
Supplementary material:

Comparative structural study of decagonal quasicrystals in the systems

Al-Cu-Me (*Me* = Co, Rh, Ir)

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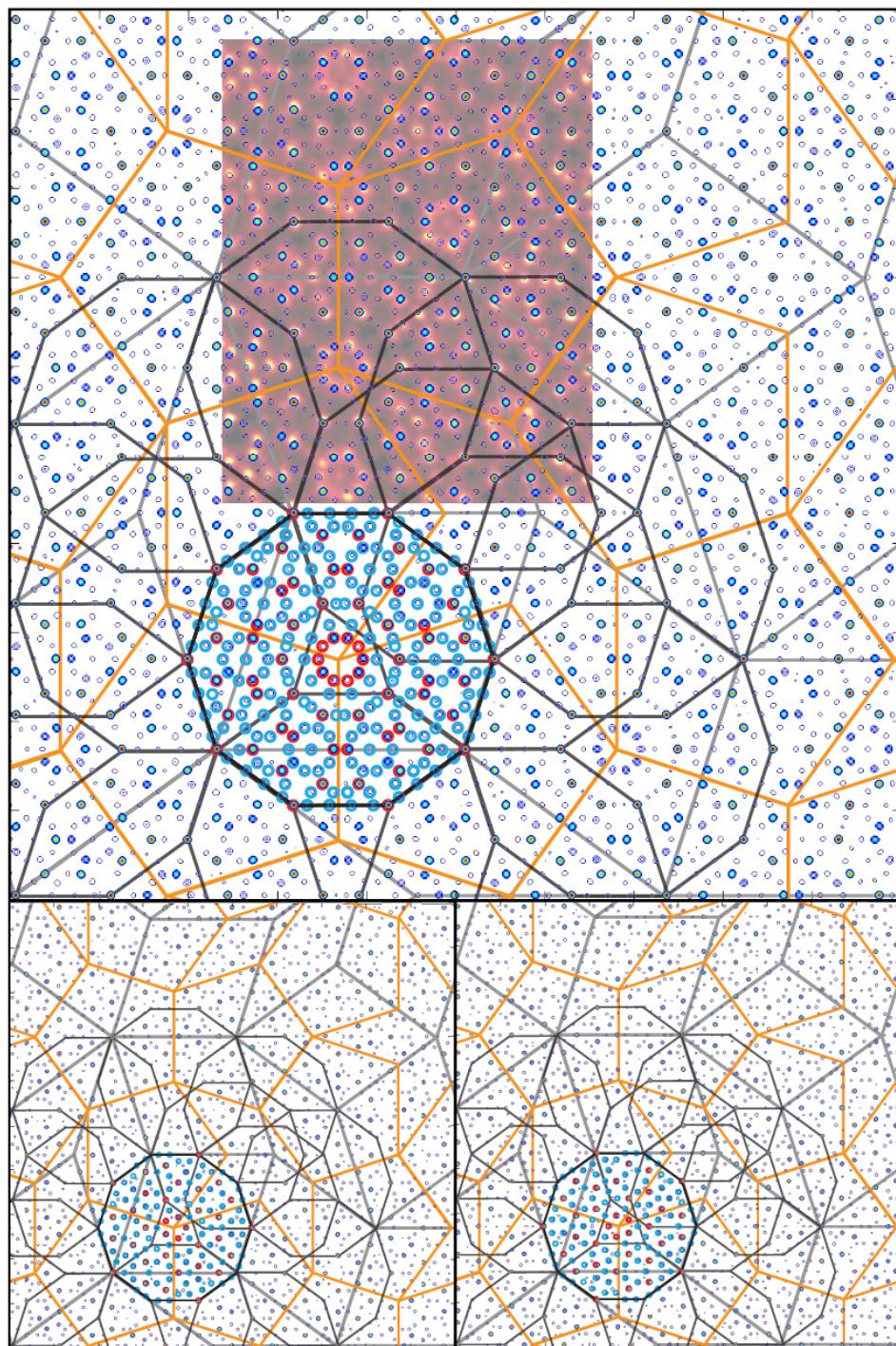
1. Electron density maps obtained from the structure solution by the charge flipping method

Figure 1 Electron density maps of d-Al-Cu-Co obtained from charge flipping: projection along the periodic axis (*top*) and sections in $z = 1/4$ and $3/4$ (*bottom*). The inset in the upper picture shows the agreement with a HAADF-STEM image taken from Taniguchi et al. (2008) *Philos. Mag.* **88** 1949. Grey lines indicate the large RPT of 27.46 \AA edge length, orange lines mark the corresponding PPT of 19.94 \AA edge length, black lines enclose the decagonal Hiraga cluster centered at the vertices of the PPT. The idealized decoration of the cluster is also shown: blue and red circles mark Al and TM (Cu/Co) atoms, respectively.

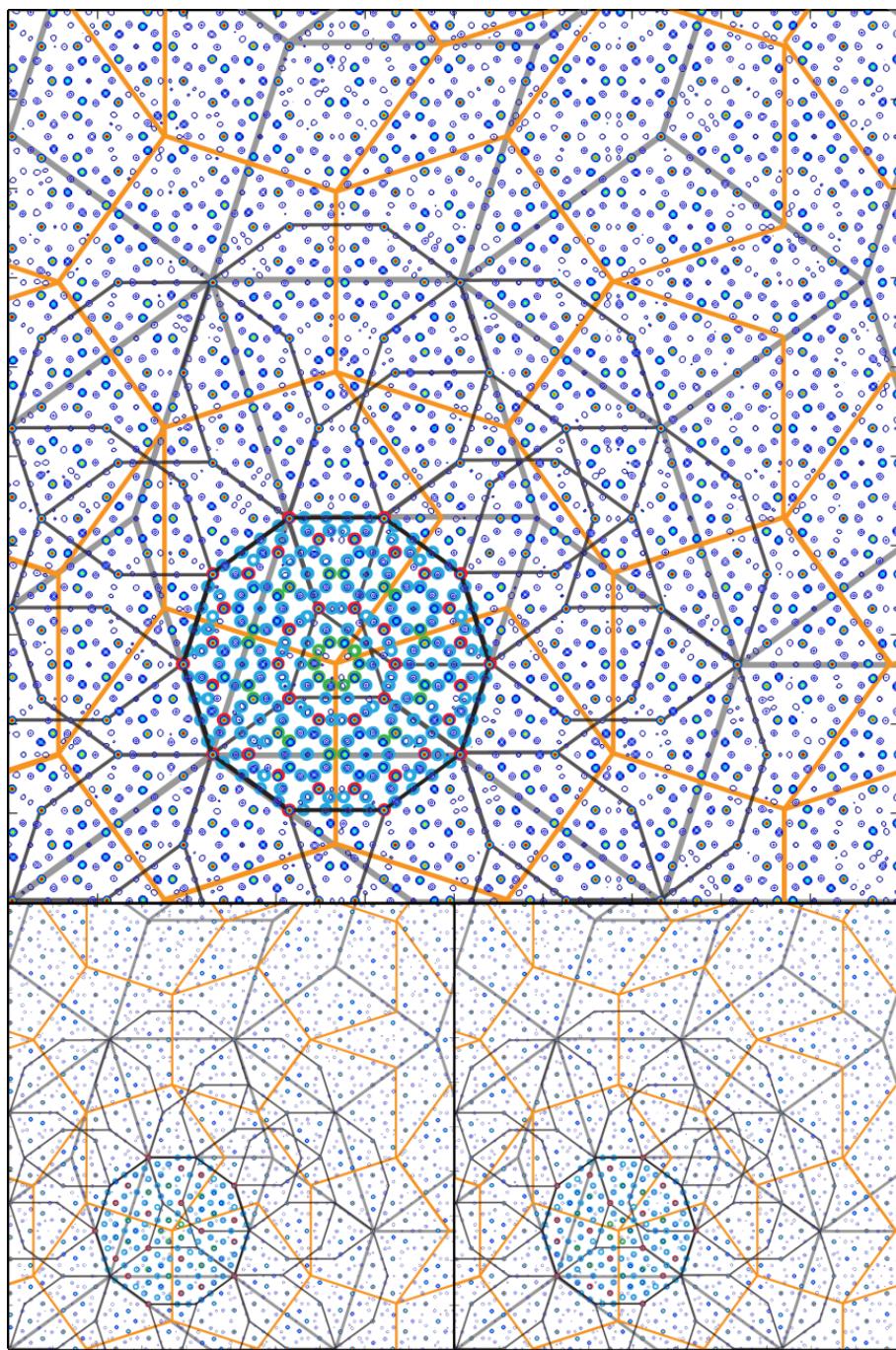


Figure 2 Electron density maps of d-Al-Cu-Rh obtained from charge flipping: projection along the periodic axis (*top*) and sections in $z = 1/4$ and $3/4$ (*bottom*). Grey lines indicate the large RPT of 27.83 \AA edge length, orange lines mark the corresponding PPT of 20.21 \AA edge length, black lines enclose the decagonal Hiraga cluster centered at the vertices of the PPT. The idealized decoration of the cluster is also shown: blue, green and red circles mark Al, Cu and Rh atoms, respectively.

