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Reusable radiochromic hackmanite with gamma exposure memory

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SUPPORTING INFO

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1. Coloration of UV- and X-ray exposed samples

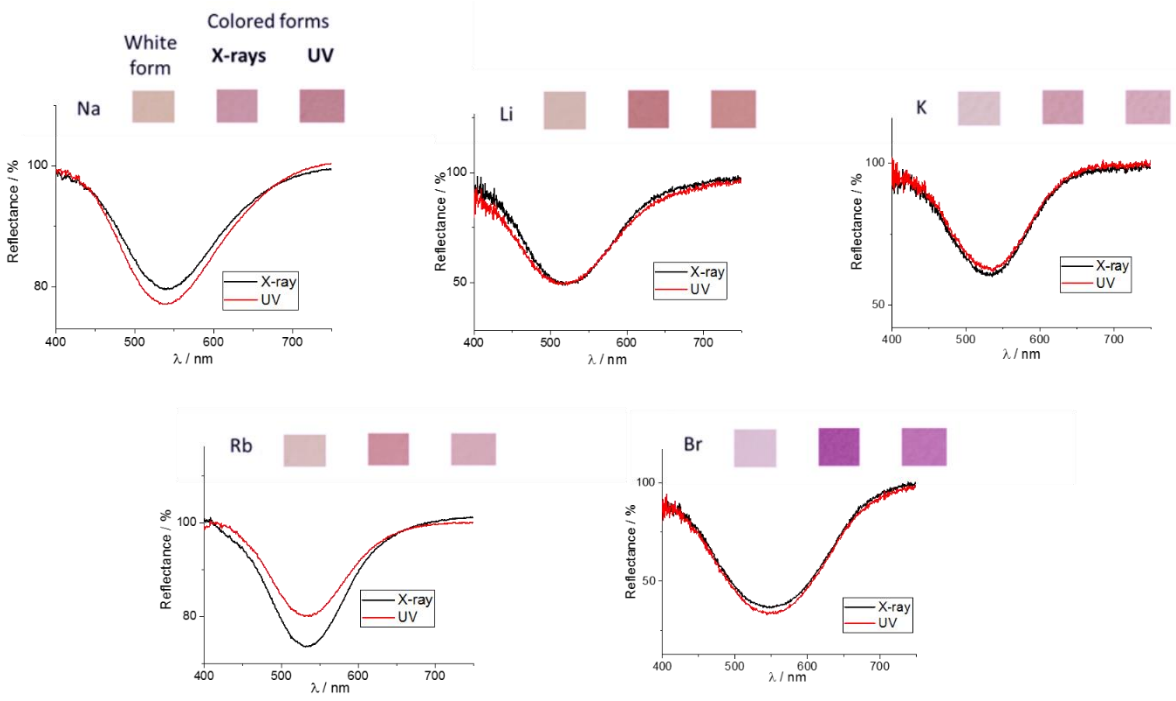

Figure S1. Photos and reflectance spectra of UV- and X-ray exposed samples.

2. X-ray powder diffraction and Rietveld Analyses

The X-ray powder diffraction patterns (Figure S2) indicate that the Na sample contains some 20 % of NaCl as impurity, while the Li sample is pure hackmanite. The K and Rb samples contain ca. 50 % of hackmanite together with the decomposition products $K(Na,K)_3Al_4Si_4O_{16}$ (i.e. nepheline) and KCl as well as $Rb_2Al_2(SiO_4)_2$ and RbCl. The Br sample contains ca. 15 % of NaBr as the only impurity.

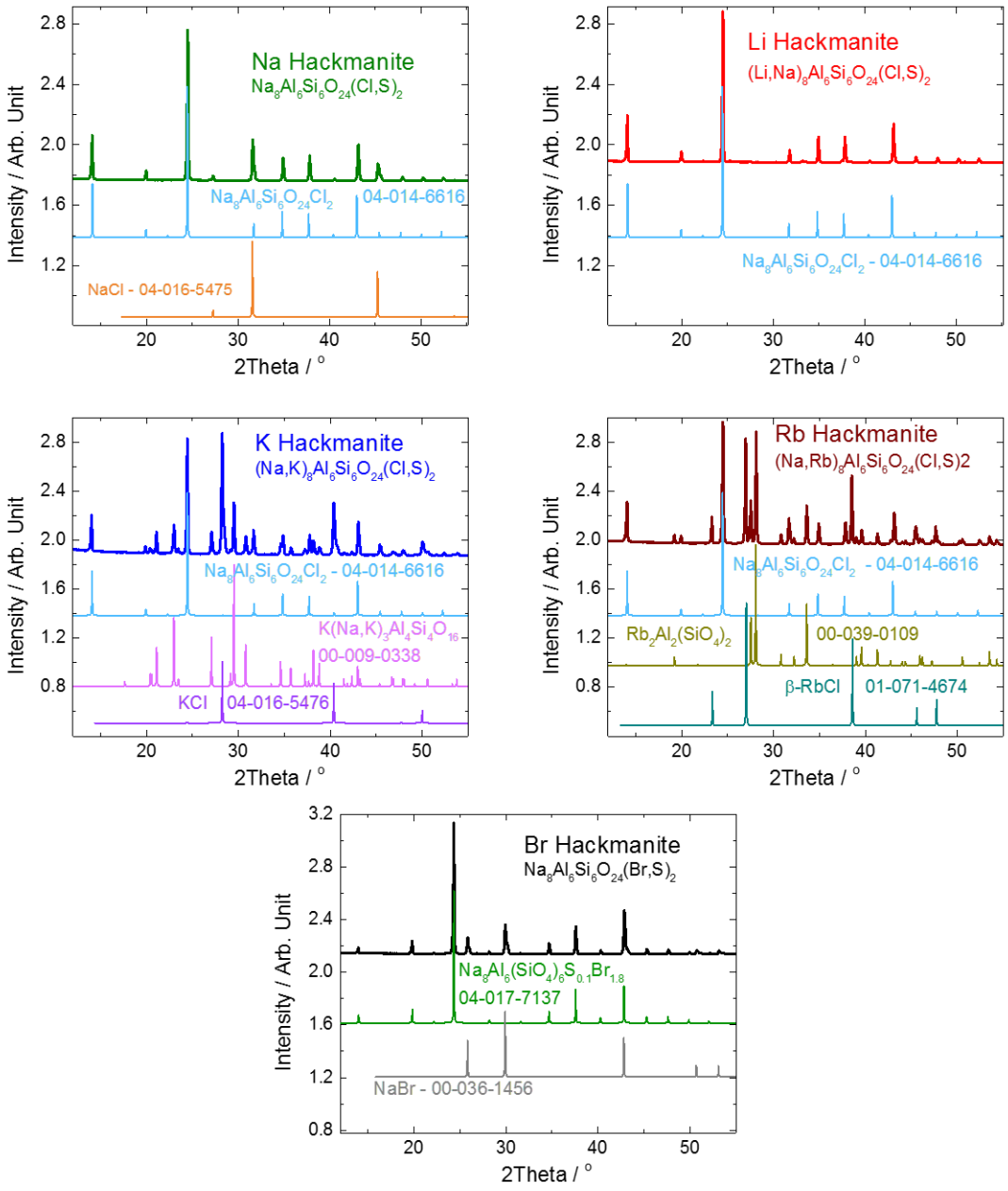

Figure S2. X-ray powder diffraction patterns of the sample powders with reference patterns. The numbers refer to entry numbers in the PDF-4+ database[1].

