Table 1. *TM subregions of AS* A. *Refined atomic temperature factors (cylindrically anisotropic, B_{xy} component in the quasiperiodic plane, B_z component along the periodic direction). Refined static displacements in the quasiperiodic plane (polar coordinates, Δr, ϕ): values given for the* F^+ *and* F^- *layers, subregions as numbered in Fig. 9; symmetry-constrained values for the other subregions and for the* $P^{\uparrow\downarrow}$ *layers. Refined static displacements along the periodic direction for the puckered layers* $P^{\uparrow\downarrow}$.

	F^-		P		F^+				
	B_{xy}	B_z	B_{xy}	B_z	B_{xy}	B_z	Δr [a]	ϕ [°]	$\lvert\Delta z\rvert$ [c]
1	1.135	0.031	1.135	0.031	1.135	0.031	-	-	-
2	-	-	0.986	0.002	-	-	0.022	333	0.004
3	-	-	2.916	0.002	0.032	0.032	0.012	149	0.030
4	7.954	0.206	1.724	0.002	-	-	0.022	238	0.021
5	0.268	0.027	0.817	0.002	0.261	0.027	0.029	95	-
6	0.032	0.036	0.544	0.002	0.032	0.036	0.012	275	0.019
7	1.532	0.124	1.556	0.002	1.555	0.124	0.033	177	0.032
8	0.033	0.200	0.032	0.002	0.050	0.203	0.099	336	0.034
9	0.032	0.027	0.032	0.002	0.032	0.027	0.037	16	0.017
10	0.037	0.042	0.565	0.002	0.114	0.044	0.046	152	0.016
11	0.032	0.032	-	-	0.032	0.032	0.088	1	-
12	0.801	0.017	0.889	0.002	0.815	0.017	0.026	45	0.011
13	7.952	0.439	-	-	7.954	0.440	0.138	10	-
14	0.880	0.211	7.954	0.440	0.923	0.212	0.061	358	0.250
15	-	-	7.954	0.002	-	-	0.086	168	0.147

Table 2. *Al subregions of AS A. Refined atomic temperature factors (cylindrically anisotropic, B_{xy} component in the quasiperiodic plane, B_z component along the periodic direction). Refined static displacements in the quasiperiodic plane (polar coordinates, Δr, ϕ): values given for the* F^+ *and* F^- *layers, subregions as numbered in Fig. 9; symmetry-constrained values for the other subregions and for the* $P^{\uparrow\downarrow}$ *layers. Refined static displacements along the periodic direction for the puckered layers* $P^{\uparrow\downarrow}$.

	F^-		P		F^+				
	B_{xy}	B_z	B_{xy}	B_z	B_{xy}	B_z	Δr [a]	ϕ [°]	Δz [c]
1	-	-	0.032	0.303	7.954	0.435	0.172	46	0.008
2	7.943	0.436	-	-	7.954	0.440	0.124	218	-
3	7.951	0.188	7.146	0.147	7.954	0.186	0.175	81	0.019
4	7.954	0.391	6.977	0.002	7.954	0.382	0.130	287	0.044
5	3.762	0.174	7.951	0.002	3.815	0.171	0.175	81	0.119
6	-	-	1.921	0.065	-	-	0.158	262	0.083
7	5.232	0.440	-	-	5.228	0.440	0.128	202	-
8	0.420	0.136	0.337	0.440	1.415	0.164	0.072	4	0.250
9	7.360	0.432	0.033	0.002	7.320	0.436	0.127	111	-
10	6.571	0.340	7.840	0.002	6.515	0.350	0.148	93	-
11	3.854	0.440	3.299	0.440	3.868	0.440	0.135	244	0.250
12	1.735	0.031	0.735	0.002	1.710	0.031	0.033	356	-
13	-	-	7.946	0.002	-	-	0.065	270	0.032
14	-	-	0.032	0.099	-	-	0.132	196	-
15	0.838	0.375	7.954	0.002	0.871	0.346	0.071	318	0.151
16	-	-	7.954	0.002	-	-	0.125	9	0.096
17	0.211	0.032	0.032	0.002	0.089	0.029	0.064	118	-
18	0.032	0.170	7.954	0.440	0.032	0.171	0.117	307	0.250
19	1.544	0.063	0.035	0.048	1.545	0.064	0.028	296	0.223
20	0.034	0.009	7.954	0.004	0.042	0.009	0.052	20	-
21	3.910	0.440	-	-	3.940	0.440	0.136	282	-
22	0.032	0.312	7.954	0.002	7.954	0.440	0.068	71	0.047
23	-	-	1.951	0.073	-	-	0.129	19	-
24	0.032	0.036	-	-	0.032	0.038	0.073	188	-
25	0.642	0.175	0.032	0.002	0.472	0.163	0.070	167	-
26	-	-	7.932	0.002	-	-	0.125	133	-
27	2.729	0.066	4.560	0.002	2.733	0.071	0.067	134	0.020
28	1.247	0.152	2.054	0.002	1.192	0.203	0.016	88	0.017
29	7.954	0.440	5.720	0.080	-	-	0.050	50	0.225
30	7.954	0.440	7.954	0.002	7.954	0.440	0.134	58	0.030
31	3.568	0.440	7.954	0.120	3.512	0.440	0.040	122	0.099
32	0.032	0.403	0.032	0.002	0.032	0.429	0.143	6	0.019
33	-	-	7.954	0.002	-	-	0.149	70	0.038
34	5.502	0.440	7.912	0.440	5.441	0.440	0.115	265	0.250
35	0.109	0.440	-	-	0.070	0.440	0.137	61	-
36	-	-	1.040	0.022	-	-	0.126	296	-
37	1.408	0.440	-	-	1.389	0.440	0.174	81	-
38	-	-	2.590	0.008	-	-	0.137	186	-

