STRUCTURAL
CHEMISTRY

Volume 76 (2020)

Supporting information for article:

LaTe1.82(1): modulated crystal structure and chemical bonding of a chalcogen-deficient rare earth metal polytelluride

Dedicated to Professor Stephen Lee on the occasion of his 65th birthday.

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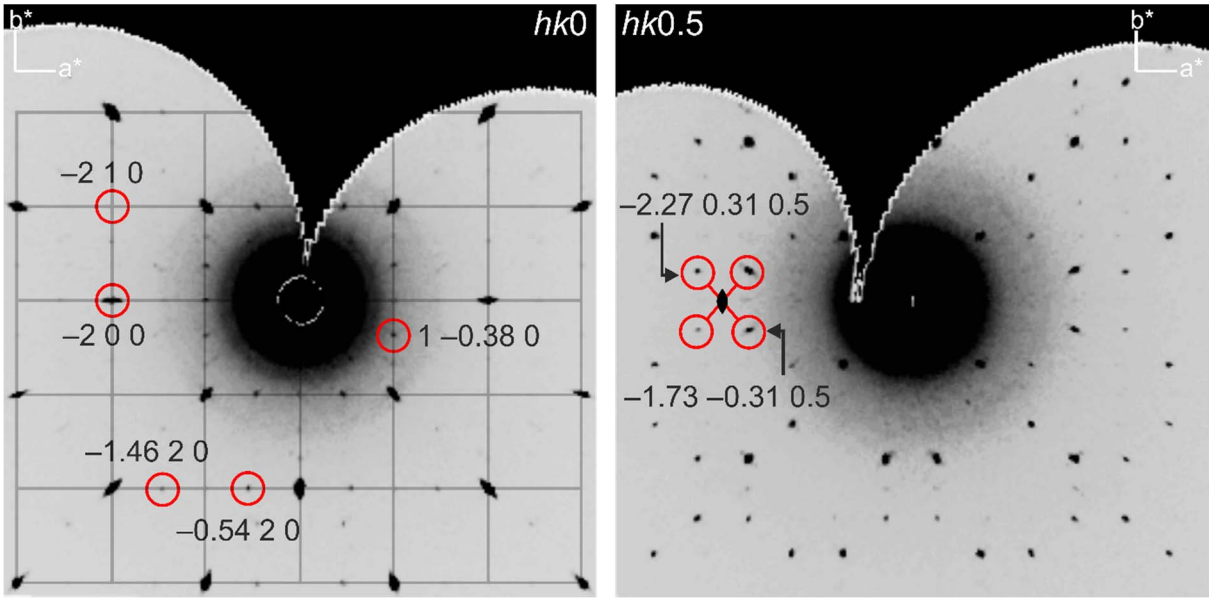

Figure S1 Reconstructed precession image of the planes *hk*0 and *hk*0.5. Miller indices correspond to the basic tetragonal cell with $a = b \approx 4.50$ Å and $c \approx 9.17$ Å (grid on left image). The *hk*0 plane shows the main reflections, which are only observed for $h + k = 2n$, and the cross-term satellite reflections. First order satellites in the *hk*0.5 plane demonstrate the wave vector component of ½ along *c** and the incompatibility with a fourfold rotational axis.

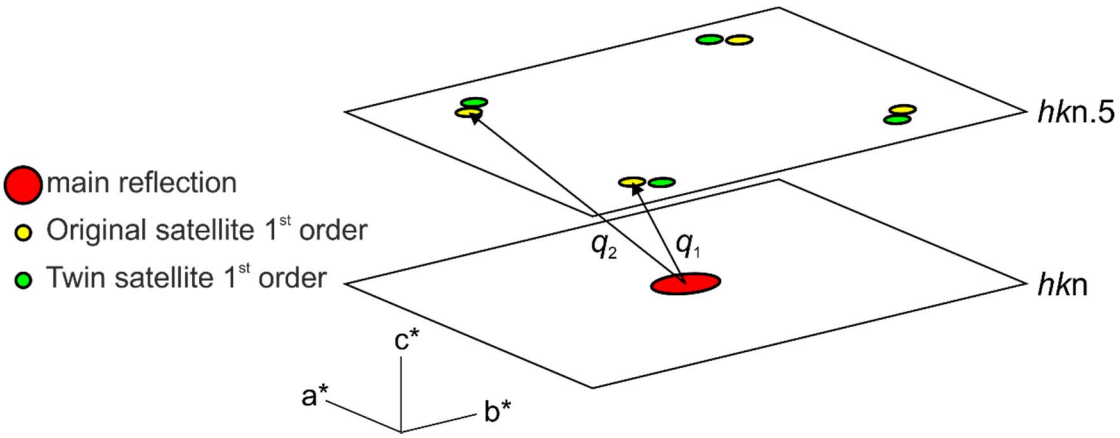

Figure S2 Sketch simulating reflections in the *hk*n.5 layers, in case of twinning (fourfold rotation axis as tin law).