The diffraction patterns measured for tape cast Na sample indicate that there is very little, if any, change in the bulk structure caused by 7 kGy gamma irradiation with Co-60 (Figure S3). However, Rietveld refinements carried out using the WinPLOTR[2] software indicated that the unit cell volume decreased minutely, which resulted in the shortening of the Na-Cl distance and the lengthening of the Na-O distance (Tables S1 and S2).

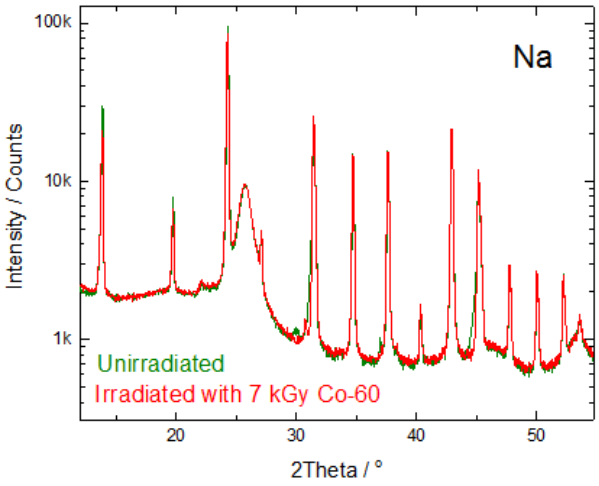

Figure S3. X-ray powder diffraction patterns of tape cast Na hackmanite sample: unirradiated (green curve) and irradiated with 7 kGy Co-60 gamma radiation (red curve). Note the logarithmic intensity scale.

Table S1. Rietveld analysis results for the unirradiated sample.

Atom	**x**	**y**	**z**	**B / Å²**
Na	0.67807(4)	0.67807(4)	0.67807(4)	3.25(1)
Al	1/4	0	1/2	2.91(2)
Si	1/4	1/2	0	0.68(2)
O	0.14988(6)	0.14186(6)	0.43963(4)	1.21(1)
Cl	0	0	0	0.98(1)
a / Å	8.88068(2)			
Na-Cl / Å	2.739(1)			
Na-O / Å	2.358(1)			
Al-O / Å	1.633(1)			
Si-O / Å	1.727(1)			
R_B / %	10.8			

Table S2. Rietveld analysis results for the sample irradiated with 7 kGy Co-60.

Atom	x	y	z	B / Å²
Na	0.67717(4)	0.67717(4)	0.67717(4)	3.23(1)
Al	1/4	0	1/2	2.30(2)
Si	1/4	1/2	0	1.00(2)
O	0.15050(5)	0.14214(5)	0.44024(4)	1.67(1)
Cl	0	0	0	1.74(1)
a / Å	8.87591(2)			
Na-Cl / Å	2.724(1)			
Na-O / Å	2.368(1)			
Al-O / Å	1.629(1)			
Si-O / Å	1.727(1)			
R_B / %	10.5			

3. Fitting of color fading curves

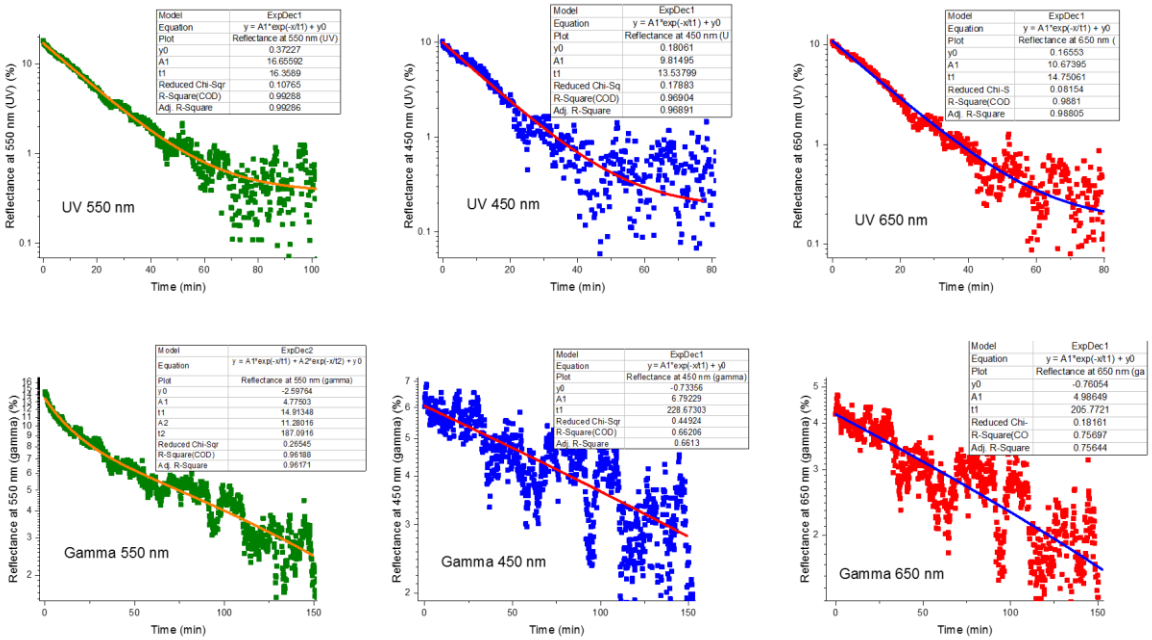

Figure S4. Tenebrescence fading curves for Na hackmanite under white light after UV (top row) and gamma irradiation (bottom row) as well as the exponential decay fits. For both cases, fading in the green (main reflection signal), blue and red regions are given.

4. Details of the hackmanite structure

Hackmanite crystallizes in the cubic space group $P\bar{4}3n$ (No. 218)[3]. Peterson[3] determined from a natural hackmanite sample, that the atomic positions are as follows: Na at (0.1778, 0.1778, 0.1778), Al at (1/4, ½, 0), Si at (1/4, 0, ½), O at (0.1390, 0.4382, 0.1498) and Cl at (0, 0, 0). The unit cell is shown in Figure S5a. The disulphide ion occupies the same site as Cl. From that same sample, the unit cell parameter was determined to be 8.877 Å.

The structure is composed of AlO_4, SiO_4 and $ClNa_4$ tetrahedra, while sodium is coordinated to three oxygen atoms and one chlorine as shown in Figure S5b. The aluminate and silicate tetrahedra are corner-sharing and they form a so-called sodalite cage, also known as a β-cage, within the unit cell. The $ClNa_4$ tetrahedron resides in the middle of the beta cage (Figure S5a).