Table 3. *TM subregions of AS* B. *Refined atomic temperature factors (cylindrically anisotropic, B_{xy} component in the quasiperiodic plane, B_z component along the periodic direction). Refined static displacements in the quasiperiodic plane (polar coordinates, Δr, ϕ): values given for the* F^+ *and* F^- *layers, subregions as numbered in Fig. 9; symmetry-constrained values for the other subregions and for the* $P^{\uparrow\downarrow}$ *layers. Refined static displacements along the periodic direction for the puckered layers* $P^{\uparrow\downarrow}$.

	F^-		P		F^+				
	B_{xy}	B_z	B_{xy}	B_z	B_{xy}	B_z	Δr [a]	ϕ [°]	Δz [c]
1	1.621	0.185	1.316	0.039	1.112	0.188	0.038	228	0.028
2	0.853	0.098	1.052	0.018	0.872	0.099	0.045	207	0.036
3	0.032	0.213	0.032	0.002	0.032	0.213	0.018	97	0.103
4	0.409	0.188	1.290	0.002	0.366	0.188	0.042	270	0.069
5	0.681	0.209	0.562	0.012	0.658	0.209	0.018	9	0.044
6	1.356	0.362	-	-	1.309	0.342	0.044	188	-
7	-	-	3.884	0.025	0.032	0.039	0.070	308	-
8	7.954	0.440	2.286	0.037	7.950	0.440	0.006	27	0.068

Table 4. *Al subregions of AS* B. *Refined atomic temperature factors (cylindrically anisotropic, B_{xy} component in the quasiperiodic plane, B_z component along the periodic direction). Refined static displacements in the quasiperiodic plane (polar coordinates, Δr, ϕ): values given for the* F^+ *and* F^- *layers, subregions as numbered in Fig. 9; symmetry-constrained values for the other subregions and for the* $P^{\uparrow\downarrow}$ *layers. Refined static displacements along the periodic direction for the puckered layers* $P^{\uparrow\downarrow}$.

