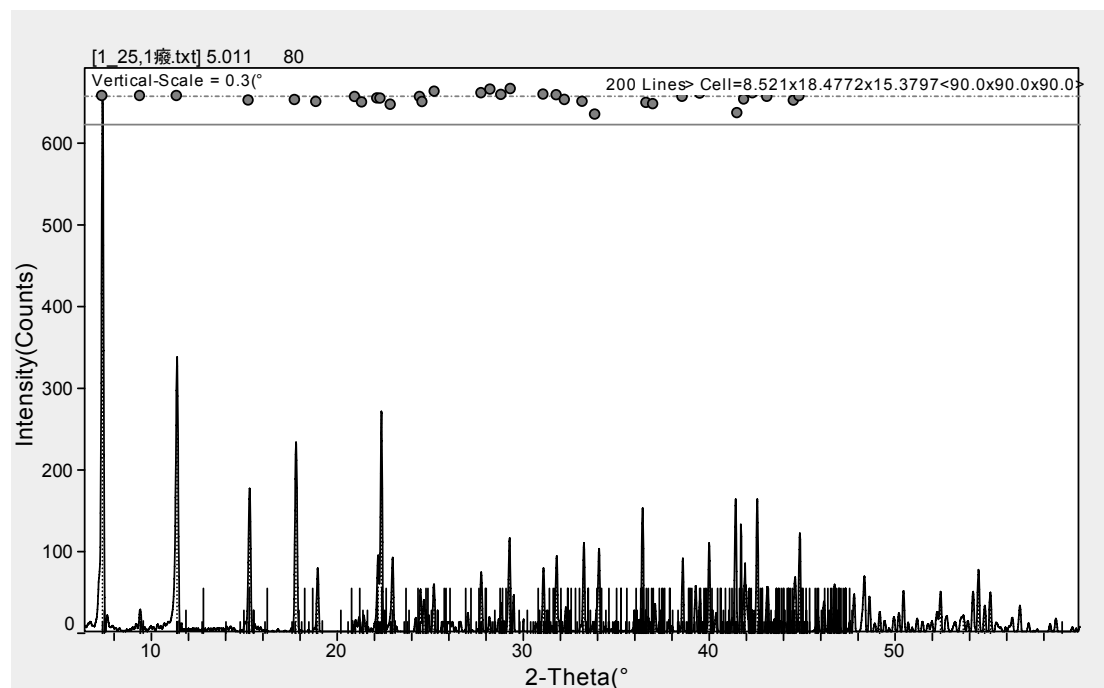Supporting information S2, Space group and unit cell obtained from XPRD patterns of complex 1 at different temperature

The space group and cell parameter obtained from XPRD patterns of 1 at 25 ^{o}C via JADE5

Pattern Indexing - Seek Miller Indices & Unit Cell [4 Hits Sorted on Figure-Of-Merit]

[1_25,1癈.txt] 5.011   809

1> fm=40, fn=12, p?=0, r?=7, C=O, Space Group=Pnma (62), a=8.528, b=15.551, c=18.778, Angle=90.00, Volume=2490.4

@ 2T(o)	h	k	l	2T(c)	Delta	d(c)	d(o)	Del-d	I%
7.375	0	1	1	7.375	0.000	11.9769	11.9769	0.0000	100.0
9.412	0	0	2	9.412	0.000	9.3889	9.3889	0.0000	3.8
-----	0	2	0	11.371	---	7.7754	---	---	
11.386	1	0	1	11.386	0.000	7.7651	7.7651	0.0000	51.1
-----	1	1	1	12.732	---	6.9472	---	---	
-----	1	0	2	14.017	---	6.3129	---	---	
-----	0	2	2	14.781	---	5.9885	---	---	
-----	1	1	2	15.134	---	5.8493	---	---	
15.295	0	1	3	15.246	-0.048	5.8066	5.7883	0.0182	26.6
-----	1	2	1	16.118	---	5.4944	---	---	
-----	1	0	3	17.561	---	5.0461	---	---	
17.779	0	3	1	17.736	-0.043	4.9967	4.9847	0.0120	35.3
-----	1	2	2	18.085	---	4.9009	---	---	
-----	1	1	3	18.470	---	4.7997	---	---	
18.950	0	0	4	18.888	-0.062	4.6945	4.6792	0.0153	10.8
-----	1	3	1	20.584	---	4.3112	---	---	

-----	2	0	0	20.814	---	4.2642	---	---	
20.982	1	2	3	20.970	-0.012	4.2328	4.2305	0.0023	0.5
21.418	2	0	1	21.350	-0.068	4.1584	4.1454	0.0130	3.0
-----	1	0	4	21.590	---	4.1126	---	---	
-----	2	1	0	21.591	---	4.1124	---	---	
-----	0	2	4	22.100	---	4.0188	---	---	
-----	2	1	1	22.109	---	4.0172	---	---	
22.198	1	3	2	22.171	-0.026	4.0061	4.0014	0.0047	14.0
-----	0	3	3	22.249	---	3.9923	---	---	
22.370	1	1	4	22.342	-0.028	3.9759	3.9710	0.0049	40.4
-----	0	4	0	22.856	---	3.8877	---	---	
22.979	2	0	2	22.886	-0.093	3.8826	3.8671	0.0154	13.1
-----	2	1	2	23.599	---	3.7669	---	---	
-----	2	2	0	23.778	---	3.7389	---	---	
-----	2	2	1	24.252	---	3.6669	---	---	
-----	0	1	5	24.362	---	3.6506	---	---	
24.476	1	2	4	24.466	-0.010	3.6354	3.6339	0.0015	7.3
24.664	1	3	3	24.600	-0.063	3.6158	3.6066	0.0092	4.3
-----	0	4	2	24.766	---	3.5919	---	---	
25.205	2	0	3	25.250	0.046	3.5241	3.5304	-0.0063	8.5
-----	1	4	1	25.604	---	3.4763	---	---	
-----	2	2	2	25.624	---	3.4736	---	---	
-----	1	0	5	25.901	---	3.4371	---	---	
-----	2	1	3	25.902	---	3.4370	---	---	
-----	1	1	5	26.537	---	3.3561	---	---	
-----	1	4	2	26.911	---	3.3103	---	---	
-----	2	3	0	27.054	---	3.2931	---	---	
-----	2	3	1	27.475	---	3.2436	---	---	
-----	1	3	4	27.665	---	3.2218	---	---	
27.740	2	2	3	27.770	0.030	3.2098	3.2132	-0.0034	10.6
28.182	2	0	4	28.250	0.067	3.1564	3.1638	-0.0074	2.3
-----	1	2	5	28.367	---	3.1436	---	---	
-----	0	0	6	28.497	---	3.1296	---	---	
-----	2	3	2	28.704	---	3.1075	---	---	
28.826	2	1	4	28.838	0.012	3.0934	3.0946	-0.0012	5.0
-----	1	4	3	28.969	---	3.0797	---	---	
-----	0	5	1	29.078	---	3.0683	---	---	
29.269	0	3	5	29.343	0.074	3.0413	3.0488	-0.0075	17.2
-----	0	4	4	29.814	---	2.9942	---	---	
-----	1	0	6	30.398	---	2.9381	---	---	
-----	2	2	4	30.541	---	2.9246	---	---	
-----	2	3	3	30.651	---	2.9144	---	---	
-----	0	2	6	30.771	---	2.9033	---	---	
-----	1	5	1	30.947	---	2.8872	---	---	