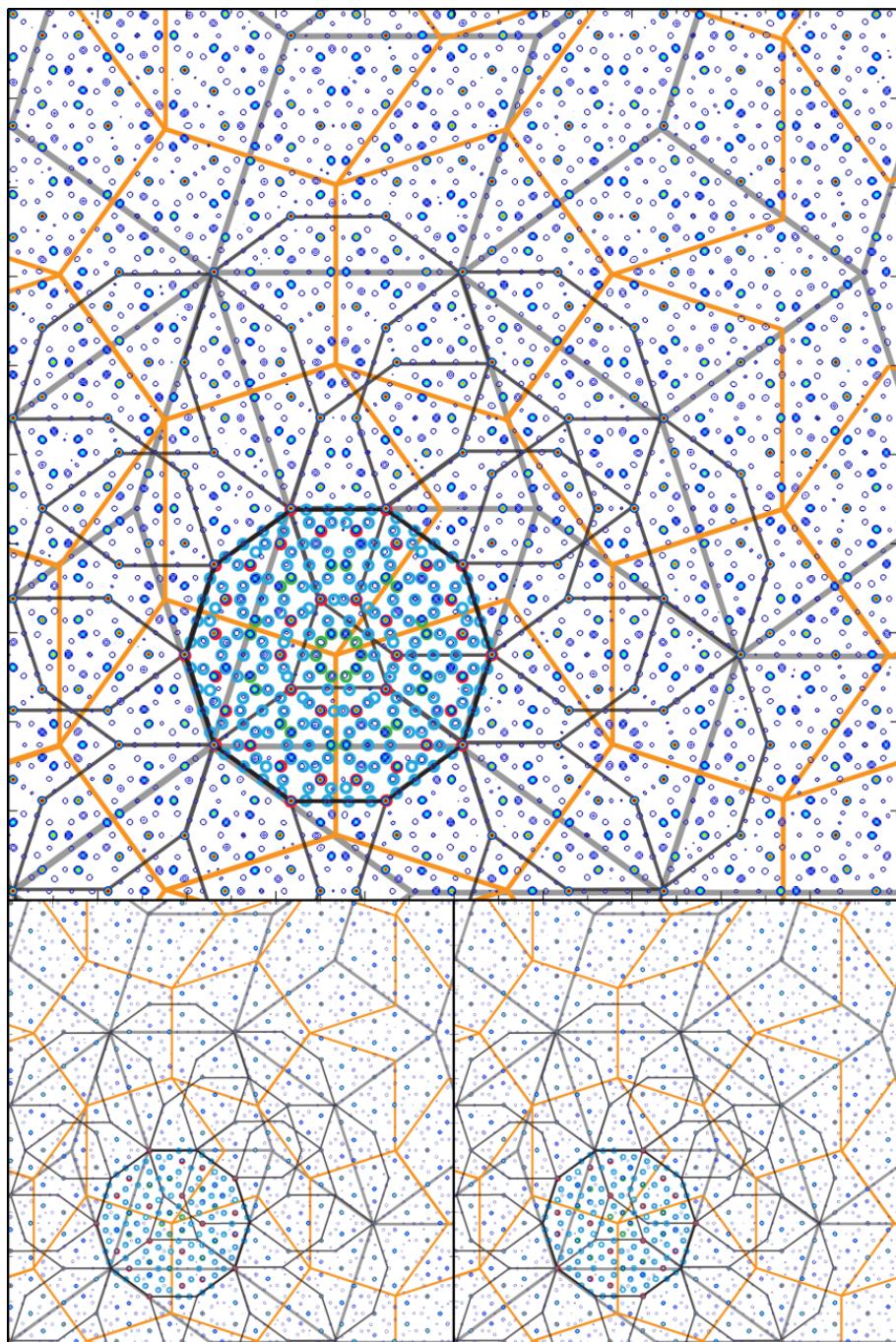


Figure 3 Electron density maps of d-Al-Cu-Ir obtained from charge flipping: projection along the periodic axis (*top*) and sections in $z = 1/4$ and $3/4$ (*bottom*). Grey lines indicate the large RPT of 27.93 \AA edge length, orange lines mark the corresponding PPT of 20.28 \AA edge length, black lines enclose the decagonal Hiraga cluster centered at the vertices of the PPT. The idealized decoration of the cluster is also shown: blue, green and red circles mark Al, Cu and Ir atoms, respectively.

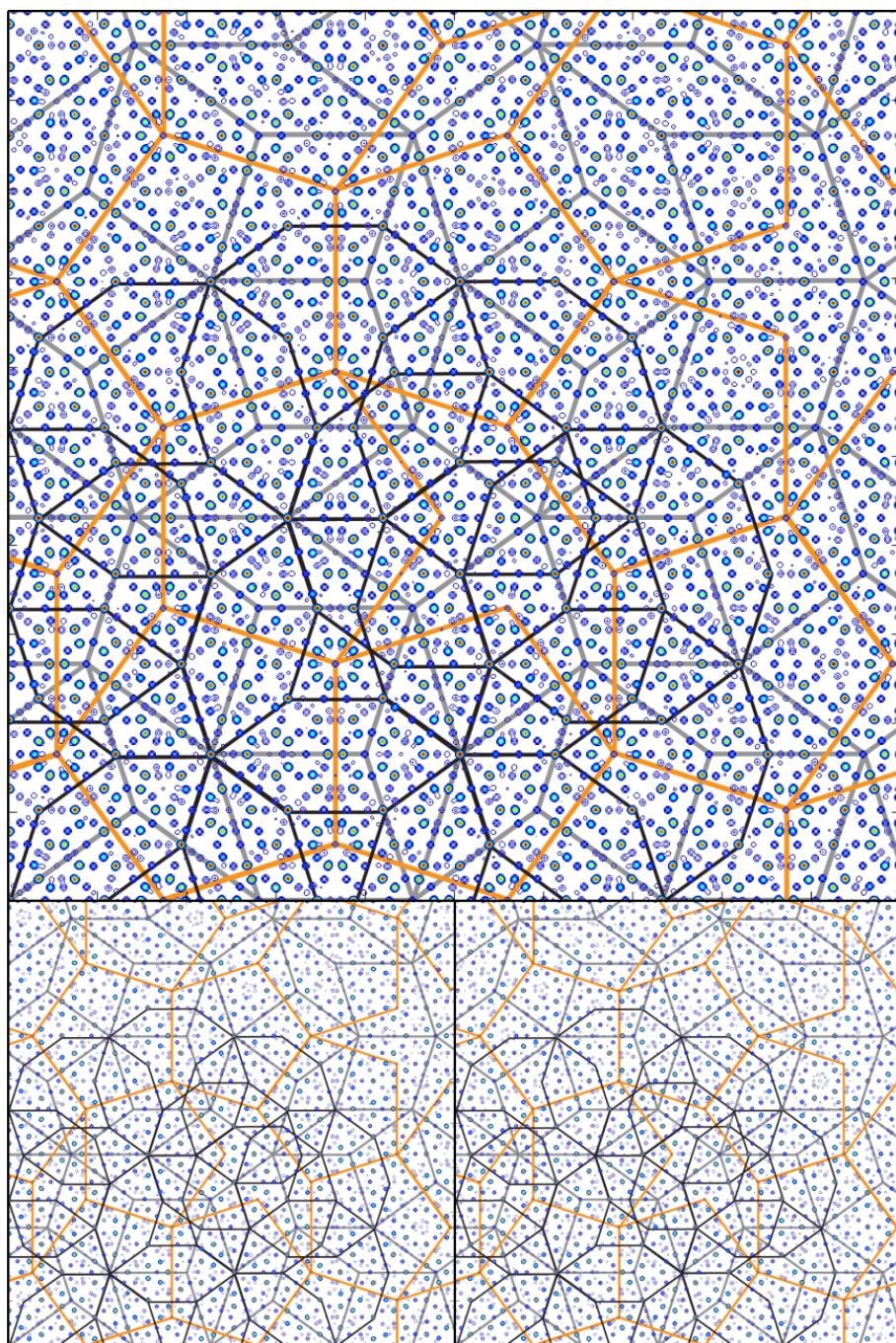
2. Electron density maps calculated from observed structure amplitudes and refined phases