	F^-		P		F^+				
	B_{xy}	B_z	B_{xy}	B_z	B_{xy}	B_z	Δr [a]	ϕ [°]	Δz [c]
1	1.030	0.202	0.032	0.002	0.620	0.204	0.069	317	0.062
2	7.954	0.284	3.011	0.002	7.954	0.284	0.087	341	0.005
3	7.954	0.440	7.954	0.002	7.954	0.440	0.126	22	0.048
4	0.032	0.188	1.318	0.002	0.032	0.189	0.046	65	0.043
5	6.265	0.361	0.032	0.438	4.808	0.348	0.091	249	0.225
6	0.450	0.187	7.954	0.308	0.359	0.186	0.034	96	-
7	-	-	2.558	0.002	-	-	0.136	151	-
8	0.032	0.141	0.262	0.007	0.032	0.141	0.038	233	0.070
9	-	-	7.953	0.032	-	-	0.168	258	0.014
10	5.177	0.440	4.079	0.003	-	-	0.083	258	0.028
11	3.285	0.206	7.954	0.002	3.292	0.206	0.046	55	0.090
12	3.761	0.388	0.032	0.002	3.850	0.390	0.065	56	0.105
13	-	-	5.700	0.028	-	-	0.175	351	-
14	0.032	0.133	1.737	0.002	0.032	0.133	0.076	5	-
15	-	-	0.032	0.026	-	-	0.007	182	0.057
16	1.194	0.438	0.032	0.002	1.130	0.439	0.032	75	0.053
17	0.032	0.066	0.032	0.002	0.032	0.063	0.064	130	-
18	0.032	0.440	2.263	0.002	0.032	0.440	0.054	73	0.051
19	-	-	2.696	0.002	-	-	0.071	249	0.025
20	1.498	0.149	0.786	0.002	1.439	0.148	0.030	62	0.090
21	0.032	0.440	1.892	0.063	-	-	0.030	304	0.049
22	0.032	0.174	0.954	0.018	0.043	0.164	0.099	294	-
23	2.789	0.252	0.379	0.002	2.809	0.251	0.043	283	0.020
24	-	-	0.327	0.002	0.500	0.440	0.036	88	0.035
25	0.032	0.440	1.744	0.002	0.032	0.440	0.112	358	0.157
26	0.663	0.070	-	-	0.400	0.068	0.164	77	-
27	0.471	0.440	0.032	0.003	2.445	0.440	0.118	111	0.088
28	1.720	0.440	7.954	0.002	1.999	0.440	0.032	137	0.051
29	0.032	0.002	-	-	0.032	0.002	0.135	359	-
30	-	-	7.954	0.002	-	-	0.158	165	-
31	-	-	1.477	0.002	0.032	0.436	0.124	214	0.135
32	0.032	0.083	0.927	0.048	1.270	0.440	0.107	48	0.008
33	3.753	0.440	7.954	0.440	3.096	0.440	0.131	335	0.225

Table 5. *TM subregions of AS* A. *Coordinates of the vertices of the asymmetric unit subregions, numbered as in Fig. 9. The coordinates* $(x_4, x_5)_V$ *are given by the four integers* $[n_1\ n_2\ n_3\ n_4]$, *and can be calculated as* $x_4 = a(\tau n_1 + n_2)/100$, $x_5 = a\chi(\tau n_3 + n_4)/100$ *(*$\chi = \sqrt{3-\tau}$, $\tau = (1+\sqrt{5})/2$*) .*

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1	[0 0 0 0]	[-8 24 0 0]	[12 -16 8 -4]	
2	[40 -60 20 -20]	[-80 140 20 -20]	[-20 40 0 20]	
3	[12 -16 8 -4]	[-8 24 0 0]	[20 -20 -20 40]	
4	[40 -60 20 -20]	[20 -20 -20 40]	[-80 140 20 -20]	
5	[-20 40 0 20]	[-80 140 20 -20]	[0 20 20 -20]	
6	[-8 24 0 0]	[20 -20 20 -40]	[-40 80 0 0]	[20 -20 -20 40]
7	[-20 40 0 20]	[60 -80 0 20]	[-40 80 40 -40]	
8	[0 20 20 -20]	[-80 140 20 -20]	[20 -20 -20 40]	
9	[20 -20 -20 40]	[-40 80 0 0]	[60 -80 40 -60]	
10	[0 20 20 -20]	[20 -20 -20 40]	[60 -80 40 -60]	
11	[-40 80 0 0]	[40 -40 0 0]	[60 -80 40 -60]	
12	[40 -40 0 0]	[-20 60 -20 40]	[0 20 20 -20]	
13	[0 20 20 -20]	[-20 60 -20 40]	[80 -100 20 -20]	
14	[40 -40 0 0]	[0 40 0 0]	[20 0 40 -60]	
15	[0 40 40 -40]	[60 -60 20 0]	[-40 100 -20 60]	

Table 6. *Al subregions of AS* A. *Coordinates of the vertices of the asymmetric unit subregions, numbered as in Fig. 9. The coordinates* $(x_4, x_5)_V$ *are given by the four integers* $[n_1\ n_2\ n_3\ n_4]$, *and can be calculated as* $x_4 = a(\tau n_1 + n_2)/100$, $x_5 = a\chi(\tau n_3 + n_4)/100$ $(\chi = \sqrt{3-\tau},\ \tau = (1+\sqrt{5})/2)$ *.*

