

Supporting information

Table S1

Indexed X-ray Diffraction Pattern of $\text{LaCa}_2\text{Cu}_2\text{GaO}_7$,
 Orthorhombic; $a = 22.359(1) \text{ \AA}$, $b = 5.480(1) \text{ \AA}$, $c = 5.390(2) \text{ \AA}$.

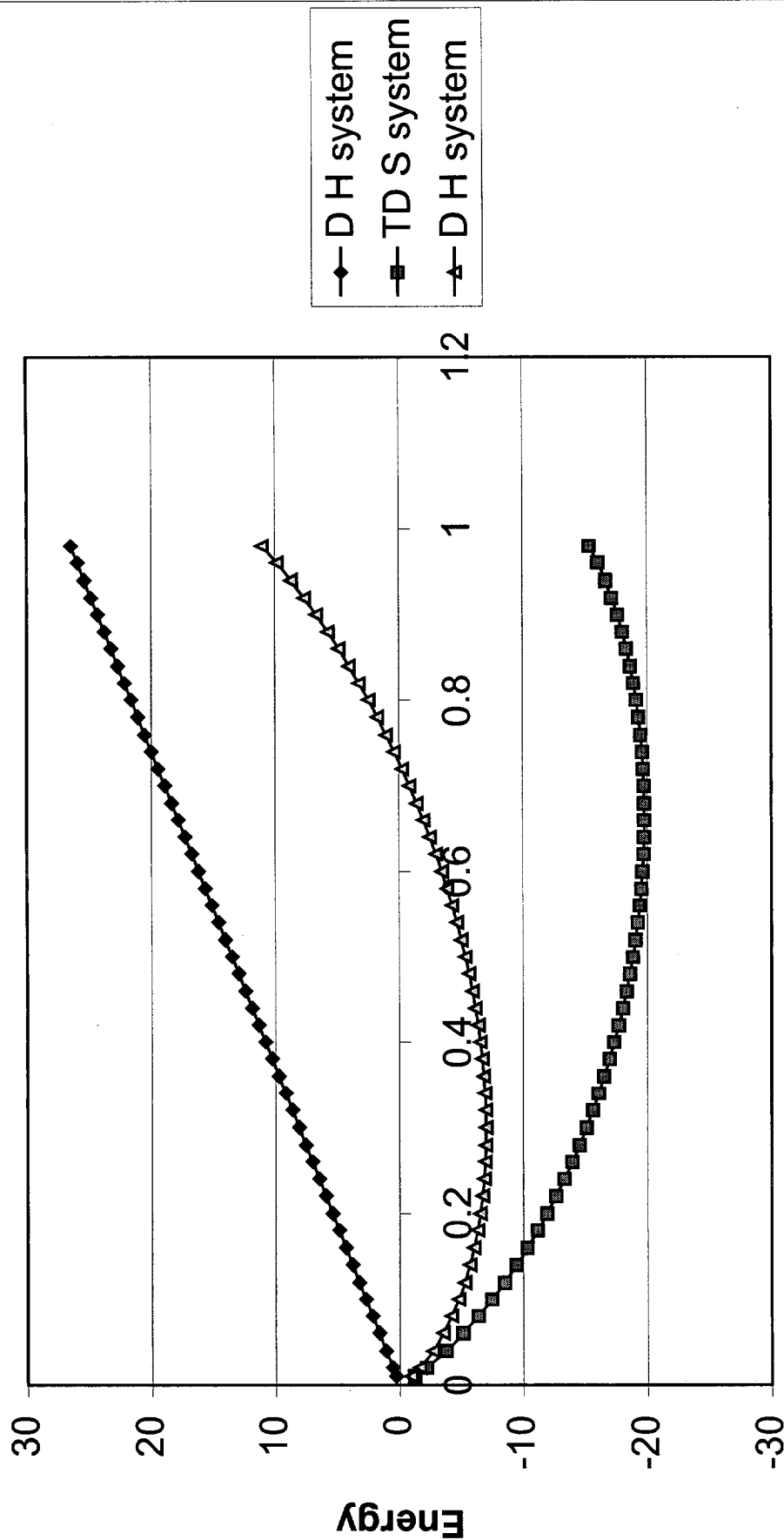
<i>hkl</i>	d_{Riet}	$\%I/I_{\text{max}}$	<i>hkl</i>	d_{Riet}	$\%I/I_{\text{max}}$
4 0 0	5.590	4	2 3 1	1.709	<1
1 1 0	5.322	1	6 2 2	1.708	<1
3 1 0	4.415	3	5 3 0	1.691	3
0 1 1	3.843	1	12 1 1	1.677	2
6 0 0	3.726	2	4 3 1	1.653	1
5 1 0	3.464	3	13 1 0	1.641	<1
4 1 1	3.167	14	4 1 3	1.633	2
7 1 0	2.759	2	14 0 0	1.597	3
0 2 0	2.740	31	7 3 0	1.586	1
0 0 2	2.695	37	6 3 1	1.569	18
6 1 1	2.675	100	11 2 1	1.562	1
2 2 0	2.661	<1	6 1 3	1.552	20