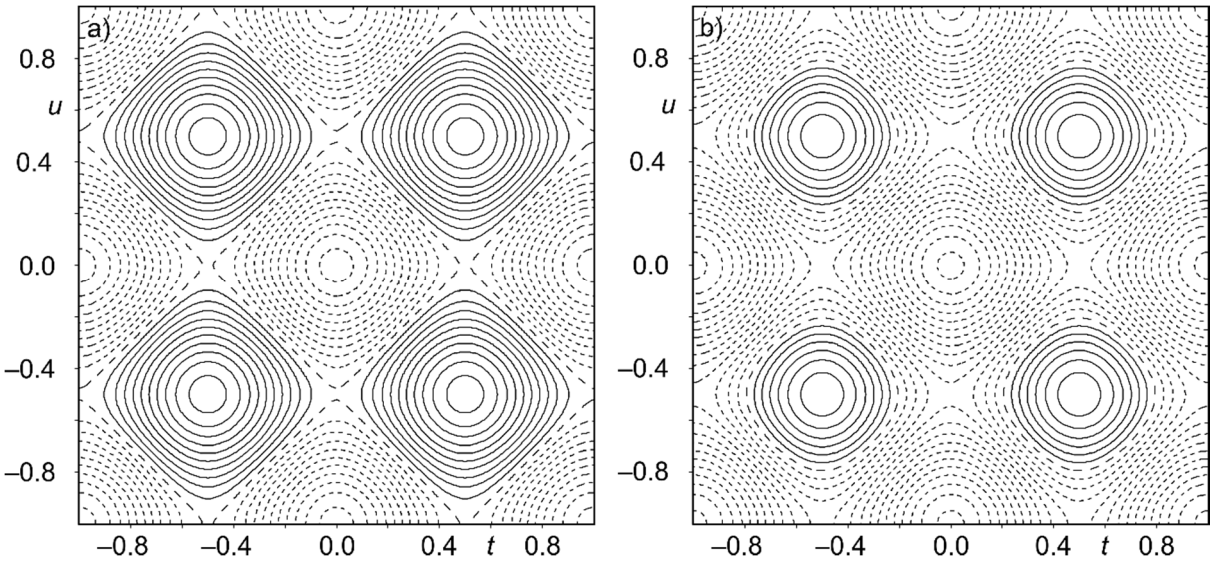

Figure S3 2D *t*-Plots of $LaTe_{1.82(1)}$. a) Position of Te2 in *dz* depending on *t* and *u*. b) Occupancy of Te2 depending on *t* and *u* with a reference level of 0.5. Both diagrams indicate a very similar behaviour along both modulation directions.

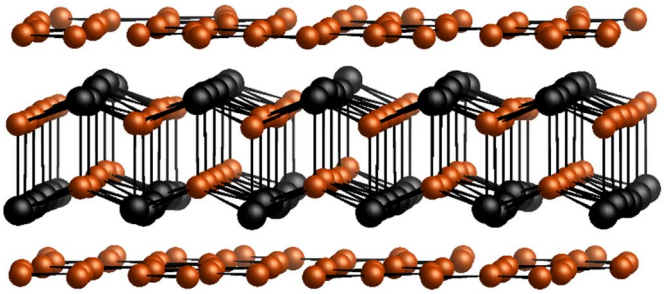

Figure S4 Approximate structure of $LaTe_{1.82(1)}$, displaying the effect of the modulation on the puckered [LaTe] layer.

Table S1 Crystallographic data and refinement details for the average structure of $LaTe_{1.82(1)}$.

Crystal data	
Chemical formula	$LaTe_{1.81(1)}$
M_r	370.50
Crystal system, space group	Tetragonal, *P*4/*nmm*
Temperature (K)	296(1)
a, *c* (Å)	4.4996 (5), 9.179 (1)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	25.18
Crystal size (mm)	0.03 × 0.02 × 0.02

Data collection	
Diffractometer	Bruker *APEX*-II CCD
Absorption correction	multi-scan, *SADBS,* (Krause *et al.*, 2015)
T_{min}, T_{max}	0.641, 0.748
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3402, 351, 289
R_{int}	0.046
θ values (°)	$\theta_{max} = 38.5$, $\theta_{min} = 2.2$
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.875
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.024, 0.057, 1.07
No. of reflections	351
No. of parameters	11
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e×Å^{-3})	3.15, −2.35

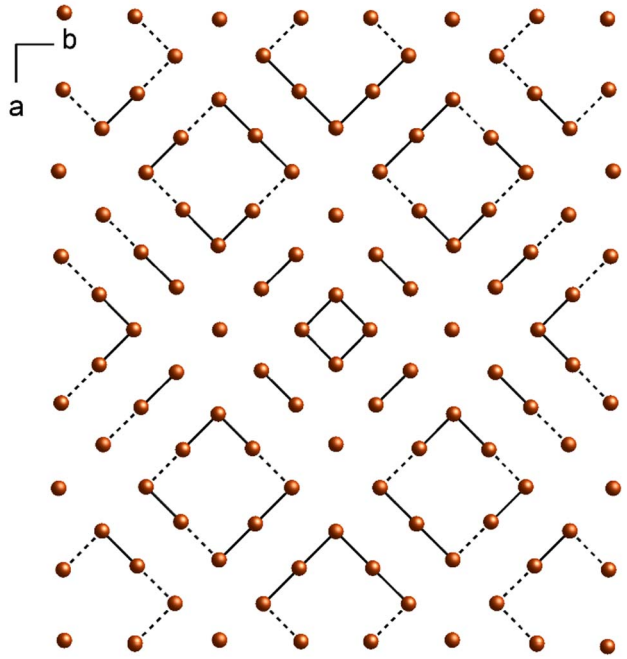

Figure S5 Section of the modulated Te layer with a cut-off occupancy at 0.45. The Te_4 artifact as result of the refinement is displayed in the center of the image.

