

Supplementary material

Supplementary tables:

Table: S3

Structure factors as phased by Charge Flipping and phases from model-Rietveld refinements for  $\delta$ -K<sub>2</sub>C<sub>2</sub>O<sub>4</sub>. Misestimated phases are noted in bold character.

#	h	k	l	Aobs(Rietveld)	A(new) CF	#	h	k	l	Aobs(Rietveld)	A(new) CF
1:	0	0	0	164.0000000	238.9100647	45:	0	4	0	-4.8764000	-10.6060133
<b>2:</b>	<b>2</b>	<b>0</b>	<b>0</b>	<b>3.0134001</b>	<b>-5.7038722</b>	46:	3	1	2	-17.1130009	-32.5020485
3:	1	1	0	2.5330000	5.3034134	47:	1	4	0	-15.5900002	-29.7830181
4:	2	1	0	-16.0879993	-31.2890129	48:	0	2	2	15.6569996	33.1681595
<b>5:</b>	<b>0</b>	<b>0</b>	<b>1</b>	<b>6.9928002</b>	<b>-11.5050087</b>	49:	7	1	0	18.0890007	35.5771599
6:	3	1	0	-24.4309998	-47.5730057	50:	1	2	2	-20.1459999	-38.7235336
7:	0	2	0	27.6410007	52.8220062	51:	5	3	0	-4.2034001	-9.1663742
8:	1	2	0	-35.5830002	-66.5720291	52:	4	3	1	-16.1429996	-31.2870178
9:	2	0	1	37.9580002	71.6449966	53:	2	4	0	12.4650002	21.6260033
10:	1	1	1	-47.1259995	-91.5930023	54:	4	0	2	-24.0879993	-47.4040031
11:	4	0	0	-46.9210014	-90.0780411	55:	2	2	2	-9.2152996	-15.7920656
12:	2	2	0	-24.5809994	-46.7090149	<b>56:</b>	<b>4</b>	<b>1</b>	<b>2</b>	<b>-0.1162900</b>	<b>27.9350071</b>
13:	2	1	1	37.0279999	71.1660080	57:	6	2	1	20.2310009	24.6800022
14:	4	1	0	44.8139992	85.6290359	58:	3	4	0	-14.4449997	-26.1124496
15:	3	2	0	-13.7559996	-24.0230007	59:	0	4	1	32.3349991	63.5001450
16:	3	1	1	51.6290016	99.9100266	60:	3	2	2	-9.1096001	-12.4199991
17:	0	2	1	-11.8430004	-17.2011337	61:	7	2	0	-8.3799000	-31.7340031
18:	1	2	1	38.2910004	74.0760117	62:	1	4	1	16.6180000	31.1960011
19:	4	0	1	26.8069992	52.3090324	63:	7	1	1	-21.7479992	-38.5701065
20:	2	2	1	-8.5502996	-15.8061800	<b>64:</b>	<b>5</b>	<b>3</b>	<b>1</b>	<b>-0.1452400</b>	<b>0.0000000</b>
21:	5	1	0	1.8773000	3.3860021	65:	8	0	0	-9.9547997	-14.6137505
22:	4	2	0	-27.0090008	-51.7140007	66:	6	3	0	11.2089996	22.5100193
23:	4	1	1	6.2609000	10.5860014	67:	2	4	1	-2.7370999	-2.5860004
24:	1	3	0	-19.8150005	-37.6690025	68:	4	4	0	11.5430002	25.9780560
25:	3	2	1	6.1704001	12.4431105	69:	8	1	0	-10.8809996	-13.8230171
26:	2	3	0	-47.2669983	-90.6240540	70:	5	1	2	2.1789000	10.6850090
27:	6	0	0	36.5690002	70.6060410	71:	4	2	2	-13.2690001	-24.8631439
28:	3	3	0	13.0570002	28.4300003	72:	1	3	2	-9.4001999	-18.3590412
29:	5	2	0	24.2059994	44.7659988	<b>73:</b>	<b>3</b>	<b>4</b>	<b>1</b>	<b>-2.7484000</b>	<b>3.7338512</b>
30:	5	1	1	-2.9844000	-8.3341026	74:	7	2	1	10.7500000	24.4511185
31:	4	2	1	-0.5973800	-2.7111077	75:	2	3	2	-23.3339996	-42.6640930
32:	6	1	0	25.0179996	55.9879990	76:	8	0	1	-15.7550001	-26.3931198
33:	0	0	2	65.0530014	95.8670883	77:	6	3	1	-11.2399998	-21.0340023
34:	1	3	1	-8.7003002	-37.6970177	78:	6	0	2	19.8449993	35.1200333
35:	2	3	1	23.1930008	45.5140533	79:	5	4	0	1.1374000	2.8140404
36:	2	0	2	-0.3554000	-5.4247985	80:	8	2	0	2.8097000	23.3410130
37:	1	1	2	3.1296999	4.2630615	81:	4	4	1	-12.6540003	-23.2530117
38:	4	3	0	21.7290001	41.9321632	82:	3	3	2	6.3541002	20.6160069
39:	6	0	1	-23.5739994	-45.7421837	83:	8	1	1	13.6840000	19.8200054
40:	2	1	2	-10.2500000	-21.5995598	84:	5	2	2	13.6199999	20.7390137
<b>41:</b>	<b>3</b>	<b>3</b>	<b>1</b>	<b>-1.5154999</b>	<b>28.0140095</b>	85:	7	3	0	-5.1683002	-13.6290960
42:	5	2	1	-36.7910004	-65.7969971	86:	6	1	2	13.0030003	22.1600132
43:	6	2	0	20.5550003	40.6030235	87:	1	5	0	-5.9830999	-13.4380169
44:	6	1	1	5.3007998	4.6340036						