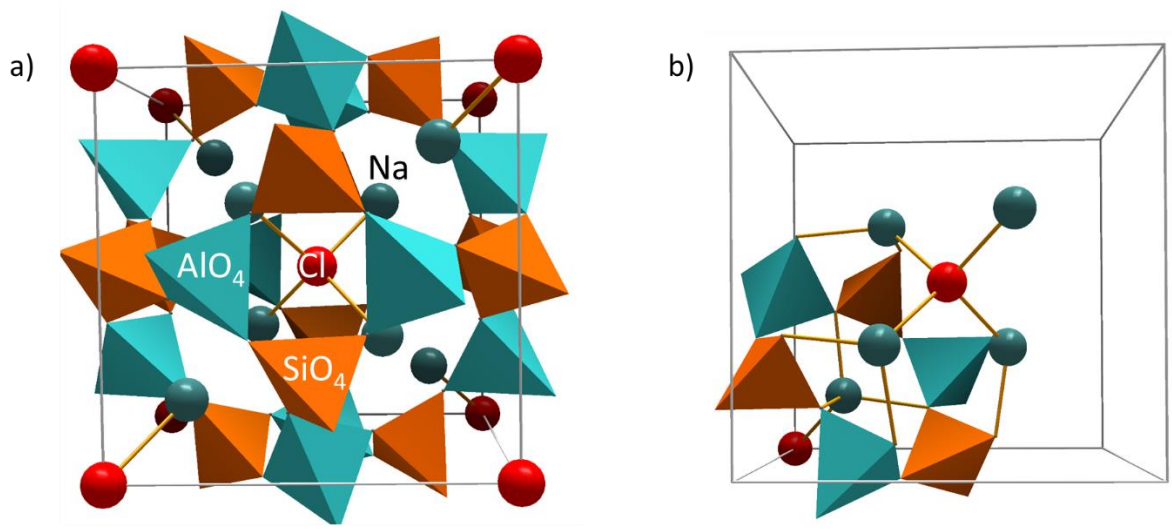

Figure S5. (a) Unit cell of hackmanite. (b) Coordination polyhedra of hackmanite in a unit cell where a part of the atoms have been removed for clarity. The color coding is the same in both (a) and (b).

5. XPS spectra before and after irradiation

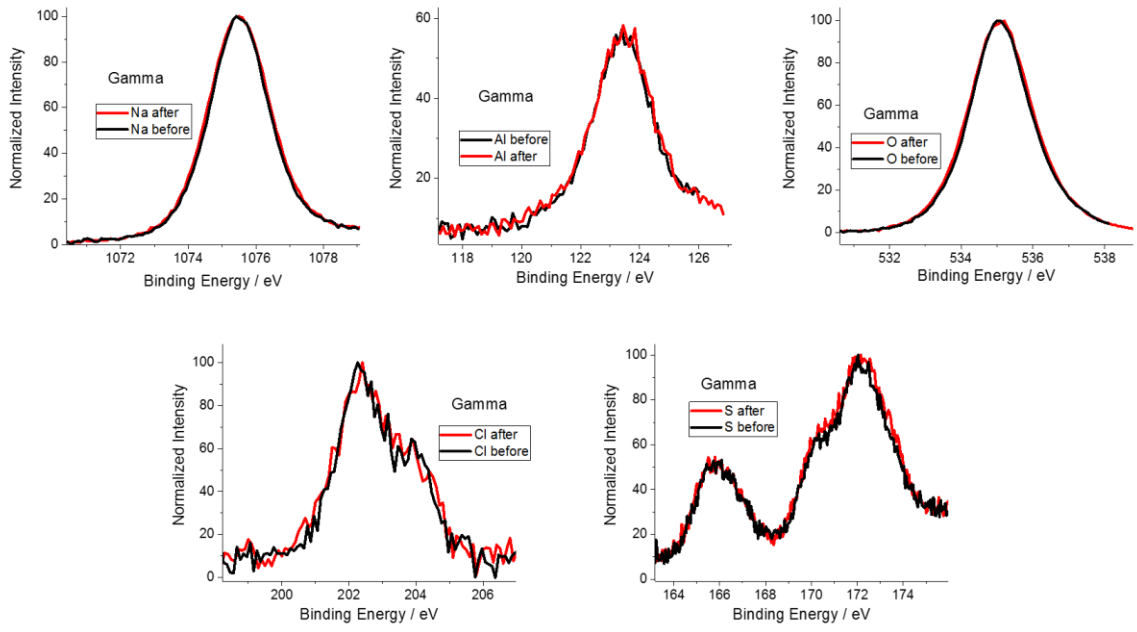

Figure S6. Normalized XPS spectra of Na hackmanite before and after gamma irradiation. Note: the spectra have been corrected for between-measurement shifts in the energy scale. The correction was done based on the shift observed for the carbon 1s peak.

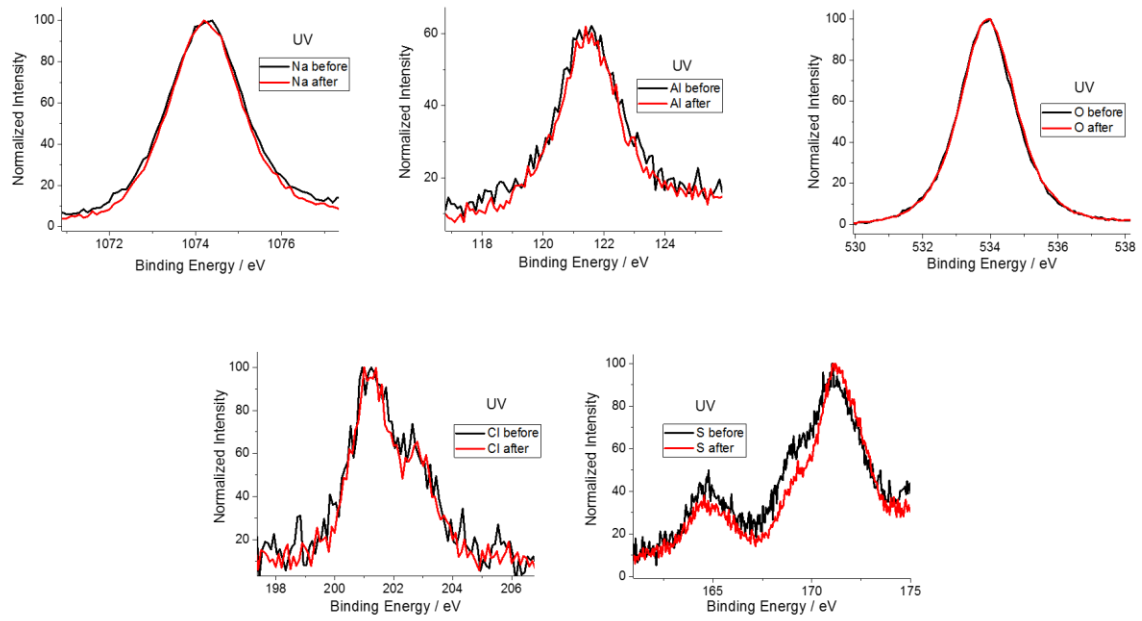

Figure S7. XPS spectra of Na hackmanite before and after UV irradiation. Note: the spectra have been corrected for between-measurement shifts in the energy scale. The correction was done based on the shift observed for the carbon 1s peak.