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1	[12 -16 8 -4]	[-8 24 0 0]	[20 -20 -20 40]	
2	[-20 40 0 20]	[-40 80 40 -40]	[20 -20 20 0]	
3	[-20 40 0 20]	[-80 140 20 -20]	[0 20 20 -20]	
4	[-8 24 0 0]	[20 -20 20 -40]	[-40 80 0 0]	[20 -20 -20 40]
5	[-20 40 0 20]	[60 -80 0 20]	[-40 80 40 -40]	
6	[0 20 20 -20]	[-80 140 20 -20]	[20 -20 -20 40]	
7	[-20 40 0 20]	[0 20 20 -20]	[60 -80 0 20]	
8	[20 -20 20 0]	[-40 80 40 -40]	[0 20 -20 60]	
9	[-40 80 40 -40]	[60 -80 0 20]	[160 -240 40 -40]	
10	[-40 80 40 -40]	[160 -240 40 -40]	[0 20 -20 60]	
11	[20 -20 20 0]	[0 20 -20 60]	[100 -140 20 0]	
12	[0 20 20 -20]	[-60 120 0 20]	[60 -80 0 20]	
13	[40 -40 0 0]	[0 20 20 -20]	[60 -80 40 -60]	
14	[0 20 -20 60]	[160 -240 40 -40]	[40 -40 40 -40]	
15	[0 20 -20 60]	[-20 60 20 0]	[100 -140 20 0]	
16	[0 20 -20 60]	[40 -40 40 -40]	[-20 60 20 0]	
17	[0 20 20 -20]	[20 0 0 20]	[-60 120 0 20]	
18	[0 20 20 -20]	[-20 60 -20 40]	[80 -100 20 -20]	
19	[20 0 0 20]	[40 -40 40 -40]	[-60 120 0 20]	
20	[0 20 20 -20]	[80 -100 20 -20]	[20 0 0 20]	
21	[40 -40 0 0]	[20 0 40 -60]	[-20 60 -20 40]	
22	[-20 60 20 0]	[40 -40 40 -40]	[20 0 0 20]	
23	[20 0 40 -60]	[-140 260 -20 40]	[-20 60 -20 40]	
24	[-40 100 20 -20]	[-20 60 -20 40]	[-140 260 -20 40]	
25	[40 -40 0 0]	[0 40 0 0]	[20 0 40 -60]	
26	[20 0 0 20]	[80 -100 20 -20]	[-40 100 20 -20]	
27	[20 0 40 -60]	[60 -60 -20 40]	[-140 260 -20 40]	
28	[60 -60 -20 40]	[-40 100 20 -20]	[-140 260 -20 40]	
29	[20 0 0 20]	[0 40 40 -40]	[-40 100 -20 60]	
30	[0 40 0 0]	[60 -60 -20 40]	[20 0 40 -60]	
31	[40 -20 20 -20]	[20 0 0 20]	[-40 100 20 -20]	
32	[0 40 40 -40]	[60 -60 20 0]	[-40 100 -20 60]	
33	[20 0 0 20]	[100 -120 0 20]	[0 40 40 -40]	
34	[0 40 0 0]	[-60 140 -20 40]	[60 -60 -20 40]	
35	[0 40 40 -40]	[40 -20 -20 60]	[60 -60 20 0]	
36	[40 -20 20 -20]	[-20 80 0 20]	[100 -120 0 20]	
37	[40 -20 -20 60]	[20 20 20 0]	[60 -60 20 0]	
38	[-20 80 0 20]	[20 20 20 0]	[40 -20 -20 60]	

Table 7. *TM subregions of AS* B. *Coordinates of the vertices of the asymmetric unit subregions, numbered as in Fig. 9. The coordinates* $(x_4, x_5)_V$ *are given by the four integers* $[n_1\ n_2\ n_3\ n_4]$*, and can be calculated as* $x_4 = a(\tau n_1 + n_2)/100$*,* $x_5 = a\chi(\tau n_3 + n_4)/100$ *(*$\chi = \sqrt{3-\tau}$*,* $\tau = (1+\sqrt{5})/2$*) .*

	8		
1	[0 0 0 0]	[-20 40 40 -60]	[40 -60 20 -20]
2	[-20 40 0 20]	[60 -80 0 20]	[-40 80 40 -40]
3	[-40 80 0 0]	[60 -80 40 -60]	[20 -20 -20 40]
4	[-40 80 0 0]	[40 -40 0 0]	[60 -80 40 -60]
5	[0 20 20 -20]	[-20 60 -20 40]	[80 -100 20 -20]
6	[20 0 0 20]	[40 -40 40 -40]	[-60 120 0 20]
7	[40 -20 20 -20]	[20 0 0 20]	[-40 100 20 -20]
8	[0 40 0 0]	[-60 140 -20 40]	[60 -60 -20 40]

Table 8. *Al subregions of AS* B. *Coordinates of the vertices of the asymmetric unit subregions, numbered as in Fig. 9. The coordinates* $(x_4, x_5)_V$ *are given by the four integers* $[n_1\ n_2\ n_3\ n_4]$*, and can be calculated as* $x_4 = a(\tau n_1 + n_2)/100$*,* $x_5 = a\chi(\tau n_3 + n_4)/100$ *(*$\chi = \sqrt{3-\tau}$*,* $\tau = (1+\sqrt{5})/2$*) .*