-----	1	1	6	30.949	---	2.8870	---	---	
31.089	2	4	0	31.105	0.015	2.8729	2.8743	-0.0014	11.4
-----	1	3	5	31.198	---	2.8646	---	---	
-----	2	4	1	31.476	---	2.8399	---	---	
-----	1	4	4	31.644	---	2.8252	---	---	
-----	2	0	5	31.722	---	2.8184	---	---	
31.803	3	0	1	31.810	0.008	2.8108	2.8114	-0.0007	13.7
-----	1	5	2	32.054	---	2.7899	---	---	
-----	0	5	3	32.110	---	2.7853	---	---	
32.294	2	1	5	32.253	-0.041	2.7732	2.7697	0.0034	4.6
-----	3	1	1	32.340	---	2.7660	---	---	
-----	1	2	6	32.552	---	2.7484	---	---	
-----	2	4	2	32.567	---	2.7472	---	---	
-----	3	0	2	32.891	---	2.7208	---	---	
33.265	2	3	4	33.204	-0.061	2.6959	2.6911	0.0048	16.4
-----	3	1	2	33.405	---	2.6801	---	---	
-----	2	2	5	33.801	---	2.6497	---	---	
-----	1	5	3	33.827	---	2.6476	---	---	
-----	0	1	7	33.882	---	2.6435	---	---	
34.080	3	2	1	33.884	-0.197	2.6434	2.6286	0.0148	15.2
-----	2	4	3	34.316	---	2.6110	---	---	
-----	0	6	0	34.579	---	2.5918	---	---	
-----	3	0	3	34.626	---	2.5884	---	---	
-----	1	4	5	34.811	---	2.5750	---	---	
-----	3	2	2	34.908	---	2.5681	---	---	
-----	1	0	7	35.037	---	2.5590	---	---	
-----	1	3	6	35.078	---	2.5560	---	---	
-----	3	1	3	35.118	---	2.5532	---	---	
-----	1	1	7	35.524	---	2.5250	---	---	
-----	2	0	6	35.552	---	2.5230	---	---	
-----	2	5	0	35.702	---	2.5128	---	---	
-----	0	6	2	35.916	---	2.4983	---	---	
-----	2	5	1	36.031	---	2.4906	---	---	
-----	2	1	6	36.033	---	2.4905	---	---	
-----	1	5	4	36.181	---	2.4807	---	---	
-----	2	3	5	36.250	---	2.4760	---	---	
-----	3	3	1	36.328	---	2.4709	---	---	
36.425	1	6	1	36.519	0.093	2.4585	2.4645	-0.0061	22.5
-----	3	2	3	36.559	---	2.4559	---	---	
36.716	2	4	4	36.642	-0.074	2.4505	2.4457	0.0048	2.6
-----	0	4	6	36.838	---	2.4379	---	---	
-----	3	0	4	36.935	---	2.4317	---	---	
-----	1	2	7	36.951	---	2.4307	---	---	
37.090	2	5	2	37.003	-0.087	2.4274	2.4219	0.0055	4.9

-----	3	3	2	37.294	---	2.4091	---	---	
-----	3	1	4	37.400	---	2.4025	---	---	
-----	2	2	6	37.443	---	2.3999	---	---	
-----	1	6	2	37.480	---	2.3976	---	---	
-----	0	5	5	37.516	---	2.3954	---	---	
-----	0	3	7	37.727	---	2.3824	---	---	
-----	0	0	8	38.315	---	2.3472	---	---	
-----	1	4	6	38.370	---	2.3440	---	---	
38.585	2	5	3	38.577	-0.008	2.3319	2.3314	0.0005	13.5
-----	3	2	4	38.768	---	2.3209	---	---	
-----	3	3	3	38.857	---	2.3157	---	---	
-----	1	5	5	39.025	---	2.3061	---	---	
-----	1	6	3	39.037	---	2.3055	---	---	
-----	1	3	7	39.230	---	2.2946	---	---	
-----	2	4	5	39.458	---	2.2818	---	---	
39.505	3	4	1	39.530	0.025	2.2778	2.2792	-0.0014	5.9
-----	2	0	7	39.661	---	2.2706	---	---	
-----	0	6	4	39.691	---	2.2690	---	---	
-----	2	3	6	39.698	---	2.2686	---	---	
-----	3	0	5	39.733	---	2.2667	---	---	
-----	1	0	8	39.798	---	2.2631	---	---	
39.998	0	2	8	40.094	0.096	2.2471	2.2522	-0.0052	16.1
-----	2	1	7	40.099	---	2.2468	---	---	
-----	3	1	5	40.171	---	2.2430	---	---	
-----	1	1	8	40.236	---	2.2395	---	---	
-----	3	4	2	40.431	---	2.2291	---	---	
-----	2	5	4	40.693	---	2.2154	---	---	
-----	2	6	0	40.704	---	2.2148	---	---	
-----	0	7	1	40.871	---	2.2061	---	---	
-----	3	3	4	40.961	---	2.2015	---	---	
-----	2	6	1	40.999	---	2.1995	---	---	
-----	1	6	4	41.133	---	2.1927	---	---	
-----	2	2	7	41.392	---	2.1796	---	---	
-----	3	2	5	41.461	---	2.1761	---	---	
41.707	1	2	8	41.525	-0.182	2.1729	2.1638	0.0091	19.8
-----	2	6	2	41.873	---	2.1556	---	---	
41.934	3	4	3	41.896	-0.038	2.1545	2.1527	0.0019	12.2
-----	1	4	7	42.246	---	2.1375	---	---	
-----	1	7	1	42.280	---	2.1358	---	---	
-----	1	5	6	42.281	---	2.1358	---	---	
42.327	4	0	0	42.357	0.030	2.1321	2.1335	-0.0014	3.2
42.583	4	0	1	42.642	0.060	2.1185	2.1213	-0.0028	24.5
-----	2	4	6	42.687	---	2.1164	---	---	
-----	4	1	0	42.773	---	2.1124	---	---	

-----	3	0	6	42.945	---	2.1043	---	---	
-----	4	1	1	43.056	---	2.0991	---	---	
43.141	1	7	2	43.132	-0.009	2.0956	2.0952	0.0004	7.9
-----	0	7	3	43.175	---	2.0936	---	---	
-----	2	5	5	43.287	---	2.0884	---	---	
-----	2	6	3	43.298	---	2.0879	---	---	
-----	3	5	1	43.354	---	2.0854	---	---	
-----	3	1	6	43.356	---	2.0853	---	---	
-----	2	3	7	43.475	---	2.0798	---	---	
-----	4	0	2	43.490	---	2.0792	---	---	
-----	3	3	5	43.542	---	2.0768	---	---	
-----	1	3	8	43.603	---	2.0740	---	---	
-----	1	6	5	43.706	---	2.0694	---	---	
-----	0	1	9	43.739	---	2.0679	---	---	
-----	3	4	4	43.879	---	2.0616	---	---	
-----	4	1	2	43.897	---	2.0608	---	---	
-----	2	0	8	43.999	---	2.0563	---	---	
-----	4	2	0	44.001	---	2.0562	---	---	
-----	3	5	2	44.191	---	2.0478	---	---	
-----	4	2	1	44.277	---	2.0440	---	---	
-----	2	1	8	44.402	---	2.0386	---	---	
-----	1	7	3	44.525	---	2.0332	---	---	
-----	0	5	7	44.568	---	2.0313	---	---	
44.621	3	2	6	44.571	-0.050	2.0312	2.0291	0.0022	8.8
-----	1	0	9	44.676	---	2.0267	---	---	
44.875	4	0	3	44.873	-0.002	2.0182	2.0181	0.0001	17.9
-----	1	1	9	45.075	---	2.0097	---	---	
-----	0	4	8	45.081	---	2.0094	---	---	
-----	4	2	2	45.100	---	2.0086	---	---	
-----	2	6	4	45.232	---	2.0031	---	---	
-----	4	1	3	45.270	---	2.0015	---	---	
-----	0	6	6	45.397	---	1.9962	---	---	
-----	0	0	12	58.977	---	1.5648	---	---	

The space group and cell parameter obtained from XPRD patterns of 1 at 80 °C via JADE5
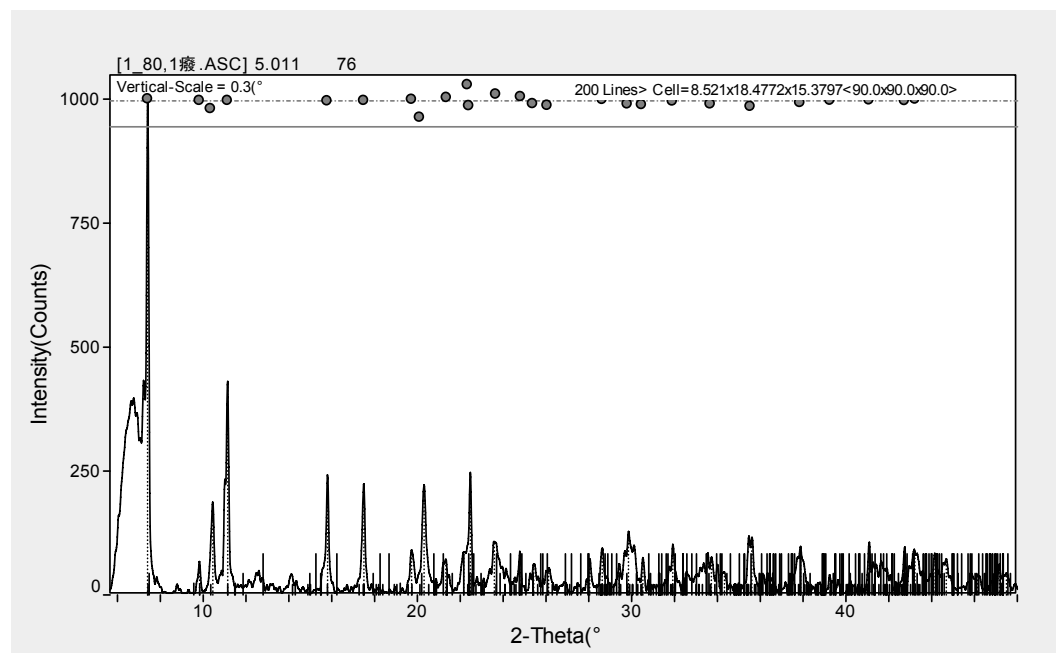
Pattern Indexing - Seek Miller Indices & Unit Cell [21 Hits Sorted on Figure-Of-Merit]