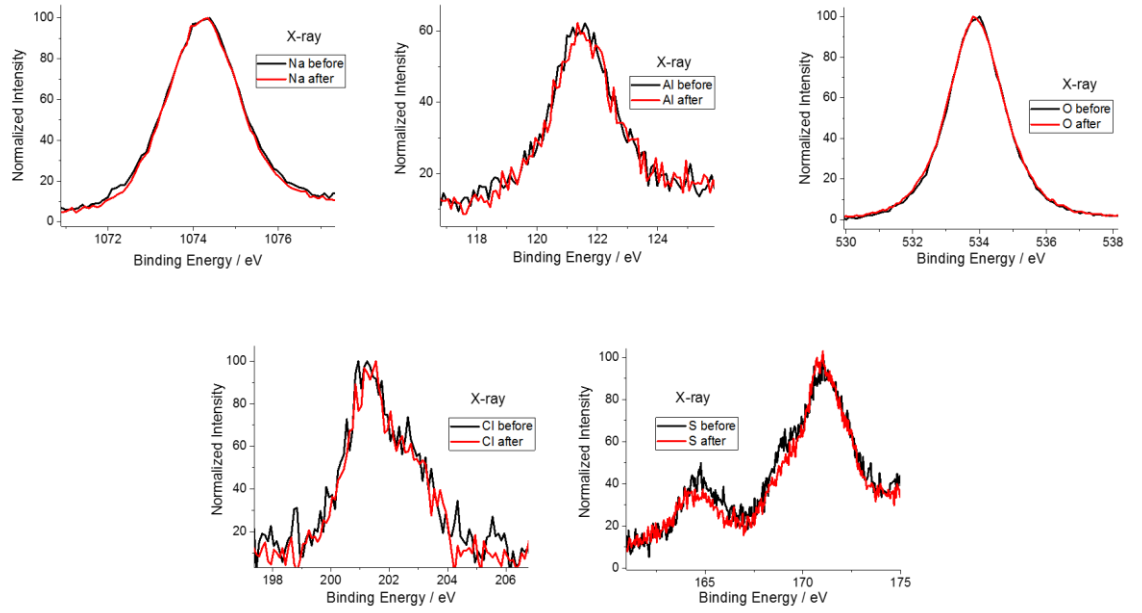

Figure S8. XPS spectra of Na hackmanite before and after X-ray irradiation. Note: the spectra have been corrected for between-measurement shifts in the energy scale. The correction was done based on the shift observed for the carbon 1s peak.

6. Fitting of XPS spectra

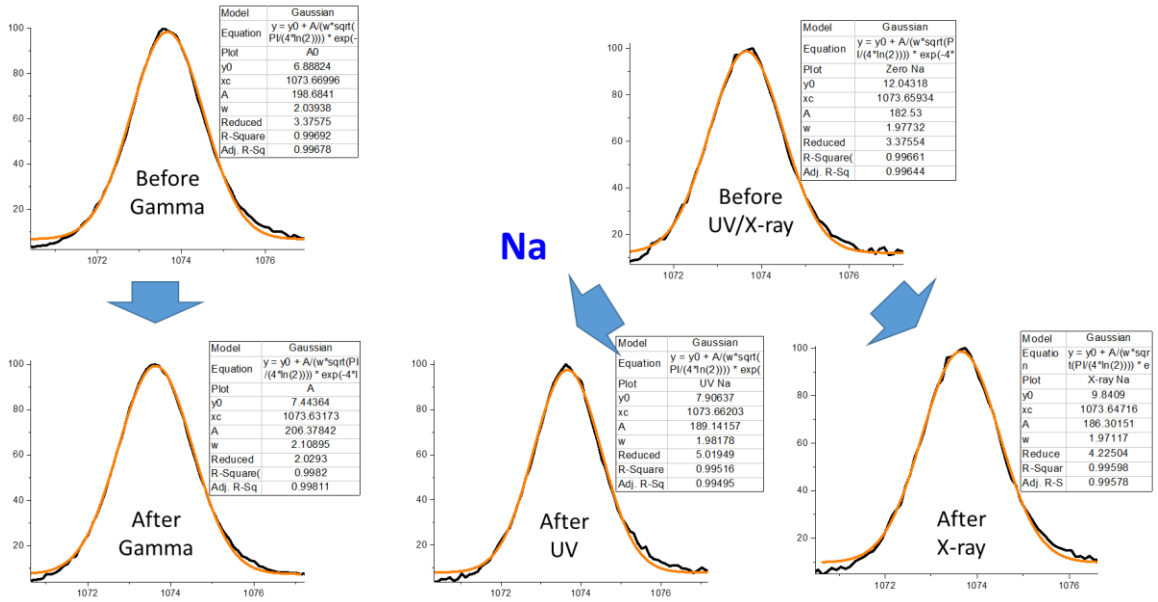

Figure S9. Fitting of the sodium (1s) XPS spectra of Na hackmanite before and after irradiation. Note: these spectra have not been corrected for between-measurement shifts in the energy scale.

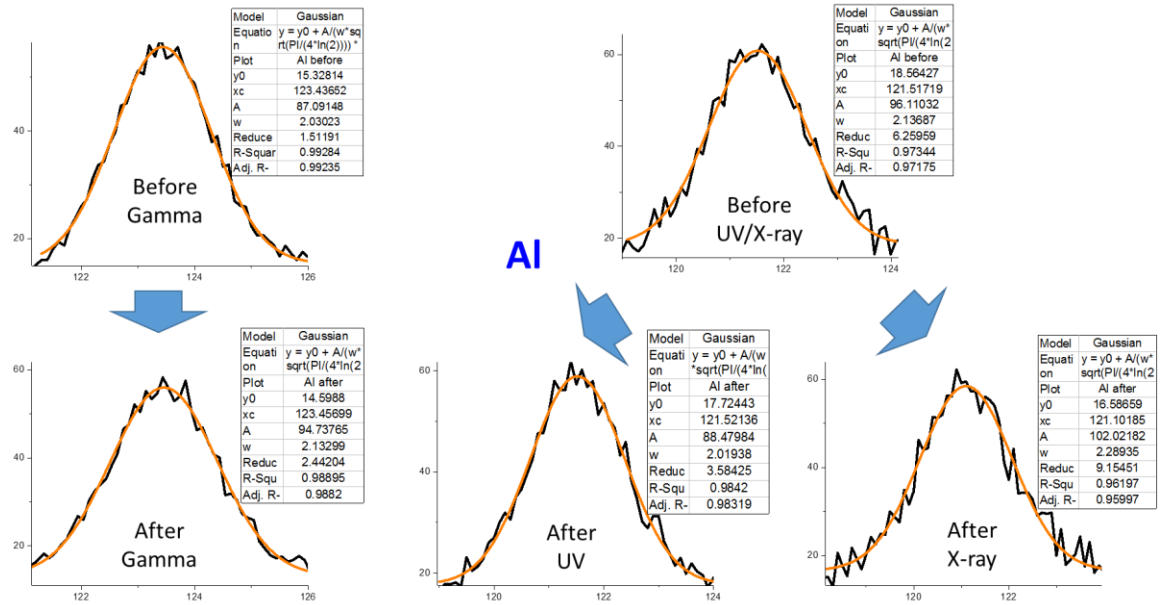

Figure S10. Fitting of the aluminium (2s) XPS spectra of Na hackmanite before and after irradiation. Note: these spectra have not been corrected for between-measurement shifts in the energy scale.

