

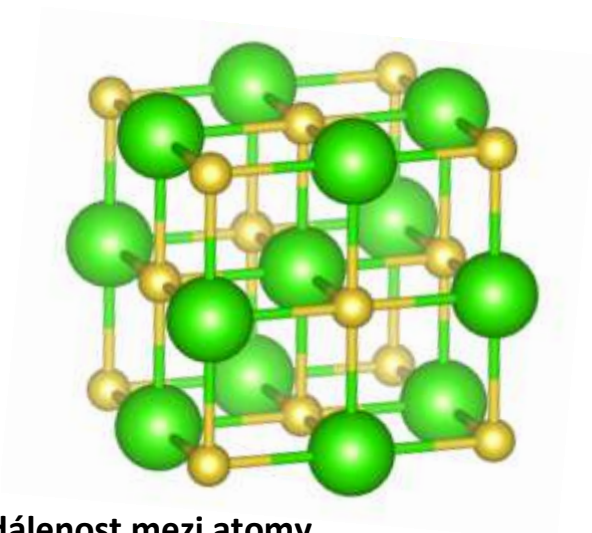
Krystalografie

Program: VESTA

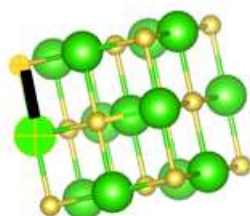
Autor: Pavla Leskotová

NaCl

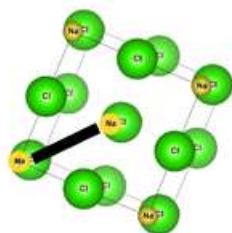
Halit



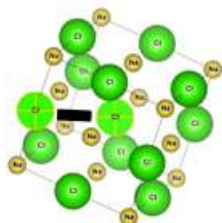
Vzdálenost mezi atomy



Na-Cl 2.72665(0) Å



Na-Na 3.85607(0) Å

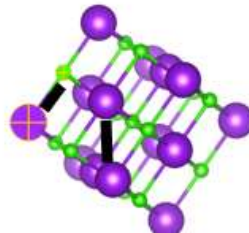
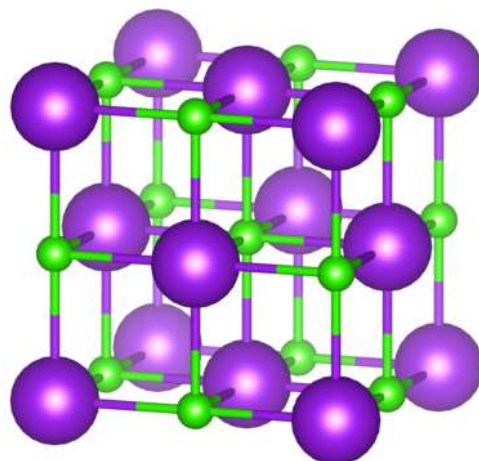


Cl-Cl 3.85607(0) Å

Na – Cl_{střed} 4.72270(0) Å

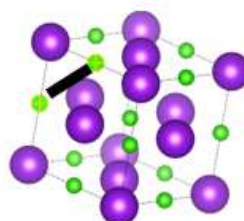
KCl

sylvín

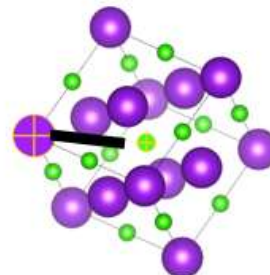


K-Cl 3.14395(0) Å

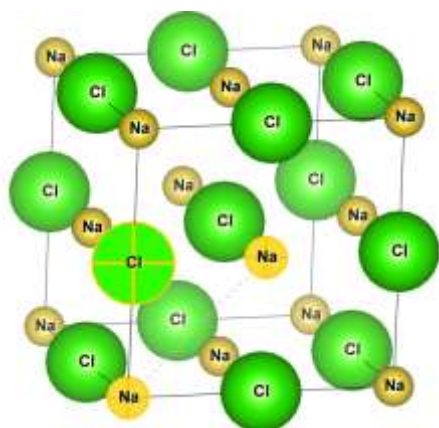
K-K 4.44622(0) Å



Cl-Cl 4.44622(0) Å



K_{roh} – Cl_{střed}
5.44548(0) Å

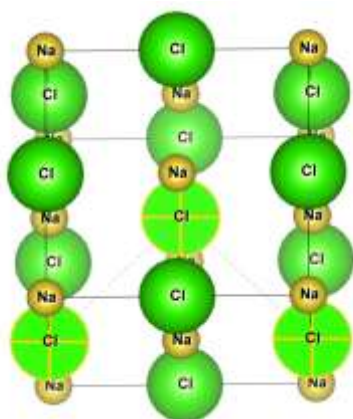


$\text{Cl}-\text{Na}_{\text{roh}}-\text{Na}_{\text{střed stěny}} = 45.0000(0)^\circ$

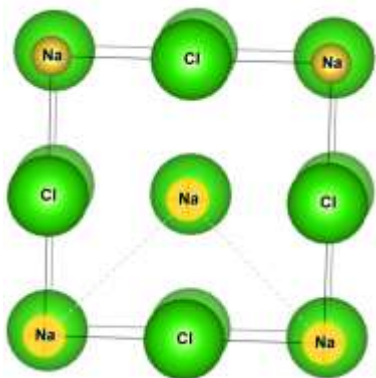
$\text{Cl}-\text{Na}-\text{Cl} = 90.0000(0)^\circ$

$\text{Cl}_{\text{spodní hrana}}-\text{Cl}_{\text{střed}}-\text{Cl}_{\text{spodní hrana}} = 60.0000(0)^\circ$

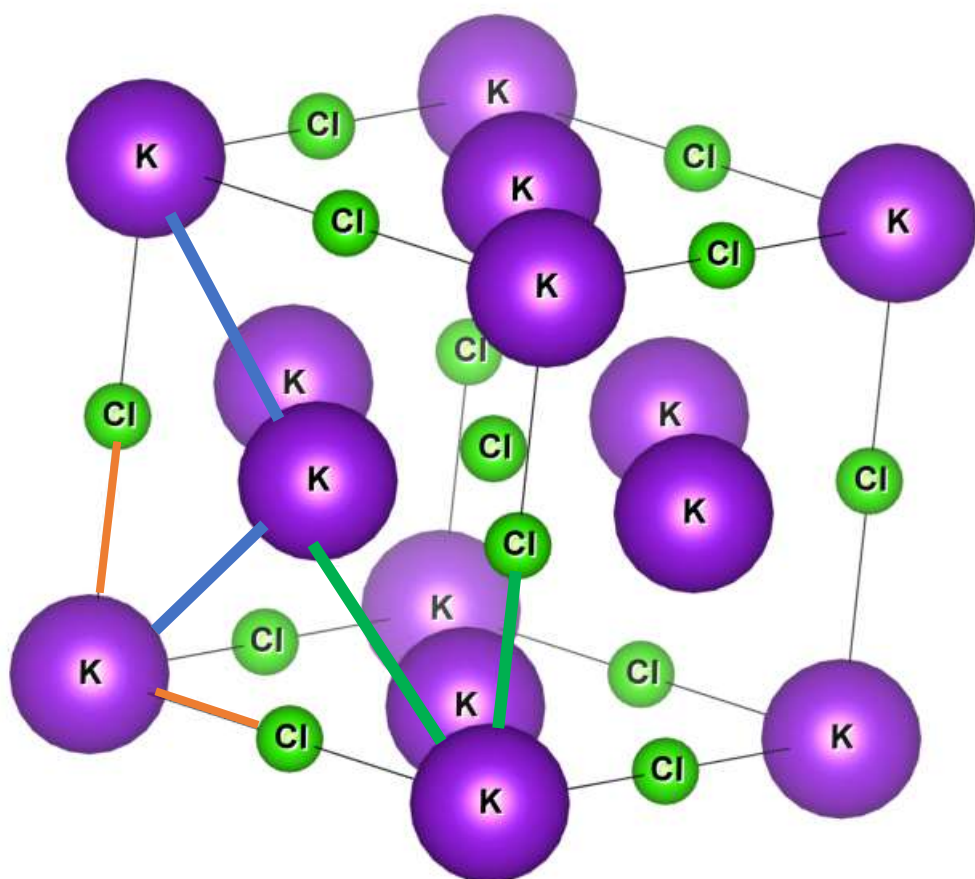
$\text{Cl}_{\text{střed hrany}}-\text{Cl}$



$\text{střed}-\text{Cl}_{\text{střed hrany}} = 90.0000(0)^\circ$



$\text{Na}_{\text{roh}}-\text{Na}_{\text{střed stěny}}-\text{Na}_{\text{roh}} = 90.0000(0)^\circ$



Cl-K-Cl 90.0000(0) deg.

