



VIZUALIZACE KRYSTALOVÉ STRUKTURY

Kieserit (kieserite) a cer (cerium)

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KCH/ACH
TUL, 1. ročník
2020

KIESERIT A CER



kieserit



cer

Úkol jsme vypracoval pomocí programu Mercury

KIESERIT

Cif data jsem našel pro jednoklonnou soustavu [3].

Prvky souměrnosti:

- body inverze

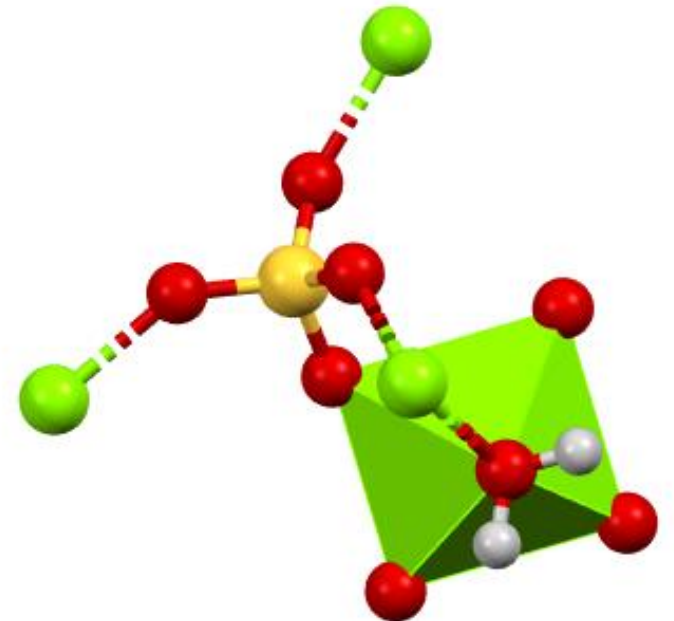
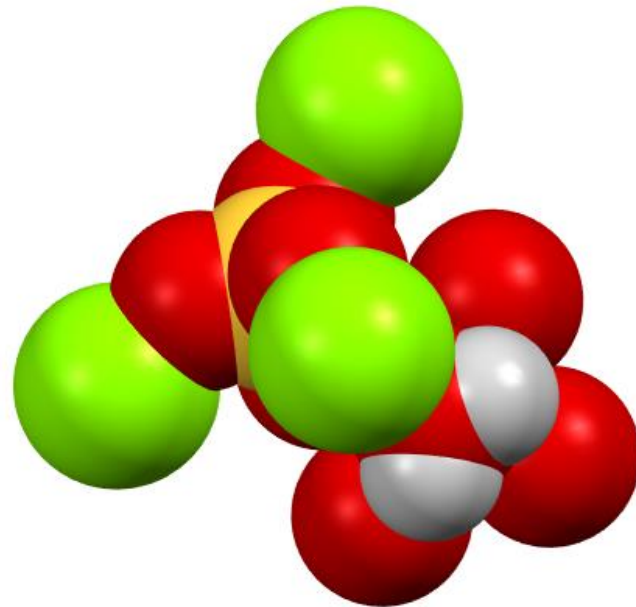
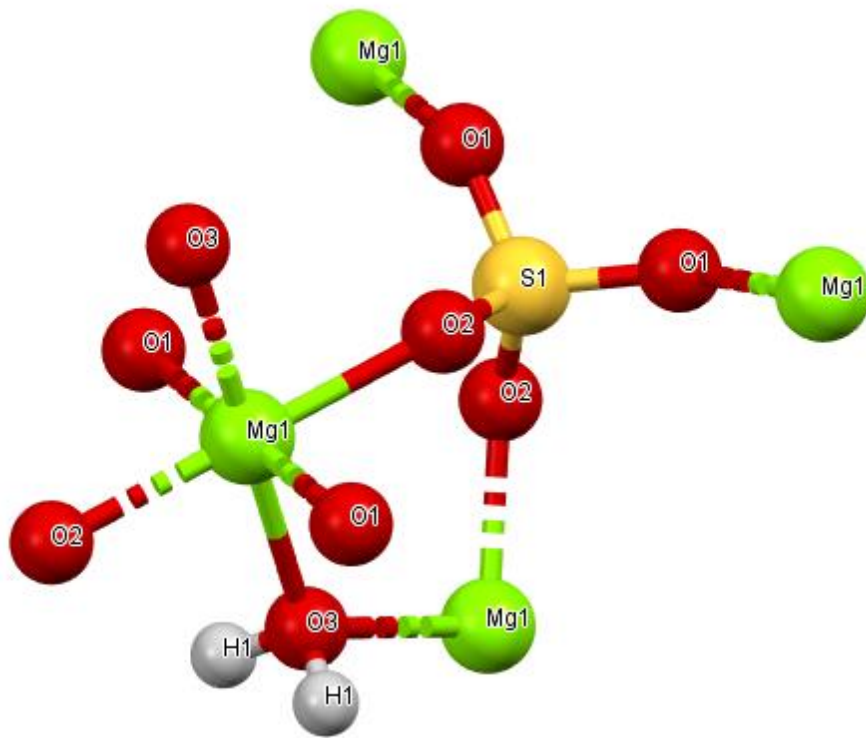
- osy rotace (dvoučetné)

- šroubové osy (dvoučetné)

- roviny zrcadlení

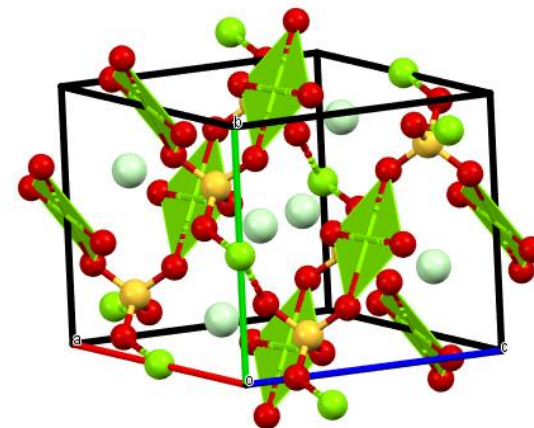
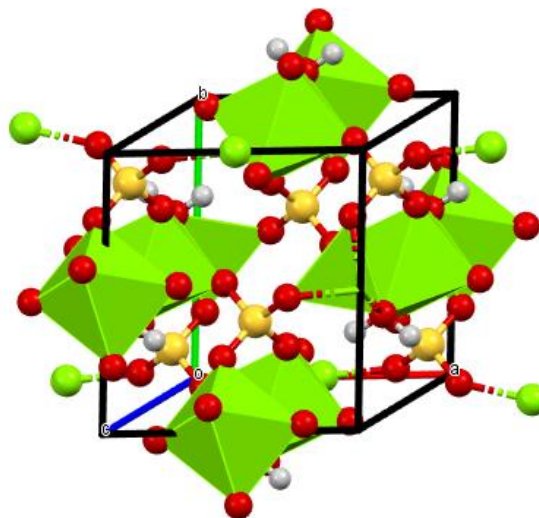
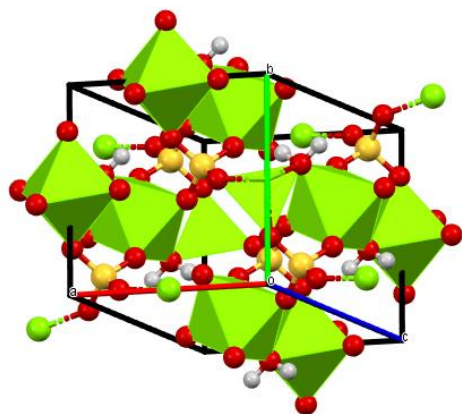
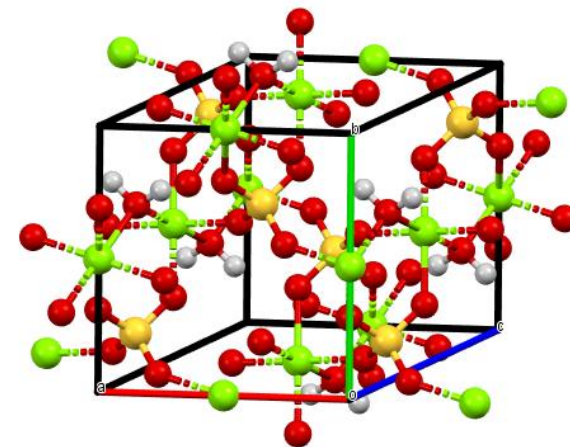
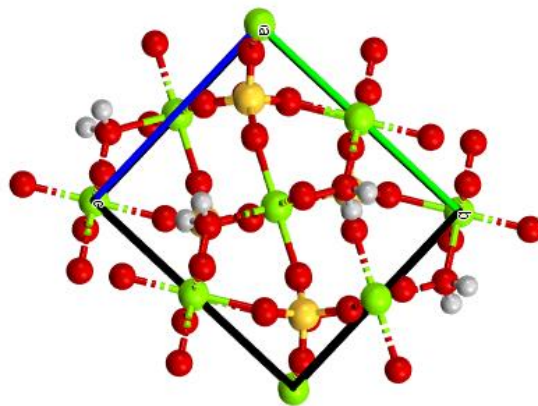
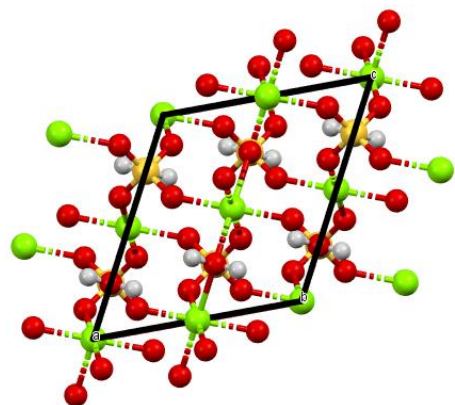
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Struktura