Figure 4 Electron density maps of d-Al-Cu-Co obtained from measured amplitudes and refined phases: projection along the periodic axis (*top*) and sections in $z = 1/4$ and $3/4$ (*bottom*). Grey lines indicate the RPT of 16.97 \AA edge length, which was used in the refinement process, orange lines mark the PPT of 19.94 \AA edge length, corresponding to the τ inflated RPT, black lines enclose the decagonal Hiraga cluster centered at the vertices of the PPT.

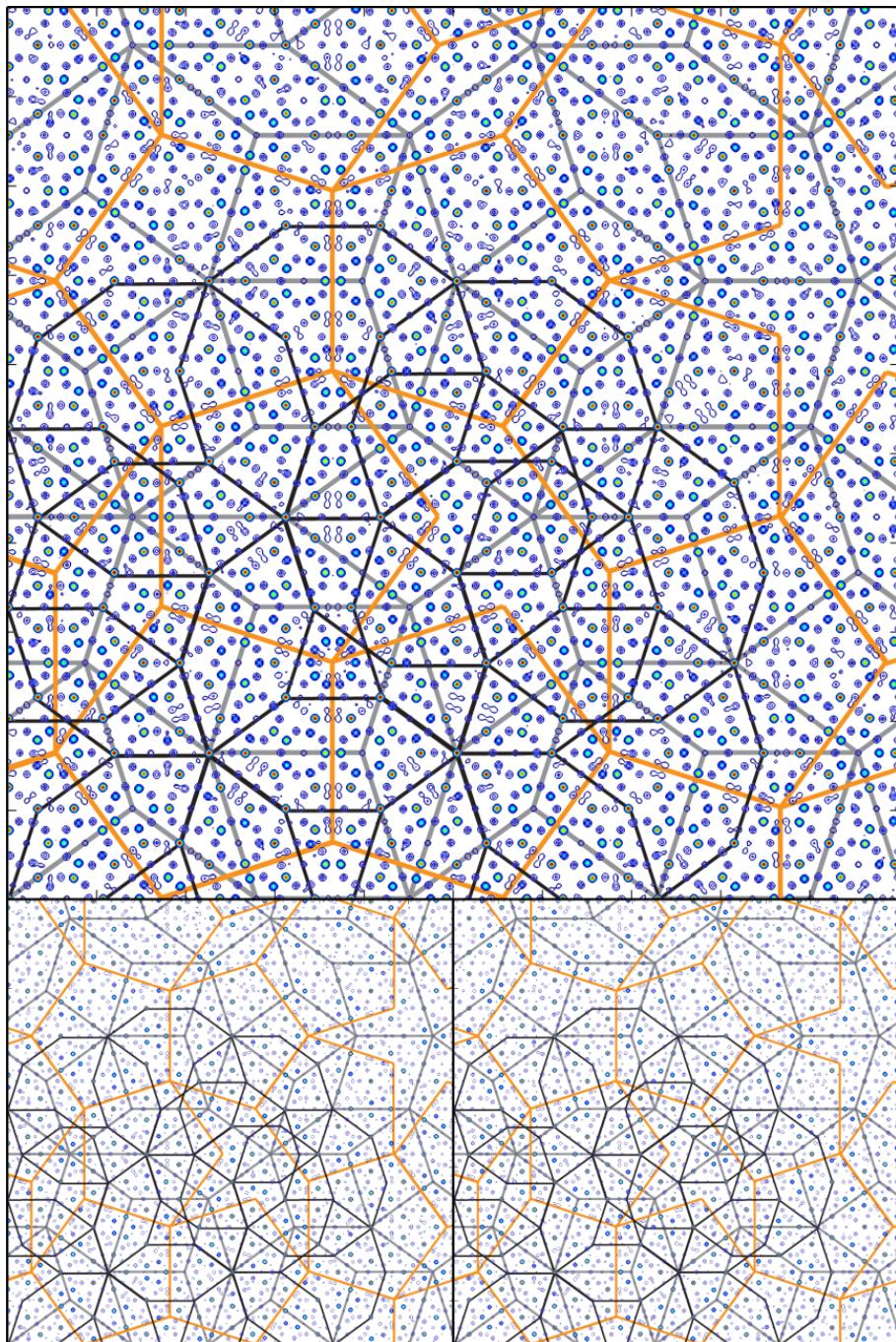


Figure 5 Electron density maps of d-Al-Cu-Co obtained from measured amplitudes and refined phases: projection along the periodic axis (*top*) and sections in $z = 1/4$ and $3/4$ (*bottom*). Grey lines indicate the RPT of 17.19 \AA edge length, which was used in the refinement process, orange lines mark the PPT of 20.21 \AA edge length, corresponding to the τ inflated RPT, black lines enclose the decagonal Hiraga cluster centered at the vertices of the PPT.