[1_80,1°C.ASC] 5.011   762

1> fm=44, fn=8, p?=0, r?=5, C=O, Space Group=Pnma (62), a=8.396, b=17.989, c=15.806, Angle=90.00, Volume=2387.2

@ 2T(o)	h	k	l	2T(c)	Delta	d(c)	d(o)	Del-d	I%
7.409	0	1	1	7.439	0.030	11.8739	11.9213	-0.0474	100.0
9.837	0	2	0	9.826	-0.011	8.9945	8.9843	0.0102	6.0
11.147	0	0	2	11.186	0.039	7.9032	7.9310	-0.0278	42.0
-----	1	0	1	11.926	---	7.4147	---	---	
12.608	1	1	1	12.903	0.295	6.8552	7.0150	-0.1598	3.6
-----	0	2	2	14.910	---	5.9369	---	---	
-----	1	0	2	15.385	---	5.7547	---	---	
-----	1	2	1	15.475	---	5.7213	---	---	
15.807	0	3	1	15.794	-0.013	5.6064	5.6019	0.0045	23.8
-----	1	1	2	16.158	---	5.4810	---	---	
17.505	0	1	3	17.525	0.020	5.0564	5.0622	-0.0058	21.9
-----	1	2	2	18.287	---	4.8474	---	---	
-----	1	3	1	19.019	---	4.6625	---	---	
19.733	0	4	0	19.724	-0.009	4.4972	4.4952	0.0020	8.5
-----	1	0	3	19.878	---	4.4628	---	---	
20.311	1	1	3	20.487	0.176	4.3315	4.3686	-0.0371	21.0
-----	2	0	0	21.146	---	4.1979	---	---	
21.330	1	3	2	21.383	0.053	4.1520	4.1621	-0.0102	5.8
-----	2	1	0	21.721	---	4.0881	---	---	
-----	2	0	1	21.888	---	4.0572	---	---	
22.165	1	2	3	22.218	0.054	3.9978	4.0073	-0.0096	7.4

-----	0	3	3	22.445	---	3.9580	---	---	
-----	2	1	1	22.445	---	3.9578	---	---	
22.470	0	0	4	22.481	0.011	3.9516	3.9534	-0.0018	23.3
-----	0	4	2	22.731	---	3.9087	---	---	
-----	1	4	1	23.111	---	3.8452	---	---	
23.592	2	2	0	23.366	-0.226	3.8040	3.7680	0.0360	8.5
-----	2	0	2	23.984	---	3.7074	---	---	
-----	2	2	1	24.043	---	3.6984	---	---	
-----	2	1	2	24.495	---	3.6310	---	---	
-----	0	2	4	24.586	---	3.6178	---	---	
24.784	1	3	3	24.849	0.066	3.5801	3.5894	-0.0094	8.0
-----	1	0	4	24.883	---	3.5754	---	---	
-----	1	4	2	25.110	---	3.5435	---	---	
-----	0	5	1	25.368	---	3.5081	---	---	
25.429	1	1	4	25.378	-0.052	3.5068	3.4997	0.0070	5.2
-----	2	3	0	25.887	---	3.4389	---	---	
26.126	2	2	2	25.974	-0.153	3.4276	3.4079	0.0197	4.7
-----	2	3	1	26.503	---	3.3603	---	---	
-----	1	2	4	26.811	---	3.3225	---	---	
-----	2	0	3	27.138	---	3.2832	---	---	
-----	1	5	1	27.534	---	3.2369	---	---	
-----	2	1	3	27.595	---	3.2299	---	---	
28.047	1	4	3	28.146	0.099	3.1678	3.1788	-0.0110	6.0
-----	2	3	2	28.278	---	3.1533	---	---	
28.625	0	1	5	28.647	0.022	3.1136	3.1159	-0.0023	8.1
-----	2	2	3	28.926	---	3.0842	---	---	
-----	1	3	4	29.053	---	3.0709	---	---	
-----	2	4	0	29.075	---	3.0687	---	---	
29.424	1	5	2	29.251	-0.173	3.0506	3.0331	0.0176	4.7
-----	2	4	1	29.630	---	3.0125	---	---	
29.850	0	6	0	29.775	-0.075	2.9982	2.9908	0.0074	11.3
-----	0	5	3	30.051	---	2.9712	---	---	
-----	0	4	4	30.079	---	2.9685	---	---	
-----	1	0	5	30.183	---	2.9585	---	---	
30.528	1	1	5	30.598	0.070	2.9193	2.9258	-0.0065	6.4
-----	2	3	3	31.029	---	2.8798	---	---	
-----	2	0	4	31.056	---	2.8773	---	---	
-----	2	4	2	31.241	---	2.8606	---	---	
-----	2	1	4	31.461	---	2.8412	---	---	
-----	1	2	5	31.815	---	2.8104	---	---	
-----	0	6	2	31.898	---	2.8032	---	---	
31.924	1	5	3	31.925	0.001	2.8009	2.8010	-0.0001	8.9
-----	1	4	4	31.951	---	2.7987	---	---	
-----	0	3	5	31.978	---	2.7964	---	---	

-----	1	6	1	32.178	---	2.7795	---	---	
-----	3	0	1	32.463	---	2.7557	---	---	
-----	2	2	4	32.648	---	2.7405	---	---	
-----	2	5	0	32.756	---	2.7318	---	---	
-----	3	1	1	32.852	---	2.7240	---	---	
-----	2	5	1	33.255	---	2.6919	---	---	
-----	1	6	2	33.679	---	2.6589	---	---	
33.725	1	3	5	33.755	0.030	2.6531	2.6554	-0.0023	6.5
-----	2	4	3	33.774	---	2.6517	---	---	
-----	3	0	2	33.954	---	2.6381	---	---	
-----	3	2	1	33.997	---	2.6348	---	---	
-----	0	0	6	34.003	---	2.6344	---	---	
34.336	3	1	2	34.328	-0.007	2.6102	2.6096	0.0006	2.8
-----	2	3	4	34.547	---	2.5941	---	---	
-----	2	5	2	34.716	---	2.5819	---	---	
-----	0	7	1	35.357	---	2.5365	---	---	
-----	1	5	4	35.364	---	2.5361	---	---	
-----	3	2	2	35.430	---	2.5314	---	---	
-----	0	2	6	35.477	---	2.5282	---	---	
-----	2	0	5	35.519	---	2.5253	---	---	
35.612	1	0	6	35.691	0.079	2.5136	2.5189	-0.0054	10.1
-----	3	3	1	35.832	---	2.5040	---	---	
-----	2	1	5	35.879	---	2.5008	---	---	
-----	1	1	6	36.049	---	2.4894	---	---	
-----	1	6	3	36.060	---	2.4887	---	---	
-----	1	4	5	36.317	---	2.4716	---	---	
-----	3	0	3	36.318	---	2.4716	---	---	
-----	3	1	3	36.671	---	2.4486	---	---	
-----	2	6	0	36.808	---	2.4398	---	---	
-----	2	2	5	36.941	---	2.4313	---	---	
-----	1	7	1	36.991	---	2.4281	---	---	
-----	2	5	3	37.038	---	2.4252	---	---	
-----	2	4	4	37.061	---	2.4237	---	---	
-----	1	2	6	37.107	---	2.4208	---	---	
-----	3	3	2	37.204	---	2.4147	---	---	
-----	2	6	1	37.260	---	2.4112	---	---	
-----	0	6	4	37.628	---	2.3885	---	---	
-----	3	2	3	37.714	---	2.3832	---	---	
37.889	0	5	5	37.854	-0.035	2.3748	2.3726	0.0021	8.9
-----	3	4	1	38.273	---	2.3497	---	---	
-----	1	7	2	38.327	---	2.3465	---	---	
-----	2	6	2	38.588	---	2.3312	---	---	
-----	2	3	5	38.655	---	2.3273	---	---	
-----	1	3	6	38.815	---	2.3181	---	---	