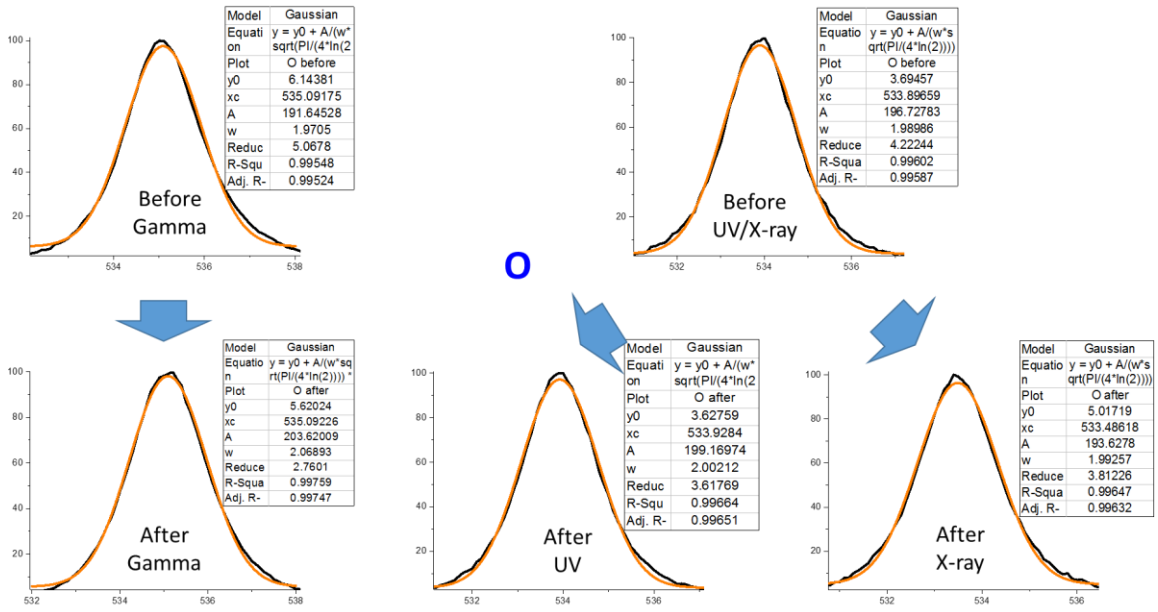

Figure S11. Fitting of the oxygen (1s) XPS spectra of Na hackmanite before and after irradiation. Note: these spectra have not been corrected for between-measurement shifts in the energy scale.

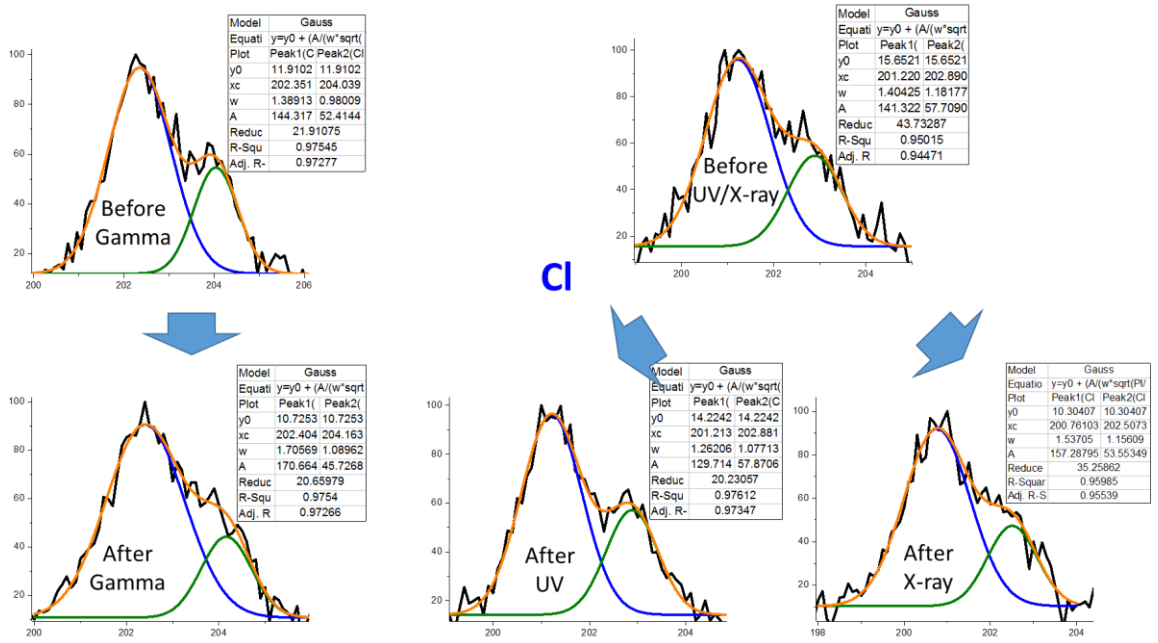

Figure S12. Fitting of the chlorine (2p) XPS spectra of Na hackmanite before and after irradiation. Note: these spectra have not been corrected for between-measurement shifts in the energy scale.

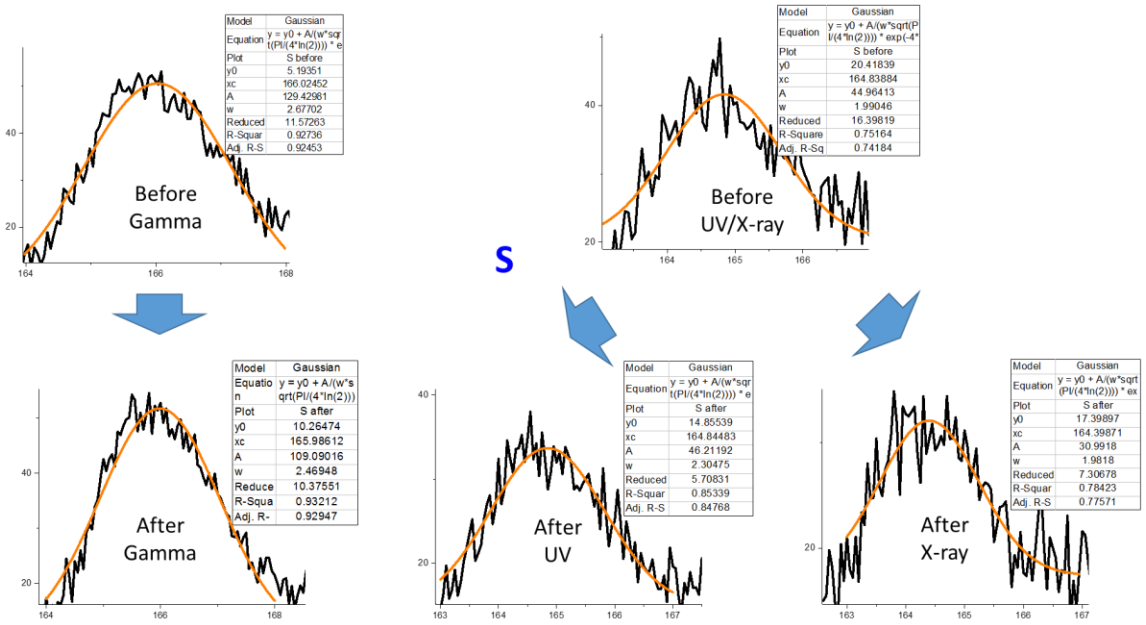

Figure S13. Fitting of the sulphur (2p, anion signals) XPS spectra of Na hackmanite before and after irradiation. Note: these spectra have not been corrected for between-measurement shifts in the energy scale.

7. Information on the natural sample

The natural hackmanite used in this work is from Koksha Valley, Afghanistan. It contains two inclusions, which are present as black spots (marked with red circles in Figure S14).