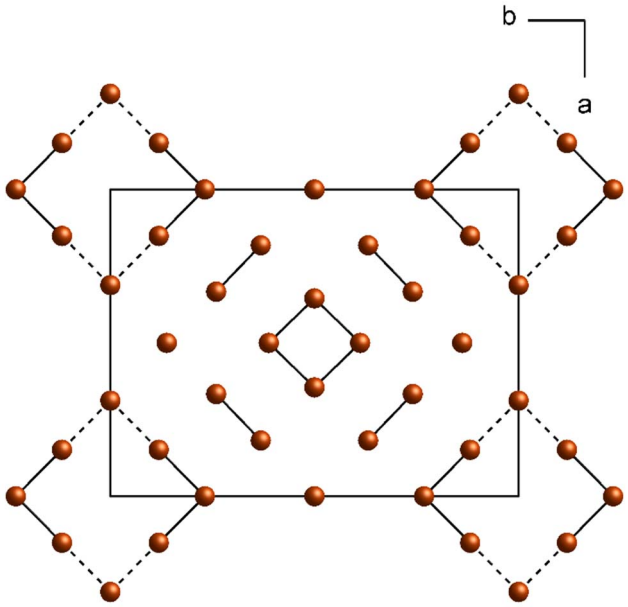

Figure S6 Structure approximant in *Amm*2 with bent Te_3 unit in the Te_8 ring and an unresolved disorder of Te_2^{2-} anions in the quadratic Te_4 fragment.

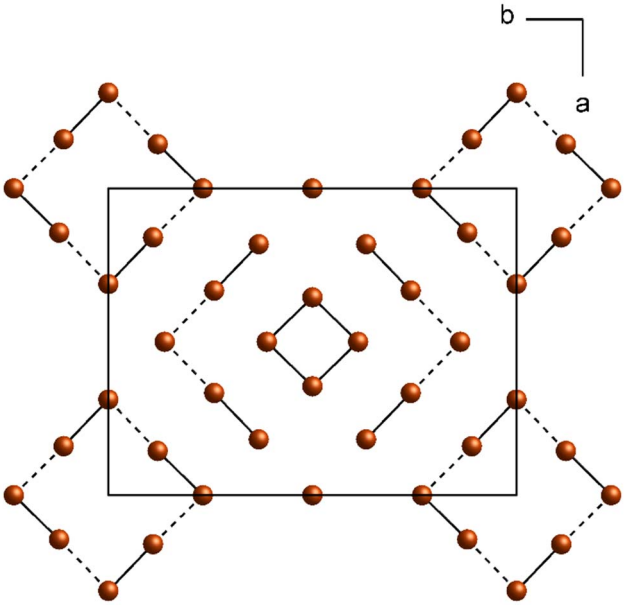

Figure S7 Structure approximant in *A*2, only showing Te_2^{2-} anions as fragments of the Te_8 ring and an unresolved disorder of Te_2^{2-} anions in the quadratic Te_4 fragment.

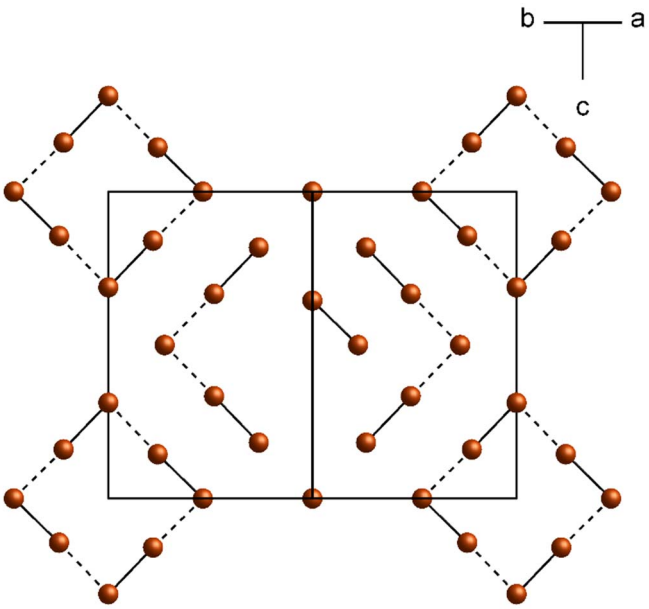

Figure S8 Structure approximant in *P*1, only showing Te_2^{2-} anions as fragments of the Te_8 ring and the resolved disorder of Te_2^{2-} anions in the center.