-----	0	7	3	38.962	---	2.3097	---	---	
39.262	1	6	4	39.181	-0.082	2.2973	2.2927	0.0046	3.1
-----	1	5	5	39.399	---	2.2851	---	---	
-----	3	3	3	39.400	---	2.2851	---	---	
-----	3	0	4	39.422	---	2.2838	---	---	
-----	3	4	2	39.573	---	2.2755	---	---	
-----	0	4	6	39.616	---	2.2731	---	---	
-----	3	1	4	39.751	---	2.2657	---	---	
-----	0	8	0	40.066	---	2.2486	---	---	
-----	2	5	4	40.094	---	2.2471	---	---	
-----	0	1	7	40.217	---	2.2405	---	---	
-----	2	0	6	40.388	---	2.2314	---	---	
-----	1	7	3	40.471	---	2.2270	---	---	
-----	2	1	6	40.711	---	2.2144	---	---	
-----	2	6	3	40.721	---	2.2139	---	---	
-----	3	2	4	40.727	---	2.2136	---	---	
-----	2	4	5	40.953	---	2.2019	---	---	
41.087	1	4	6	41.105	0.018	2.1941	2.1951	-0.0009	9.8
-----	2	7	0	41.151	---	2.1918	---	---	
-----	3	5	1	41.231	---	2.1877	---	---	
-----	1	0	7	41.372	---	2.1806	---	---	
-----	2	7	1	41.563	---	2.1710	---	---	
-----	3	4	3	41.663	---	2.1660	---	---	
-----	2	2	6	41.668	---	2.1657	---	---	
-----	1	1	7	41.689	---	2.1647	---	---	
-----	0	8	2	41.728	---	2.1628	---	---	
-----	1	8	1	41.950	---	2.1518	---	---	
-----	3	3	4	42.312	---	2.1343	---	---	
-----	3	5	2	42.455	---	2.1274	---	---	
-----	1	2	7	42.628	---	2.1192	---	---	
42.750	0	3	7	42.755	0.005	2.1132	2.1134	-0.0002	8.7
-----	2	7	2	42.779	---	2.1120	---	---	
-----	1	6	5	42.911	---	2.1059	---	---	
-----	4	0	0	43.060	---	2.0989	---	---	
-----	3	0	5	43.135	---	2.0955	---	---	
-----	1	8	2	43.158	---	2.0944	---	---	
43.226	2	3	6	43.225	-0.001	2.0913	2.0912	0.0001	7.7
-----	1	7	4	43.324	---	2.0867	---	---	
-----	4	1	0	43.366	---	2.0848	---	---	
-----	3	1	5	43.441	---	2.0814	---	---	
-----	4	0	1	43.457	---	2.0807	---	---	
-----	2	6	4	43.560	---	2.0760	---	---	
-----	2	5	5	43.760	---	2.0670	---	---	
-----	4	1	1	43.761	---	2.0669	---	---	

-----	1	5	6	43.904	---	2.0605	---	---	
44.161	1	3	7	44.157	-0.004	2.0493	2.0491	0.0002	7.2
-----	4	2	0	44.277	---	2.0440	---	---	
-----	3	2	5	44.350	---	2.0408	---	---	
-----	3	5	3	44.433	---	2.0372	---	---	
-----	3	4	4	44.453	---	2.0363	---	---	
-----	3	6	1	44.625	---	2.0289	---	---	
-----	4	0	2	44.631	---	2.0286	---	---	
44.689	4	2	1	44.665	-0.024	2.0271	2.0261	0.0010	5.9
-----	2	7	3	44.746	---	2.0237	---	---	
-----	4	1	2	44.929	---	2.0158	---	---	
-----	1	8	3	45.112	---	2.0081	---	---	
-----	2	4	6	45.332	---	1.9989	---	---	
-----	0	7	5	45.447	---	1.9941	---	---	
-----	2	0	7	45.579	---	1.9886	---	---	
-----	0	9	1	45.716	---	1.9830	---	---	
-----	2	8	0	45.736	---	1.9822	---	---	
-----	4	3	0	45.762	---	1.9811	---	---	
-----	3	6	2	45.775	---	1.9805	---	---	
-----	0	6	6	45.813	---	1.9790	---	---	
-----	4	2	2	45.815	---	1.9789	---	---	
-----	3	3	5	45.834	---	1.9781	---	---	
-----	2	1	7	45.872	---	1.9766	---	---	
-----	0	0	8	45.891	---	1.9758	---	---	
-----	2	8	1	46.114	---	1.9668	---	---	
46.135	4	3	1	46.141	0.006	1.9657	1.9659	-0.0002	2.9
-----	1	4	7	46.230	---	1.9621	---	---	
-----	0	2	10	59.312	---	1.5568	---	---	
-----	1	1	10	59.700	---	1.5476	---	---	

The space group and cell parameter obtained from XPRD patterns of 1 at 190 °C via JADE5
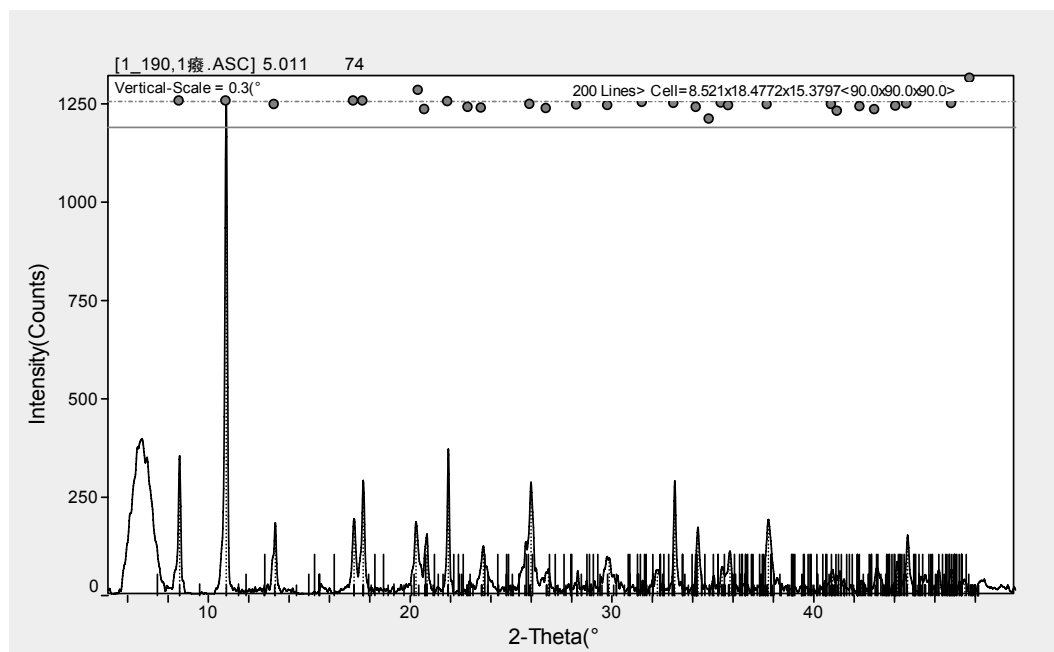
Pattern Indexing - Seek Miller Indices & Unit Cell [48 Hits Sorted on Figure-Of-Merit]

[1_190,1°C.ASC] 5.011   740

29> fm=39, fn=9, p?=0, r?=6, C=M, Space Group=P21/c (14), a=5.320, b=16.232, c=13.771, Angle=104.71, Volume=1150.3

@ 2T(o)	h	k	l	2T(c)	Delta	d(c)	d(o)	Del-d	I%
8.580	0	1	1	8.580	0.000	10.2967	10.2967	0.0000	27.5
10.892	0	2	0	10.892	0.000	8.1160	8.1160	0.0000	100.0
-----	0	2	1	12.762	---	6.9307	---	---	
13.324	0	0	2	13.283	-0.040	6.6598	6.6399	0.0199	13.9
-----	0	1	2	14.363	---	6.1614	---	---	
-----	0	2	2	17.209	---	5.1484	---	---	
17.218	1	0	0	17.218	0.000	5.1459	5.1459	0.0000	14.9
17.677	-1	1	1	17.677	0.000	5.0133	5.0133	0.0000	22.3
-----	0	3	1	17.678	---	5.0129	---	---	
-----	1	1	0	18.069	---	4.9053	---	---	
-----	-1	0	2	18.913	---	4.6884	---	---	
-----	-1	1	2	19.693	---	4.5042	---	---	
-----	-1	2	1	20.070	---	4.4205	---	---	
20.294	1	2	0	20.418	0.124	4.3460	4.3722	-0.0262	14.2
-----	0	1	3	20.724	---	4.2826	---	---	
20.837	1	1	1	20.739	-0.098	4.2795	4.2596	0.0199	11.2
-----	0	3	2	21.139	---	4.1994	---	---	
-----	-1	2	2	21.875	---	4.0597	---	---	
21.893	0	4	0	21.884	-0.008	4.0580	4.0565	0.0015	29.0
-----	0	2	3	22.811	---	3.8951	---	---	