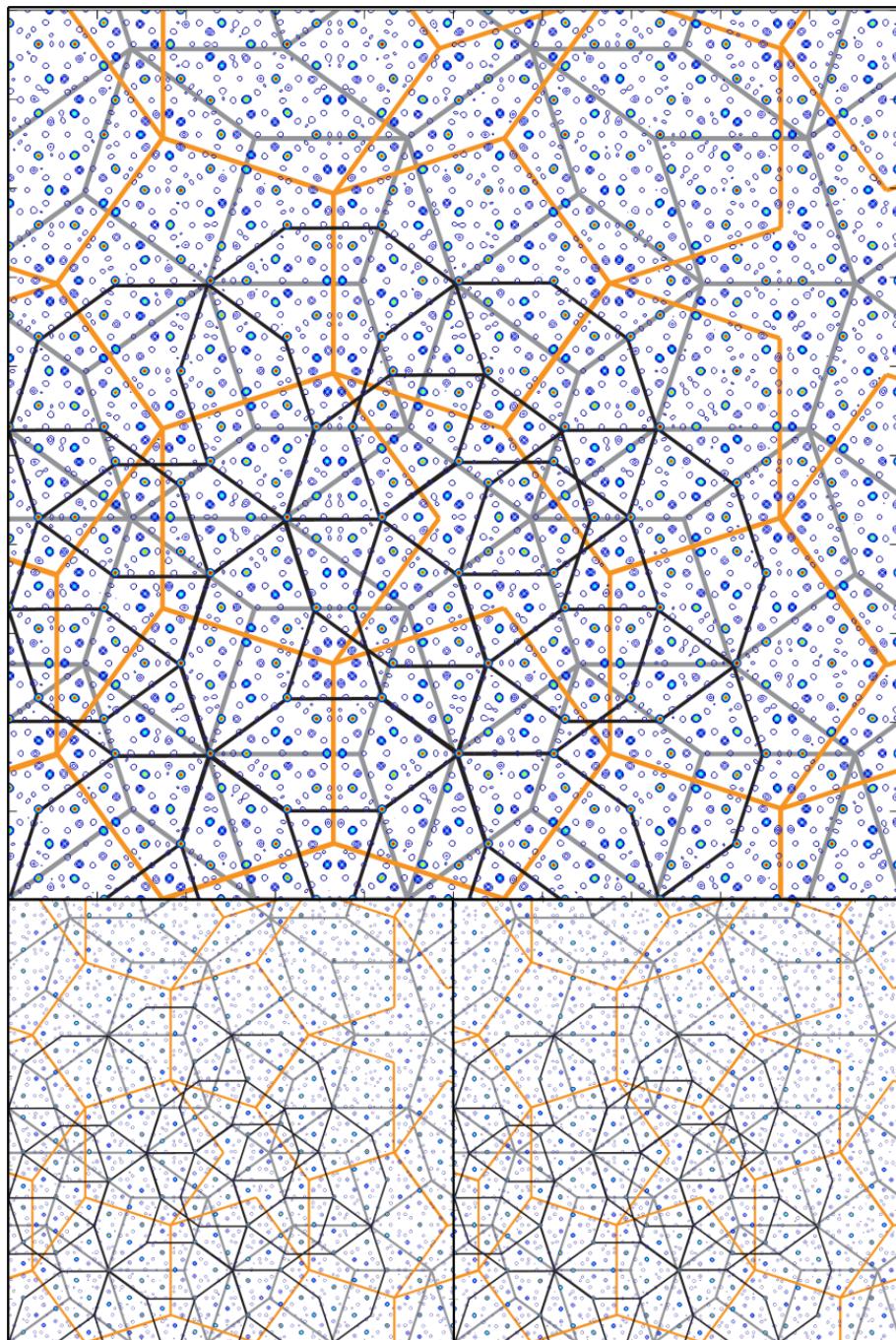


Figure 6 Electron density maps of d-Al-Cu-Ir obtained from measured amplitudes and refined phases: projection along the periodic axis (*top*) and sections in $z = 1/4$ and $3/4$ (*bottom*). Grey lines indicate the RPT of 17.26 \AA edge length, which was used in the refinement process, orange lines mark the PPT of 20.28 \AA edge length, corresponding to the τ inflated RPT, black lines enclose the decagonal Hiraga cluster centered at the vertices of the PPT.

3. Values of the refined parameters

Tables 1-3 list the structural parameters for all three DQC structures. In the first column, T stands for thin rhomb and F for the thick one. The parameters are given for the asymmetric unit of each kind of rhomb in one chosen orientation. The full decoration of one rhomb can be obtained by applying the mirror plane operations (there is a mirror plane along the long diagonal of the thick rhomb and along the short diagonal of the thin one, there are also mirror planes within the atomic planes at $z = 1/4$ and $3/4$). The atomic decoration of the other possible orientations of rhombs can be obtained by applying the 10_5 screw axis rotations.

Some parameters are given without standard deviations (STD). If only the position STDs are not given, then this is due to the fact that these positions were fixed (e.g. atoms decorating the vertices of rhombi have x and y coordinates fixed, most atoms have the z coordinate fixed, for atoms at the edges of the rhombs the y coordinate is constrained to the value of x and thus no STD is given for the y coordinate). If no STDs are given for some atoms, this is due to the constraints from the matching rules for the atoms at the edges of rhombs. In that case, in the second column, in the parenthesis, the number of the equivalent atom is given.

Table 1 Refined parameters for d-Al-Cu-Co

	x [Å]	y [Å]	z [Å]	SOF	p(TM)	b _{xy} [Å ²]	b _{zz} [Å ²]				
T 1	0.0000	0.0000	1.031	1.000	1.000	1.304	9.1E-02	0.133	4.1E-02		
T 2	2.5586	1.1E-02	0.0000	1.031	1.000	0.000	2.392	1.4E-01			
T 3	8.0104	9.4E-04	0.0000	1.031	1.000	0.000	2.171	2.0E-01			
T 4	0.7757	1.6E-03	2.3872	1.031	0.500	0.000	1.699	8.5E-02			
T 5	2.5022	6.1E-03	7.6563	7.1E-03	1.031	0.427	1.7E-02	0.000	2.627	2.4E-01	
T 6	4.5337	2.2E-03	13.9532		1.031	1.000	1.000	0.209	2.1E-02	1.236	1.1E-01
T 7	5.2434		16.1375		1.781	3.0E-02	0.500	0.000	3.488	1.7E-01	
T 8	7.2462		9.9735		1.031	1.000	1.000	3.566	1.4E-01	2.069	1.4E-01
T 9	8.0898	3.9E-03	7.3771		1.031	0.500	0.000	0.446	4.5E-02		
T 10	9.7020	1.6E-03	2.4152		1.031	1.000	0.000	1.351	1.4E-01		
T 11	2.6042	8.2E-03	4.2058	1.2E-02	1.031	1.000	0.627	4.4E-02	0.164	3.5E-02	
T 12	4.2624	8.6E-03	6.0481	5.8E-03	1.031	1.000	1.000	0.447	3.1E-02	0.506	5.6E-02
T 13	4.5120	3.4E-03	1.5917	6.8E-03	1.031	1.000	0.473	3.8E-02	0.002	2.6E-03	
T 14	5.2641	4.1E-03	11.4911	7.5E-03	1.031	0.500	0.000	0.738	6.6E-02		
T 15	5.3833	8.4E-03	8.4016	7.0E-03	1.031	1.000	0.000	0.097	1.7E-02		
T 16	5.2434		3.8095		2.303	3.8E-02	0.500	0.000	0.390	2.7E-02	
T 17	7.2026	3.9E-03	6.3614	3.3E-02	1.031	0.500	1.000	0.001	1.6E-03		
T 18	7.0832	9.8E-03	2.7387	1.5E-02	1.031	1.000	0.000	0.024	1.1E-02		
T 19	3.7327	1.6E-02	0.0000		3.092	1.000	0.000	0.011	7.6E-03		
T 20 (7)	10.4868		0.0000		2.341	0.500	0.000	3.488			
T 21	1.2582	1.0E-03	3.8724		3.092	1.000	1.000	0.883	5.3E-02	0.408	2.9E-02
T 22	3.2406		9.9735		3.092	1.000	0.000	1.506	9.0E-02		
T 23	3.9821	1.2E-03	12.2594		3.092	1.000	1.000	0.329	2.6E-02	1.562	1.1E-01
T 24	6.0179	1.0E-03	13.7560		3.092	1.000	0.000	0.814	9.8E-02		
T 25	7.7145	4.5E-04	8.5323		2.729	1.1E-02	0.500	1.000	0.008	3.2E-03	
T 26	8.5235	1.6E-03	6.0422		3.092	1.000	1.000	0.236	2.1E-02	0.110	2.0E-02
T 27	3.3503	9.9E-03	5.2533	2.7E-03	3.092	1.000	0.000	2.020	2.2E-01		
T 28	3.2653	4.4E-03	2.3375	3.9E-03	3.092	1.000	0.000	2.073	1.7E-01		