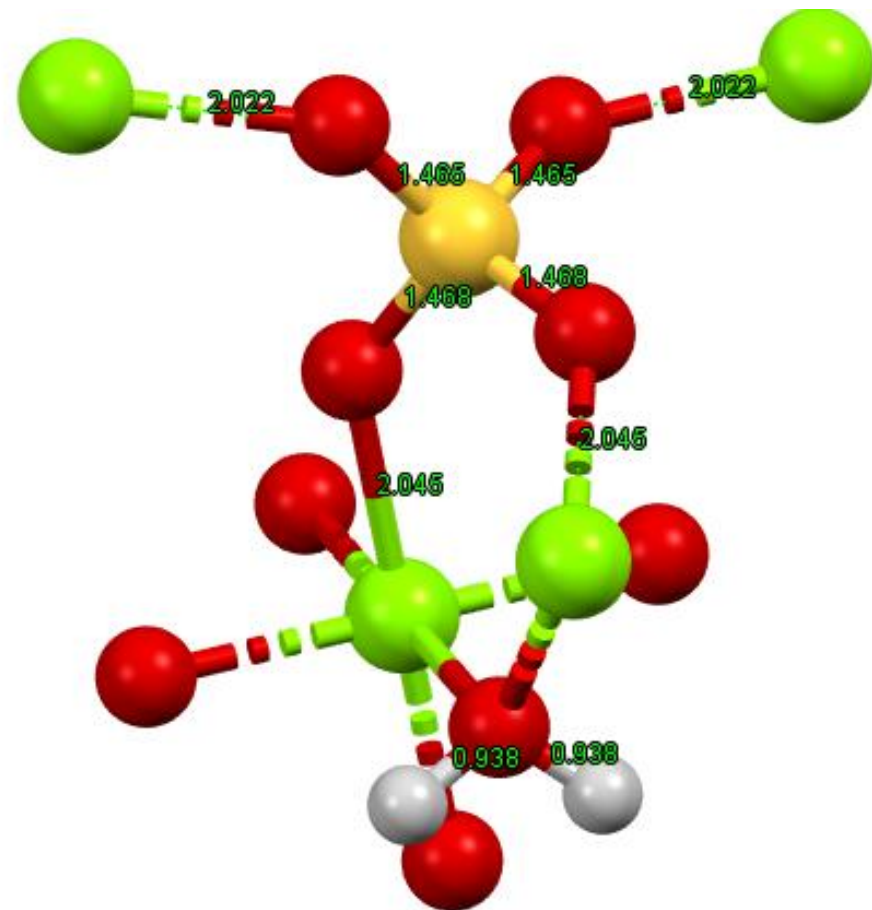
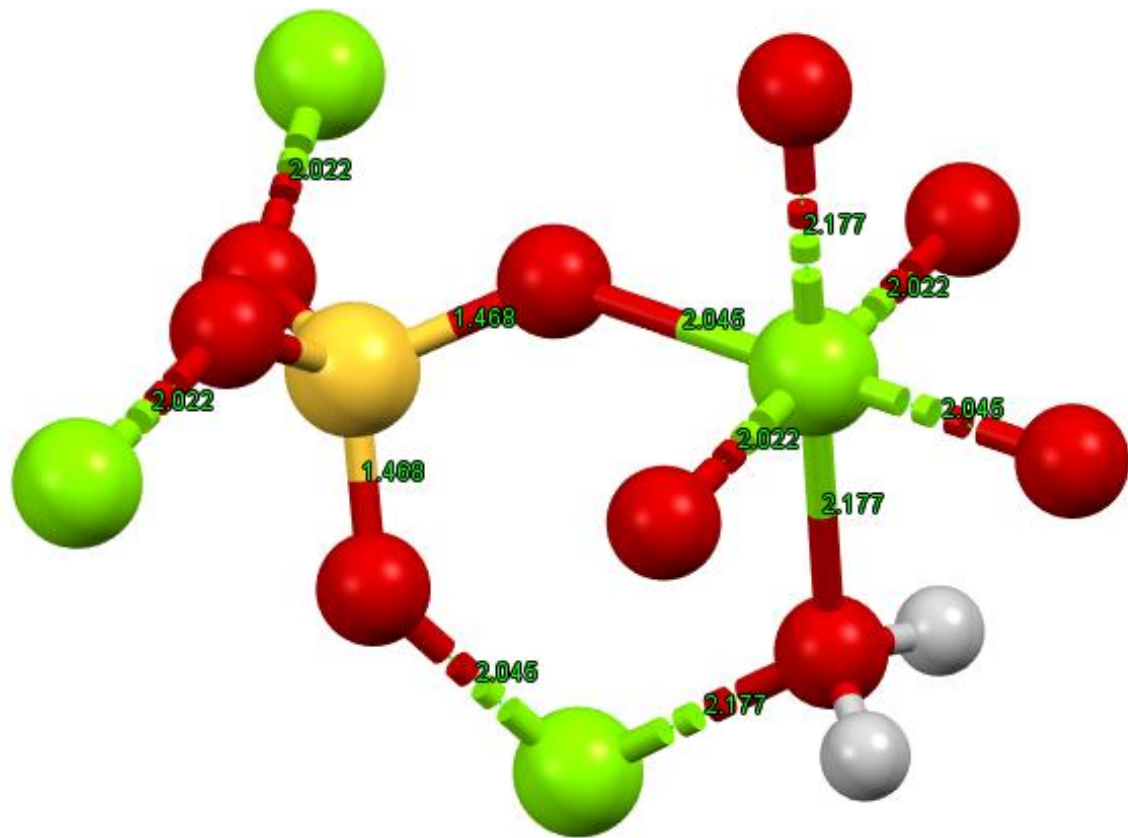
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Základní buňka



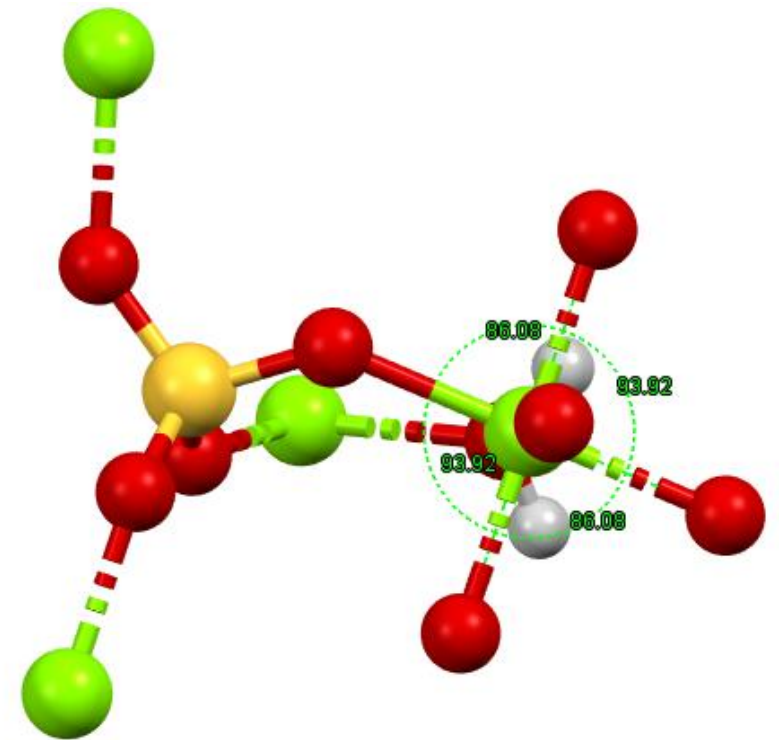
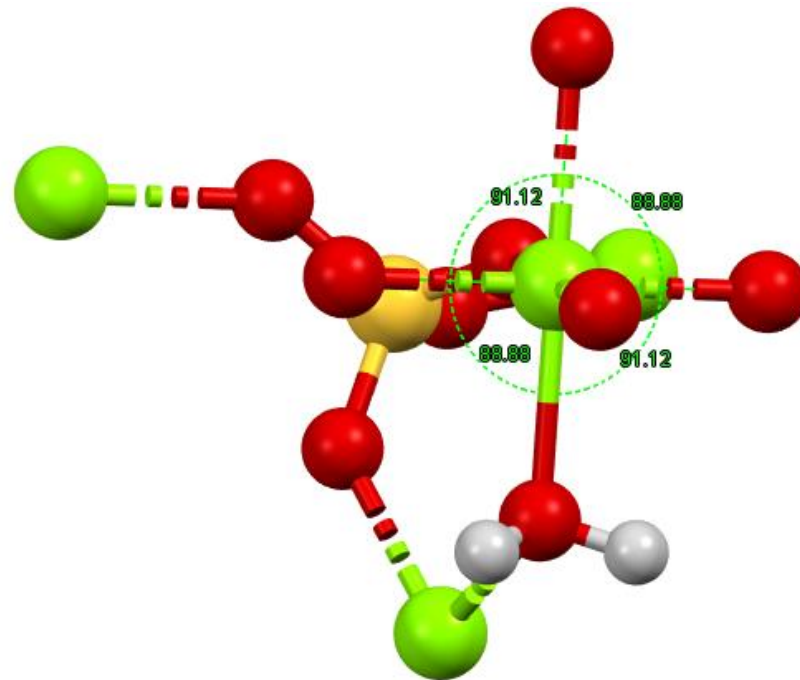
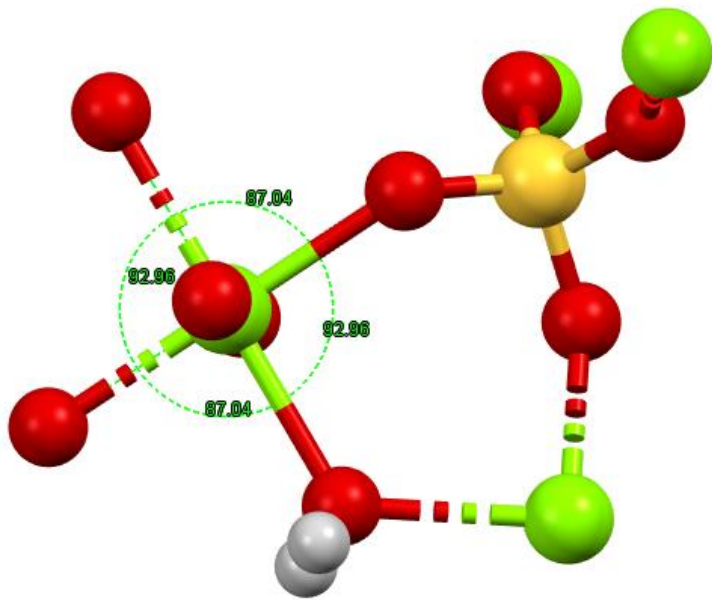
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Délky vazeb



