (at.%): Sr 20.1(3), La 19.8(2), Ga 60.1(5). Sample was provided by Kucheyko, S., Moscow State Univ., Russia. Pattern taken at 22 C. Single-crystals of Sr La Ga3 O7 were grown by Czochralski method. To replace 22-1436.															
Color: Colorless															
Strong Lines: 2.98/X 1.84/3 2.55/2 3.21/2 1.59/2 2.67/1 3.89/1 1.44/1 1.83/1 1.55/1															
101 Lines, Wavelength to Compute Theta = 1.54056Å(Cu), 1% Type = Peak Area															
#	d(nm)	I(f)	(h k l)	2-Theta	#	d(nm)	I(f)	(h k l)	2-Theta	#	d(nm)	I(f)	(h k l)	2-Theta	
1	0.56975	3.0	(1 1 0)	15.540	35	0.15941	15.0	(2 1 3)	57.791	69	0.11488	0.0	(6 2 2)	84.208	
2	0.53334	1.0	(0 0 1)	16.608	36	0.15761	2.0	(4 1 2)	58.515	70	0.11443	5.0	(5 2 3)	84.618	
3	0.44469	1.0	(1 0 1)	19.950	37	0.15464	7.0	(3 3 2)	59.751	71	0.11377	1.0	(5 4 2)	85.224	
4	0.40264	2.0	(2 0 0)	22.058	38	0.15145	2.0	(5 1 1)	61.144	72	0.11169	1.0	(6 4 0)	87.210	
5	0.38930	12.0	(1 1 1)	22.824	39	0.15079	2.0	(2 2 3)	61.437	73	0.11117	1.0	(4 0 4)	87.723	
6	0.36023	1.0	(2 1 0)	24.694	40	0.14923	2.0	(4 2 2)	62.150	74	0.11063	0.0	(7 2 0)	88.262	
7	0.32137	18.0	(2 0 1)	27.736	41	0.14822	1.0	(3 0 3)	62.621	75	0.11012	1.0	(4 1 4)	88.770	
8	0.29848	100.0	(2 1 1)	29.911	42	0.14577	1.0	(3 1 3)	63.798	76	0.10933	1.0	(6 4 1)	89.586	
9	0.28474	4.0	(2 2 0)	31.390	43	0.14401	10.0	(5 2 1)	64.674	77	0.10909	1.0	(3 3 4)	89.832	
10	0.26665	14.0	(0 0 2)	33.581	44	0.14238	2.0	(4 4 0)	65.502	78	0.10832	1.0	(7 2 1)	90.651	
11	0.25471	22.0	(3 1 0)	35.206	45	0.13909	1.0	(3 2 3)	67.258	79	0.10715	1.0	(4 2 4)	91.924	
12	0.25309	3.0	(1 0 2)	35.438	46	0.13814	1.0	(5 3 0)	67.783	80	0.10619	1.0	(6 1 3)	93.004	
13	0.25120	1.0	(2 2 1)	35.714	47	0.13788	1.0	(4 3 2)	67.926	81	0.10576	2.0	(7 3 0)	93.494	
14	0.24147	2.0	(1 1 2)	37.204	48	0.13756	1.0	(4 4 1)	68.107	82	0.10482	1.0	(1 1 5)	94.590	
15	0.23976	1.0	(3 0 1)	37.479	49	0.13589	0.0	(5 1 2)	69.059	83	0.10476	0.0	(7 1 2)	94.667	
16	0.22987	1.0	(3 1 1)	39.156	50	0.13421	4.0	(6 0 0)	70.050	84	0.10351	1.0	(6 2 3)	96.175	
17	0.22230	2.0	(2 0 2)	40.547	51	0.13333	3.0	(0 0 4)	70.583	85	0.10307	1.0	(2 0 5)	96.715	
18	0.21431	5.0	(2 1 2)	42.129	52	0.13240	0.0	(6 1 0)	71.150	86	0.10269	2.0	(5 4 3)	97.202	
19	0.20605	2.0	(3 2 1)	43.905	53	0.13147	4.0	(4 1 3)	71.732	87	0.10226	3.0	(2 1 5)	97.752	
20	0.20133	5.0	(4 0 0)	44.989	54	0.13044	1.0	(5 2 2)	72.387	88	0.10125	0.0	(6 5 1)	99.066	
21	0.19534	3.0	(4 1 0)	46.449	55	0.12977	2.0	(3 3 3)	72.821	89	0.09989	1.0	(7 4 0)	100.914	