T 29	4.1338	6.4E-03	7.6650	3.2E-03	3.092	1.000	1.000	0.164	2.1E-02
T 30	5.7071	2.2E-03	9.9735		3.092	1.000	0.000	1.774	1.1E-01
T 31	6.0550	5.6E-03	6.1732	3.0E-03	3.092	1.000	0.000	2.109	8.4E-02
T 32	6.0136	1.6E-03	1.5975	1.0E-02	3.092	1.000	0.000	0.930	1.2E-01
T 33	7.9352	1.3E-02	3.7665	4.3E-03	3.092	1.000	0.000	0.050	9.6E-03
T 34	8.3929	5.5E-03	1.4551		3.092	1.000	1.000	1.899	1.3E-01
T 35	1.1274		0.8191		3.092	0.400	0.000	3.975	2.8E-01
F 36 (1)	0.0000		0.0000		1.031	1.000	1.000	1.304	0.133
F 37	-6.5332	4.2E-03	0.0000		1.356	9.8E-03	0.500	1.000	0.055
F 38	-8.8011	7.8E-03	0.0000		1.031	1.000	1.000	1.225	3.7E-02
F 39	-14.3553	8.2E-03	0.0000		1.031	1.000	0.330	3.0E-02	0.000
F 40	-21.0024	4.9E-03	0.0000		1.031	1.000	0.000	1.239	1.1E-01
F 41	-23.4196	2.7E-03	0.0000		1.031	1.000	1.000	0.008	4.2E-03
F 42 (4)	-2.0307		1.4754		1.031	0.500	0.000	1.699	
F 43 (5)	-6.5083		4.7457		1.031	0.427	0.000	2.627	
F 44 (6)	-11.8693		8.6236		1.031	1.000	1.000	0.209	1.236
F 45 (7)	-13.7274		9.9735		1.781	0.500	0.000	3.488	
F 46 (26)	-18.8672		6.2393		1.031	1.000	1.000	0.236	0.110
F 47 (25)	-20.9853		4.7003		1.393	0.500	1.000	0.008	
F 48 (24)	-25.4271		1.4732		1.031	1.000	0.000	0.814	
F 49	-4.6124	6.7E-03	1.1367	1.3E-02	1.031	1.000	0.000	0.001	1.6E-03
F 50	-7.4374	7.6E-03	2.2361	4.7E-03	1.031	1.000	0.663	2.7E-02	0.010
F 51	-9.3550	7.4E-03	3.8496	3.6E-03	1.490	1.8E-02	0.500	0.000	0.010
F 52	-11.8793	2.8E-02	0.1700	3.9E-02	1.031	0.500	0.000	0.001	1.0E-03
F 53	-11.1489	9.5E-03	6.2227	4.7E-03	1.031	1.000	0.000	0.507	3.0E-02
F 54	-11.7491	2.4E-03	3.8245	1.3E-03	1.031	1.000	1.000	0.014	3.9E-03
F 55	-13.8327	8.4E-03	5.2966	3.8E-03	1.031	1.000	0.000	2.489	1.5E-01
F 56	-13.7498	3.6E-03	2.4748	9.6E-03	1.031	0.687	2.7E-02	0.000	1.546
F 57	-14.3301	6.5E-03	7.7682	6.0E-03	1.031	1.000	1.000	0.006	2.6E-03
F 58	-16.2883	6.0E-03	2.4141	4.2E-03	1.031	1.000	1.000	3.542	1.4E-01
F 59	-16.3869	7.6E-03	6.0830	6.5E-03	1.031	1.000	0.000	2.229	2.0E-01
F 60	-18.1867	4.6E-03	3.9187	8.7E-03	1.031	1.000	0.000	2.627	1.1E-01
F 61	-18.9701	4.0E-04	1.4628	1.5E-03	1.031	1.000	0.000	0.017	5.1E-03
F 62	-4.0550	5.9E-03	0.0000		3.092	1.000	0.000	1.891	1.5E-01
F 63	-10.4959	2.9E-03	0.0000		3.092	1.000	1.000	1.545	7.7E-02
F 64	-12.8696	1.0E-02	0.0000		3.092	1.000	0.000	2.840	1.1E-01
F 65	-19.5391	8.6E-03	0.0000		3.092	1.000	0.000	1.315	7.9E-02
F 66	-25.1605	9.1E-03	0.0000		3.092	1.000	1.000	1.796	1.1E-01
F 67 (7)	-27.4548		0.0000		2.341	0.500	0.000	3.488	
F 68 (21)	-3.2940		2.3932		3.092	1.000	1.000	0.883	0.408
F 69 (22)	-8.4840		6.1640		3.092	1.000	0.000	1.506	
F 70 (23)	-10.4252		7.5743		3.092	1.000	1.000	0.329	1.562
F 71 (10)	-15.7819		8.4808		3.092	1.000	0.000	1.351	
F 72 (9)	-20.0027		5.4142		3.092	0.500	0.000	0.446	
F 73(8)	-22.2113		3.8095		3.092	1.000	1.000	3.566	2.069
F 74	-5.8176	7.1E-03	2.3595	1.5E-03	3.092	1.000	0.000	1.601	1.6E-01
F 75	-7.7190		3.8095		3.092	1.000	1.000	0.985	5.9E-02
F 76	-8.4723	2.6E-03	1.4071	4.8E-03	3.092	1.000	0.000	2.427	9.7E-02
F 77	-10.4862	5.0E-04	4.8447	9.5E-03	3.092	0.500	0.334	1.7E-02	0.748
F 78	-11.8824	2.5E-02	2.1486	1.2E-02	3.092	1.000	0.000	3.781	1.5E-01
F 79	-12.9466	2.7E-03	7.6036	2.3E-03	3.092	1.000	0.000	1.520	7.6E-02
F 80	-12.8778	5.9E-03	4.5930	6.9E-03	3.092	1.000	0.000	0.757	6.1E-02
F 81	-14.8182	5.9E-03	6.0337	5.2E-03	3.092	1.000	1.000	1.227	6.1E-02
F 82	-14.9956	2.1E-03	1.3907	3.9E-03	3.092	1.000	1.000	0.335	2.3E-02
F 83	-15.8731	7.1E-03	3.9717	8.1E-03	3.092	1.000	0.000	0.343	3.8E-02
F 84	-17.6133	1.0E-02	6.0485	8.1E-03	3.092	0.500	0.000	0.004	3.6E-03
F 85	-17.6469	6.0E-03	2.1466	6.2E-03	3.092	1.000	0.000	0.802	4.0E-02
F 86	-20.2943	6.9E-03	2.3642	2.3E-03	3.092	1.000	0.000	2.263	1.1E-01
F 87	-23.3228	1.0E-02	1.4560	4.8E-04	3.092	1.000	0.000	0.340	2.7E-02

F 88	-21.4351	3.7E-02	2.3544	1.031	1.000	0.000	0.594	6.5E-02
F 89	-1.3770		0.0000	3.092	0.400	0.000	3.209	2.9E-01
F 90	-16.8300		0.0000	1.031	0.500	0.000	0.010	9.5E-04
F 91 (90)	-16.8300		0.0000	3.092	0.500	0.000	0.010	