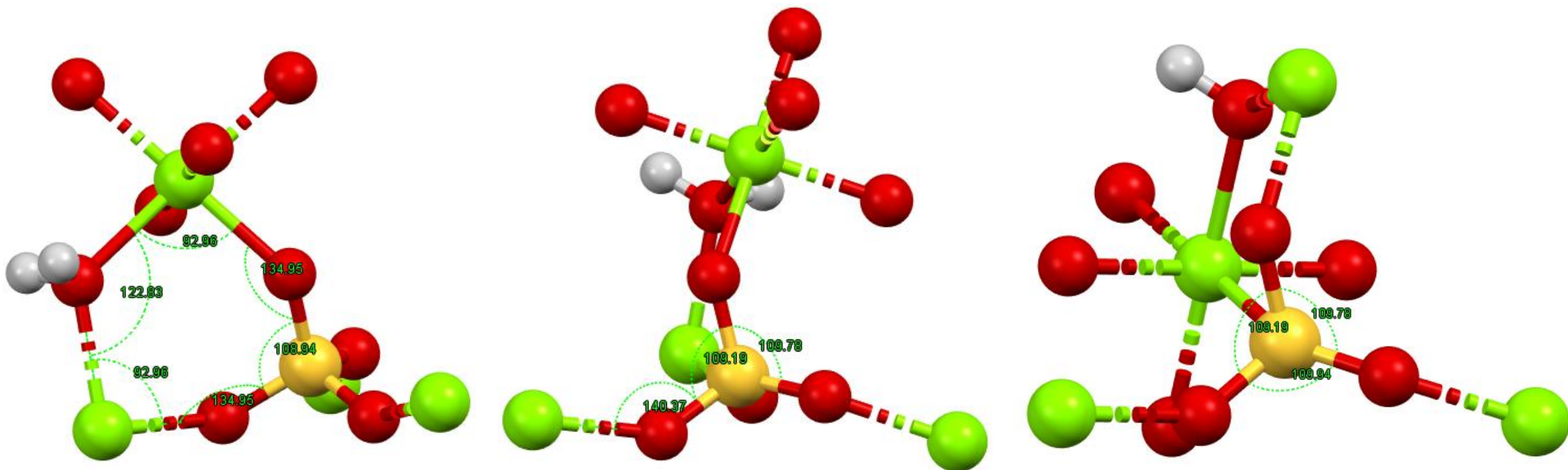
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Vazebné úhly



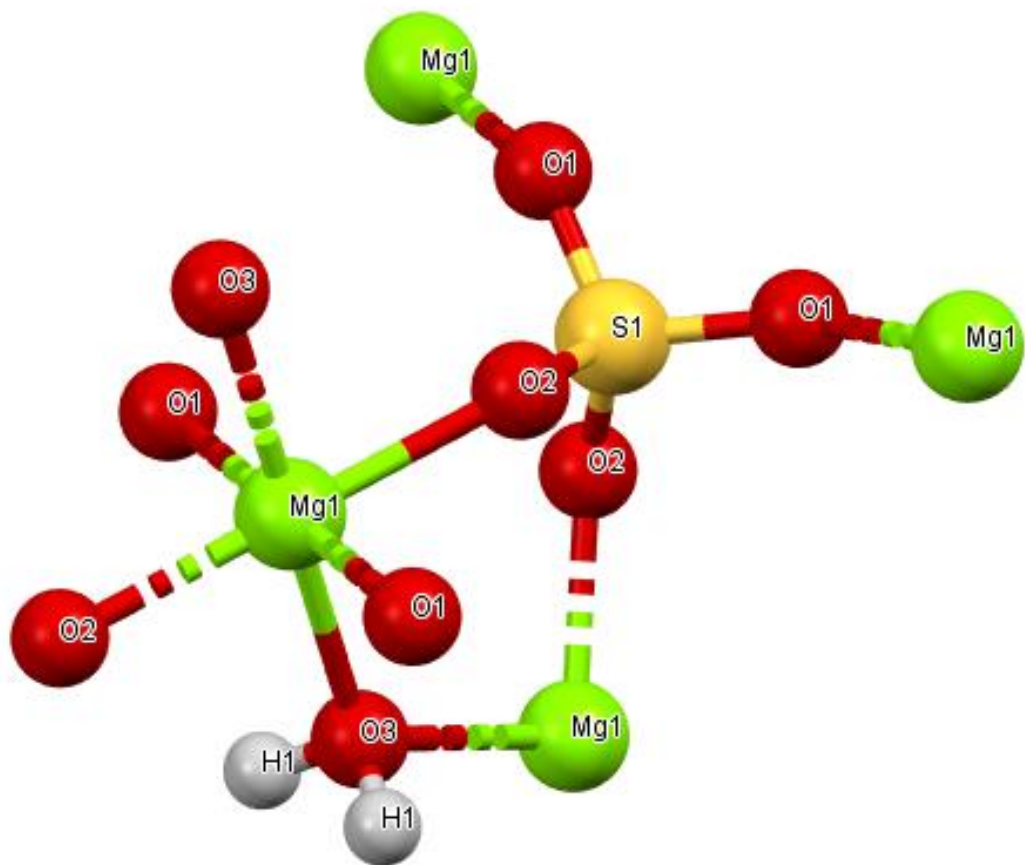
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Vazebné úhly