		33	
1	[0 0 0 0]	[-20 40 40 -60]	[40 -60 20 -20]
2	[0 0 0 0]	[-40 80 0 0]	[-20 40 40 -60]
3	[40 -60 20 -20]	[-80 140 20 -20]	[-20 40 0 20]
4	[40 -60 20 -20]	[-20 40 40 -60]	[20 -20 -20 40]
5	[-20 40 0 20]	[-40 80 40 -40]	[20 -20 20 0]
6	[-20 40 0 20]	[-80 140 20 -20]	[0 20 20 -20]
7	[-20 40 0 20]	[60 -80 0 20]	[-40 80 40 -40]
8	[0 20 20 -20]	[-80 140 20 -20]	[20 -20 -20 40]
9	[-40 80 0 0]	[60 -80 40 -60]	[20 -20 -20 40]
10	[20 -20 20 0]	[-40 80 40 -40]	[0 20 -20 60]
11	[0 20 20 -20]	[20 -20 -20 40]	[60 -80 40 -60]
12	[-40 80 40 -40]	[60 -80 0 20]	[160 -240 40 -40]
13	[20 -20 20 0]	[0 20 -20 60]	[100 -140 20 0]
14	[-40 80 0 0]	[40 -40 0 0]	[60 -80 40 -60]
15	[0 20 20 -20]	[-60 120 0 20]	[60 -80 0 20]
16	[40 -40 40 -40]	[160 -240 40 -40]	[60 -80 0 20]
17	[0 20 -20 60]	[-20 60 20 0]	[100 -140 20 0]
18	[20 0 0 20]	[40 -40 40 -40]	[-60 120 0 20]
19	[0 20 20 -20]	[80 -100 20 -20]	[20 0 0 20]
20	[40 -40 0 0]	[20 0 40 -60]	[-20 60 -20 40]
21	[-20 60 20 0]	[40 -40 40 -40]	[20 0 0 20]
22	[20 0 40 -60]	[-140 260 -20 40]	[-20 60 -20 40]
23	[40 -40 0 0]	[0 40 0 0]	[20 0 40 -60]
24	[20 0 0 20]	[80 -100 20 -20]	[-40 100 20 -20]
25	[-40 100 -20 60]	[60 -60 20 0]	[-20 60 20 0]
26	[20 0 40 -60]	[60 -60 -20 40]	[-140 260 -20 40]
27	[60 -60 -20 40]	[-40 100 20 -20]	[-140 260 -20 40]
28	[20 0 0 20]	[0 40 40 -40]	[-40 100 -20 60]
29	[0 40 0 0]	[60 -60 -20 40]	[20 0 40 -60]
30	[40 -20 20 -20]	[20 0 0 20]	[-40 100 20 -20]
31	[60 -60 -20 40]	[40 -20 20 -20]	[-40 100 20 -20]
32	[60 -60 -20 40]	[-60 140 -20 40]	[40 -20 20 -20]
33	[40 -20 20 -20]	[-20 80 0 20]	[100 -120 0 20]