Table 2 Refined parameters for d-Al-Cu-Rh

	x [Å]	y [Å]	z [Å]	SOF	p(Cu)	p(Rh)	b _{xy} [Å ²]	b _{zz} [Å ²]
T 1	0.0000	0.0000	1.070	0.0E+00 1.000	0	1	0.360	2.2E-02 0.613 3.7E-02
T 2	2.5397	4.1E-03	0.0000	1.070 0.0E+00 1.000	0	0	2.518	2.3E-01
T 3	8.0439	7.2E-03	0.0000	1.070 0.0E+00 1.000	0	0	1.560	1.2E-01
T 4	0.7965	1.9E-03	2.4513	1.070 0.0E+00 1.000	0	0	1.819	1.8E-01
T 5	2.4963	3.0E-03	7.6338	7.6E-03 1.070 0.0E+00 1.000	0	0	0.405	4.5E-02
T 6	4.5698	1.3E-03	14.0645	1.070 0.0E+00 1.000	1	0	0.898	4.5E-02 1.202 6.0E-02
T 7	5.3119		16.3485	2.282 2.4E-02 0.364 2.2E-02	1	0	1.156	4.6E-02
T 8	7.3333	3.8E-04	10.1273	1.070 0.0E+00 1.000	0	1	0.530	2.6E-02 0.601 3.0E-02
T 9	8.1092	1.9E-03	7.7394	2.5E-03 1.070 0.0E+00 1.000	0	0	2.629	1.3E-01
T 10	9.7580	2.7E-03	2.6647	0.0E+00 1.070 0.0E+00 1.000	0	0	0.596	4.2E-02
T 11	3.0247	8.8E-03	3.7667	4.6E-03 1.070 0.0E+00 1.000	1	0	1.538	7.7E-02
T 12	4.5660	1.7E-03	6.0103	7.0E-03 1.070 0.0E+00 1.000	0	1	0.003	1.2E-03 1.036 5.2E-02
T 13	4.5021	3.5E-03	1.6588	7.4E-03 1.070 0.0E+00 1.000	0	0	1.158	6.9E-02
T 14	5.2459	5.3E-03	11.6340	5.0E-03 1.070 0.0E+00 1.000	0	0	1.432	1.1E-01
T 15	5.3322	2.4E-03	8.5476	5.8E-03 1.070 0.0E+00 1.000	0	0	0.602	4.8E-02
T 16	5.3034	8.5E-04	3.9024	2.6E-03 2.330 2.5E-02 0.500	0	1	0.447	2.7E-02 0.765 3.8E-02
T 17	7.2262	5.7E-03	5.4216	4.4E-03 1.070 0.0E+00 1.000	1	0	2.121	1.1E-01 0.367 3.7E-02
T 18	7.3866	2.3E-03	2.5346	4.5E-03 1.070 0.0E+00 1.000	0	1	0.707	3.5E-02 0.746 4.5E-02
T 19	4.2644	1.0E-02	0.0000	3.209 0.0E+00 1.000	1	0	1.828	1.3E-01 1.017 8.1E-02
T 20 (7)	10.6239		0.0000	1.997 0.0E+00 0.364	1	0	1.156	
T 21	1.2656	4.6E-04	3.8950	3.209 0.0E+00 1.000	0	1	0.372	1.9E-02 0.914 4.6E-02
T 22	3.3008	1.4E-03	10.1590	2.672 2.1E-02 0.500	0	0	1.492	6.0E-02
T 23	4.0372	8.3E-04	12.4251	3.209 0.0E+00 1.000	1	0	0.819	4.1E-02 0.706 4.2E-02
T 24	6.1029	1.1E-03	13.9142	3.209 0.0E+00 1.000	0	0	1.285	6.4E-02
T 25	7.8008	4.0E-03	8.6154	2.9E-03 3.209 0.0E+00 1.000	0	0	2.905	2.0E-01
T 26	8.6158	6.3E-04	6.1802	3.209 0.0E+00 1.000	0	1	0.100	7.0E-03 0.341 2.0E-02
T 27	3.3553	5.1E-03	5.3756	3.4E-03 3.209 0.0E+00 1.000	0	0	0.471	3.3E-02
T 28	3.2897	1.8E-03	2.3862	7.0E-04 3.209 0.0E+00 1.000	0	0	2.879	2.0E-01
T 29	3.8403	8.7E-03	7.7418	2.1E-03 3.209 0.0E+00 1.000	1	0	0.003	1.7E-03 0.318 3.2E-02
T 30	5.8833	6.5E-03	10.1730	6.9E-03 3.209 0.0E+00 0.500	0	0	0.648	5.8E-02
T 31	6.0270	4.2E-03	6.3613	7.0E-03 3.209 0.0E+00 1.000	0	0	0.923	6.5E-02
T 32	6.1446	4.6E-03	1.6206	7.3E-03 3.209 0.0E+00 1.000	0	0	0.548	4.4E-02
T 33	7.8886	5.5E-03	3.7602	5.9E-03 3.209 0.0E+00 1.000	0	0	1.339	9.4E-02
T 34	8.7012	5.3E-03	1.3761	4.9E-03 3.209 0.0E+00 1.000	1	0	0.502	3.5E-02 1.315 7.9E-02
T 35	1.2836	4.1E-02	0.7744	8.1E-02 3.209 0.0E+00 0.400	0	0	2.456	1.7E-01
T 36	5.3119		16.3485	1.070 0.0E+00 0.210 8.4E-03	1	0	1.945	5.8E-02
T 37 (36)	10.6239		0.0000	3.209 0.0E+00 0.210	1	0	1.945	
F 38 (1)	0.0000		0.0000	1.070 0.0E+00 1.000	0	1	0.360	0.613
F 39	-6.3760	7.6E-03	0.0000	2.308 2.5E-02 0.358 2.1E-02	0	1	1.325	6.6E-02
F 40	-8.8246	1.0E-02	0.0000	1.070 0.0E+00 1.000	0	0	0.518	4.1E-02
F 41	-14.8067	3.7E-03	0.0000	1.070 0.0E+00 1.000	0	1	0.381	1.9E-02
F 42	-21.2698	2.9E-03	0.0000	1.070 0.0E+00 1.000	0	0	3.053	2.1E-01
F 43	-23.6839	2.9E-03	0.0000	1.070 0.0E+00 1.000	0	1	1.157	4.6E-02 1.029 6.2E-02
F 44	-2.0624	4.0E-03	1.5311	5.7E-03 1.070 0.0E+00 1.000	0	0	2.318	1.9E-01
F 45	-6.3868	9.0E-03	4.6418	7.7E-03 1.070 0.0E+00 1.000	0	0	0.377	4.1E-02
F 46 (6)	-11.9640		8.6924	1.070 0.0E+00 1.000	1	0	0.898	1.202
F 47 (7)	-13.9068		10.1039	2.282 0.0E+00 0.364	1	0	1.156	
F 48 (26)	-19.1640		6.2843	1.070 0.0E+00 1.000	0	1	0.100	0.341
F 49 (24)	-25.7430		1.5045	1.070 0.0E+00 1.000	0	0	1.285	