KIESERIT

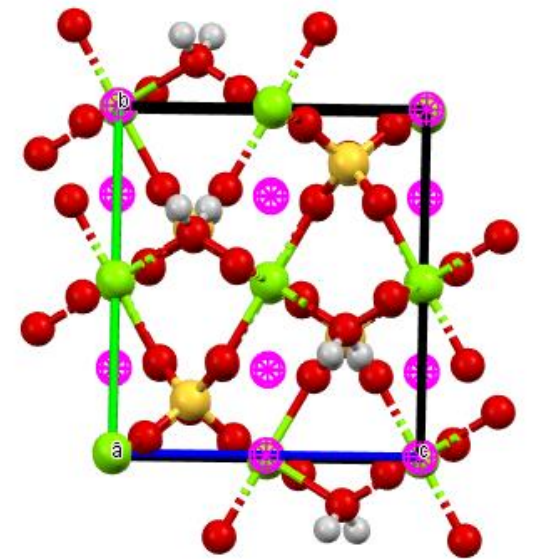
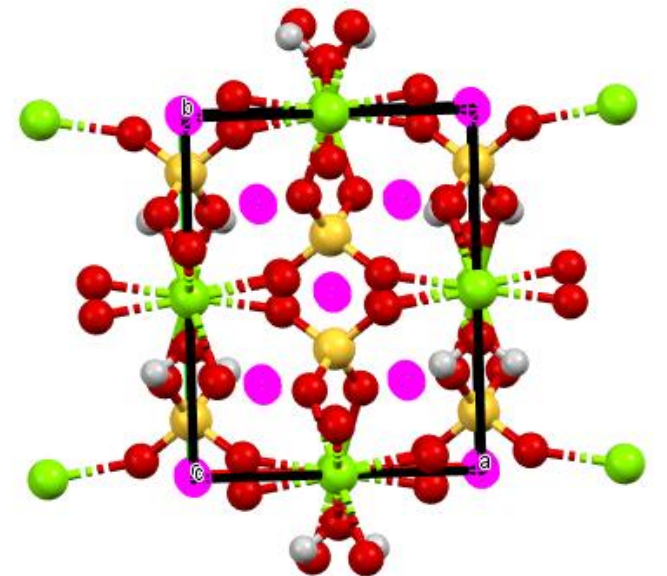
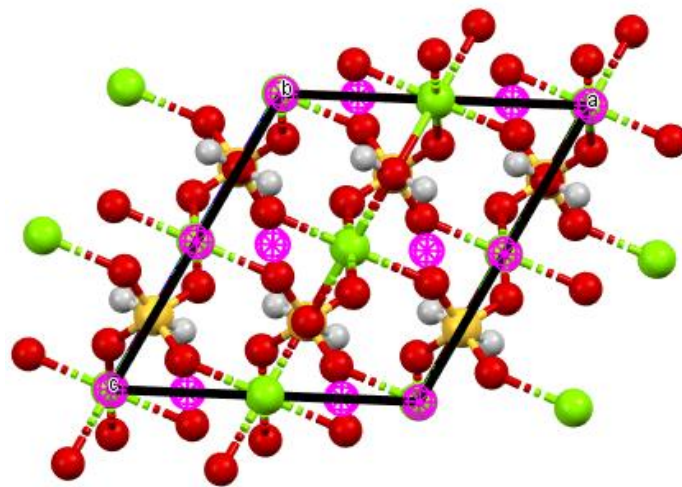
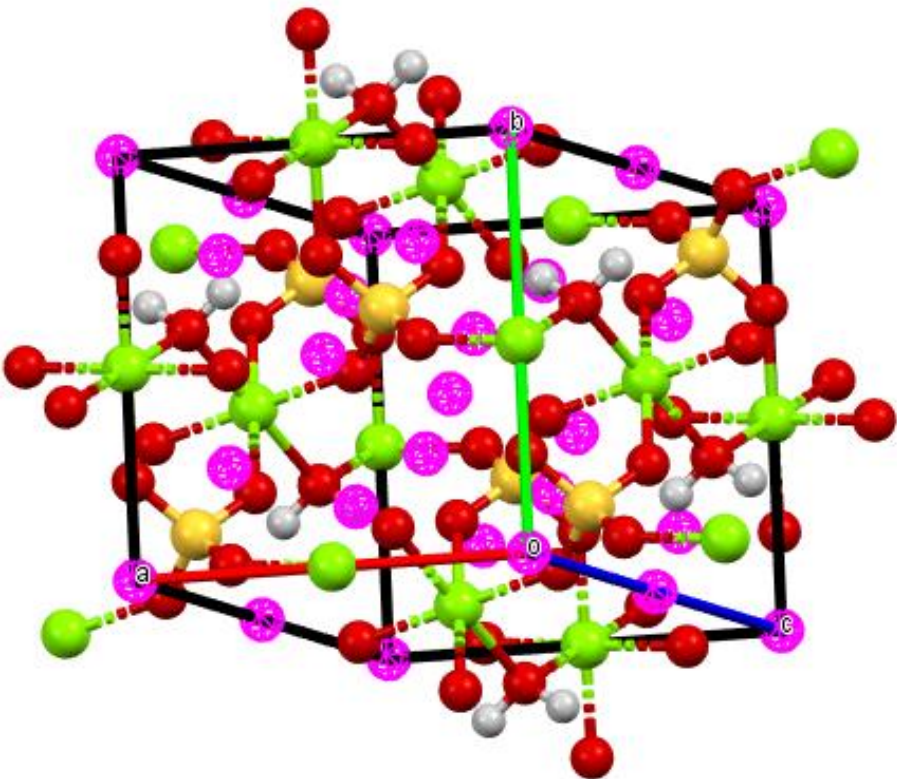
Koordinační čísla



Mg1:	6
S1:	4
O1:	2
O2:	2
O8:	4
H1:	1

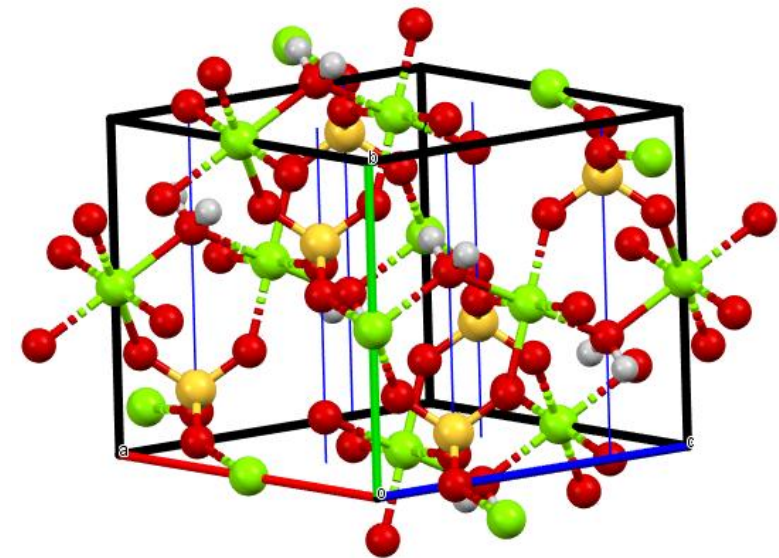
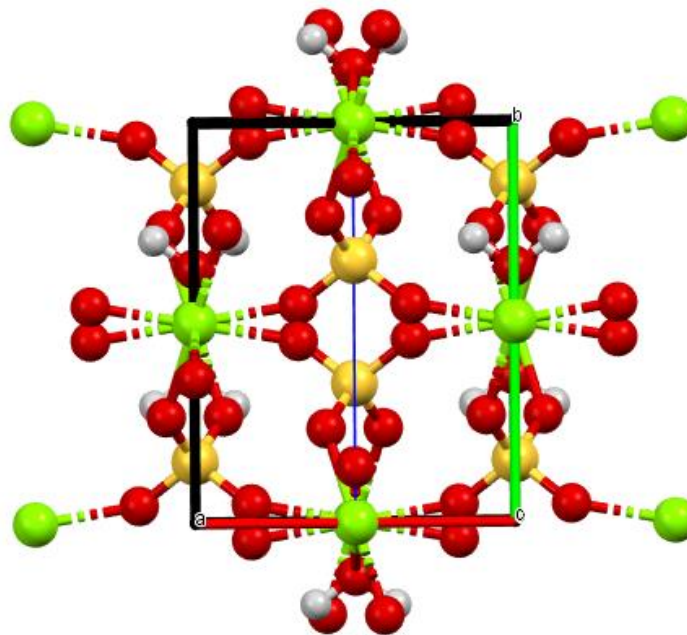
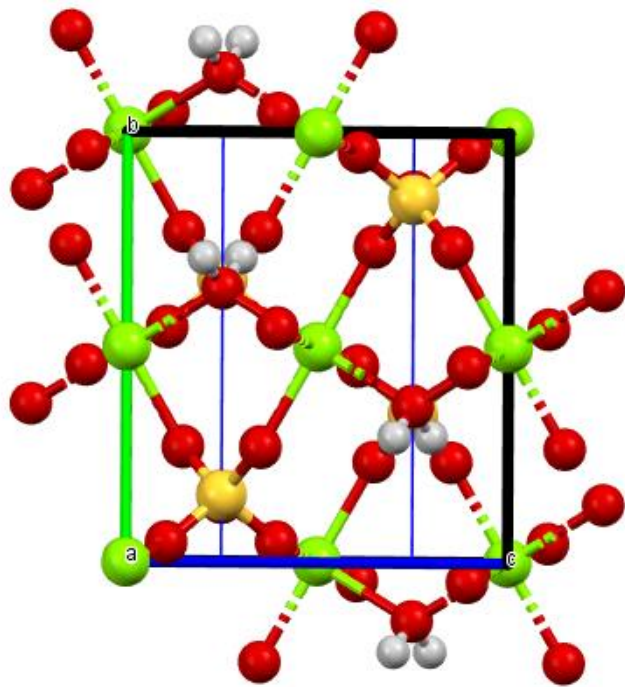
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Body inverze