-----	1	2	1	22.825	---	3.8928	---	---	
22.962	0	4	1	22.890	-0.071	3.8818	3.8700	0.0119	1.8
-----	-1	1	3	23.529	---	3.7779	---	---	
23.626	-1	3	1	23.544	-0.082	3.7756	3.7626	0.0129	9.2
-----	1	3	0	23.844	---	3.7288	---	---	
-----	1	0	2	24.377	---	3.6484	---	---	
-----	1	1	2	24.995	---	3.5596	---	---	
-----	-1	3	2	25.112	---	3.5432	---	---	
-----	-1	2	3	25.399	---	3.5039	---	---	
-----	0	4	2	25.686	---	3.4654	---	---	
-----	0	3	3	25.938	---	3.4322	---	---	
25.989	1	3	1	25.950	-0.039	3.4306	3.4256	0.0050	21.6
-----	0	0	4	26.750	---	3.3299	---	---	
26.856	1	2	2	26.768	-0.088	3.3277	3.3170	0.0107	4.6
-----	0	1	4	27.317	---	3.2620	---	---	
-----	-1	4	1	27.720	---	3.2155	---	---	
-----	-1	0	4	27.953	---	3.1892	---	---	
-----	1	4	0	27.978	---	3.1864	---	---	
-----	-1	3	3	28.258	---	3.1555	---	---	
28.316	0	5	1	28.271	-0.044	3.1541	3.1492	0.0049	4.0
-----	-1	1	4	28.499	---	3.1294	---	---	
-----	0	2	4	28.959	---	3.0807	---	---	
-----	-1	4	2	29.079	---	3.0683	---	---	
-----	1	3	2	29.505	---	3.0250	---	---	
-----	0	4	3	29.803	---	2.9954	---	---	
29.865	1	4	1	29.814	-0.052	2.9943	2.9893	0.0051	6.5
-----	-1	2	4	30.081	---	2.9683	---	---	
-----	1	1	3	30.218	---	2.9551	---	---	
-----	0	5	2	30.610	---	2.9182	---	---	
31.537	0	3	4	31.521	-0.016	2.8359	2.8345	0.0014	1.6
-----	1	2	3	31.723	---	2.8183	---	---	
-----	-1	4	3	31.864	---	2.8061	---	---	
32.245	-1	5	1	32.361	0.116	2.7642	2.7738	-0.0096	4.1
-----	-1	3	4	32.563	---	2.7475	---	---	
-----	1	5	0	32.585	---	2.7457	---	---	
-----	1	4	2	32.987	---	2.7131	---	---	
33.113	0	6	0	33.085	-0.028	2.7053	2.7031	0.0022	22.4
-----	-1	5	2	33.549	---	2.6690	---	---	
-----	0	6	1	33.781	---	2.6512	---	---	
-----	-2	0	2	33.988	---	2.6355	---	---	
-----	0	1	5	34.078	---	2.6288	---	---	
-----	1	3	3	34.098	---	2.6273	---	---	
-----	-1	1	5	34.166	---	2.6222	---	---	
-----	0	5	3	34.187	---	2.6206	---	---	

-----	-2	1	1	34.194	---	2.6201	---	---	
34.268	1	5	1	34.197	-0.071	2.6199	2.6146	0.0053	13.1
-----	-2	1	2	34.447	---	2.6014	---	---	
-----	0	4	4	34.823	---	2.5742	---	---	
35.049	2	0	0	34.840	-0.209	2.5730	2.5581	0.0149	3.1
-----	2	1	0	35.289	---	2.5412	---	---	
35.459	0	2	5	35.436	-0.024	2.5311	2.5294	0.0016	4.8
-----	-1	2	5	35.521	---	2.5252	---	---	
-----	-2	2	1	35.548	---	2.5233	---	---	
-----	1	0	4	35.609	---	2.5191	---	---	
-----	-1	4	4	35.780	---	2.5075	---	---	
-----	-2	2	2	35.793	---	2.5067	---	---	
35.849	0	6	2	35.796	-0.053	2.5064	2.5028	0.0036	8.0
-----	-2	1	3	36.022	---	2.4912	---	---	
-----	-1	5	3	36.025	---	2.4910	---	---	
-----	1	1	4	36.050	---	2.4893	---	---	
-----	2	2	0	36.608	---	2.4527	---	---	
-----	1	5	2	37.036	---	2.4253	---	---	
-----	1	4	3	37.198	---	2.4151	---	---	
-----	-2	2	3	37.318	---	2.4076	---	---	
-----	-1	6	1	37.331	---	2.4068	---	---	
-----	1	2	4	37.346	---	2.4059	---	---	
-----	1	6	0	37.529	---	2.3946	---	---	
-----	0	3	5	37.604	---	2.3900	---	---	
-----	2	1	1	37.630	---	2.3884	---	---	
-----	-1	3	5	37.685	---	2.3850	---	---	
37.753	-2	3	1	37.711	-0.042	2.3834	2.3808	0.0026	14.5
-----	-2	3	2	37.943	---	2.3694	---	---	
-----	-2	0	4	38.367	---	2.3442	---	---	
-----	-1	6	2	38.383	---	2.3432	---	---	
-----	0	5	4	38.704	---	2.3245	---	---	
-----	2	3	0	38.720	---	2.3236	---	---	
-----	-2	1	4	38.781	---	2.3201	---	---	
-----	2	2	1	38.880	---	2.3144	---	---	
-----	0	6	3	38.953	---	2.3102	---	---	
-----	1	6	1	38.961	---	2.3098	---	---	
-----	-2	3	3	39.398	---	2.2852	---	---	
-----	0	7	1	39.410	---	2.2845	---	---	
-----	1	3	4	39.424	---	2.2837	---	---	
-----	-1	5	4	39.580	---	2.2751	---	---	
-----	-1	0	6	39.902	---	2.2574	---	---	
-----	-2	2	4	40.001	---	2.2521	---	---	
-----	-1	1	6	40.303	---	2.2359	---	---	
-----	0	4	5	40.472	---	2.2270	---	---	

-----	-1	4	5	40.548	---	2.2230	---	---	
-----	-2	4	1	40.573	---	2.2217	---	---	
-----	-1	6	3	40.604	---	2.2200	---	---	
-----	0	0	6	40.606	---	2.2199	---	---	
-----	2	0	2	40.639	---	2.2182	---	---	
-----	-2	4	2	40.791	---	2.2103	---	---	
-----	1	5	3	40.885	---	2.2054	---	---	
40.932	2	3	1	40.892	-0.040	2.2051	2.2030	0.0021	4.3
-----	0	1	6	41.001	---	2.1995	---	---	
-----	2	1	2	41.033	---	2.1978	---	---	
41.305	0	7	2	41.188	-0.117	2.1899	2.1840	0.0059	4.1
-----	-1	2	6	41.486	---	2.1749	---	---	
-----	1	6	2	41.521	---	2.1731	---	---	
-----	2	4	0	41.523	---	2.1730	---	---	
-----	-2	3	4	41.968	---	2.1510	---	---	
-----	-2	4	3	42.164	---	2.1415	---	---	
-----	0	2	6	42.167	---	2.1413	---	---	
-----	1	4	4	42.188	---	2.1403	---	---	
-----	2	2	2	42.199	---	2.1397	---	---	
42.375	1	1	5	42.310	-0.065	2.1344	2.1312	0.0031	2.1
-----	-2	1	5	42.529	---	2.1239	---	---	
-----	-1	7	1	42.557	---	2.1225	---	---	
-----	1	7	0	42.735	---	2.1141	---	---	
43.142	0	6	4	43.043	-0.099	2.0997	2.0951	0.0046	4.9
-----	-1	3	6	43.398	---	2.0834	---	---	
-----	1	2	5	43.448	---	2.0811	---	---	
-----	-1	7	2	43.504	---	2.0785	---	---	
-----	2	4	1	43.580	---	2.0751	---	---	
-----	-2	2	5	43.662	---	2.0714	---	---	
-----	-1	6	4	43.847	---	2.0631	---	---	
-----	0	5	5	43.930	---	2.0593	---	---	
-----	-1	5	5	44.001	---	2.0562	---	---	
-----	0	7	3	44.019	---	2.0554	---	---	
-----	-2	5	1	44.024	---	2.0552	---	---	
-----	1	7	1	44.026	---	2.0551	---	---	
-----	0	3	6	44.055	---	2.0538	---	---	
44.145	2	3	2	44.086	-0.059	2.0524	2.0498	0.0026	6.0
-----	-2	5	2	44.229	---	2.0461	---	---	
-----	-2	4	4	44.603	---	2.0298	---	---	
44.656	0	8	0	44.622	-0.034	2.0290	2.0275	0.0015	11.3
-----	2	5	0	44.915	---	2.0164	---	---	
-----	1	6	3	45.051	---	2.0107	---	---	
-----	0	8	1	45.165	---	2.0059	---	---	
-----	1	3	5	45.293	---	2.0005	---	---	