2 0 2	2.620	1	12 2 0	1.541	4
4 2 0	2.460	1	12 0 2	1.533	4
1 2 1	2.428	2	1 2 3	1.499	1
4 0 2	2.428	1	3 3 2	1.482	1
3 1 2	2.300	<1	14 1 1	1.475	4
8 1 1	2.260	24	3 2 3	1.473	<1
10 0 0	2.236	6	9 3 0	1.472	<1
6 2 0	2.207	2	8 3 1	1.471	6
6 0 2	2.184	1	10 2 2	1.457	4
5 1 2	2.127	1	8 1 3	1.457	5
8 2 0	1.956	2	5 3 2	1.432	2
7 2 1	1.940	1	5 2 3	1.424	<1
8 0 2	1.940	2	16 0 0	1.397	<1
10 1 1	1.933	1	14 2 0	1.380	2
7 1 2	1.928	1	14 0 2	1.374	2
0 2 2	1.921	38	0 4 0	1.370	4
2 2 2	1.894	2	10 3 1	1.368	1
12 0 0	1.863	9	7 3 2	1.367	1
4 2 2	1.817	3	2 4 0	1.360	1
3 3 0	1.774	1	7 2 3	1.360	<1
9 2 1	1.742	2	10 1 3	1.357	<1
10 2 0	1.732	3	0 0 4	1.348	5
0 3 1	1.730	<1	12 2 2	1.338	8
10 0 2	1.721	3			