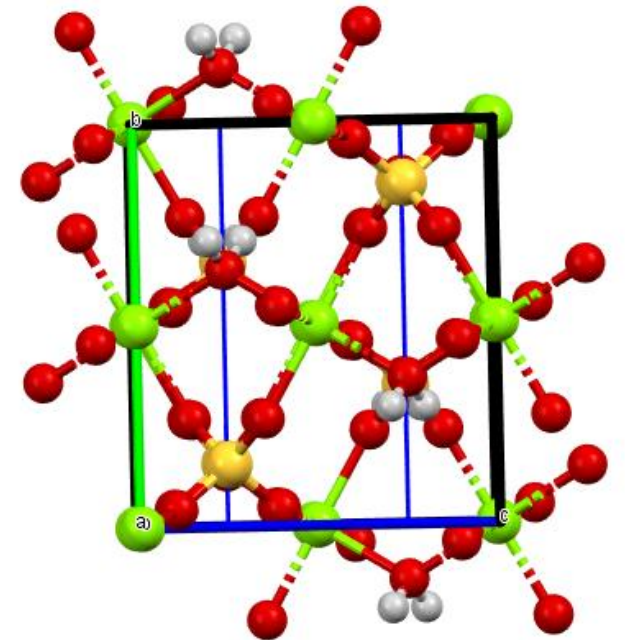
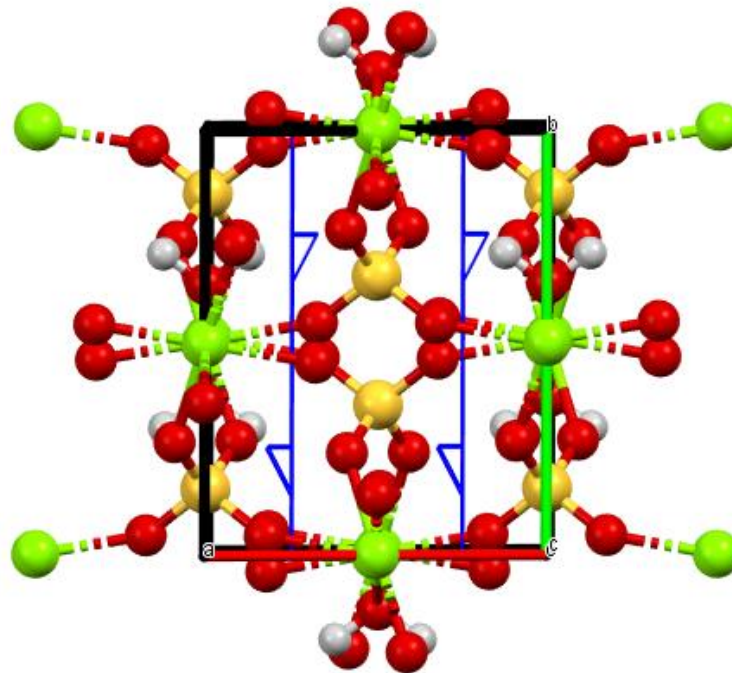
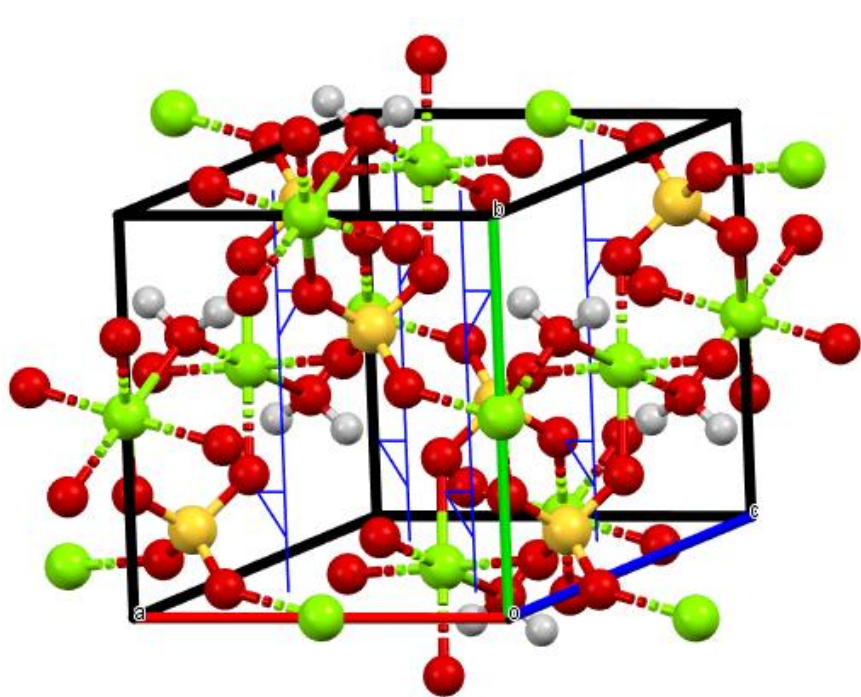
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Dvoučtetné osy rotace (2-fold proper rotation axes)



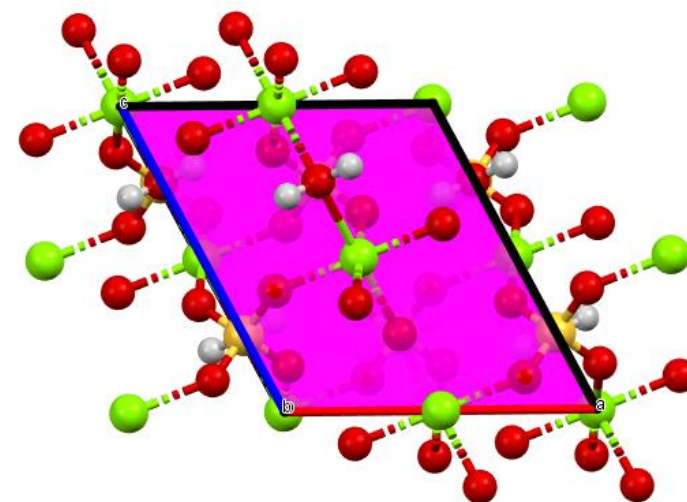
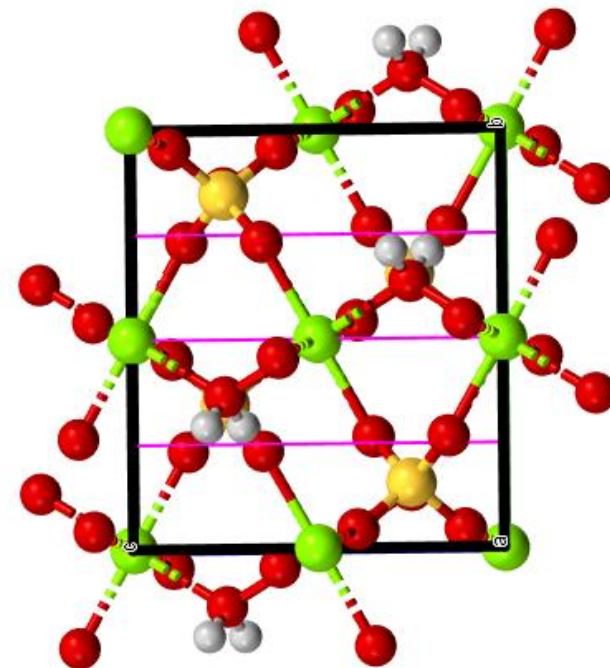
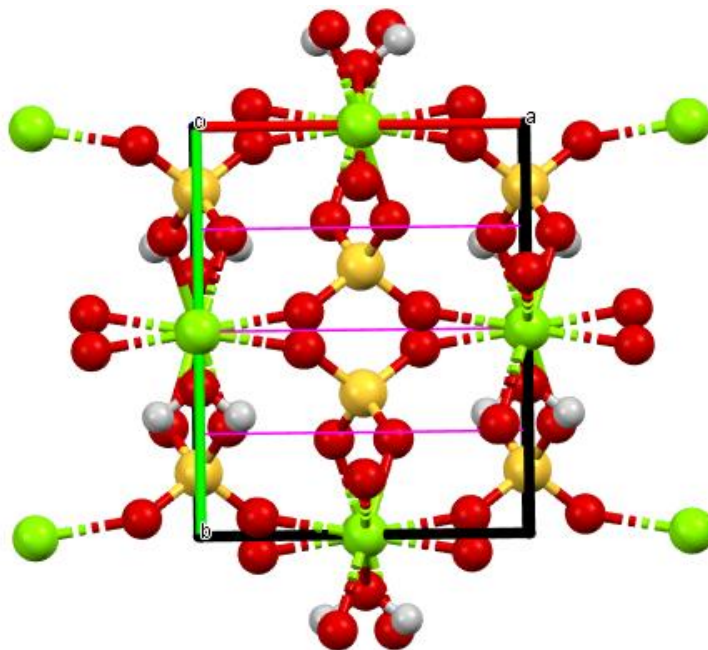
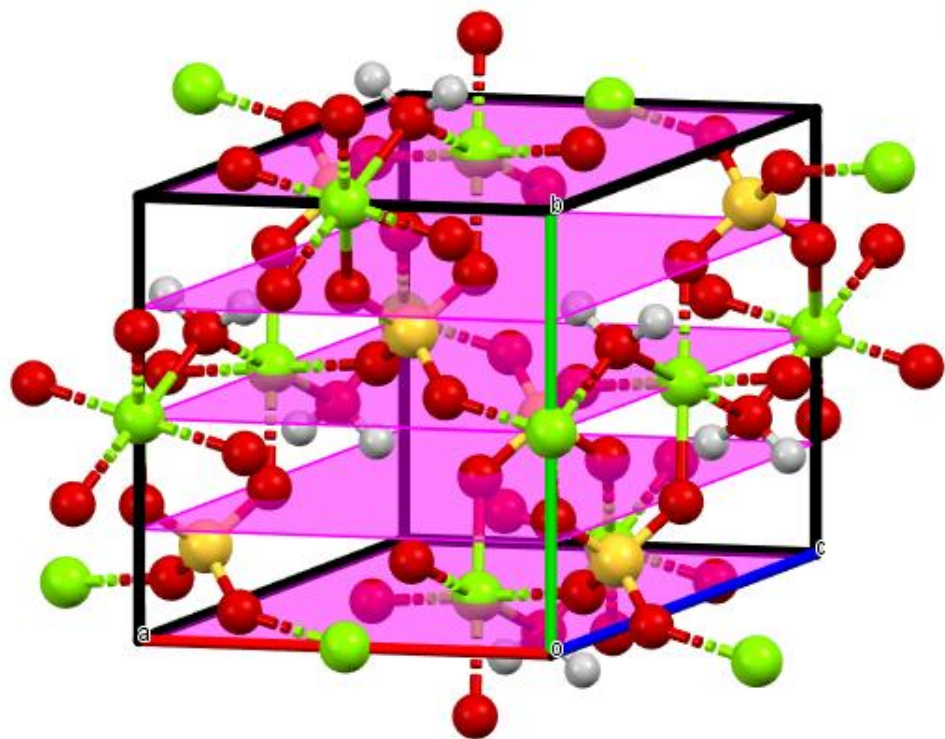
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Dvoučelné šroubové osy (2-fold screw axes)