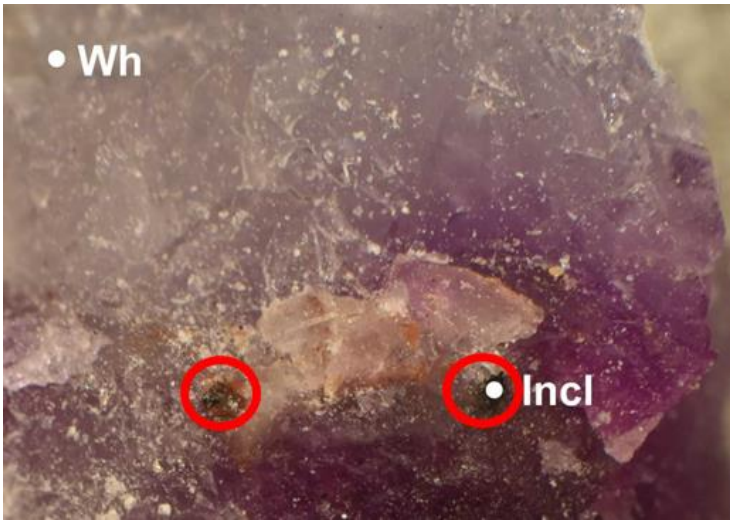

Figure S14. Photo of the natural hackmanite sample. The red circles show two inclusions. The points marked with “Wh” and “Incl” are those used for the analyses in this work.

The composition of the inclusions was analysed with EDX. The results (Tables S3 and S4) suggest that the one on the right side of Figure S14 is U/Th oxide and the one on the left is iron oxide.

Table S3. EDX results for the inclusion on the right side of Figure S14 (marked with "Incl).

Element	App Conc.	Intensity Corrn.	Weight%	Weight% Sigma	Atomic%
C K	1.76	1.5177	1.15	0.05	63.21
O K	0.46	0.6010	0.76	0.06	31.29
Th M	0.44	0.9057	0.49	0.04	1.38
U M	1.30	0.8749	1.49	0.05	4.12
Totals			3.89		

Table S4. EDX results for the inclusion on the left side of Figure S14.

Element	App Conc.	Intensity Corrn.	Weight%	Weight% Sigma	Atomic%
C K	1.24	0.6837	1.80	0.08	38.71
O K	3.03	0.9344	3.25	0.08	52.32
Mg K	0.02	0.5233	0.03	0.01	0.37
Si K	0.03	0.7604	0.03	0.01	0.30
Fe K	1.51	0.8385	1.80	0.04	8.29
Totals			6.92		

8. Cyclic repeatability of the "gamma memory" functionality

The Na sample that had received a dose of 7 kGy was tested for repeatability of 10 cycles of 5 min bleaching and 3 min UV exposure. Bleaching was done with a LOT/QD LS0500 solar simulator lamp employing a Standa ZS-19 filter to block wavelengths below 400 nm. The solar lamp was operated at 110000 lx (measured with a Hagner E4-X Luxmeter). UV exposure was obtained with a 4 W Analytic Jena UVLS-24 AL 254 nm UV lamp operated at 5.8 mW/cm^2 (measured with an Opsytec Dr. Gröbel Radiometer RM 12).

The results show that the shape of the reflectance curve does not change (except by experimental uncertainty due to the need for moving the sample for bleching and UV exposure) during the repeated cycles and that the width of the signal is always clearly higher than for the reference sample that has not been exposed to gamma radiation (Figure S15a).

A similar test with 5 cycles was done for the natural sample using 535 and 275 nm lasers for bleaching and coloring, respectively (Figure S15b). Difference curves were calculated with the "Wh" point's (see Figure S14) reflectance curve as reference. The results show that the signal of the Na_3V_{Cl} entity remains in the cycles (Figure S15b). There is a slight change in intensity and position of the curves, but these are caused by the fact that the sample must be moved between the measurements; and because of the differences in the surface roughness of the sample that will affect if the measurements are not always done exactly at the same spot.

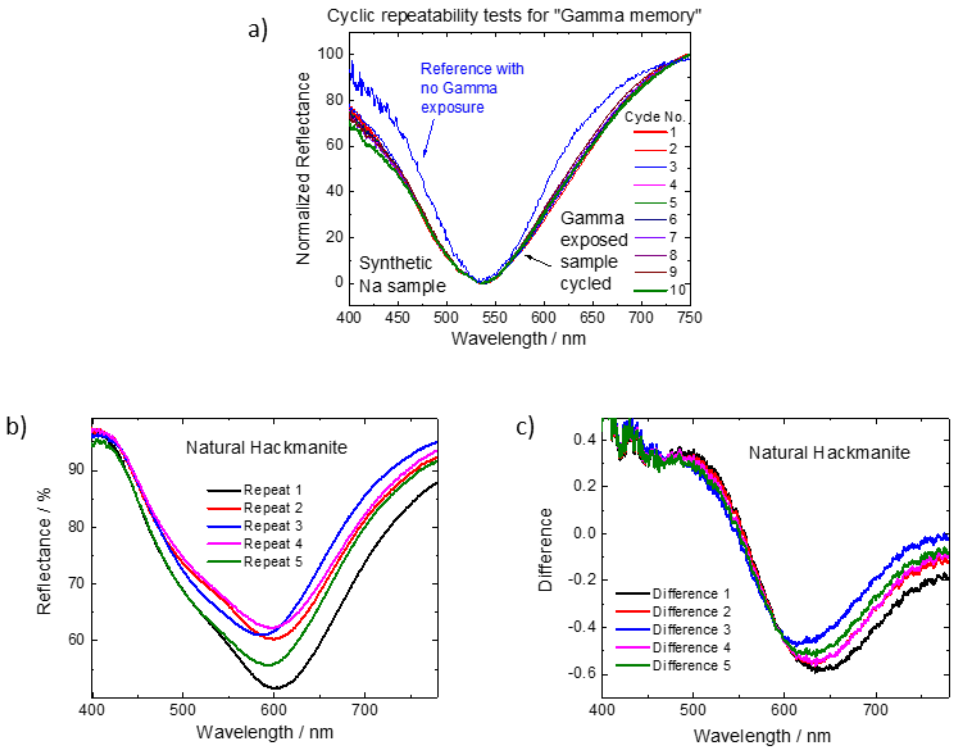

Figure S15. (a) Normalized reflectance spectra of synthetic Na hackmanite (previously exposed to 7 kGy of gamma radiation) after 1 to 10 cycles of bleaching and UV exposure. The curves of the first and last cycle are plotted with a thicker line than the others to show that there is only experimental variation in the signal width. (b) Reflectance spectra of the natural hackmanite sample measured at the inclusion point after repeated optical bleaching - UV pumping cycles. (c) Differences between the spectra measured at the inclusion and at the white point.

9. XYZ structures for TD-DFT calculations

The atoms in italics are treated with pseudopotentials and no basis functions.

F-center in Na_4V_{Cl}

117

Al	2.206330	0.000220	-4.414916
Al	2.206330	-0.000220	4.414916
Al	-2.206330	-0.000220	-4.414916
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Na	-2.839710	-2.839710	-2.839710
Na	2.839710	2.839710	-2.839710
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O	-3.830408	-1.237864	1.324391
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O	-3.179919	-0.585434	5.734455
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F-center in Na_3V_{Cl}

116

Na	-2.854000	-2.847520	-2.838557

Na	-2.797301	2.868894	2.816075
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Na	2.908687	-2.851292	2.798681
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O	-3.819176	1.232130	-1.343042
O	-3.809564	-1.250143	1.343356
O	-3.232294	-0.611243	-3.140057
O	-3.183943	0.609558	3.106058
O	-3.183211	0.601865	-5.734985
O	-3.176773	-0.598159	5.719002
O	-3.123309	-3.210598	-0.590378
O	-3.116359	3.168257	0.583758
O	-3.075407	-5.654483	0.594474
O	-3.057931	5.642381	-0.551536
O	-1.331885	-3.802136	1.252453
O	-1.319853	3.800901	-1.231993
O	-1.310424	4.917057	1.271238
O	-1.295109	-4.993273	-1.209171
O	-1.258487	1.334659	-3.807601
O	-1.215560	-1.289979	-5.006525
O	-1.193071	-1.294653	3.787184
O	-1.173914	1.256071	5.039405
O	-0.614388	-3.129653	-3.229071
O	-0.594803	5.721303	-3.181680