Table. S4:

Structure factors as phased by Charge Flipping and phases from model-Rietveld refinements for  $\alpha$ -Rb<sub>2</sub>C<sub>2</sub>O<sub>4</sub>, misestimated phases are noted in bold character.

#	h	k	l	Aobs(Rietveld)	A(new)	CF	#	h	k	l	Aobs(Rietveld)	A(new)	CF
1:	0	0	0	236.0000000	134.2151337		27:	3	0	3	1.6794000	1.0344716	
2:	1	0	0	13.0860004	13.6420708		28:	4	-1	1	7.9661002	8.5576134	
3:	1	0	1	-18.7099991	-19.0650101		29:	4	-2	2	-1.7093000	-0.9707072	
4:	0	0	2	-18.0359993	-22.2150002		30:	3	-1	4	9.7334003	10.6500959	
5:	1	0	2	69.7160034	80.1482086		31:	4	-1	2	12.6110001	13.7002611	
6:	2	-1	0	89.8479996	96.3066864		32:	2	0	5	0.7053900	0.0000000	
7:	2	0	0	9.9511003	10.4750128		<b>33:</b>	<b>4</b>	<b>0</b>	<b>0</b>	<b>-0.4313100</b>	<b>0.0000000</b>	
8:	2	0	1	39.8470001	44.8750000		34:	3	0	4	10.3450003	14.2876244	
9:	2	-1	2	7.8256001	8.7197285		35:	4	0	1	-8.0698004	-3.6343029	
10:	1	0	3	12.5489998	13.5610304		36:	0	0	6	6.6808000	3.2751982	
11:	2	0	2	48.6160011	54.2050781		37:	4	-1	3	-2.5727999	-2.6989009	
12:	3	-1	0	14.8590002	16.8050041		38:	1	0	6	10.6960001	11.5991507	
13:	0	0	4	43.3940010	49.0321388		39:	4	0	2	9.5144997	10.5262547	
14:	3	-1	1	-20.3279991	-22.4558277		<b>40:</b>	<b>3</b>	<b>-1</b>	<b>5</b>	<b>0.0000000</b>	<b>-1.8313316</b>	
15:	2	0	3	-15.0439997	-16.8491096		<b>41:</b>	<b>5</b>	<b>-2</b>	<b>0</b>	<b>1.7722000</b>	<b>-2.9327164</b>	
16:	1	0	4	21.1720009	23.2641029		42:	4	-2	4	8.0486002	9.3960247	
17:	3	-1	2	24.8059998	26.3800945		43:	5	-2	1	-4.3994002	-5.3071871	
18:	3	0	0	34.9099998	39.8081169		44:	2	-1	6	5.1424999	4.0898819	
19:	3	0	1	-1.6693000	-4.0348983		45:	4	0	3	1.7538000	0.3334095	
20:	2	-1	4	25.7759991	28.3970890		46:	4	-1	4	2.4296000	2.2001324	
21:	3	0	2	1.7146000	2.3073726		47:	3	0	5	-0.4364400	-0.9777243	
22:	3	-1	3	6.0221000	6.2977710		48:	2	0	6	5.0688000	4.6376033	
23:	2	0	4	11.9870005	12.6600456		49:	5	-2	2	4.4713998	5.2794118	
24:	4	-2	0	27.9869995	30.7490997		50:	5	-1	0	5.2947998	4.2498899	
25:	1	0	5	0.4902800	0.0000000		51:	5	-1	1	0.0000000	0.0000000	
26:	4	-1	0	3.7921000	4.2217216		<b>52:</b>	<b>5</b>	<b>-1</b>	<b>2</b>	<b>0.5385700</b>	<b>-4.1698542</b>	