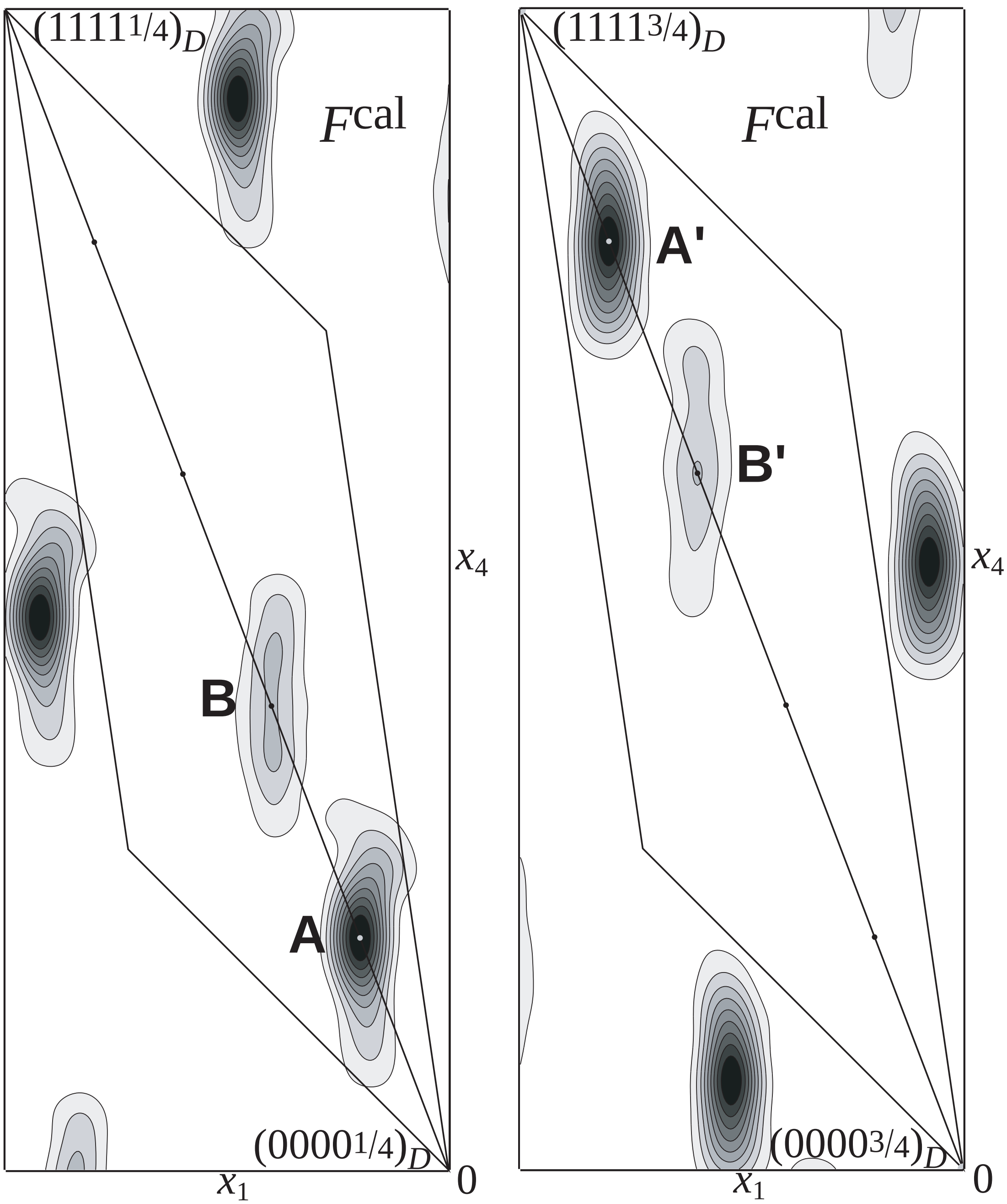

Fig. 1. Average 4 Å structure ($P\overline{1}0$). Left : $F^{\rm cal}$ Fourier map, plane $(x_1, 0, c/4, x_4, 0)_V$, bounded projection $0 < x_3 < c/2$. Note the profiles of AS A, B, with the deformation due to static ADPs.
Right : As above, in the plane $(x_1, 0, c/4, x_4, 0)_V$. The profiles of AS A′, B′ are visible.