-----	2	1	3	45.307	---	1.9999	---	---	
-----	-2	3	5	45.501	---	1.9919	---	---	
-----	-2	5	3	45.517	---	1.9912	---	---	
-----	-1	7	3	45.519	---	1.9911	---	---	
-----	1	5	4	45.540	---	1.9902	---	---	
-----	-1	4	6	45.967	---	1.9727	---	---	
46.202	1	7	2	46.357	0.155	1.9570	1.9632	-0.0062	4.1
-----	2	2	3	46.386	---	1.9559	---	---	
-----	0	4	6	46.595	---	1.9476	---	---	
-----	2	4	2	46.625	---	1.9464	---	---	
-----	-2	0	6	46.730	---	1.9423	---	---	
-----	0	8	2	46.764	---	1.9409	---	---	
-----	-1	1	7	46.806	---	1.9393	---	---	
46.881	2	5	1	46.852	-0.029	1.9375	1.9364	0.0011	3.9
-----	-2	1	6	47.083	---	1.9285	---	---	
47.492	0	7	4	47.756	0.264	1.9029	1.9129	-0.0099	2.1
-----	1	4	5	47.782	---	1.9019	---	---	
-----	-2	5	4	47.820	---	1.9005	---	---	
-----	-1	2	7	47.859	---	1.8991	---	---	
-----	0	6	5	47.883	---	1.8982	---	---	
-----	-1	6	5	47.950	---	1.8957	---	---	
-----	-2	6	1	47.971	---	1.8949	---	---	
-----	-2	4	5	47.981	---	1.8945	---	---	
-----	-1	8	1	48.007	---	1.8936	---	---	
-----	0	1	7	48.106	---	1.8899	---	---	
-----	-2	2	6	48.131	---	1.8889	---	---	
-----	2	3	3	48.143	---	1.8885	---	---	
-----	-2	6	2	48.163	---	1.8878	---	---	
-----	-1	0	8	53.314	---	1.7169	---	---	
-----	-1	1	8	53.635	---	1.7074	---	---	
-----	-1	2	8	54.590	---	1.6797	---	---	
-----	0	0	8	55.116	---	1.6650	---	---	
55.503	0	1	8	55.429	-0.073	1.6563	1.6543	0.0020	2.4
56.146	-1	3	8	56.158	0.012	1.6365	1.6368	-0.0003	2.0
-----	0	2	8	56.364	---	1.6310	---	---	
-----	-2	0	8	57.770	---	1.5946	---	---	
-----	0	3	8	57.901	---	1.5913	---	---	
-----	-2	1	8	58.074	---	1.5870	---	---	
-----	-1	4	8	58.307	---	1.5812	---	---	
-----	-2	2	8	58.982	---	1.5647	---	---	

The space group and cell parameter obtained from XPRD patterns of complex 1 via JADE5 after 1 was cooled down to room temperature and exposed to air for 48 hours
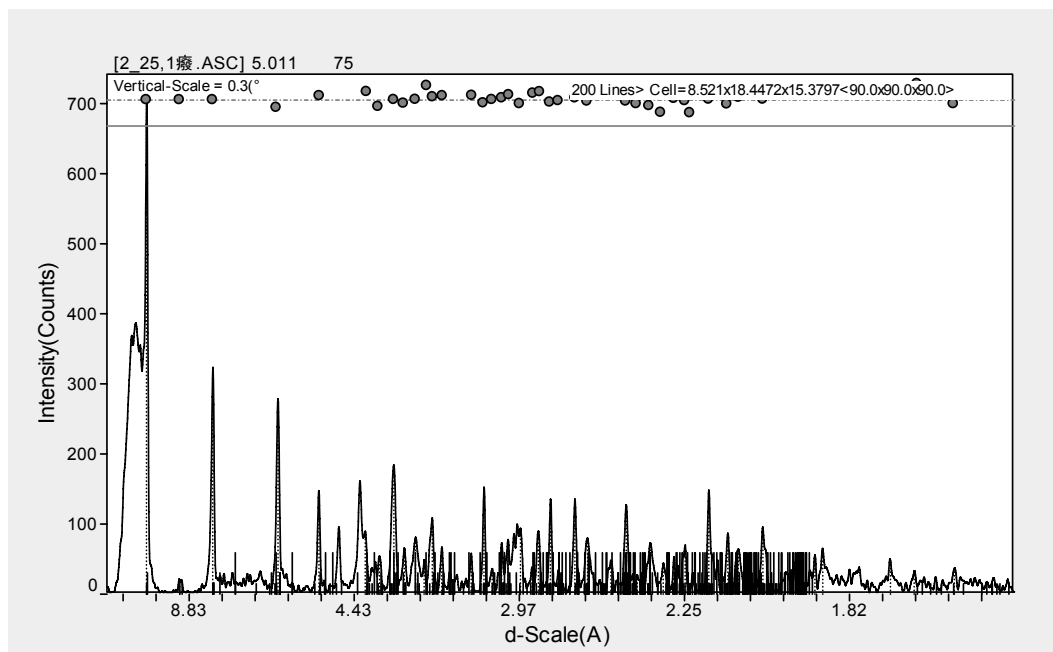
Pattern Indexing - Seek Miller Indices & Unit Cell [36 Hits Sorted on Figure-Of-Merit]

[2_25,1癈.ASC] 5.011   759

8> fm=48, fn=9, p?=0, r?=10, C=O, Space Group=Pnma (62), a=8.485, b=15.392, c=18.743, Angle=90.00, Volume=2447.9

@ 2T(o)	h	k	l	2T(c)	Delta	d(c)	d(o)	Del-d	I%
7.426	0	1	1	7.426	0.000	11.8951	11.8951	0.0000	100.0
9.429	0	0	2	9.429	0.000	9.3714	9.3714	0.0000	2.4
11.438	1	0	1	11.438	0.000	7.7300	7.7300	0.0000	44.9
-----	0	2	0	11.488	---	7.6960	---	---	
-----	1	1	1	12.805	---	6.9078	---	---	
-----	1	0	2	14.068	---	6.2900	---	---	
-----	0	2	2	14.883	---	5.9475	---	---	
-----	1	1	2	15.204	---	5.8226	---	---	
15.381	0	1	3	15.293	-0.088	5.7889	5.7560	0.0330	38.5
-----	1	2	1	16.239	---	5.4539	---	---	
-----	1	0	3	17.614	---	5.0310	---	---	
17.862	0	3	1	17.910	0.047	4.9486	4.9616	-0.0129	20.4
-----	1	2	2	18.200	---	4.8703	---	---	
-----	1	1	3	18.539	---	4.7820	---	---	
-----	0	0	4	18.923	---	4.6857	---	---	
20.668	1	3	1	20.762	0.094	4.2748	4.2940	-0.0192	10.9
-----	2	0	0	20.921	---	4.2426	---	---	
-----	1	2	3	21.080	---	4.2111	---	---	
21.535	2	0	1	21.456	-0.078	4.1379	4.1231	0.0149	5.9