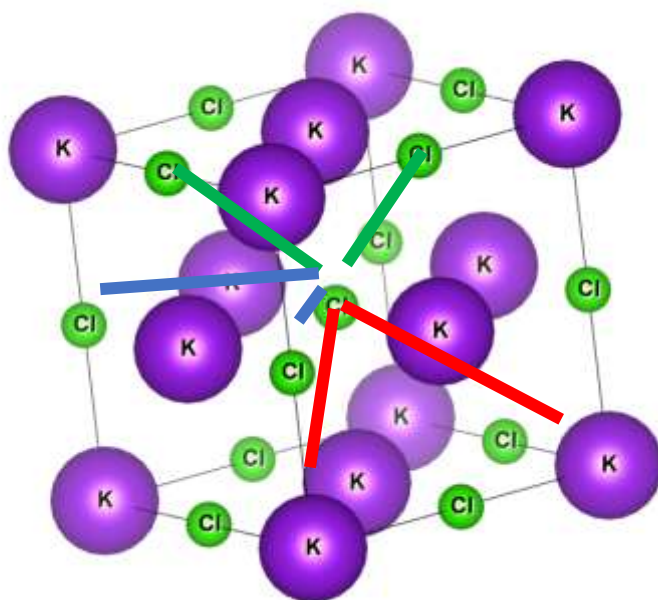
Cl-K-K = 45.0000(0) deg.

K-K-K = 90.0000(0) deg

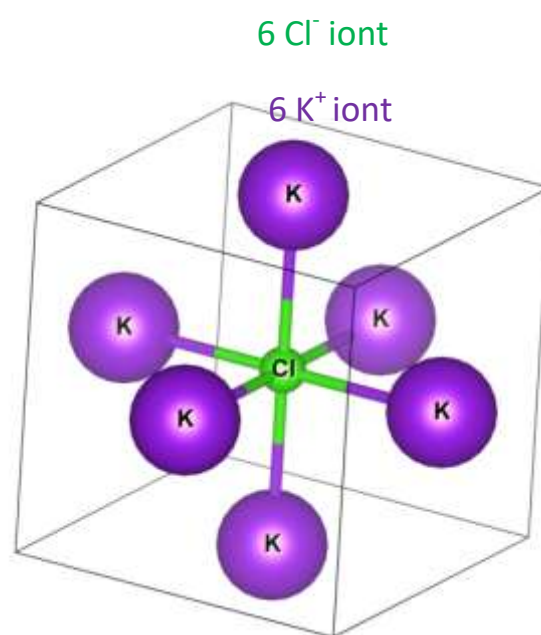
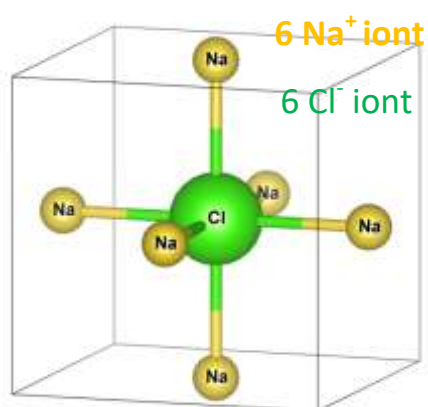
K-Cl-K = 70.5288(0) deg.

Cl-Cl-Cl = 60.0000(0) deg.

Cl-Cl-Cl = 90.0000(0) deg.



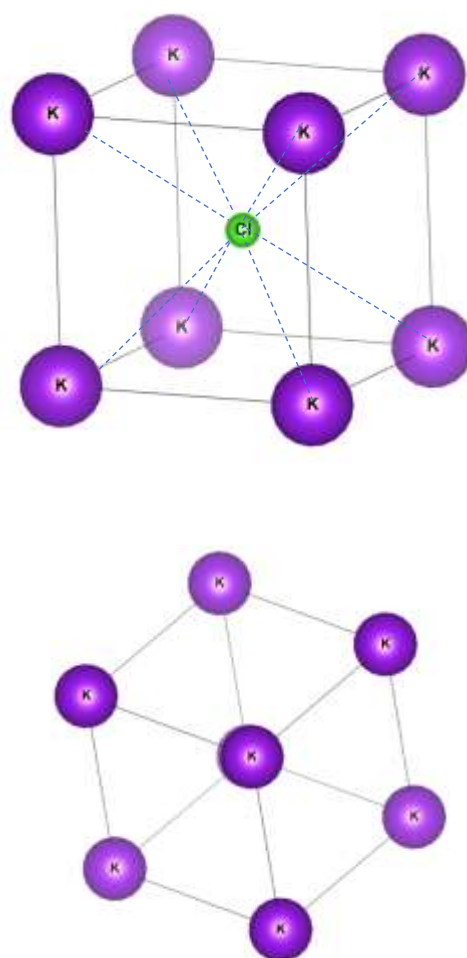
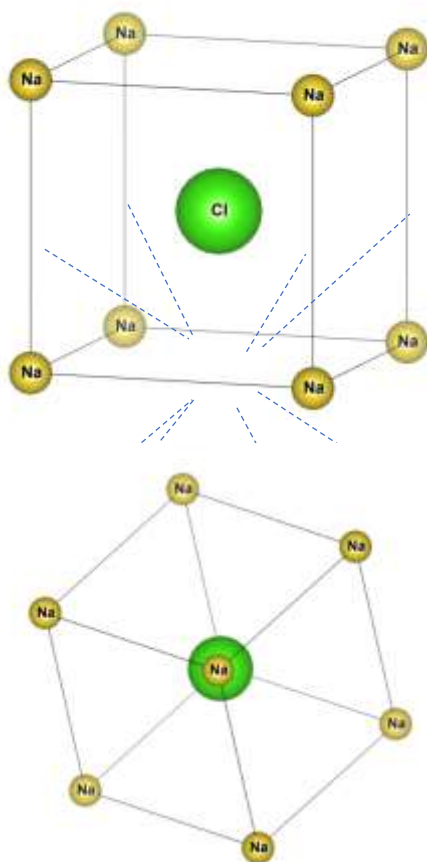
Koordinální číslo



Symetrie

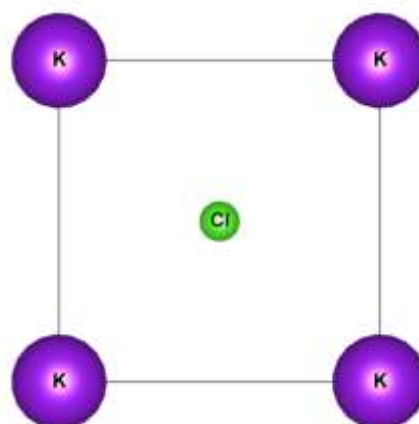
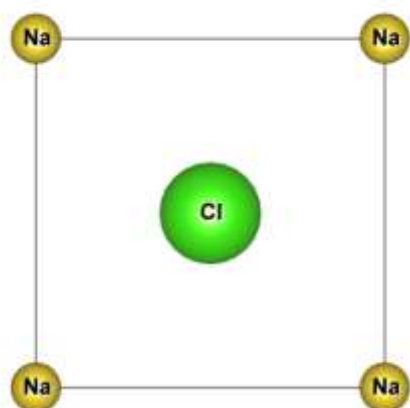
6

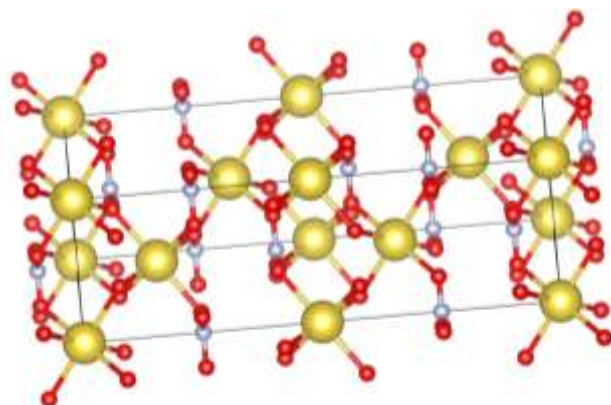
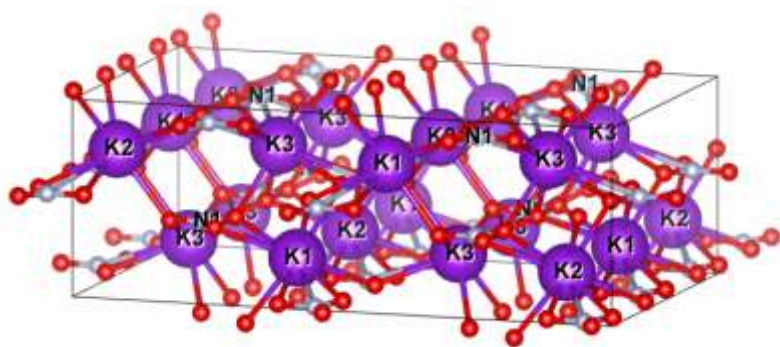
Střed symetrie