F 50	-4.6361	6.0E-03	2.1137	1.9E-02	1.070	0.0E+00	0.500		1	0	1.595	9.6E-02		
F 51	-7.3212	9.9E-04	2.3483	1.5E-03	1.070	0.0E+00	1.000		0	1	0.479	2.4E-02	0.777	3.9E-02
F 52	-9.3599	1.3E-03	3.7798	4.0E-03	1.070	0.0E+00	1.000		0	0	0.352	2.8E-02		
F 53	-11.0593	3.5E-03	6.3166	4.3E-03	1.070	0.0E+00	1.000		0	0	1.476	8.9E-02		
F 54	-11.9363	1.8E-03	3.7885	2.1E-03	1.070	0.0E+00	1.000		0	1	0.848	3.4E-02	0.907	4.5E-02
F 55	-13.9801	3.7E-03	5.5451	8.5E-03	1.070	0.0E+00	1.000		0	0	0.129	1.9E-02		
F 56	-13.9290	2.9E-03	2.3985	2.3E-03	1.070	0.0E+00	1.000		0	0	4.016	2.4E-01		
F 57	-14.6245	3.4E-03	7.9063	5.6E-03	1.070	0.0E+00	1.000		1	0	0.305	1.8E-02	1.634	8.2E-02
F 58	-16.6454	4.6E-03	6.3172	5.1E-03	1.070	0.0E+00	1.000		0	0	1.668	8.3E-02		
F 59	-18.4747	3.4E-03	3.8037	3.3E-03	1.070	0.0E+00	1.000		0	0	1.933	9.7E-02		
F 60	-19.1821	1.8E-03	1.3261	4.4E-03	1.070	0.0E+00	1.000		1	0	0.578	2.9E-02	1.548	7.7E-02
F 61	-4.1588	7.1E-03	0.0000		3.209	0.0E+00	1.000		0	0	3.669	2.2E-01		
F 62	-10.5847	2.7E-03	0.0000		3.209	0.0E+00	1.000		0	1	2.285	9.1E-02	2.285	9.1E-02
F 63	-13.1862	4.4E-03	0.0000		3.209	0.0E+00	1.000		0	0	2.022	1.4E-01		
F 64	-18.9032	2.4E-02	0.0000		3.209	0.0E+00	1.000		0	0	1.604	8.0E-02		
F 65	-25.5190	6.4E-03	0.0000		3.209	0.0E+00	1.000		1	0	1.072	5.4E-02	1.588	9.5E-02
F 66 (7)	-27.8137	0.0000		1.997	0.0E+00	0.364			1	0	1.156			
F 67 (21)	-3.3133	2.4073		3.209	0.0E+00	1.000			0	1	0.372		0.914	
F 68 (2)	-8.6417	6.2786		2.672	0.0E+00	0.500			0	0	1.492			
F 69 (23)	-10.5695	7.6792		3.209	0.0E+00	1.000			1	0	0.819		0.706	
F 70 (10)	-16.1736	8.4570		3.209	0.0E+00	1.000			0	0	0.596			
F 71 (9)	-20.4903	5.3207		3.209	0.0E+00	1.000			0	0	2.629			
F 72 (8)	-22.5215	3.8449		3.209	0.0E+00	1.000			0	1	0.530		0.601	
F 73	-5.9118	6.0E-03	2.6326	9.9E-03	3.209	0.0E+00	1.000		0	0	1.112	7.8E-02		
F 74	-8.0049	5.6E-03	4.0208	4.8E-03	3.209	0.0E+00	1.000		1	0	0.142	1.4E-02	0.564	3.9E-02
F 75	-8.6347	3.2E-03	1.6490	7.0E-03	3.209	0.0E+00	1.000		0	0	1.259	7.6E-02		
F 76	-10.6457	1.5E-03	5.0037	7.0E-03	3.209	0.0E+00	1.000		0	0	0.302	2.4E-02		
F 77	-11.3706	3.4E-03	2.4063	2.5E-03	3.209	0.0E+00	1.000		0	0	3.351	1.7E-01		
F 78	-13.0790	4.2E-03	7.6970	2.4E-03	3.209	0.0E+00	1.000		0	0	1.810	9.0E-02		
F 79	-15.0300	3.9E-03	6.1799	1.9E-03	3.209	0.0E+00	1.000		0	1	0.422	2.5E-02	0.784	3.9E-02
F 80	-15.1933	7.5E-03	1.5793	1.4E-02	3.209	0.0E+00	0.401	2.0E-02	0	0	3.269	3.3E-01		
F 81	-16.0699	8.0E-03	3.9301	5.0E-03	3.209	0.0E+00	1.000		0	0	3.344	1.7E-01		
F 82	-17.8200	7.6E-03	6.0245	8.8E-03	3.209	0.0E+00	0.500		1	0	1.590	8.0E-02		
F 83	-17.9186	1.8E-03	2.5478	4.9E-03	3.209	0.0E+00	1.000		0	1	0.458	1.8E-02	1.070	4.3E-02
F 84	-20.4447	2.2E-03	2.4024	1.9E-03	3.209	0.0E+00	1.000		0	0	0.637	3.8E-02		
F 85	-23.3140	3.4E-03	1.3855	5.3E-03	3.209	0.0E+00	1.000		0	0	1.832	1.1E-01		
F 86	-21.9062	2.1E-02	2.2204	6.6E-03	1.070	0.0E+00	1.000		0	0	0.132	1.6E-02		
F 87	-1.5760	4.7E-02	0.0000		3.209	0.0E+00	0.400		0	0	1.582	1.1E-01		
F 88	-11.9399	2.5E-02	0.2286	3.7E-02	1.070	0.0E+00	1.000		0	0	0.162	2.6E-02		
F 89	-16.8396	1.3E-02	1.4581	2.8E-02	1.070	0.0E+00	1.000		0	0	1.786	1.1E-01	1.669	1.2E-01
F 90	-13.4259	8.8E-03	4.0225	2.2E-02	3.209	0.0E+00	1.000		0	0	0.422	3.4E-02		
F 91	-6.5033	4.4E-03	0.0000		1.517	1.8E-02	0.142	2.8E-01	0	1	0.031	1.5E-03		
F 92 (36)	-13.9068	0.0E+00	10.1039		1.070	0.0E+00	0.210		1	0	1.945			
F 93 (36)	-27.8137	0.0E+00	0.0000		3.209	0.0E+00	0.210		1	0	1.945			

Table 3 Refined parameters for d-Al-Cu-Ir

	x [Å]	y [Å]	z [Å]	SOF	p(Cu)	p(Rh)	b _{xy} [Å ²]	b _{zz} [Å ²]				
T 1	0.0000	0.0000	1.065	1.000	0.000	1.000	0.186	1.5E-02	1.159	5.8E-02		
T 2	2.6296	9.0E-03	0.0000	1.065	1.000	0.000	0.000	2.405	3.4E-01			
T 3	8.1852	5.3E-03	0.0000	1.065	1.000	0.000	0.000	0.211	3.4E-02			
T 4	0.7824	1.1E-03	2.4079	1.065	1.000	0.000	0.000	1.349	1.5E-01			
T 5	2.4972	1.6E-03	7.6857	1.065	1.000	0.000	0.000	0.815	7.3E-02			
T 6	4.6091	2.2E-03	14.1855	1.065	1.000	1.000	0.000	1.736	8.7E-02	1.403	1.1E-01	
T 7	5.3325	16.4118	2.299	2.5E-02	0.500	1.000	0.000	0.998	5.0E-02			
T 8	7.3914	8.8E-04	10.0752	1.065	1.000	0.000	1.000	1.634	4.9E-02	0.729	3.6E-02	
T 9	9.8525	3.1E-03	2.5006	1.065	1.000	0.000	0.000	3.705	2.2E-01			