O	-0.591816	3.085225	-5.644862
O	-0.580073	-5.702979	3.189326
O	-0.543617	3.065343	3.242210
O	-0.474822	-2.992664	5.671574
O	5.749785	-3.117830	-0.539201
O	5.733452	3.186453	0.577492
O	5.628407	0.577981	3.141768
O	5.623335	-0.574908	-3.080422
O	4.973314	1.230270	-1.289543
O	4.886467	-1.269415	1.418534
O	3.856364	1.265597	1.352910
O	3.800595	-1.220800	-1.296975
O	3.172592	0.593794	-3.099672
O	3.172062	-0.582208	-5.736244
O	3.163980	-0.524455	3.211730
O	3.163627	3.281718	-0.641102
O	3.128641	0.508172	5.671733
O	3.098522	-3.217465	0.585614
O	3.092940	5.710226	0.553176
O	3.077781	-5.659451	-0.605626
O	1.388018	3.883740	1.254597
O	1.330515	-3.813375	-1.264315
O	1.307257	1.280243	3.961724
O	1.299188	5.013126	-1.225522
O	1.293049	-1.229934	4.918515
O	1.290707	-5.007525	1.197088
O	1.247632	-1.354431	-3.825586
O	1.197417	1.286786	-4.997150
O	0.647242	-3.098167	3.187275
O	0.607605	3.077453	5.698614
O	0.596707	3.105240	-3.197073
O	0.587571	-5.731616	-3.185355
O	0.577104	-3.086255	-5.669830
O	0.571885	5.703044	3.198597
Si	-4.422292	-0.006293	-2.209402
Si	-4.402093	-0.003911	2.208437
Si	-2.200562	-4.408220	0.010556
Si	-2.191738	4.379849	0.013682
Si	-0.013569	2.200745	-4.402471
Si	-0.004212	-2.208339	-4.423466
Si	4.394090	0.050232	2.228720
Si	4.388898	0.010785	-2.188045
Si	2.220151	4.442011	-0.001981

Si	2.209034	0.026162	4.403334
Si	2.192768	-4.421625	-0.026778
Si	0.029616	-2.177242	4.364217
Si	0.022963	2.191139	4.468936
Cl-Bq	-0.383031	-0.387112	-0.436294
Al	-6.628520	-0.000493	-4.406704
Al	-6.613993	0.003096	4.411785
Al	-4.400459	-6.619329	0.003352
Al	-4.392894	6.605665	0.015695
Al	-0.008415	4.411946	-6.607035
Al	6.635131	-0.015843	4.426294
Al	6.599813	0.010974	-4.398189
Al	4.431115	6.648814	-0.012154
Al	4.409269	-6.610754	-0.009185
Al	0.023420	-4.389785	6.608364
Al	0.003208	4.420473	6.641351
Al	0.003184	-4.420279	-6.626801
Si	-6.618418	4.401409	0.002252
Si	-6.616114	-4.410577	0.009237
Si	-4.415590	0.009117	-6.616267
Si	-4.406113	-0.001813	6.612880
Si	-0.007400	6.607288	4.412861
Si	-0.006083	-6.621296	-4.411496
Si	6.619897	4.418109	-0.003324
Si	6.613490	-4.384689	0.017512
Si	4.403458	0.001992	-6.623060
Si	4.394912	-0.043117	6.607638
Si	0.011635	-6.609976	4.404514
Si	0.005768	6.616490	-4.399577

S_2^-:

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Al	2.220737	0.005600	-4.441186
Al	2.206019	-0.002448	4.417736
Al	0.007185	4.439429	2.218547
Al	-2.206957	-0.010073	-4.421597
Al	-2.221996	0.002574	4.424076
Al	-4.437141	2.212647	0.003339
Al	4.437463	2.224225	0.003021
Al	0.022059	-4.456286	2.216182
Al	-4.431891	-2.220594	0.001231

Al	4.417987	-2.214474	-0.007944
Al	-0.024602	-4.456823	-2.222013
Al	-0.002523	4.423377	-2.211991
Na	1.687471	1.721972	1.693076
Na	-1.744163	-1.807623	1.702615
Na	1.707488	-1.813830	-1.751328
Na	-1.677488	1.671705	-1.680636
Na	-2.816099	-2.833841	-2.817402
Na	2.815594	2.830248	-2.796964
Na	2.816079	-2.827953	2.814503
Na	-2.794729	2.828467	2.817772
O	1.235170	1.319798	-5.011351
O	1.256984	1.352592	3.882187
O	-1.235225	-1.334906	-4.996059
O	-1.276861	-1.353133	3.875529
O	1.222793	-1.322233	4.983368
O	1.272750	-1.352012	-3.908319
O	-1.235582	1.316594	4.992808
O	-1.241125	1.327738	-3.870279
O	-5.013936	1.225525	1.315104
O	3.878873	1.270528	1.346714
O	1.372689	-5.031748	1.282312
O	1.356226	3.894412	1.264254
O	4.983731	-1.230431	1.309321
O	-3.903410	-1.270420	1.357814
O	-1.379339	-5.027299	-1.290777
O	-1.345326	3.863845	-1.254857
O	-4.995023	-1.243955	-1.322833
O	3.875843	-1.267172	-1.363573
O	-1.318789	4.989342	1.235563
O	-1.285009	-3.927595	1.200960
O	4.991046	1.229954	-1.314582
O	-3.869304	1.245728	-1.328535
O	1.316367	4.995505	-1.234080
O	1.281939	-3.928398	-1.206450
O	5.736205	-3.196542	-0.573090
O	-3.090894	5.675210	-0.572221
O	-3.081961	-3.176125	-0.547087
O	-5.756691	3.180939	-0.587380
O	3.120827	-5.664016	-0.579063
O	3.160932	3.256733	-0.563367
O	-5.741667	-3.208104	0.572952
O	3.078249	5.715820	0.572648

O	3.077335	-3.178328	0.547336
O	5.776423	3.172500	0.585804
O	-3.123652	-5.664925	0.573340
O	-3.131134	3.210365	0.571635
O	5.672239	-0.563302	-3.106851
O	-3.200211	-0.576931	5.740816
O	-3.166235	-0.573736	-3.081359
O	-0.584246	5.746544	-3.181829
O	-0.567145	-3.117942	5.653809
O	-0.545769	-3.090905	-3.169219
O	-5.647639	0.563687	-3.110007
O	3.193519	0.561046	5.732560
O	3.201117	0.575930	-3.120421
O	-0.583802	-5.747522	3.205776
O	-0.582238	3.091595	-5.678021
O	-0.559878	3.160119	3.249396
O	-5.679267	-0.567899	3.114319
O	3.202493	-0.578734	-5.751593
O	3.164454	-0.568787	3.078660
O	0.580464	-5.747394	-3.212466
O	0.575311	3.075286	5.711794
O	0.568982	3.119862	-3.214433
O	5.651961	0.554453	3.111869
O	-3.191848	0.568955	-5.731963
O	-3.208508	0.573972	3.107674
O	0.584982	5.774659	3.173676
O	0.562509	-3.128755	-5.663808
O	0.551262	-3.094386	3.164212
Si	2.221607	4.453873	0.004972
Si	-2.219858	-4.453796	-0.020251
Si	-2.215974	4.427735	0.000061
Si	0.001378	2.213308	-4.439118
Si	0.003372	2.222008	4.449085
Si	-4.445903	-0.000678	2.219744
Si	0.005391	-2.224567	-4.434574
Si	-0.010592	-2.219797	4.418431
Si	-4.419662	-0.006371	-2.209864
Si	4.430230	0.001733	-2.221191
Si	2.215921	-4.454238	0.015879
Si	4.417747	0.001640	2.209629
S	-0.654622	0.472095	0.751530
S	0.788242	0.466531	-0.645881
Al	-6.626169	-0.009119	-4.428206