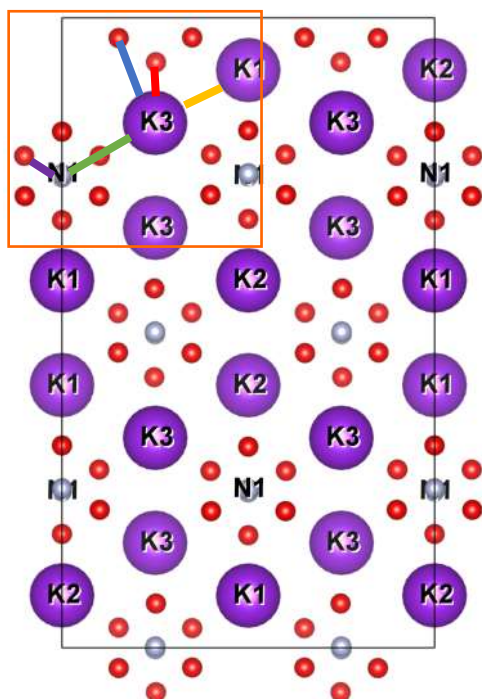
Rovina symetrie

Pohled zepředu/zboku/svrchu





Vzdálenost mezi atomy



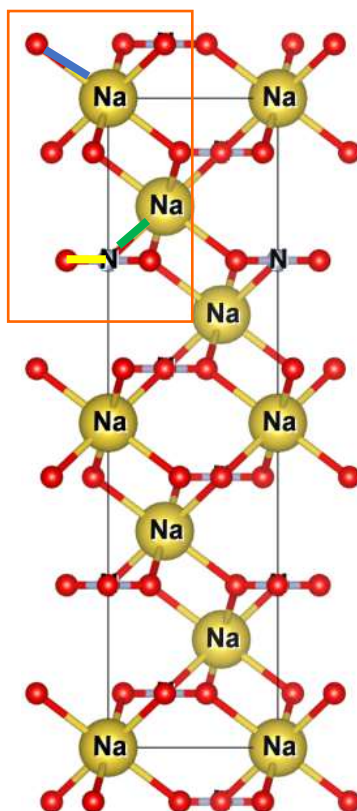
$\text{O}_6\text{-K}_3$ 2.88078(0) Å

$\text{O}_7\text{-K}_3$ = 4.58437(0) Å

$\text{N}_1\text{-K}_3$ = 3.27988(0) Å

N1-O1 = 1.24147(0) Å

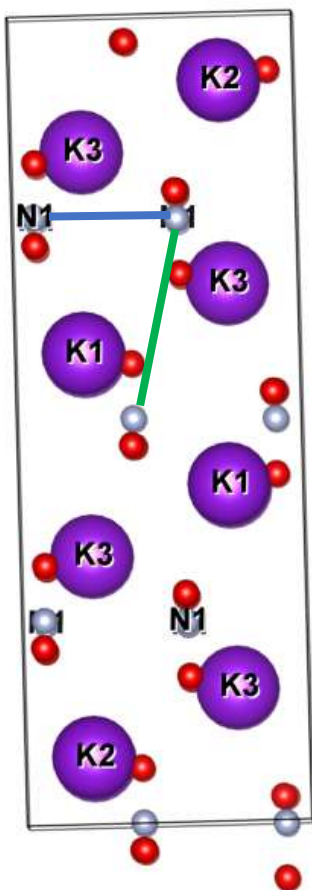
K1-K3 = 4.43450(0) Å



Na-O = 2.40379(0) Å

Na-N = 3.24545(0) Å

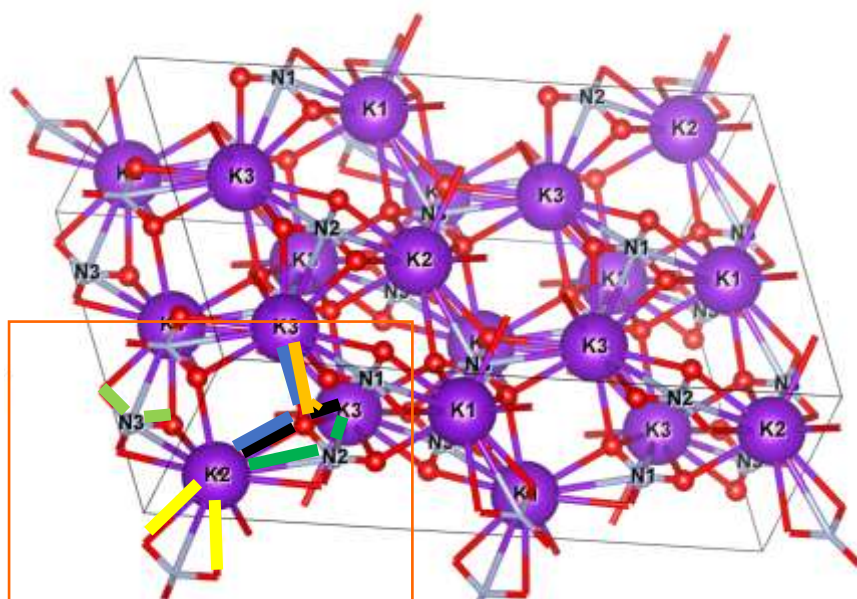
N-O = 1.24215(0) Å



$N_1-N_2 = 3.22321(0) \text{ \AA}$

$N_2-N_3 = 5.35613(0) \text{ \AA}$

Úhly

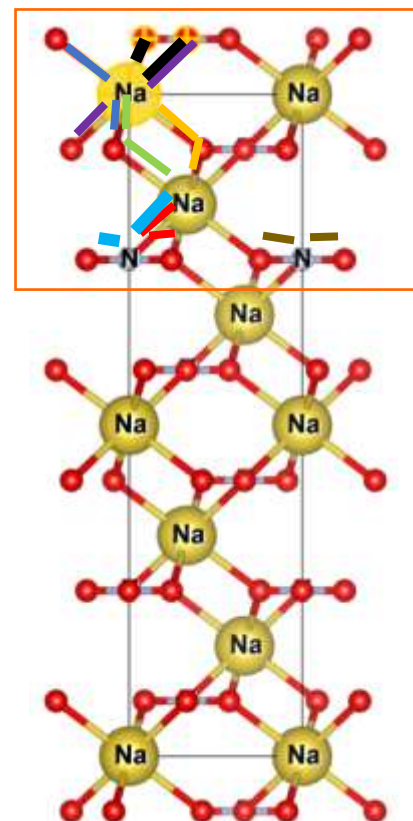


O4-K3-O2 = 44.1161(0) deg.

O4-N3-O2 = 119.6598(0) deg.

K2-N2-K3 = 108.8502(0) deg.

K2-O4-K3 = 133.9531(0) deg.



O-Na-O = 89.4259(0) deg.

O-Na-O = 90.5741(0) deg.

O-Na-O = 180.0000(0) deg.

Na-O-Na = 114.9268(0) deg.

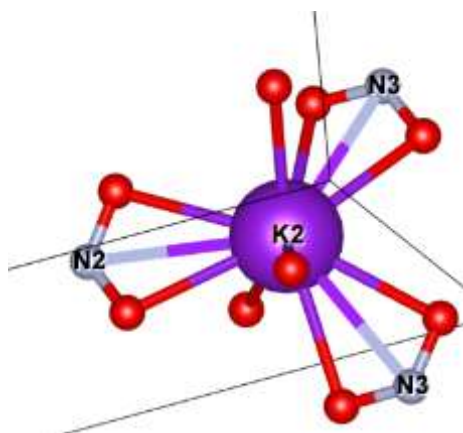
Na-O-Na = 52.9503(0) deg.

Na-N-O = 90.0000(0) deg.

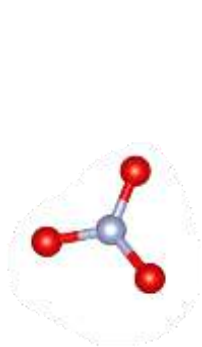
Na-N-O = 141.3607(0) deg.

O-N-O = 120.0000(0) deg.

Koordinální číslo



Každý atom K^+ je spojen s 3 NO_3^- takže koordinální číslo je 6. Na kladně nabitý iont N^{+V} se vážou 3 záporně nabitý ionty O^- .