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Roviny zrcadlení (mirror planes)



CER

Podle Wikipedie [4] existují 4 alotropické modifikace ceru: α , β , γ , δ :

α : kubická plošně centrovaná (fcc), pod $-150\text{ }^{\circ}\text{C}$

β : dvojitá hexagonální (dhcp), $20-(-150)\text{ }^{\circ}\text{C}$

γ : kubická plošně centrovaná (fcc), $726-20\text{ }^{\circ}\text{C}$ (dle zdroje pokojová teplota)

δ : kubická tělesově centrovaná (bcc), nad $726\text{ }^{\circ}\text{C}$

Cif data jsem našel jen pro kubickou plošně centrovanou [5] a jednodílnou soustavu [6]. Dle zdroje [6] se má jednat o hexagonální soustavu (hcp), tvar buňky v programu Mercury tomu ale neodpovídá. Z rozdílnosti prvků souměrnosti u kieseritu a „jednodílného“ ceru vyvozují, že se nejspíše opravdu jedná o hexagonální cer.

CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Prvky souměrnosti:

- body inverze

- osy rotace (dvoučetné, trojčetné, čtyřčetné)

- šroubové osy (dvoučetné, trojčetné, čtyřčetné)

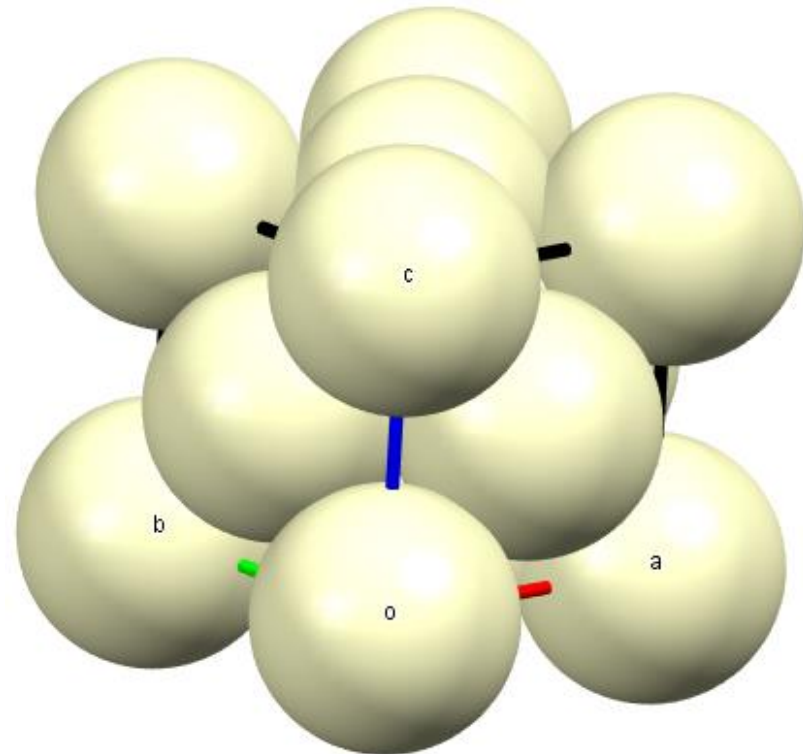
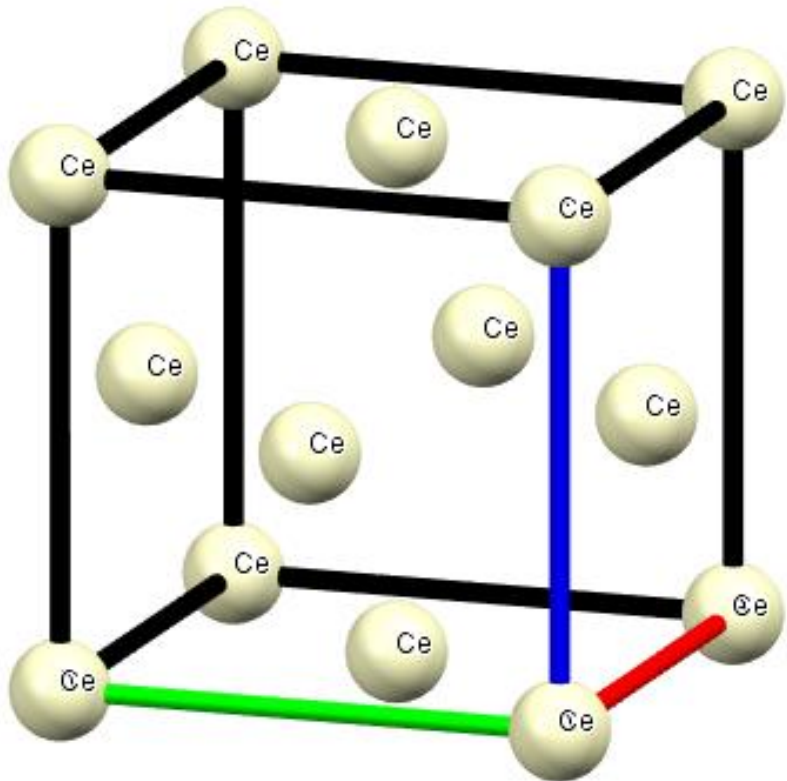
- rotačně inverzní osy (trojčetné, čtyřčetné)