Table: S5

Structure factors as phased by Charge Flipping and phases from model-Rietveld refinements for  $\alpha$ -Rb<sub>2</sub>CO<sub>3</sub>, misestimated phases are noted in bold character

#	h	k	l	Aobs(Rietveld)	A(new)	CF	#	h	k	l	Aobs(Rietveld)	A(new)	CF	
1:	0	0	0	208.0000000	128.3709259		<b>24:</b>	<b>1</b>	<b>0</b>	<b>5</b>	<b>0.4514900</b>	<b>-2.8657849</b>		
2:	1	0	0	14.0290003	13.3820219		25:	4	-2	0	32.4790001	31.9925900		
3:	1	0	1	-20.3729992	-19.0250015		26:	3	0	3	2.9786000	3.2847557		
4:	0	0	2	-13.5129995	-15.6959991		27:	4	-1	0	-3.7706001	-3.7707899		
5:	1	0	2	67.6220016	68.2571259		28:	4	-1	1	13.3879995	13.1246080		
6:	2	-1	0	99.1460037	100.1400452		29:	4	-2	2	-6.0335002	-6.8442211		
7:	2	0	0	0.9791700	0.3016227		30:	3	-1	4	9.0197001	8.8150940		
8:	2	0	1	37.0209999	37.3670578		31:	2	0	5	1.4218000	11.9200668		
<b>9:</b>	<b>2</b>	<b>-1</b>	<b>2</b>	<b>2.2138000</b>	<b>-1.6331875</b>		32:	4	-1	2	14.1040001	11.6842155		
10:	1	0	3	4.9020000	4.4877882		33:	0	0	6	8.2104998	8.2198191		
11:	2	0	2	44.7050018	44.9491463		34:	3	0	4	8.7907000	8.3983097		
12:	0	0	4	36.2210007	36.3160744		35:	4	0	0	0.1316200	1.4669420		
13:	3	-1	0	11.9139996	12.3630009		36:	1	0	6	7.0058999	8.9006538		
14:	3	-1	1	-22.2819996	-21.9660797		37:	4	0	1	-9.1363001	-8.5093908		
15:	1	0	4	19.7819996	16.2133121		38:	4	-1	3	-2.4379001	-2.2543015		
16:	2	0	3	-11.9200001	-16.1644058		<b>39:</b>	<b>3</b>	<b>-1</b>	<b>5</b>	<b>0.0000000</b>	<b>-4.7598143</b>		
17:	3	-1	2	22.1840000	21.6062183		40:	4	0	2	8.3900003	4.6508756		
18:	3	0	0	38.5559998	37.8990059		41:	2	-1	6	6.5739999	6.3596287		
19:	3	0	1	-6.9622998	-7.4066305		42:	4	-2	4	6.8866000	6.6784711		
20:	2	-1	4	19.9489994	19.5730419		43:	5	-2	0	-2.2193999	-0.7704080		
<b>21:</b>	<b>3</b>	<b>0</b>	<b>2</b>	<b>-0.6895800</b>	<b>0.0000000</b>		44:	2	0	6	5.1206999	7.0712643		
22:	2	0	4	10.8290005	8.0241690		45:	5	-2	1	-5.4492002	-7.1267767		
23:	3	-1	3	6.1686001	8.0061560									