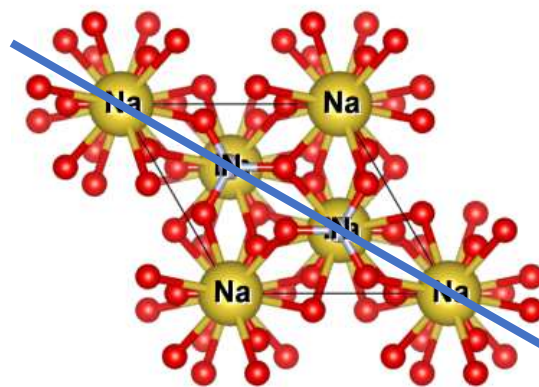
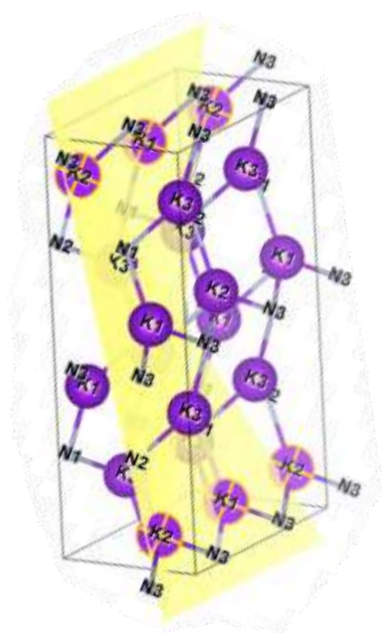


Kolem každého kationtu Na^+ leží na přímce 2 anionty NO_3^- . Proto koordinální číslo je 6

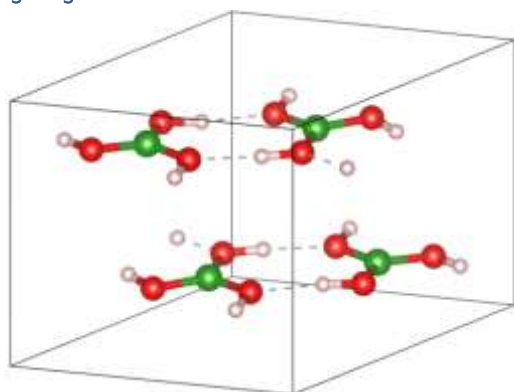
Na každá kationt N^{+V} se váže 3 O^- . Proto koordinální číslo je 3

Symetrie

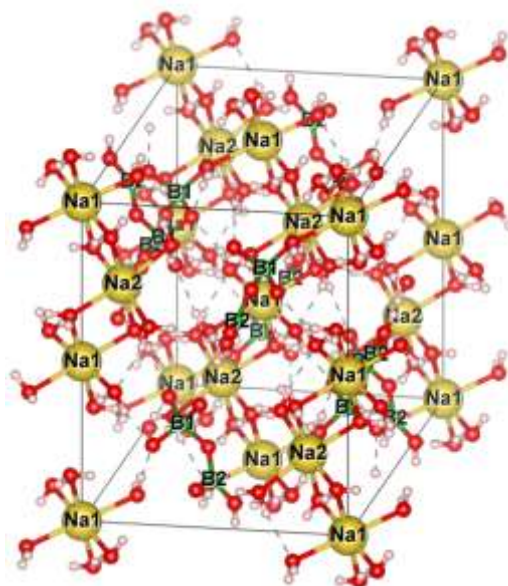
Rovina symetrie



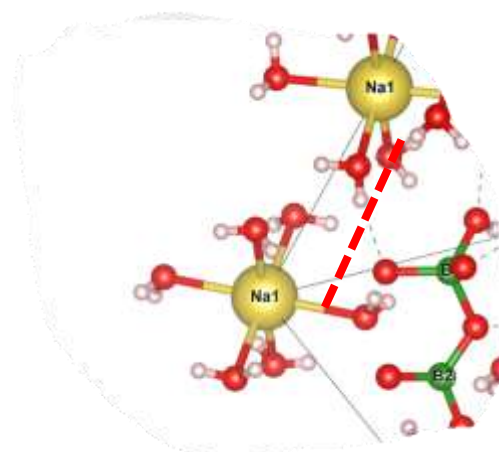
H₃BO₃

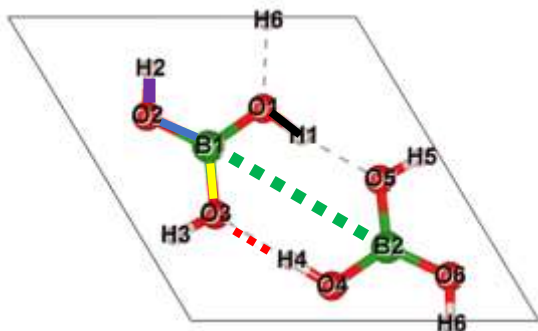


Borax



Vzdálenosti



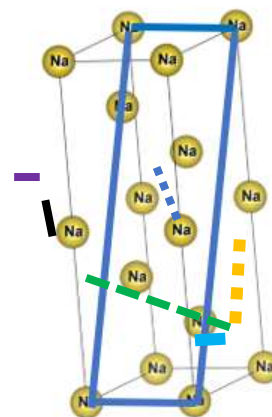


$B1-O2 = 1.37058(0) \text{ \AA}$ $B1-B2 = 4.06993(0) \text{ \AA}$

$B1-O3 = 1.36757(0) \text{ \AA}$ $H1-O5 = 1.75334(0) \text{ \AA}$

$O2-H2 = 0.95917(0) \text{ \AA}$

$O1-H1 = 0.96002(0) \text{ \AA}$



$O7-Na1 = 2.41210(0) \text{ \AA}$

$O7-H7 = 0.82734(0) \text{ \AA}$

$H8-O1 = 1.93575(0) \text{ \AA}$

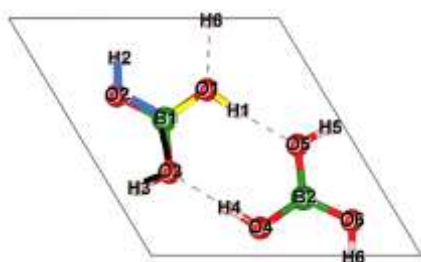
$Na1-B2 = 5.23371(0) \text{ \AA}$

$B1-B2 = 2.43050(0) \text{ \AA}$

$Na1-Na1 = 6.10555(0) \text{ \AA}$

$B2-O3 = 1.37568(0) \text{ \AA}$

Úhly

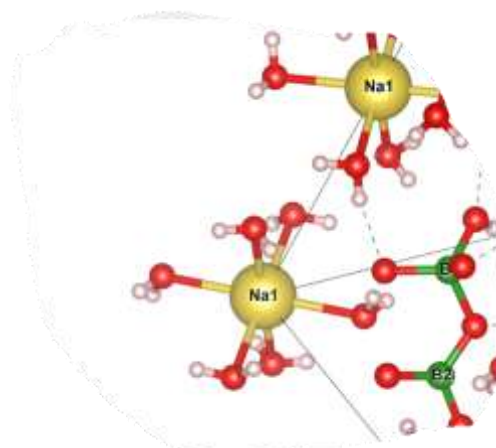


$H2-O2-B1 =$

$110.9687(0) \text{ deg.}$

$H3-O3-B1 = 112.8965(0) \text{ deg.}$

$B1-O1-H1 = 110.1946(0) \text{ deg.}$



$O8-Na1-O7 = 88.2828(0) \text{ deg.}$

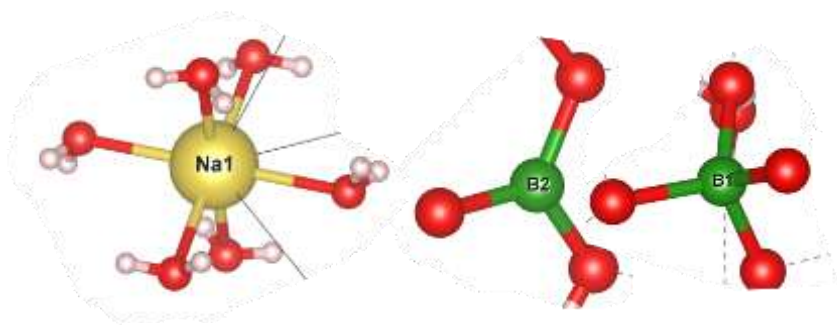
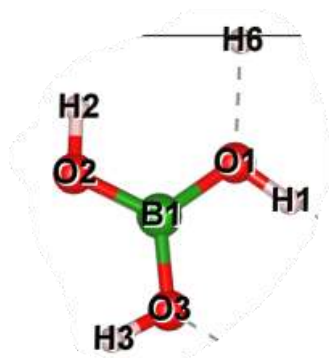
$O3-B2-O2 = 122.4380(0) \text{ deg.}$

$B2-O2-B1 = 116.5935(0) \text{ deg.}$

$H7A-O7-H7B = 99.6899(0) \text{ deg.}$

$O1-B1-O4 = 111.7155(0) \text{ deg.}$

Koordinální číslo



Na kladném iontu Na^+ je navázaných 6 molekul vody.