22	0.19465	3.0	(2 2 2)	46.623	56	0.12850	1.0	(6 1 1)	73.659	90	0.09989	1.0	(2 2 5)	100.914	
23	0.18985	5.0	(3 3 0)	47.875	57	0.12652	0.0	(4 2 3)	75.008	91	0.09952	0.0	(5 2 4)	101.425	
24	0.18922	1.0	(3 0 2)	48.043	58	0.12580	0.0	(5 4 0)	75.509	92	0.09892	1.0	(8 0 1)	102.279	
25	0.18837	1.0	(4 0 1)	48.275	59	0.12559	1.0	(4 4 2)	75.663	93	0.09832	2.0	(7 3 2)	103.154	
26	0.18417	25.0	(3 1 2)	49.447	60	0.12502	1.0	(2 1 4)	76.065	94	0.09819	3.0	(8 1 1)	103.338	
27	0.18342	9.0	(4 1 1)	49.662	61	0.12386	1.0	(6 2 1)	76.911	95	0.09732	1.0	(4 4 4)	104.651	
28	0.18010	3.0	(4 2 0)	50.643	62	0.12265	1.0	(5 3 2)	77.809	96	0.09592	1.0	(5 3 4)	106.845	
29	0.17884	4.0	(3 3 1)	51.026	63	0.12242	2.0	(5 4 1)	77.983	97	0.09490	1.0	(6 6 0)	108.524	
30	0.17121	1.0	(3 2 2)	53.474	64	0.12073	1.0	(2 2 4)	79.287	98	0.09458	2.0	(6 4 3)	109.067	
31	0.17064	0.0	(4 2 1)	53.667	65	0.11990	3.0	(6 0 2)	79.944	99	0.09458	2.0	(6 0 4)	109.067	
32	0.16969	1.0	(1 1 1)	53.993	66	0.11940	1.0	(3 0 4)	80.351	100	0.09423	1.0	(4 0 5)	109.652	
33	0.16262	2.0	(2 0 3)	56.544	67	0.11864	0.0	(6 1 2)	80.969	101	0.09392	0.0	(7 2 3)	110.206	
34	0.16068	2.0	(4 0 2)	57.290	68	0.11810	6.0	(3 1 4)	81.416						
Simulation Parameters: Fixed-Slit Intensities, Two-Theta Range = 13.54/112.21/0.02, FWHM = 0.1															
o Scale(Å)															

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VITA

Miss Ratanakorn Teerasarunyanon was born on January 16, 1989 in Nakorn Pathom, Thailand. She graduated with Bachelor's Degree in Chemistry (2nd class honor) from Faculty of Science, Silpakorn University in 2010. She continued the Master's degree in program of Chemistry (Inorganic Chemistry), Faculty of Science, Chulalongkorn University in 2011 and completed in 2013.

PRESENTATIONS

October 21-23, 2013.

Poster Presentation: "Effects of Calcium Doping on Electrical Properties of $\text{La}_{1.6}\text{Sr}_{0.4}\text{Ni}_{0.9}\text{Co}_{0.1}\text{O}_4$ Materials for SOFCs" The 39th congress on science and technology of Thailand (STT39), BITEC Bangna, Bangkok, Thailand.

January 8-10, 2014.

Poster Presentation: "Electrical Conductivity of $\text{La}_{1.6}\text{Sr}_{0.4}\text{Ni}_{0.9}\text{Co}_{0.1}\text{O}_4$ Oxide Doped with Calcium" The 9th Mathematics and Physical Science Graduate Congress at University of Malaya, Malaysia.

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