- skluzové roviny

- roviny zrcadlení

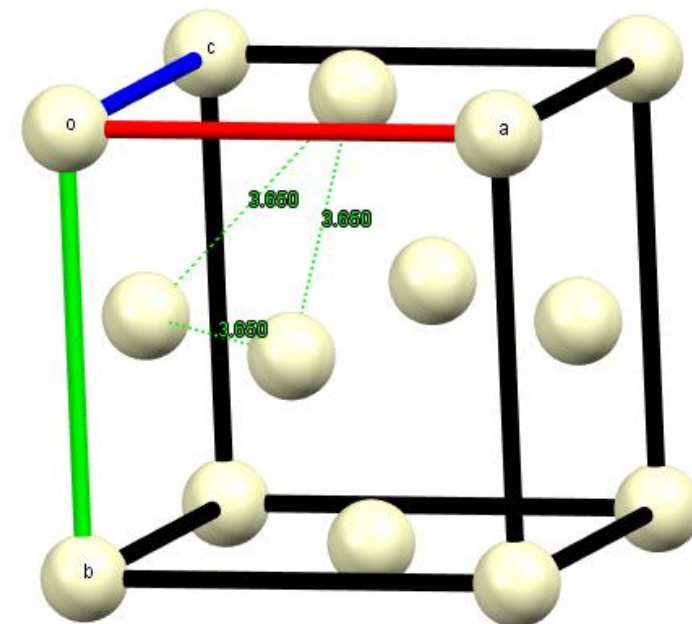
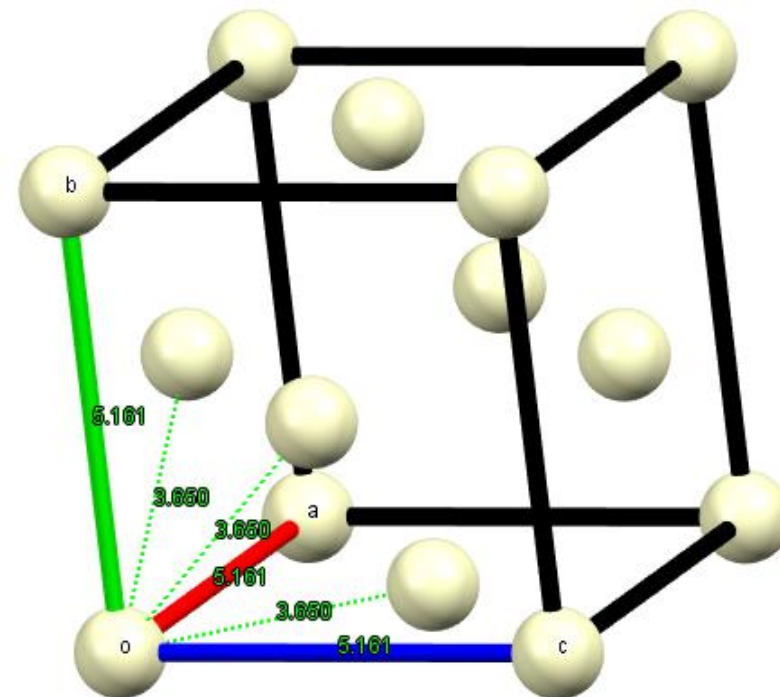
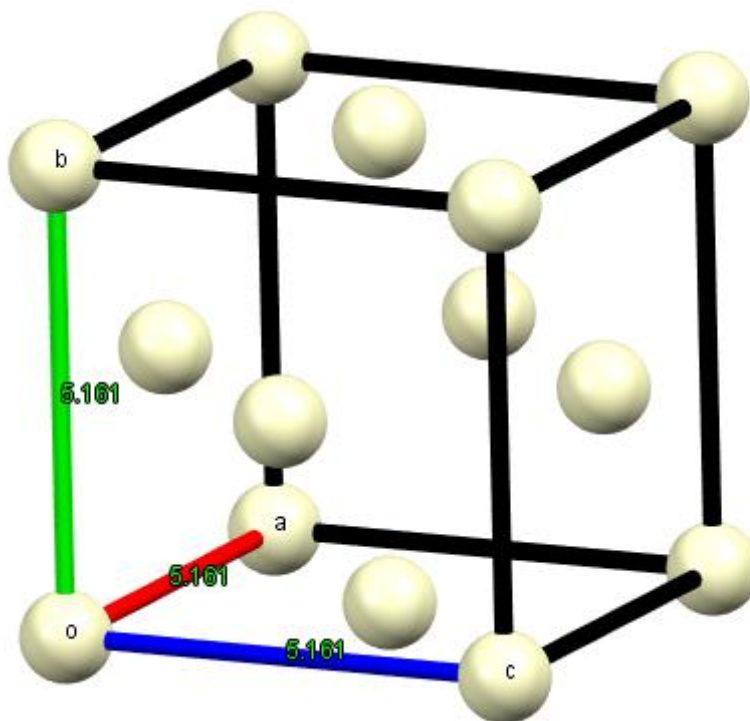
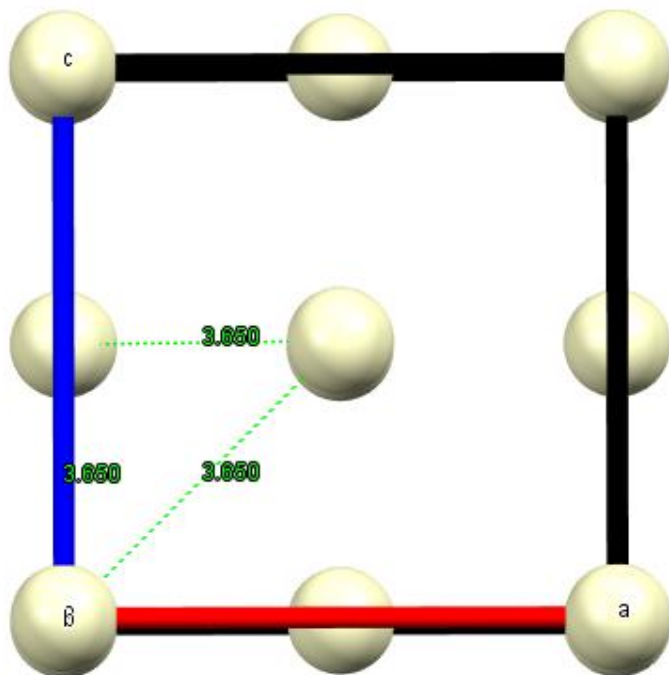
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Základní buňka



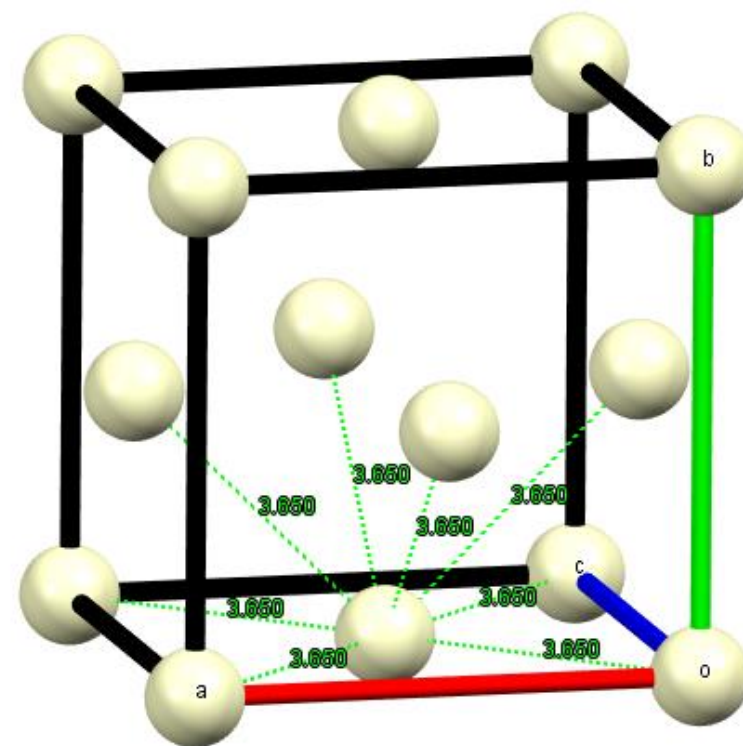
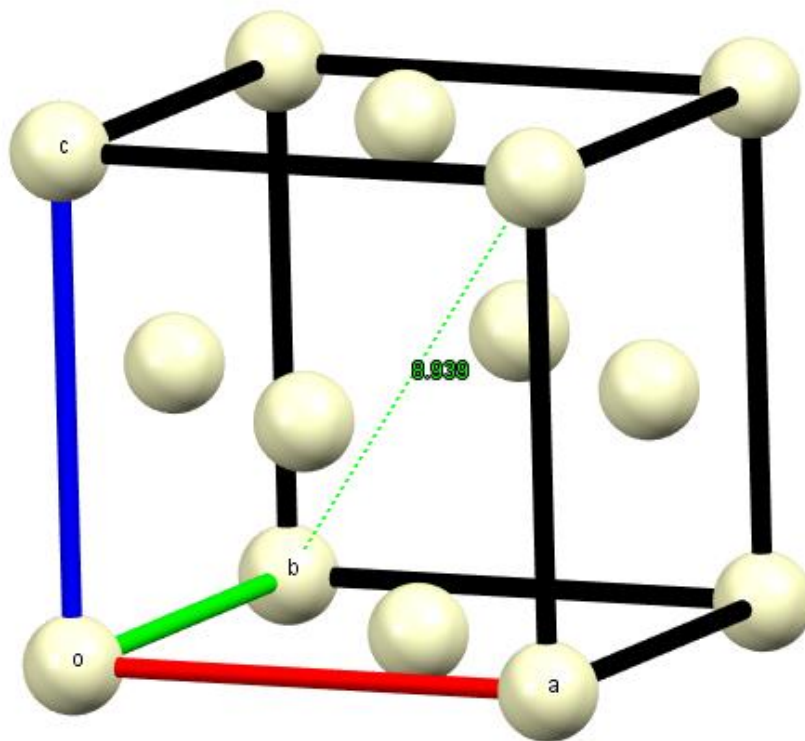
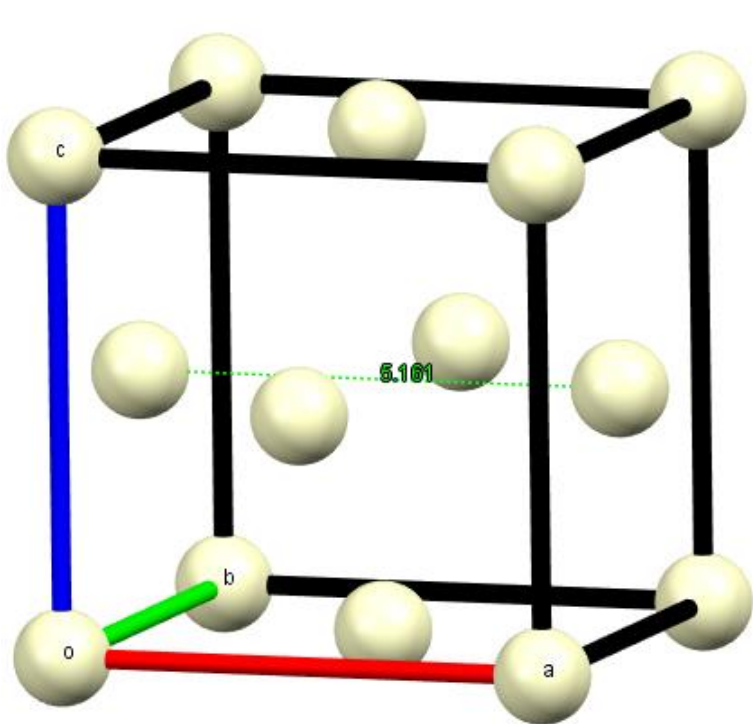
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Délky vazeb