Proto koordinační číslo je 6

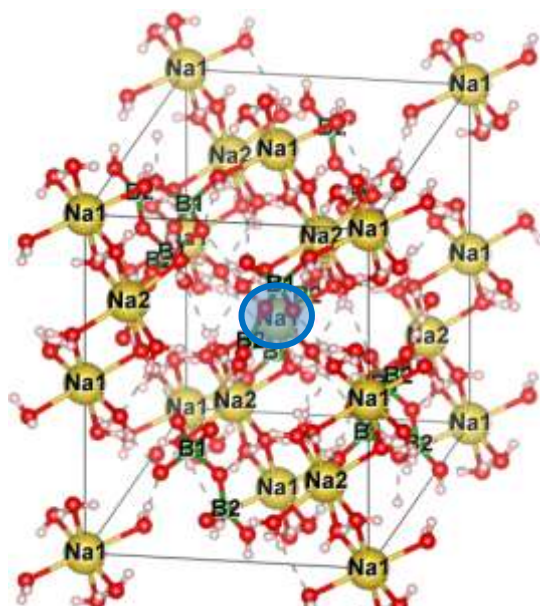
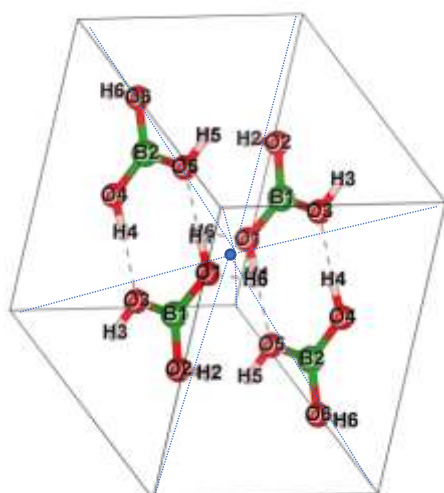
Na kationtu B jsou navázány 3 nebo 4 atomy kyslíku O.

Proto koordinační číslo je 3 nebo 4.

Na kladném kationtu B^{+3} jsou navázány 3 atomy kyslíku O

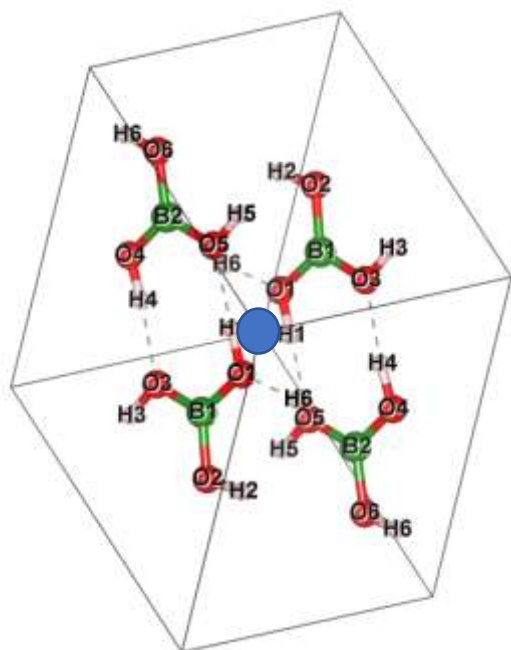
Proto koordinační číslo je 3

Prvky symetrie



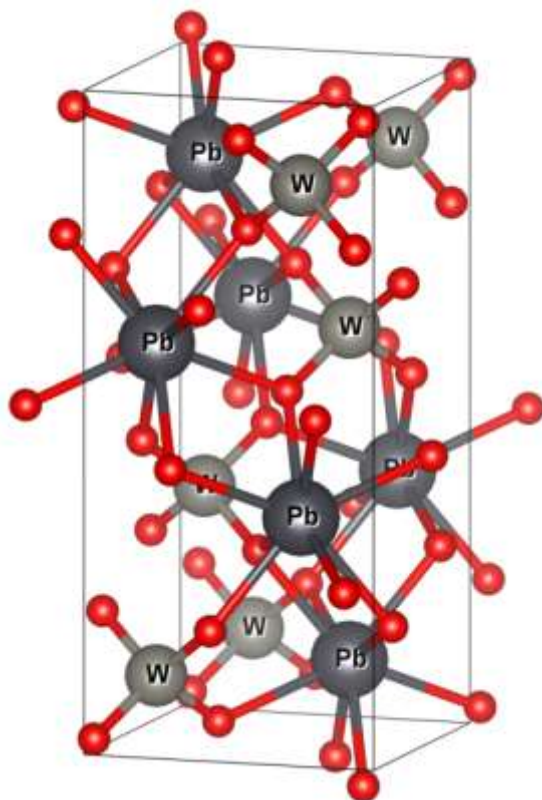
Střed symetrie – centrální atom Na^+

Střed symetrie (uprostřed buňky)

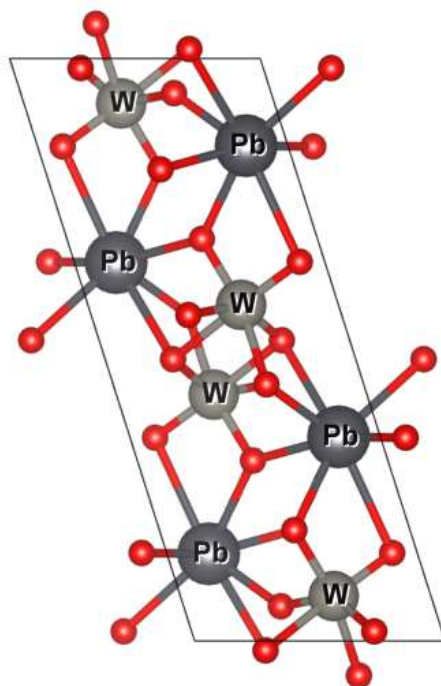


Osa symetrie

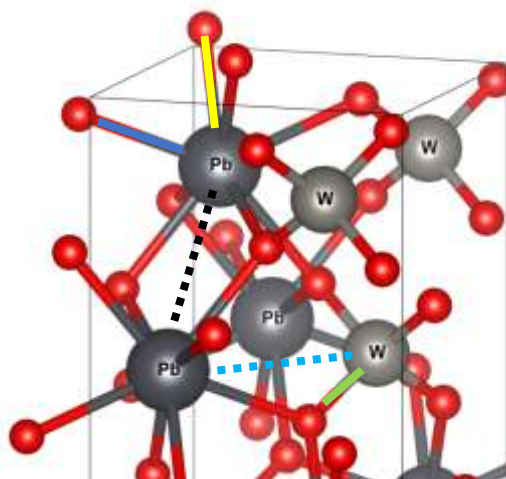
Stolzit



Raspit



Vzdálenost mezi atomy



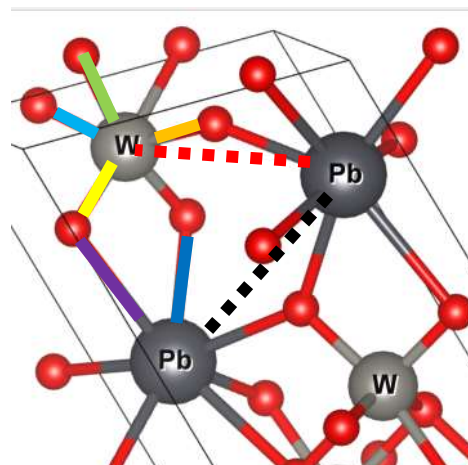
Pb-O = 2.65654(0) Å

Pb-O = 2.61326(0) Å

W-O = 1.77562(0) Å

Pb-Pb = 4.07124(0) Å

Pb-W = 3.86773(0) Å



O4-Pb = 2.47460(0) Å

O3-Pb = 2.86445(0) Å

W-O2 = 2.06538(0) Å

O1-W = 1.92028(0) Å

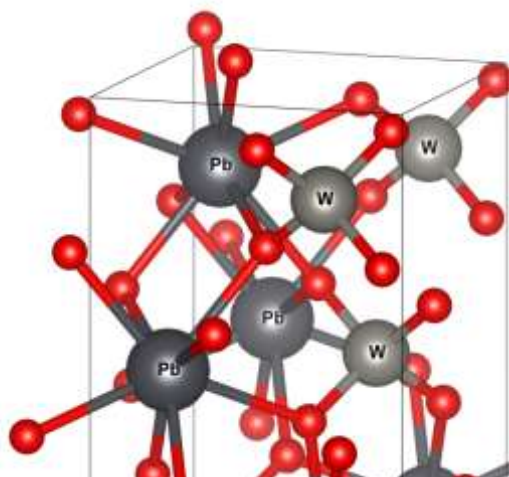
W-O3 = 1.74584(0) Å

O2-W = 1.96938(0) Å

Pb-Pb = 4.60733(0) Å

W-Pb = 4.02572(0) Å

Úhly



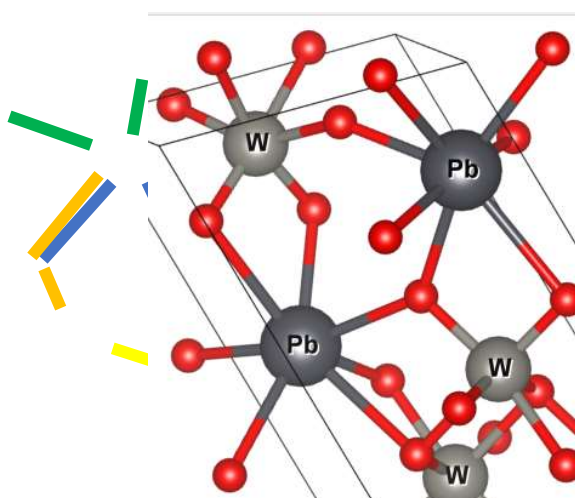
O-Pb-O = 78.8343(0) deg.