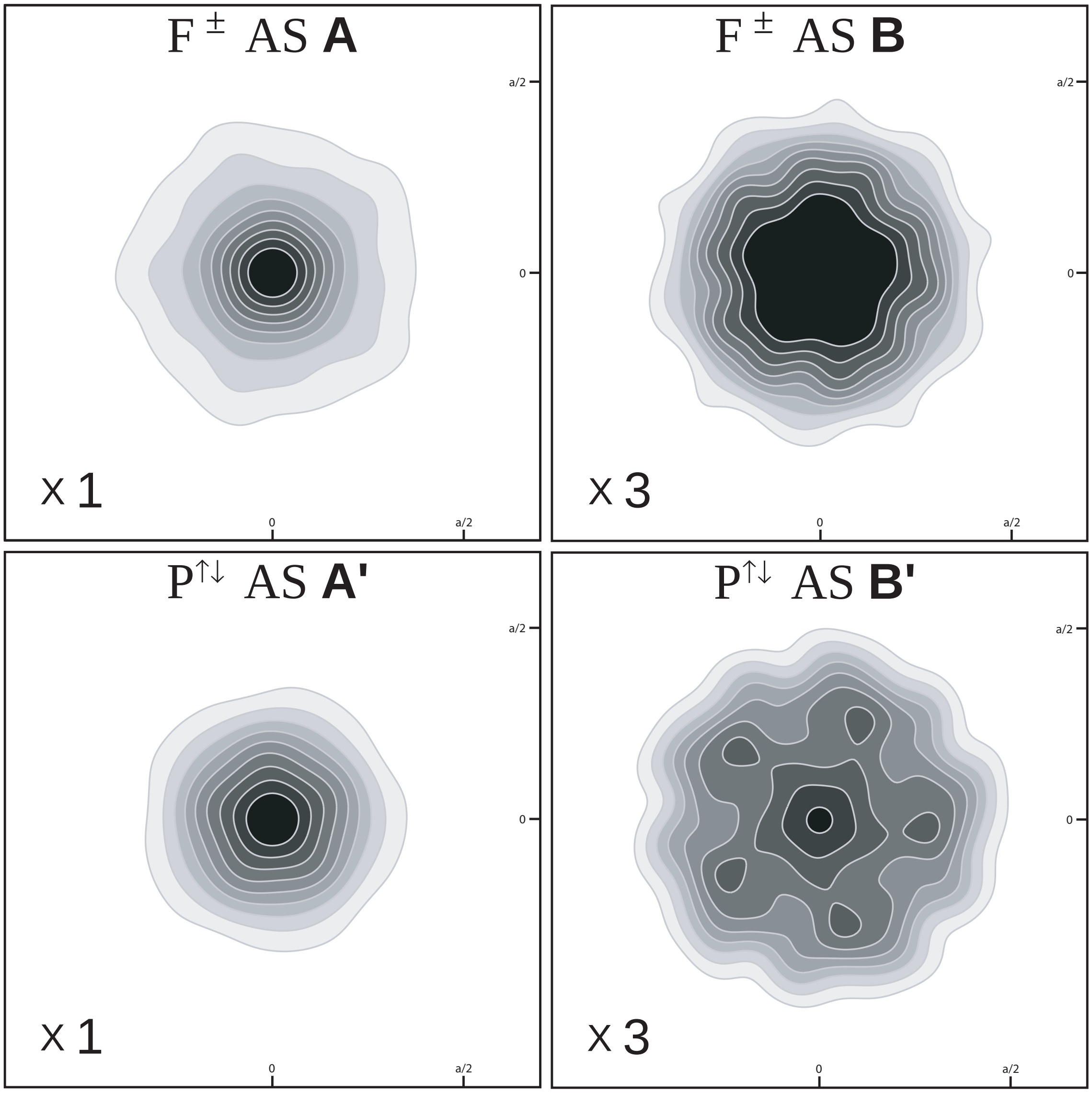

Fig. 2. Average 4 Å structure ($P\overline{10}$). Left, up: F^{cal} Fourier map, plane $(0,0,0,x_4,x_5)_V + (1/5,1/5,1/5,1/5,1/4)_D$, bounded projection $0 < x_3 < c/2$: AS A of layer(s) $\mathrm{F}^{\pm}$. Contour levels 10%, 20%, ... , 90%. 100% is the value in the center.

Left, down: F^{cal} Fourier map, plane $(0,0,0,x_4,x_5)_V + (4/5,4/5,4/5,4/5,3/4)_D$, bounded projection $c/2 < x_3 < c$: AS A′ of layer(s) $\mathrm{P}^{\uparrow\downarrow}$. Contour levels 10%, 20%, ... , 90% (same scale as above).

Right, up: F^{cal} Fourier map, plane $(0,0,0,x_4,x_5)_V + (2/5,2/5,2/5,2/5,1/4)_D$, bounded projection $0 < x_3 < c/2$: AS B of layer(s) $\mathrm{F}^{\pm}$. Contour levels 3.33%, 6.67%, ... , 30% (same scale as above).

Right, down: F^{cal} Fourier map, plane $(0,0,0,x_4,x_5)_V + (3/5,3/5,3/5,3/5,3/4)_D$, bounded projection $c/2 < x_3 < c$: AS B′ of layer(s) $\mathrm{P}^{\uparrow\downarrow}$. Contour levels 3.33%, 6.67%, ... , 30% (same scale as above).