Table S2Selected Bond lengths (Å) and angles (°) for LaCa₂Cu₂GaO₇

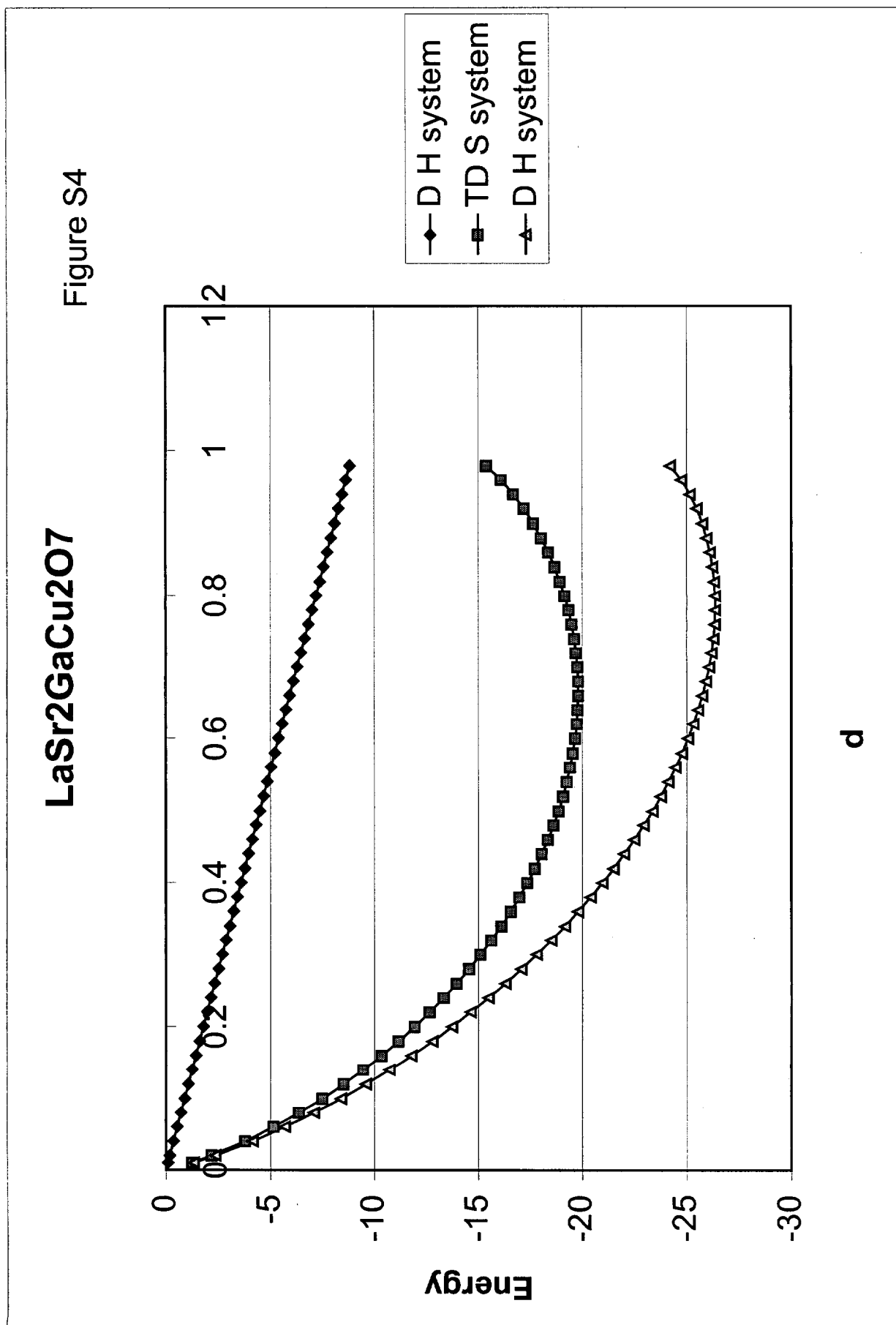
Atoms	XRD Refinement	Neutron Refinement
	Bond Lengths	Bond Lengths
Cu-O1	1.897	1.91392(3)
	1.934	1.92671(3)
Cu-O2	1.923	1.91242(3)
	1.941	1.94738(3)
Cu-O3	2.421	2.34535(4)
Ga-O3	1.730 x 2	1.80898(2) x 2
Ga-O4	1.841	1.89581(3)
	2.038	1.98444(4)
A1-O1	2.510 x 2	2.55495(3) x 2
	2.613 x 2	2.57758(3) x 2
A1-O2	2.467 x 2	2.43030(2) x 2
	2.476 x 2	2.45264(3) x 2
A2-O1	2.505	2.53461(3)
	2.617	2.60936(3)
A2-O2	2.552	2.56917(3)
	2.564	2.64477(3)
A2-O3	2.456	2.40877(4)
	2.610	2.65091(4)
	2.994	3.22426(6)
A2-O4	2.456	2.42359(3)
	Angles	Angles
O1-Cu-O1	89.6	89.151(2)
O1-Cu-O2	88.1	91.096(2)
	93.9	91.096(2)
	176.3	177.393(0)
	177.2	177.393(0)
O2-Cu-O3	88.5	88.592(2)
O3-Ga-O3	127.2	128.966(1)
O3-Ga-O4	105.3	104.129(0)
	106.8	106.214(1)
O4-Ga-O4	103.2	105.078(1)