O-Pb-O = 67.4240(0) deg.

Pb-O-W = 120.2269(0) deg.

Pb-O-Pb = 101.1657(0) deg.

O-W-O = 108.0811(0) deg.



O4-Pb-O3 = 57.6892(0) deg.

W-O3-Pb = 97.4731(0) deg.

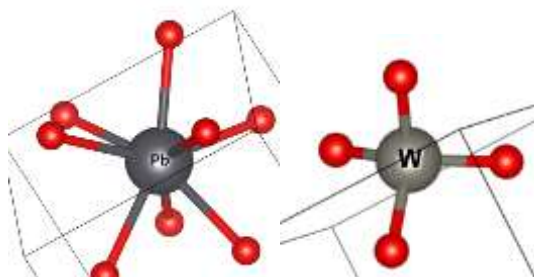
W-O4-Pb = 109.9686(0) deg.

Pb-O2-W = 139.9372(0) deg.

O2-W-O1 = 85.2220(0) deg.

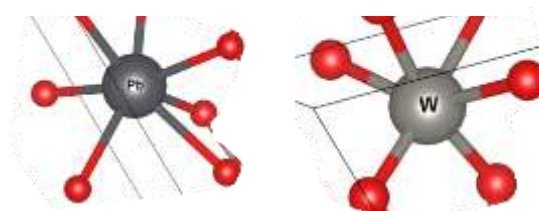
O1-Pb-O1 = 72.7504(0) deg.

Koordinální číslo



Kationt Pb^{+2} je spojen s 8 kyslíky. Proto koordinální číslo je 8.

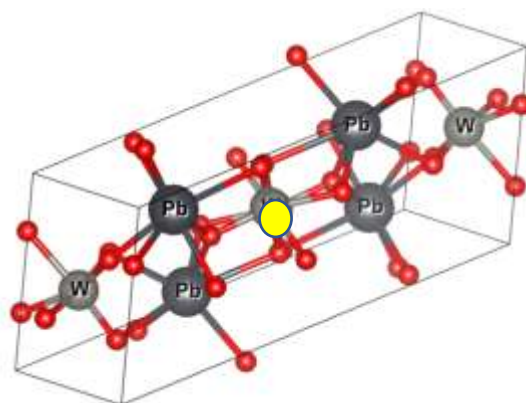
Kationt W^{+6} je spojen s 4 kyslíky. Proto koordinální číslo je 4.



Kationt Pb^{+2} je spojen s 7 kyslíky. Proto koordinální číslo je 7.

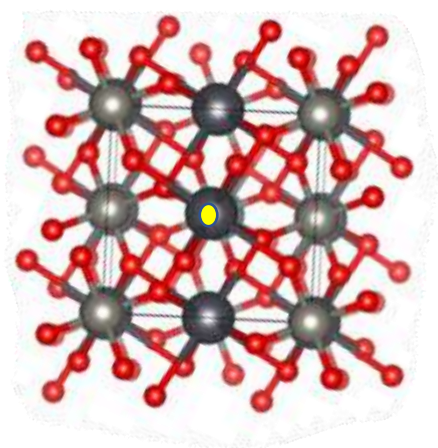
Kationt W^{+6} je spojen s 6 kyslíky. Proto koordinální číslo je 6.

Prvky symetrie

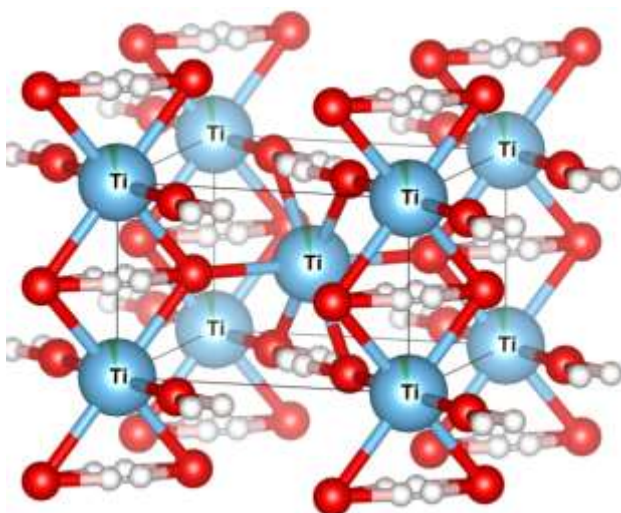


Střed symetrie leží uprostřed
elementární buňky

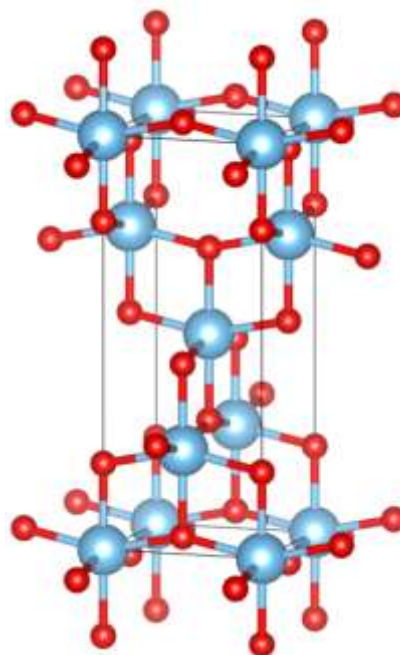
Osa symetrie prochází středem



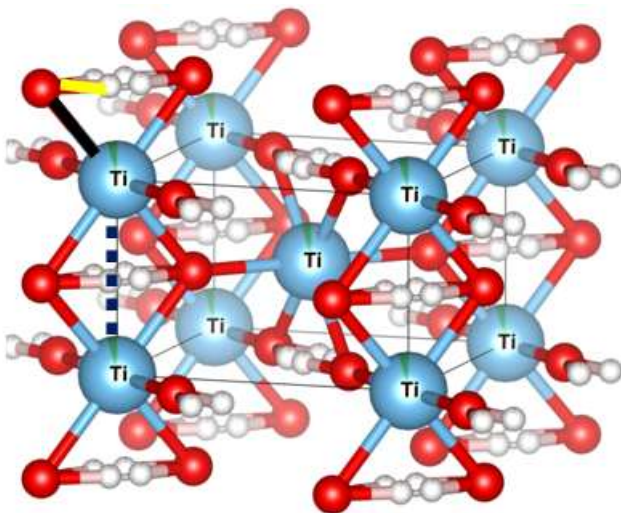
Rutil



Anatas



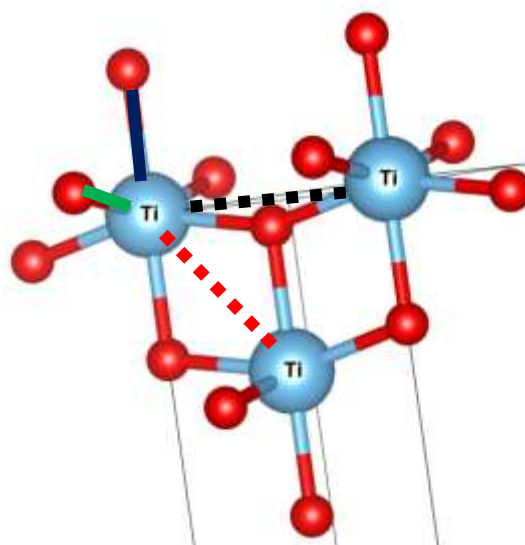
Vzdálenost mezi atomy



Ti-O = 1.94676(0) Å

O-H = 1.04157(0) Å

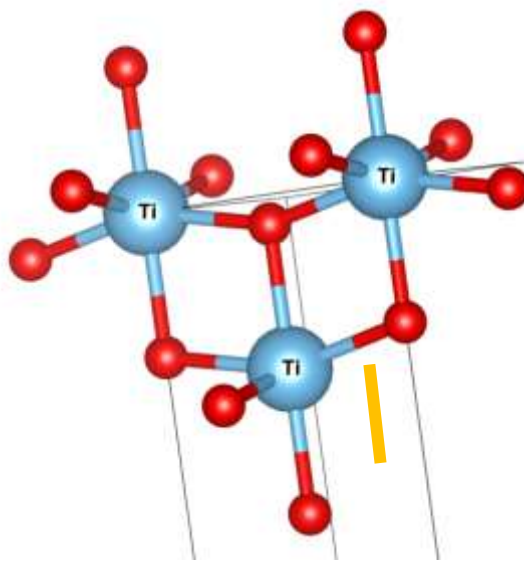
Ti-Ti = 2.95400(0) Å

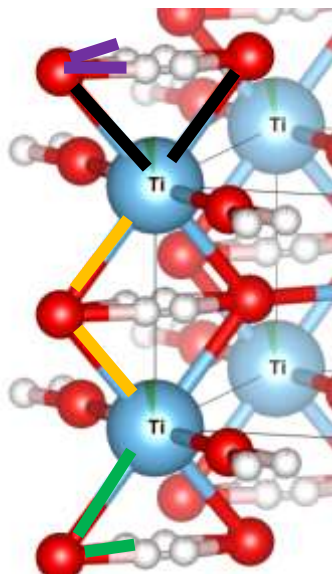


Ti-O = 1.97955(0) Å

Ti-O = 1.93387(0) Å

Úhly mezi atomy



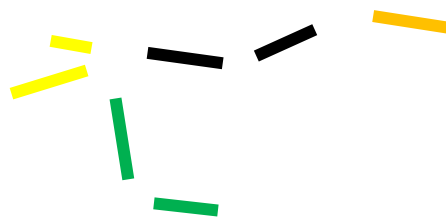


O-Ti-O = 81.3013(0) deg.