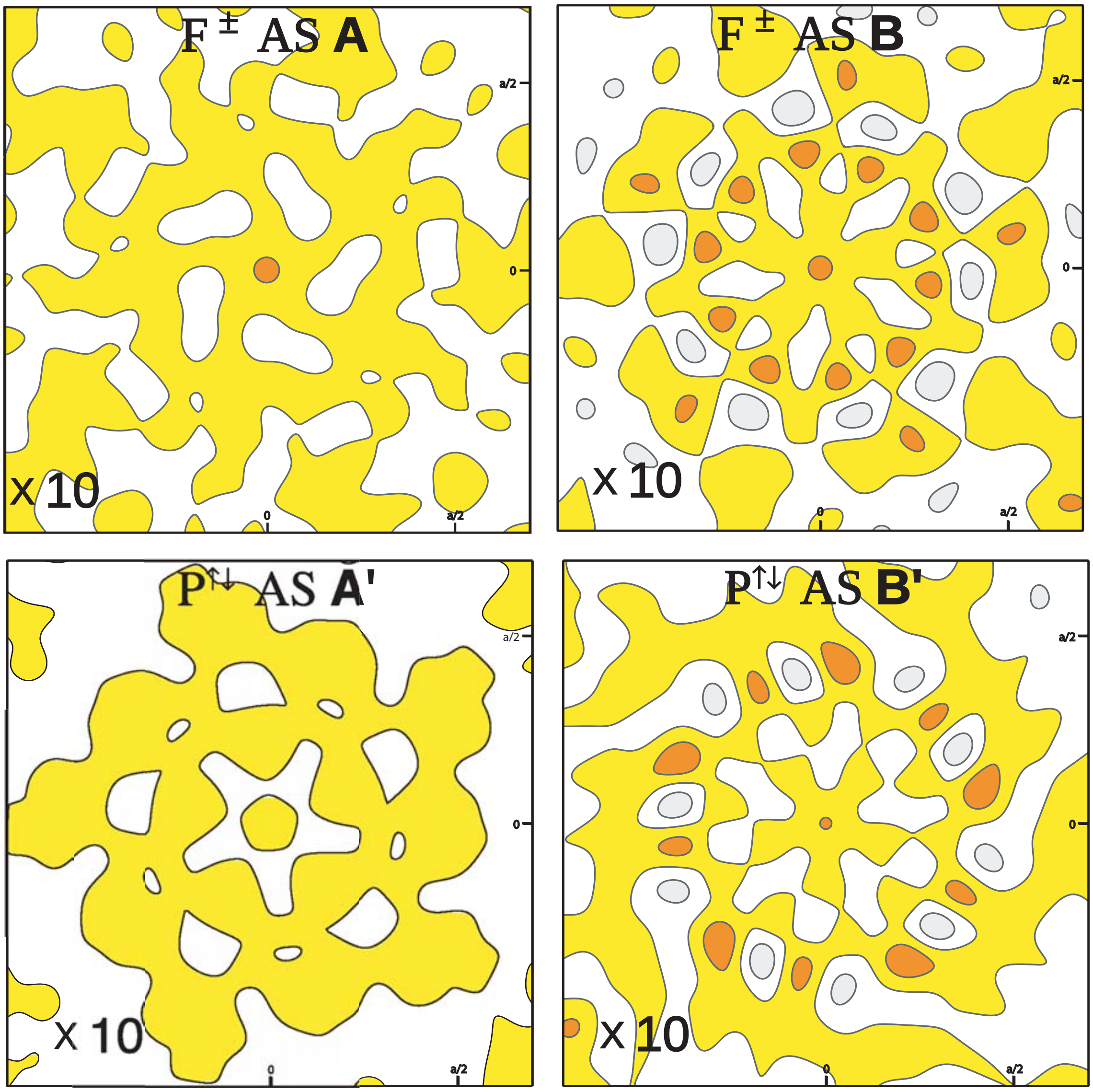

Fig. 3. Average 4 Å structure ($P\overline{10}$). Left, up: $F^{\rm dif}$ Fourier map, plane $(0,0,0,x_4,x_5)_V + (1/5,1/5,1/5,1/5,1/4)_D$, bounded projection $0 < x_3 < c/2$: AS A of layer(s) $\mathrm{F}^{\pm}$. Contour levels: -2% < orange <-1%< yellow <0%< white <1%< grey <2% (same scale as $F^{\rm cal}$).
Left, down: $F^{\rm dif}$ Fourier map, plane $(0,0,0,x_4,x_5)_V + (4/5,4/5,4/5,4/5,3/4)_D$, bounded projection $c/2 < x_3 < c$: AS A′ of layer(s) $\mathrm{P}^{\uparrow\downarrow}$. Contour levels as above.
Right, up: $F^{\rm dif}$ Fourier map, plane $(0,0,0,x_4,x_5)_V + (2/5,2/5,2/5,2/5,1/4)_D$, bounded projection $0 < x_3 < c/2$: AS B of layer(s) $\mathrm{F}^{\pm}$. Contour levels as above.
Right, down: $F^{\rm dif}$ Fourier map, plane $(0,0,0,x_4,x_5)_V + (3/5,3/5,3/5,3/5,3/4)_D$, bounded projection $c/2 < x_3 < c$: AS B′ of layer(s) $\mathrm{P}^{\uparrow\downarrow}$. Contour levels as above.