Al	-6.642744	0.008431	4.438775
Al	6.638508	0.011067	-4.431865
Al	-4.441467	-6.642064	-0.004239
Al	4.440528	-6.636933	0.000900
Al	0.000891	4.424357	-6.631167
Al	-4.424974	6.627806	0.004432
Al	4.430199	6.641793	-0.001075
Al	0.009087	-4.433961	6.631805
Al	-0.001493	4.425206	6.641894
Al	6.628853	-0.013481	4.431412
Al	-0.011270	-4.444010	-6.641687
Si	-6.638457	-4.432098	-0.010587
Si	-6.632717	4.417885	0.004059
Si	6.631841	-4.422453	0.010345
Si	-0.006297	-6.645337	-4.436195
Si	0.003348	-6.640748	4.432682
Si	4.431811	0.007951	-6.638561
Si	0.004463	6.625341	-4.416791
Si	-4.419036	-0.010763	-6.629052
Si	-4.426024	0.010221	6.633668
Si	6.637075	4.419782	-0.004642
Si	-0.001850	6.633916	4.422107
Si	4.421468	-0.014340	6.629898

S_3^-:

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Al	-4.446447	2.203211	-0.025273
Al	-4.425547	-2.221405	-0.010455
Al	-2.264290	-0.008276	-4.469083
Al	-2.185931	-0.009197	4.401312
Al	-0.030125	4.449596	2.230087
Al	-0.006902	-4.427726	2.207622
Al	4.446446	2.203211	0.025272
Al	4.425547	-2.221405	0.010454
Al	2.264289	-0.008276	4.469082
Al	2.185931	-0.009197	-4.401312
Al	0.030124	4.449596	-2.230087
Al	0.006902	-4.427726	-2.207623
Na	-2.870803	-2.859940	-2.873232
Na	-2.788819	2.822296	2.784906
Na	-1.917686	1.948418	-1.912208

Na	-1.594635	-1.625755	1.594810
Na	2.870803	-2.859940	2.873231
Na	2.788819	2.822296	-2.784907
Na	1.917686	1.948418	1.912208
Na	1.594635	-1.625755	-1.594811
O	-5.777073	0.549012	-3.100278
O	-5.754670	3.206302	-0.562753
O	-5.753453	-3.179235	0.585868
O	-5.623642	-0.567083	3.105834
O	-5.014676	-1.231914	-1.316197
O	-4.979255	1.213731	1.296880
O	-3.972107	1.289625	-1.427793
O	-3.843053	-1.270164	1.327374
O	-3.328675	-0.587894	-3.218534
O	-3.211367	0.577170	-5.804416
O	-3.175653	-0.567336	5.717543
O	-3.145987	-3.243725	-0.601610
O	-3.141063	0.568950	3.061750
O	-3.128037	5.665386	-0.560215
O	-3.085245	3.152829	0.505672
O	-3.085169	-5.679955	0.584800
O	-1.399595	4.997435	1.308231
O	-1.346576	1.385186	-3.971839
O	-1.341622	-3.847818	1.245448
O	-1.302835	-5.009681	-1.220996
O	-1.287069	3.955607	-1.213086
O	-1.250952	-1.319345	-4.992480
O	-1.232553	-1.354084	3.843798
O	-1.195605	1.296963	4.986976
O	-0.598955	-5.750625	3.174030
O	-0.598838	-3.158204	-3.234629
O	-0.568782	-3.076002	5.685659
O	-0.565097	5.744128	-3.218533
O	-0.545227	3.135617	-5.683926
O	-0.511606	3.067508	3.172758
O	5.777073	0.549012	3.100277
O	5.754670	3.206302	0.562753
O	5.753453	-3.179235	-0.585868
O	5.623641	-0.567083	-3.105835
O	5.014676	-1.231914	1.316196
O	4.979254	1.213731	-1.296881
O	3.972107	1.289625	1.427792
O	3.843053	-1.270164	-1.327374

O	3.328675	-0.587894	3.218533
O	3.211366	0.577170	5.804415
O	3.175652	-0.567336	-5.717544
O	3.145986	-3.243725	0.601609
O	3.141063	0.568950	-3.061751
O	3.128037	5.665386	0.560214
O	3.085245	3.152829	-0.505673
O	3.085168	-5.679955	-0.584801
O	1.399595	4.997435	-1.308231
O	1.346575	1.385186	3.971839
O	1.341622	-3.847818	-1.245448
O	1.302834	-5.009681	1.220995
O	1.287069	3.955607	1.213086
O	1.250952	-1.319345	4.992480
O	1.232553	-1.354084	-3.843799
O	1.195604	1.296963	-4.986977
O	0.598954	-5.750625	-3.174031
O	0.598838	-3.158204	3.234629
O	0.568782	-3.076002	-5.685660
O	0.565096	5.744128	3.218533
O	0.545227	3.135617	5.683925
O	0.511605	3.067508	-3.172759
Si	-4.505350	-0.008283	-2.256229
Si	-4.395481	-0.011276	2.197034
Si	-2.226119	4.447081	0.018779
Si	-2.213195	-4.435068	-0.000742
Si	-0.032077	2.214784	-4.451252
Si	-0.016293	-2.220306	-4.429233
Si	4.505349	-0.008283	2.256229
Si	4.395481	-0.011276	-2.197034
Si	2.226119	4.447081	-0.018779
Si	2.213195	-4.435068	0.000741
Si	0.032076	2.214784	4.451251
Si	0.016293	-2.220306	4.429232
S	-1.145299	-0.561234	-1.149354
S	1.145299	-0.561234	1.149354
S	0.000000	0.588030	0.000000
Al	-6.688031	-0.015440	-4.461593
Al	-6.604075	0.006754	4.422373
Al	-4.447443	6.644006	0.009153
Al	-4.423861	-6.625048	0.004109
Al	-0.018561	4.455128	6.653658
Al	-0.008423	-4.416202	-6.630469

Al	6.688030	-0.015440	4.461592
Al	6.604074	0.006754	-4.422374
Al	4.447442	6.644006	-0.009153
Al	4.423860	-6.625048	-0.004110
Al	0.018561	4.455128	-6.653659
Al	0.008422	-4.416202	6.630469
Si	-6.646214	4.433880	0.015575
Si	-6.630449	-4.412061	-0.011775
Si	-4.453952	-0.015141	-6.665372
Si	-4.401928	0.012310	6.616843
Si	-0.015279	6.648297	4.441092
Si	-0.006099	-6.621553	4.413227
Si	6.646213	4.433880	-0.015575
Si	6.630448	-4.412061	0.011775
Si	4.453952	-0.015141	6.665372
Si	4.401928	0.012310	-6.616844
Si	0.015278	6.648297	-4.441092
Si	0.006098	-6.621553	-4.413227

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