LaCa₂GaCu₂O₇

Figure S3

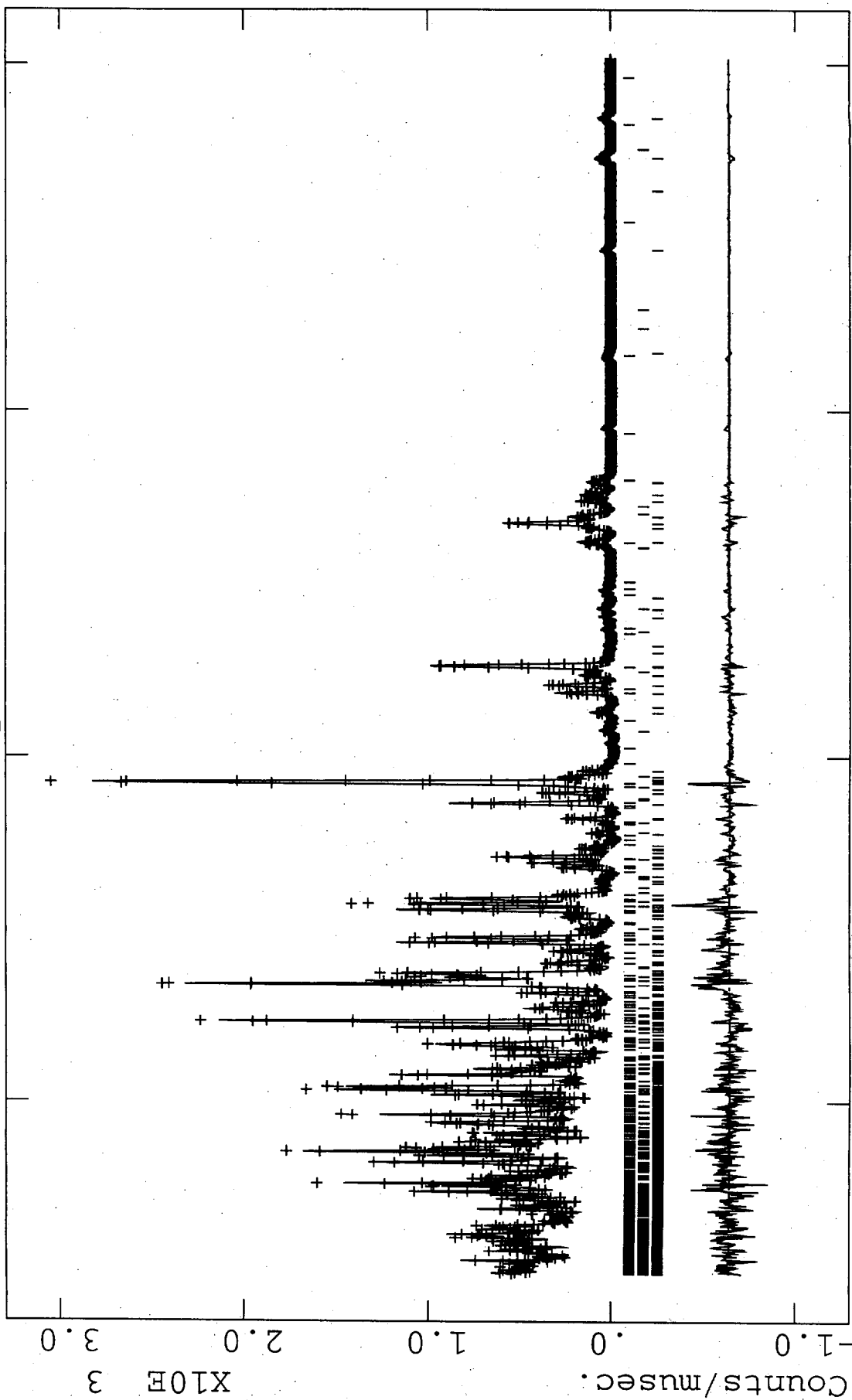


d



LaCa2Cu2GaO7 Figure S5 Hist 1

Bank 1, 2-Theta 144.8, L-S cycle 1071 Obsd. and Diff. Profiles



D-spacing, Å

Figure S6