Ti-O-Ti = 98.6987(0) deg.

Ti-O-H = 50.8830(0) deg.

H-O-H = 28.8514(0) deg.



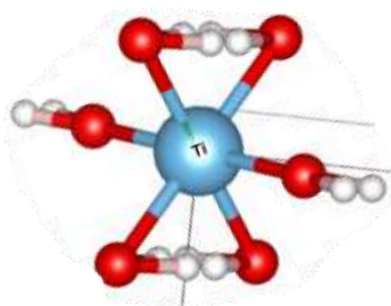
Ti-O-Ti = 156.1843(0) deg.

Ti-O-Ti = 101.9078(0) deg.

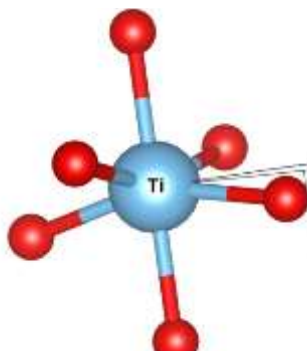
O-Ti-O = 101.9078(0) deg.4

O-Ti-O = 92.4401(0) deg.

Koordinační číslo



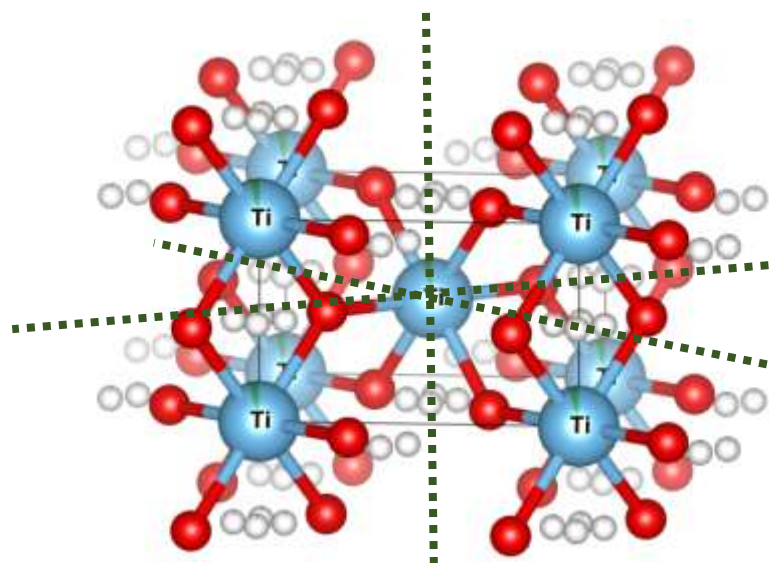
Každý atom Ti^{+4} je navázán na 6 atomů kyslíku O. Proto koordinační číslo je 6.



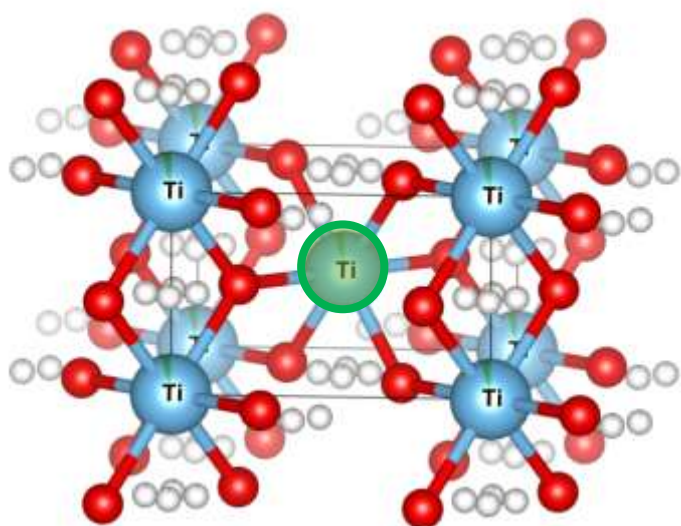
Každý kationt Ti^{+4} je navázán na 6 atomů kyslíku. Proto koordinační číslo je 6

Prvky symetrie

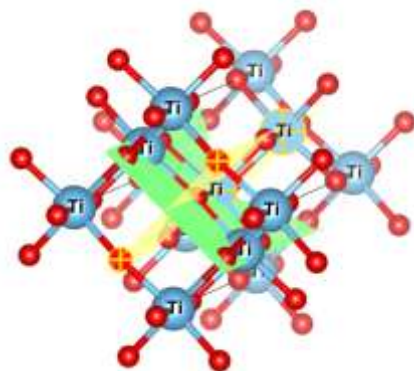
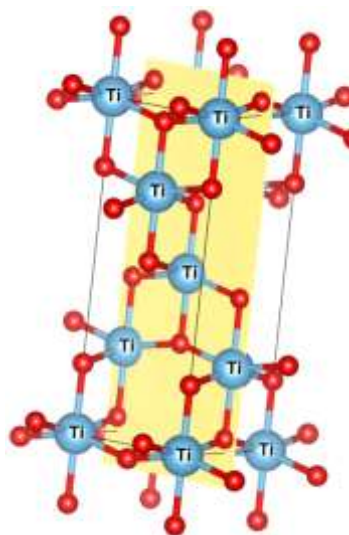
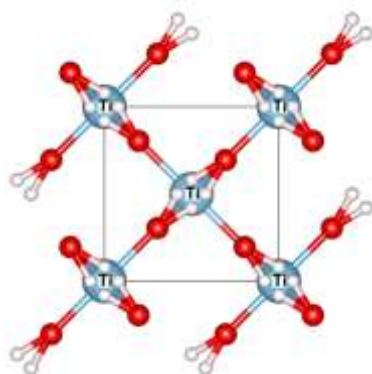
Osy symetrie