-----	1	0	4	21.647	---	4.1019	---	---	
-----	2	1	0	21.710	---	4.0901	---	---	
-----	0	2	4	22.193	---	4.0023	---	---	
-----	2	1	1	22.228	---	3.9961	---	---	
-----	1	3	2	22.343	---	3.9758	---	---	
22.402	0	3	3	22.404	0.002	3.9650	3.9654	-0.0003	24.8
-----	1	1	4	22.413	---	3.9635	---	---	
23.032	2	0	2	22.992	-0.040	3.8650	3.8583	0.0067	7.2
-----	0	4	0	23.094	---	3.8480	---	---	
23.712	2	1	2	23.716	0.004	3.7486	3.7492	-0.0006	9.3
-----	2	2	0	23.930	---	3.7155	---	---	
24.239	2	2	1	24.403	0.164	3.6445	3.6688	-0.0242	5.4
-----	0	1	5	24.420	---	3.6421	---	---	
-----	1	2	4	24.572	---	3.6198	---	---	
24.731	1	3	3	24.764	0.034	3.5922	3.5970	-0.0048	13.6
-----	0	4	2	24.995	---	3.5596	---	---	
25.309	2	0	3	25.355	0.046	3.5098	3.5161	-0.0062	8.4
-----	2	2	2	25.773	---	3.4539	---	---	
-----	1	4	1	25.842	---	3.4448	---	---	
-----	1	0	5	25.964	---	3.4289	---	---	
-----	2	1	3	26.017	---	3.4220	---	---	
-----	1	1	5	26.612	---	3.3468	---	---	
27.093	1	4	2	27.144	0.051	3.2825	3.2885	-0.0060	7.5
-----	2	3	0	27.253	---	3.2696	---	---	
-----	2	3	1	27.672	---	3.2209	---	---	
27.860	1	3	4	27.823	-0.037	3.2038	3.1997	0.0041	20.8
-----	2	2	3	27.916	---	3.1934	---	---	
28.353	2	0	4	28.354	0.002	3.1450	3.1452	-0.0002	4.0
-----	1	2	5	28.474	---	3.1321	---	---	
-----	0	0	6	28.551	---	3.1238	---	---	
-----	2	3	2	28.898	---	3.0871	---	---	
28.930	2	1	4	28.953	0.022	3.0813	3.0837	-0.0023	9.1
-----	1	4	3	29.194	---	3.0565	---	---	
29.321	0	5	1	29.378	0.057	3.0377	3.0435	-0.0058	9.1
-----	0	3	5	29.486	---	3.0268	---	---	
30.069	0	4	4	30.024	-0.045	2.9738	2.9694	0.0043	11.6
-----	1	0	6	30.468	---	2.9315	---	---	
-----	2	2	4	30.684	---	2.9113	---	---	
30.765	2	3	3	30.841	0.076	2.8969	2.9038	-0.0070	3.7
-----	0	2	6	30.867	---	2.8945	---	---	
-----	1	1	6	31.029	---	2.8797	---	---	
31.157	1	5	1	31.249	0.092	2.8600	2.8682	-0.0082	11.0
-----	1	3	5	31.352	---	2.8508	---	---	
-----	2	4	0	31.358	---	2.8503	---	---	

-----	2	4	1	31.728	---	2.8179	---	---	
-----	2	0	5	31.829	---	2.8092	---	---	
31.889	1	4	4	31.861	-0.028	2.8064	2.8040	0.0024	18.1
-----	3	0	1	31.974	---	2.7968	---	---	
-----	1	5	2	32.351	---	2.7650	---	---	
32.381	2	1	5	32.369	-0.012	2.7635	2.7625	0.0010	4.0
-----	0	5	3	32.395	---	2.7614	---	---	
-----	3	1	1	32.512	---	2.7517	---	---	
-----	1	2	6	32.661	---	2.7395	---	---	
-----	2	4	2	32.815	---	2.7269	---	---	
-----	3	0	2	33.054	---	2.7078	---	---	
33.367	2	3	4	33.390	0.022	2.6813	2.6831	-0.0017	18.0
-----	3	1	2	33.577	---	2.6668	---	---	
-----	2	2	5	33.943	---	2.6389	---	---	
-----	0	1	7	33.956	---	2.6379	---	---	
-----	3	2	1	34.080	---	2.6286	---	---	
34.132	1	5	3	34.117	-0.015	2.6258	2.6247	0.0011	9.9
-----	2	4	3	34.560	---	2.5932	---	---	
-----	3	0	3	34.788	---	2.5767	---	---	
-----	0	6	0	34.947	---	2.5653	---	---	
-----	1	4	5	35.022	---	2.5600	---	---	
-----	3	2	2	35.103	---	2.5543	---	---	
-----	1	0	7	35.115	---	2.5534	---	---	
-----	1	3	6	35.231	---	2.5453	---	---	
-----	3	1	3	35.288	---	2.5413	---	---	
35.544	1	1	7	35.611	0.067	2.5190	2.5236	-0.0046	5.8
-----	2	0	6	35.662	---	2.5155	---	---	
-----	2	5	0	36.016	---	2.4916	---	---	
-----	2	1	6	36.152	---	2.4826	---	---	
-----	0	6	2	36.276	---	2.4743	---	---	
-----	2	5	1	36.344	---	2.4699	---	---	
-----	2	3	5	36.434	---	2.4640	---	---	
36.478	1	5	4	36.462	-0.016	2.4622	2.4611	0.0011	17.0
-----	3	3	1	36.562	---	2.4556	---	---	
-----	3	2	3	36.752	---	2.4434	---	---	
-----	2	4	4	36.881	---	2.4351	---	---	
-----	1	6	1	36.887	---	2.4348	---	---	
-----	0	4	6	37.036	---	2.4253	---	---	
-----	1	2	7	37.064	---	2.4235	---	---	
37.141	3	0	4	37.097	-0.044	2.4215	2.4187	0.0028	2.5
-----	2	5	2	37.312	---	2.4080	---	---	
-----	3	3	2	37.526	---	2.3947	---	---	
-----	3	1	4	37.570	---	2.3921	---	---	
-----	2	2	6	37.587	---	2.3910	---	---	

-----	0	5	5	37.784	---	2.3790	---	---	
-----	1	6	2	37.843	---	2.3754	---	---	
37.940	0	3	7	37.870	-0.070	2.3738	2.3696	0.0042	9.1
-----	0	0	8	38.389	---	2.3429	---	---	
38.723	1	4	6	38.577	-0.146	2.3319	2.3234	0.0084	4.8
-----	2	5	3	38.881	---	2.3144	---	---	
-----	3	2	4	38.960	---	2.3098	---	---	
-----	3	3	3	39.087	---	2.3026	---	---	
-----	1	5	5	39.299	---	2.2907	---	---	
39.368	1	3	7	39.383	0.015	2.2860	2.2868	-0.0008	6.4
-----	1	6	3	39.394	---	2.2854	---	---	
-----	2	4	5	39.692	---	2.2689	---	---	
-----	2	0	7	39.776	---	2.2643	---	---	
-----	3	4	1	39.812	---	2.2623	---	---	
-----	2	3	6	39.880	---	2.2586	---	---	
-----	1	0	8	39.885	---	2.2584	---	---	
-----	3	0	5	39.895	---	2.2578	---	---	
40.048	0	6	4	40.036	-0.011	2.2502	2.2496	0.0006	9.1
-----	0	2	8	40.202	---	2.2413	---	---	
-----	2	1	7	40.222	---	2.2402	---	---	
-----	1	1	8	40.331	---	2.2344	---	---	
40.491	3	1	5	40.341	-0.151	2.2339	2.2260	0.0080	3.1
-----	3	4	2	40.711	---	2.2145	---	---	
-----	2	5	4	40.991	---	2.1999	---	---	
-----	2	6	0	41.083	---	2.1952	---	---	
-----	3	3	4	41.189	---	2.1898	---	---	
-----	0	7	1	41.306	---	2.1839	---	---	
-----	2	6	1	41.377	---	2.1803	---	---	
41.477	1	6	4	41.483	0.006	2.1750	2.1753	-0.0003	20.1
-----	2	2	7	41.538	---	2.1723	---	---	
-----	1	2	8	41.644	---	2.1670	---	---	
-----	3	2	5	41.653	---	2.1665	---	---	
-----	3	4	3	42.173	---	2.1410	---	---	
-----	2	6	2	42.248	---	2.1374	---	---	
-----	1	4	7	42.451	---	2.1276	---	---	
-----	1	5	6	42.550	---	2.1229	---	---	
42.632	4	0	0	42.583	-0.049	2.1213	2.1190	0.0023	10.6
-----	1	7	1	42.717	---	2.1150	---	---	
-----	4	0	1	42.868	---	2.1079	---	---	
-----	2	4	6	42.918	---	2.1055	---	---	
-----	4	1	0	43.006	---	2.1015	---	---	
-----	3	0	6	43.109	---	2.0967	---	---	
43.261	4	1	1	43.289	0.027	2.0884	2.0896	-0.0012	7.5
-----	3	1	6	43.527	---	2.0775	---	---	