T	10	3.0327	1.1E-02	3.8027	5.7E-03	1.065		1.000	1.000	0.000	1.812	1.3E-01	1.380	1.9E-01
T	11	4.6648	5.5E-03	6.1242	5.8E-03	1.065		1.000	1.000	0.000	0.001	1.2E-03	0.712	6.4E-02
T	12	4.6717	7.0E-03	1.7639	1.1E-02	1.065		1.000	1.000	0.000	0.802	6.4E-02	0.678	8.8E-02
T	13	5.3380	2.4E-03	11.6590	4.7E-03	1.065		1.000	0.000	0.000	1.884	2.1E-01		
T	14	5.3764	6.2E-03	8.6278	4.2E-03	1.065		1.000	0.000	0.000	0.279	5.6E-02		
T	15	5.3066	2.3E-03	3.8448	3.0E-03	2.380	2.6E-02	0.500	1.000	0.000	0.109	2.0E-02		
T	16	8.0811	2.8E-02	5.1684	9.3E-03	1.065		0.500	0.000	0.000	0.849	7.6E-02		
T	17	7.4698	3.0E-03	2.5997	6.2E-03	1.065		1.000	0.000	1.000	0.198	1.6E-02	0.767	4.6E-02
T	18	4.2046	3.9E-03	0.0000		3.194		1.000	0.000	1.000	0.001	9.4E-04	1.314	7.9E-02
T	19 (7)	10.6650		0.0000		1.960		0.500	1.000	0.000	0.998			
T	20	1.2465	4.9E-04	3.8363		3.194		1.000	0.000	1.000	0.661	2.6E-02	0.660	3.3E-02
T	21	3.3055	9.9E-04	10.1734		2.756	2.2E-02	0.500	0.000	0.000	0.004	3.1E-03		
T	22	4.0409	9.8E-04	12.4368		3.194		1.000	0.000	1.000	1.457	5.8E-02	1.186	4.7E-02
T	23	6.1234	1.6E-03	13.9774		3.194		1.000	0.000	0.000	2.502	2.3E-01		
T	24	7.8040	4.6E-03	8.8053		3.194		0.500	0.000	0.000	1.542	1.4E-01		
T	25	8.6585	9.1E-04	6.1754		3.194		1.000	0.000	1.000	0.846	3.4E-02	0.384	2.7E-02
T	26	3.1594	1.4E-02	5.5701	1.5E-02	3.194		1.000	0.000	0.000	2.051	1.4E-01		
T	27	3.2578	4.9E-03	2.4610	7.3E-03	3.194		1.000	0.000	0.000	0.759	8.4E-02		
T	28	4.1002	2.1E-03	7.8717	4.9E-03	3.194		1.000	0.709	2.1E-02	0.291	0.405	2.8E-02	
T	29	5.6174	9.8E-03	9.9512	1.2E-02	3.194		1.000	0.000	0.000	0.359	4.0E-02		
T	30	6.1211	3.6E-03	6.2753	2.7E-03	3.194		1.000	0.000	0.000	1.328	1.6E-01		
T	31	6.2541	8.6E-03	1.5031	4.6E-03	3.194		1.000	0.000	0.000	0.992	8.9E-02		
T	32	7.8308	5.4E-03	3.9446	7.7E-03	3.194		1.000	0.000	0.000	2.604	1.8E-01		
T	33	8.6328	9.4E-04	1.3032	7.1E-03	3.194		1.000	1.000	0.000	0.000	7.8E-04	1.620	1.3E-01
T	34	0.9840	2.9E-02	0.7778	6.5E-02	3.194		0.400	0.000	0.000	4.889	2.9E-01		
F	35 (1)	0.0000		0.0000		1.065		1.000	0.000	1.000	0.186		1.159	
F	36	-6.5554	3.6E-03	0.0000		2.185	3.4E-02	0.500	1.000	0.000	1.495	1.0E-01		
F	37	-8.6230	1.5E-02	0.0000		1.065		1.000	0.000	0.000	3.040	4.0E-01		
F	38	-14.5552	7.3E-03	0.0000		1.065		1.000	0.000	0.000	1.534	1.1E-01	0.767	7.7E-02
F	39	-21.3215	1.7E-03	0.0000		1.065		1.000	0.000	0.000	0.001	1.8E-03		
F	40	-23.8022	1.8E-03	0.0000		1.065		1.000	0.000	1.000	0.879	4.4E-02	0.545	3.8E-02
F	41	-2.0882	8.2E-03	1.5082	4.8E-03	1.065		1.000	0.000	0.000	2.348	2.1E-01		
F	42 (5)	-6.5379		4.7500		1.065		1.000	0.000	0.000	0.815			
F	43 (6)	-12.0669		8.7671		1.065		1.000	1.000	0.000	1.736		1.403	
F	44 (7)	-13.9606		10.1430		2.299		0.500	1.000	0.000	0.998			
F	45 (25)	-19.2138		6.3264		1.065		1.000	0.000	1.000	0.846		0.384	
F	46 (24)	-21.4509		4.7010		1.065		0.500	0.000	0.000	1.542			
F	47 (23)	-25.8506		1.5045		1.065		1.000	0.000	0.000	2.502			
F	48	-7.2391	3.9E-03	2.4113	1.2E-03	1.065		1.000	0.357	1.1E-02	0.643	0.356	1.8E-02	
F	49	-9.4037	8.1E-04	3.8082	5.3E-03	1.065		1.000	0.000	0.000	0.635	5.1E-02		
F	50	-11.1920	5.1E-03	6.3714	6.2E-03	1.065		1.000	0.000	0.000	0.613	5.5E-02		
F	51	-11.9599	1.4E-03	3.7994	2.2E-03	1.065		1.000	0.000	1.000	0.124	8.7E-03	0.810	4.1E-02
F	52	-14.0724	7.8E-03	2.4076	2.2E-03	1.065		1.000	0.000	0.000	1.552	1.1E-01		
F	53	-14.5553	7.3E-03	7.7667	1.6E-03	1.065		1.000	1.000	0.000	1.842	9.2E-02	0.867	6.9E-02
F	54	-16.4950	1.7E-03	2.1763	8.7E-03	1.065		1.000	1.000	0.000	0.227	2.3E-02	1.489	1.0E-01
F	55	-16.6541	7.3E-03	6.3696	8.1E-03	1.065		1.000	0.000	0.000	1.169	9.4E-02		
F	56	-18.4590	3.9E-03	3.8450	2.9E-03	1.065		1.000	0.000	0.000	1.577	1.1E-01		
F	57	-19.1493	5.8E-03	1.3231	6.3E-03	1.065		1.000	1.000	0.000	0.354	3.2E-02	0.969	6.8E-02
F	58	-22.1412	2.8E-02	2.3615	5.9E-03	1.065		0.500	0.000	0.000	0.750	9.7E-02		
F	59	-4.1123	4.3E-03	0.0000		3.194		1.000	0.000	0.000	0.715	7.9E-02		
F	60	-10.6251	2.0E-03	0.0000		3.194		1.000	0.000	1.000	0.479	2.4E-02	0.651	3.9E-02
F	61	-13.2382	5.0E-03	0.0000		3.194		1.000	0.000	0.000	0.510	5.6E-02		
F	62	-19.9133	8.4E-03	0.0000		3.194		1.000	1.000	0.000	0.991	5.9E-02		
F	63	-25.6120	8.3E-03	0.0000		3.194		1.000	1.000	0.000	0.118	1.9E-02	0.796	8.0E-02
F	64 (7)	-27.9213		0.0000		1.960		0.500	1.000	0.000	0.998			
F	65 (20)	-3.2634		2.3710		3.194		1.000	0.000	1.000	0.661		0.660	
F	66 (21)	-8.6540		6.2875		2.756		0.500	0.000	0.000	0.004			
F	67 (22)	-10.5793		7.6864		3.194		1.000	0.000	1.000	1.457		1.186	
F	68 (9)	-16.0879		8.5975		3.194		1.000	0.000	0.000	3.705			

F	69	-20.5169	6.0E-03	5.2098	1.7E-02	3.194	0.500	0.000	0.000	1.663	1.3E-01		
F	70 (8)	-22.5311		3.9162		3.194	1.000	0.000	1.000	1.634		0.729	
F	71	-5.9197	7.4E-03	2.4394	3.6E-03	3.194	1.000	0.000	0.000	1.765	1.1E-01		
F	72	-7.9617	4.5E-03	3.9504	3.8E-03	3.194	1.000	1.000	0.000	0.073	1.3E-02	1.552 1.4E-01	
F	73	-8.6098	2.0E-03	1.4897	2.1E-03	3.194	1.000	0.000	0.000	1.431	1.3E-01		
F	74	-10.4885	7.1E-03	4.8747	4.3E-03	3.194	1.000	1.000	0.000	0.126	1.8E-02	0.509 4.6E-02	
F	75	-11.4849	7.1E-03	2.5185	7.4E-03	3.194	1.000	0.000	0.000	2.126	1.5E-01		
F	76	-13.1479	3.5E-03	7.7406	1.7E-03	3.194	1.000	0.000	0.000	1.691	1.0E-01		
F	77	-13.6048	1.7E-02	3.7696	3.1E-02	3.194	1.000	0.000	0.000	1.847	1.1E-01		
F	78	-15.0647	4.6E-03	6.1891	2.4E-03	3.194	1.000	0.000	1.000	0.617	2.5E-02	0.786 3.9E-02	
F	79	-15.3424	7.4E-03	1.2819	9.9E-03	3.194	1.000	0.000	0.000	0.656	5.9E-02		
F	80	-15.9249	8.7E-03	3.8890	2.8E-03	3.194	0.710	3.5E-02	0.000	0.000	3.433	2.1E-01	
F	81	-17.8670	6.5E-03	6.1778	5.5E-03	3.194	0.500	1.000	0.000	0.030	8.3E-03		
F	82	-17.9712	3.2E-03	2.3737	1.5E-03	3.194	1.000	0.266	1.1E-02	0.734	1.846	5.5E-02	
F	83	-20.3756	1.1E-02	2.3523	7.2E-03	3.194	1.000	0.000	0.000	2.884	2.0E-01		
F	84	-23.4581	6.4E-03	1.3681	8.9E-03	3.194	1.000	0.000	0.000	1.964	1.4E-01		
F	85	-1.3131	1.1E-01	0.0000		3.194	0.400	0.000	0.000	4.915	3.4E-01		
F	86	-12.1033	1.9E-02	1.0608	1.3E-02	1.065	0.500	0.540	2.2E-02	0.460	0.836	5.0E-02	
F	87	-14.2670	1.5E-02	5.1515	1.4E-02	1.065	1.000	0.000	0.000	2.544	1.8E-01		
F	88	-4.7163	9.7E-03	2.3366	2.6E-02	1.065	0.500	1.000	0.000	0.013	1.3E-03		
F	89	-6.5725		0.0000		1.493	0.000	0.000	0.000	2.237			
F	90	-17.3487		0.0000		2.423	4.1E-02	0.230	1.8E-02	0.000	0.096	2.3E-02	
F	91	-17.3487		0.0000		1.836	0.230	0.000	0.000	0.096			