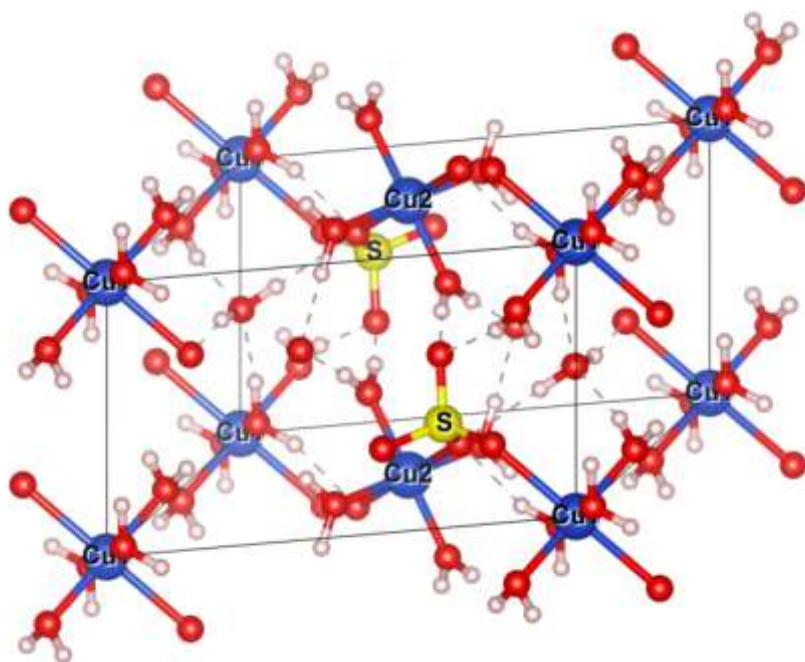
Střed symetrie



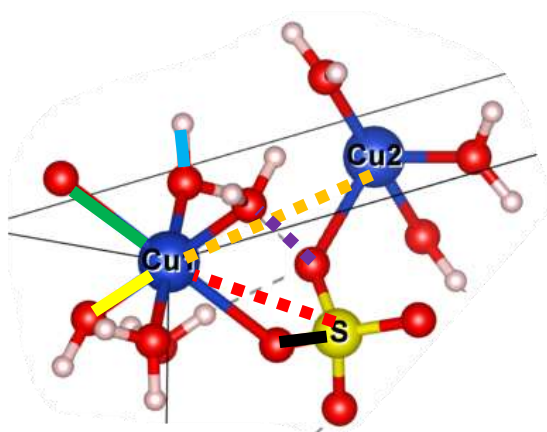
Rovina symetrie



Modrá skalice



Vzdálenosti



Cu1-O1 = 2.38583(0) Å

O6-S = 9.68513(0) Å

O5-Cu1 = 1.97484(0) Å

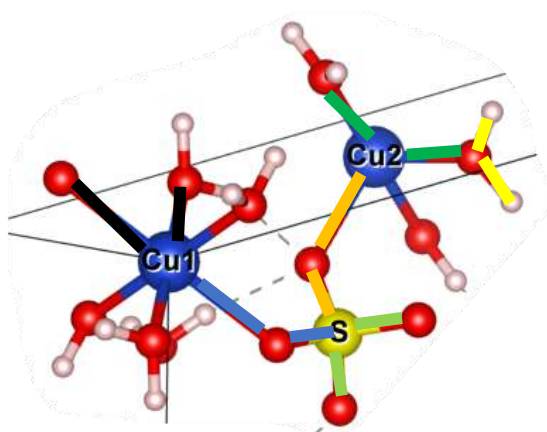
H6B-O6 = 0.98292(0) Å

Cu1-S = 3.56057(0) Å

Cu2-Cu1 = 5.56893(0) Å

O2-H6A = 1.89683(0) Å

Úhly mezi vazby



$\text{Cu1-O1-S} = 132.6202(0) \text{ deg.}$

$\text{O4-S-O3} = 109.0796(0) \text{ deg.}$

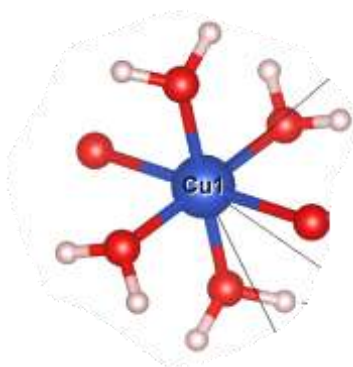
$\text{Cu2-O2-S} = 138.8253(0) \text{ deg.}$

$\text{O6-Cu1-O1} = 88.6073(0) \text{ deg.}$

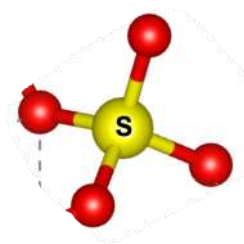
$\text{O7-Cu2-O8} = 90.2697(0) \text{ deg.}$

$\text{H8A-O8-H8B} = 110.2048(0) \text{ deg.}$

Koordinační číslo



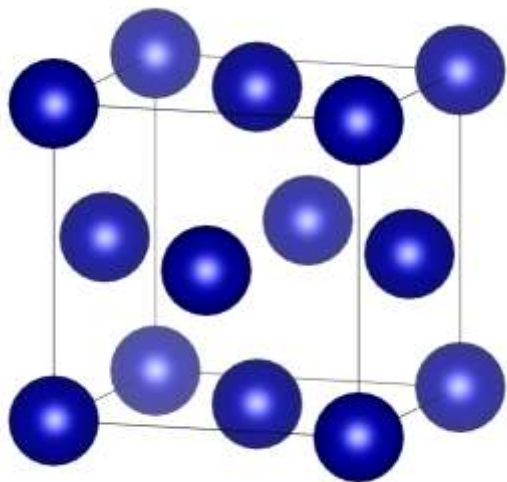
Atom mědi Cu^{+2} je navázán na 6 atomů kyslíku. Proto koordinační číslo je 6



Atom síry S^{+6} je navázán na 4 atomy kyslíku. Proto koordinační číslo je 4.

Kobalt

krychlová struktura



Vzdálenost

Co-Co = 2.50881(0) Å

Co-Co = 2.50881(0) Å

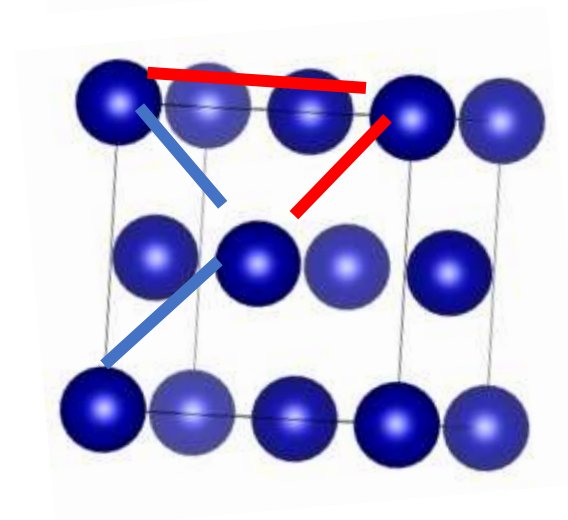
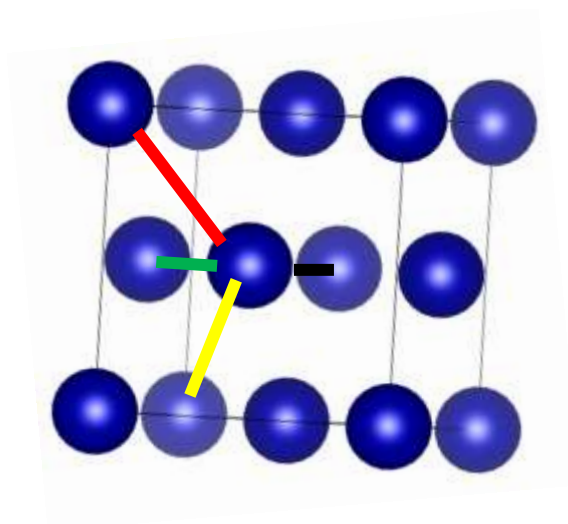
Co-Co = 4.34539(0) Å

Co-Co = 3.54800(0) Å

Úhel

Co-Co-Co = 90.0000(0) deg.

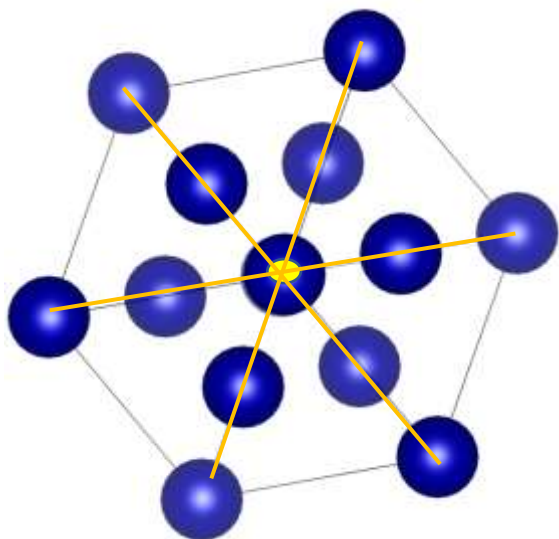
Co-Co-Co = 45.0000(0) deg.



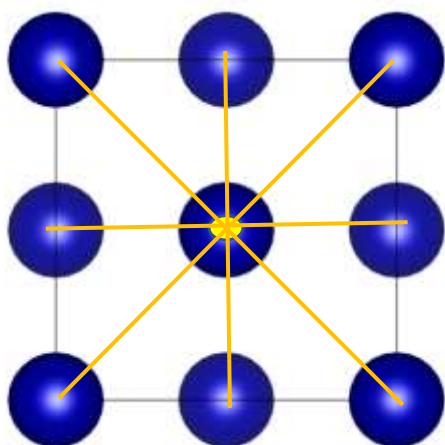
Prvky symetrie

Osa symetrie

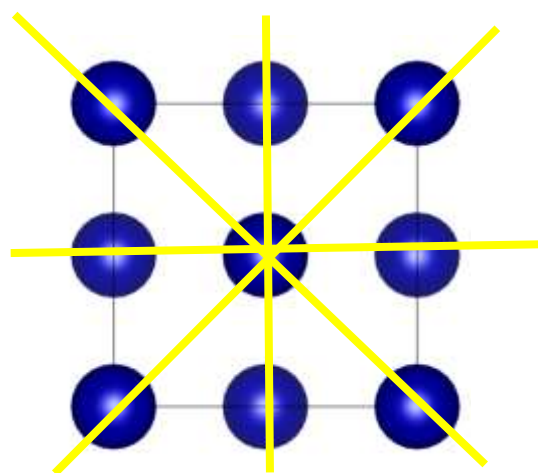
Trojčetná osa procházející středem



Čtyřčetné osy symetrie procházející středem



Rovina symetrie



Pohled zepředu/zboku/svrchu

Dvojčetné osy symetrie