-----	1	7	2	43.566	---	2.0757	---	---	
-----	2	5	5	43.581	---	2.0750	---	---	
-----	0	7	3	43.600	---	2.0742	---	---	
-----	2	3	7	43.658	---	2.0716	---	---	
-----	2	6	3	43.668	---	2.0711	---	---	
-----	3	5	1	43.692	---	2.0700	---	---	
-----	4	0	2	43.715	---	2.0690	---	---	
-----	1	3	8	43.759	---	2.0670	---	---	
-----	3	3	5	43.769	---	2.0666	---	---	
-----	0	1	9	43.832	---	2.0637	---	---	
-----	1	6	5	44.048	---	2.0541	---	---	
-----	2	0	8	44.120	---	2.0509	---	---	
-----	4	1	2	44.129	---	2.0505	---	---	
-----	3	4	4	44.153	---	2.0495	---	---	
-----	4	2	0	44.253	---	2.0451	---	---	
-----	3	5	2	44.526	---	2.0332	---	---	
-----	4	2	1	44.530	---	2.0330	---	---	
-----	2	1	8	44.531	---	2.0330	---	---	
44.756	3	2	6	44.763	0.007	2.0229	2.0232	-0.0003	12.5
-----	1	0	9	44.773	---	2.0225	---	---	
-----	0	5	7	44.825	---	2.0203	---	---	
-----	1	7	3	44.953	---	2.0148	---	---	
-----	4	0	3	45.098	---	2.0087	---	---	
-----	1	1	9	45.179	---	2.0053	---	---	
-----	0	4	8	45.278	---	2.0011	---	---	
-----	4	2	2	45.352	---	1.9980	---	---	
-----	4	1	3	45.502	---	1.9918	---	---	
-----	2	6	4	45.596	---	1.9879	---	---	
-----	0	6	6	45.727	---	1.9825	---	---	
53.921	0	1	11	54.108	0.187	1.6936	1.6990	-0.0054	3.8
-----	0	4	10	54.404	---	1.6850	---	---	
-----	1	0	11	54.915	---	1.6705	---	---	
-----	1	1	11	55.265	---	1.6608	---	---	
-----	1	4	10	55.557	---	1.6528	---	---	
56.353	1	2	11	56.307	-0.046	1.6325	1.6313	0.0012	4.0
-----	0	3	11	56.894	---	1.6171	---	---	
-----	1	3	11	58.014	---	1.5885	---	---	
-----	2	0	11	58.309	---	1.5811	---	---	
-----	1	5	10	58.634	---	1.5732	---	---	
-----	2	1	11	58.646	---	1.5729	---	---	
-----	2	4	10	58.927	---	1.5660	---	---	
-----	0	0	12	59.098	---	1.5619	---	---	
-----	2	2	11	59.648	---	1.5488	---	---	

Supporting information 3, XRPD patterns of dehydration and rehydration for complex 1 at different cycles.
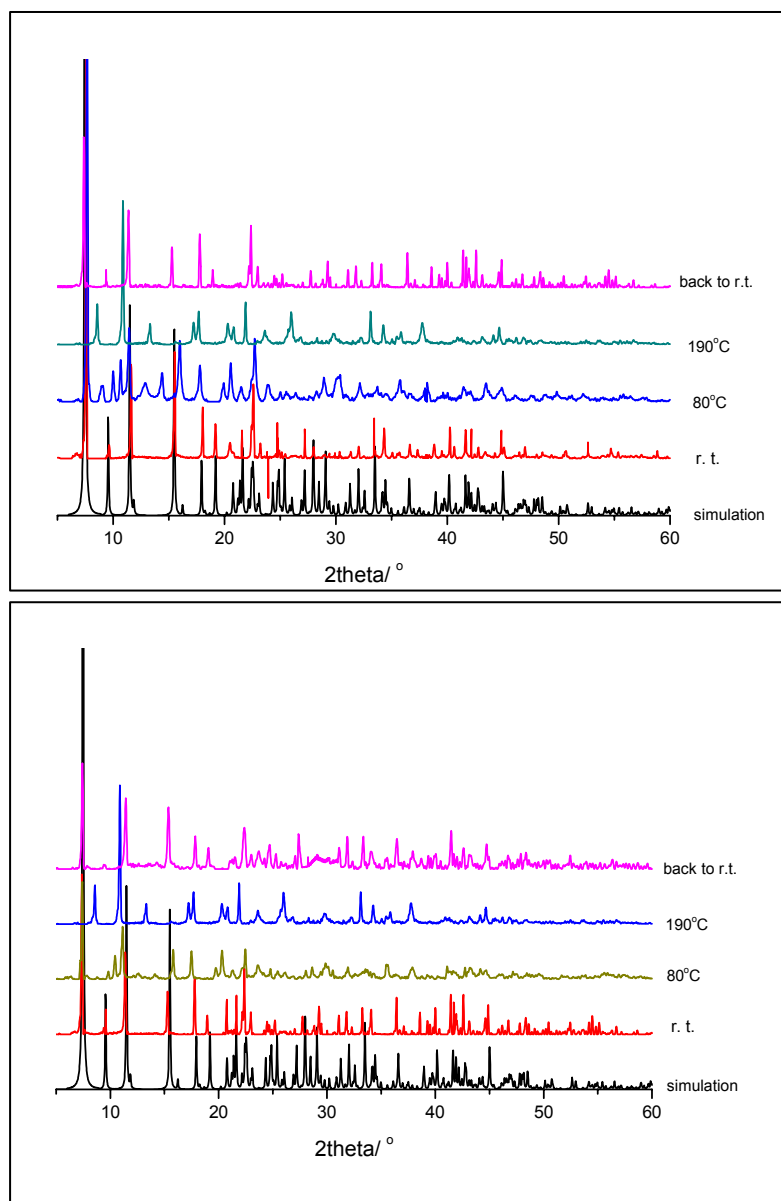
Fig. The first (up) and second (down) cycle of XRPD patterns of dehydration and rehydration for complex **1**.

Supporting information 4, Synthesis and X-ray crystallography of complex 1

Synthesis: Complex **1** was prepared as follows: An aqueous reaction mixture was prepared by dissolving H_3L (0.044 g, 0.25 mmol), $NaHCO_3$ (0.022 g, 0.25 mmol), and $La(NO_3)_3$ (0.108g, 0.25 mmol) in 18 mL of de-ionized water. Its pH was adjusted to 6.4 with 1.0 M NaOH. The resulting mixture was transferred to a 25-mL Teflon-lined vessel (Parr) and heated at 150°C for 1000 min. Cooling of the reaction mixture to room temperature at a rate of 5°C per hour afforded colourless crystalline solids as the product (yield: 0.027g; 27% based on La). Anal. Calcd (%) for $C_{11}H_{22}La_2N_4O_{20}$: C, 16.42; H, 2.24; N, 6.96. Found: C, 16.37; H, 2.37; N, 6.93.

X-ray Crystallography: Data collection was performed on a Bruker SMART Apex CCD diffractometer at 223 K for complex **1**. Absorption corrections were applied by using the multiscan program SADABS.[1] The structures were solved by direct methods, and non-hydrogen atoms, except for O4w and O5w, were refined anisotropically by least-squares on F^2 using the SHELXTL program.[2] The O4w and O5w refined isotropically is due to their disorder, and no improvement can be achieved in the anisotropic thermal parameters by modelling disorder and/or using appropriate restraints, although the occupancies of these atoms are correct. The hydrogen atoms of organic ligands were generated geometrically (C-H, 0.96 Å, N-H = 0.87), while those for O1w to O5w are generated by using restraints on the O-H bond lengths and H-O-H bond angles and the fixing of the hydrogen atom U value to be 1.5 U(eq) of the parent oxygen atom. Generating the hydrogen atoms for O6w/O6w' is failure, due to its anisotropic thermal parameters large enough even after modelling the disorder of the atom.

Crystal data are: $C_{11}H_{22}La_2N_4O_{20}$, orthorhombic, space group *Pnma, a =* 8.521(2), *b* = 18.477(4), *c* = 15.380(4) Å, *V* = 2421.4(10) Å^3, *Z* = 4, ρ_{calcd} = 2.217g·cm^{-3}, *M* = 808.15, μ(Mo *K*α) = 3.579 mm^{-1}, T = 223 K. R_{int} = 0.0513, R_1 = 0.0595 (*I* > 2σ(*I*)), wR_2 = 0.1204 (all data) are obtained based on the 12529 reflections measured (of which, 2460 are independent and 2254 are observed) and 173

parameters.