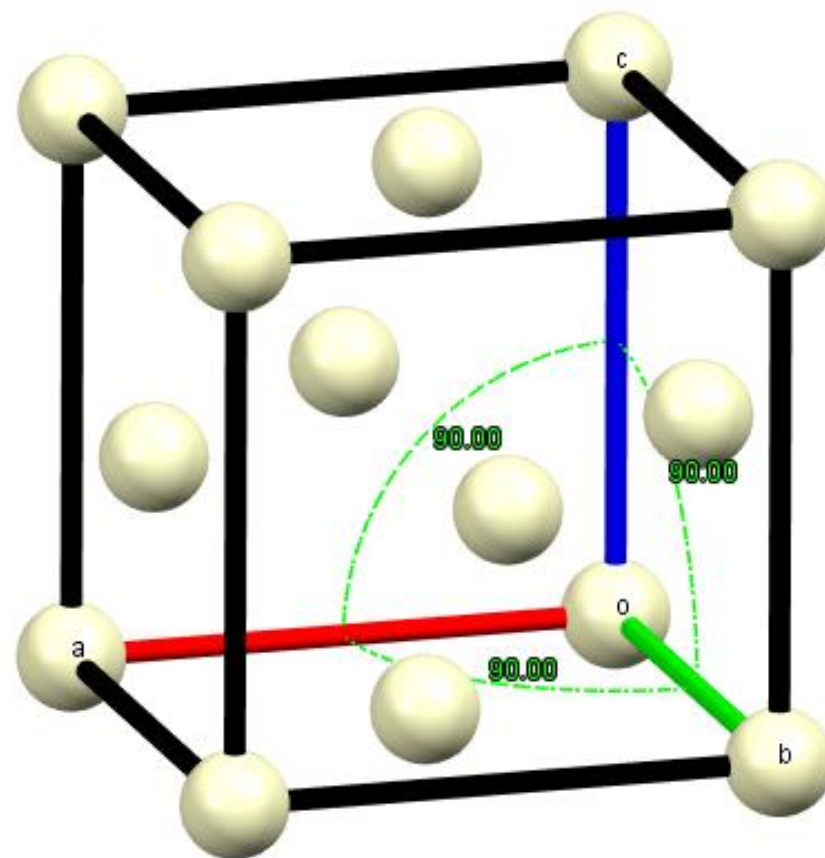
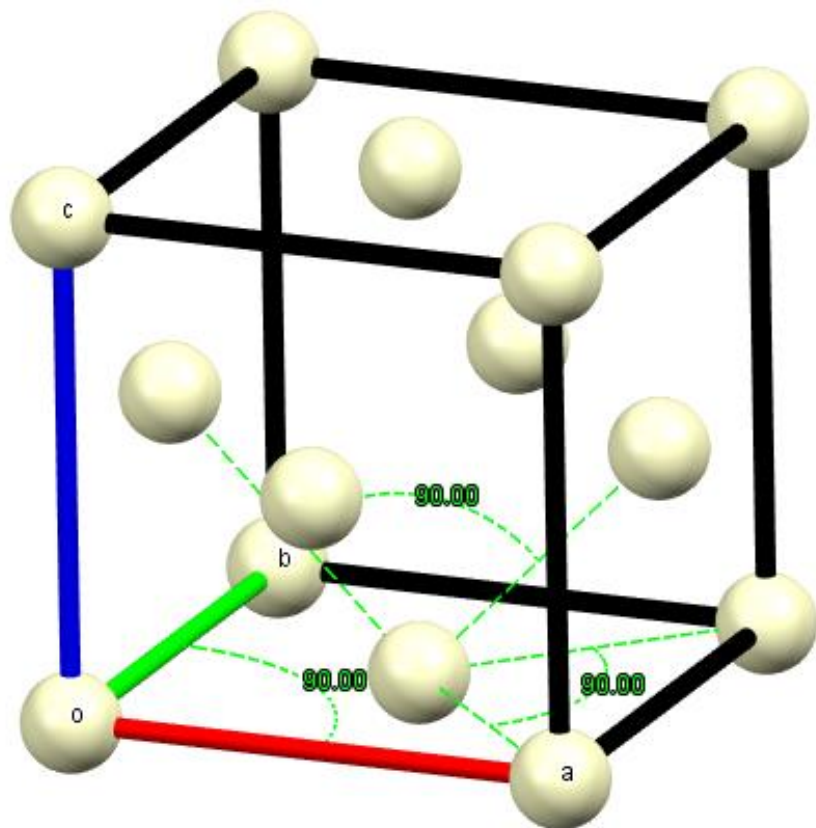
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Délky vazeb



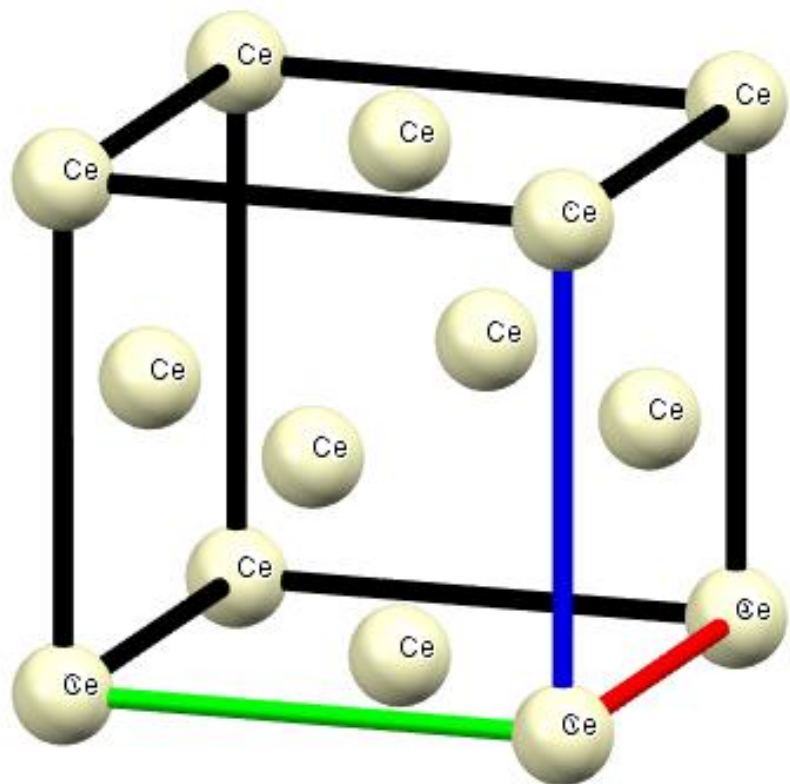
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Vazebné úhly



CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Koordinační čísla

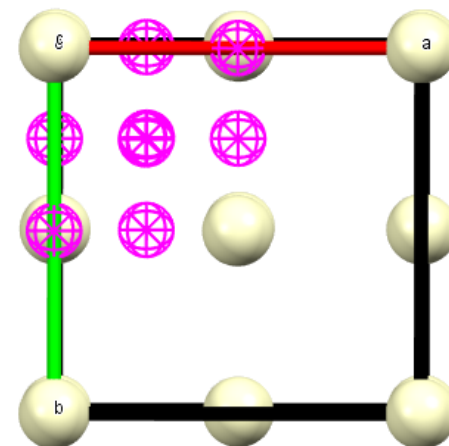
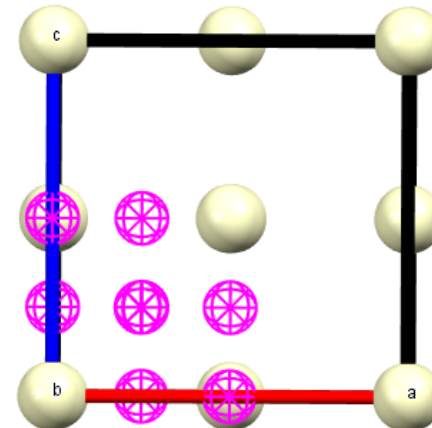
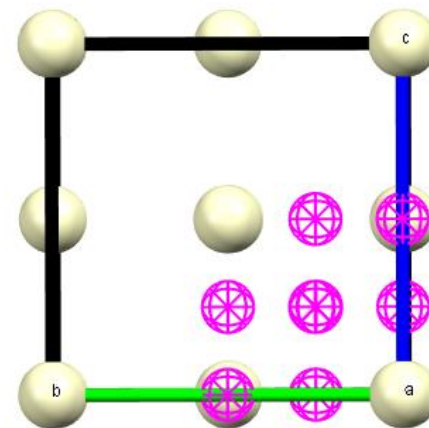
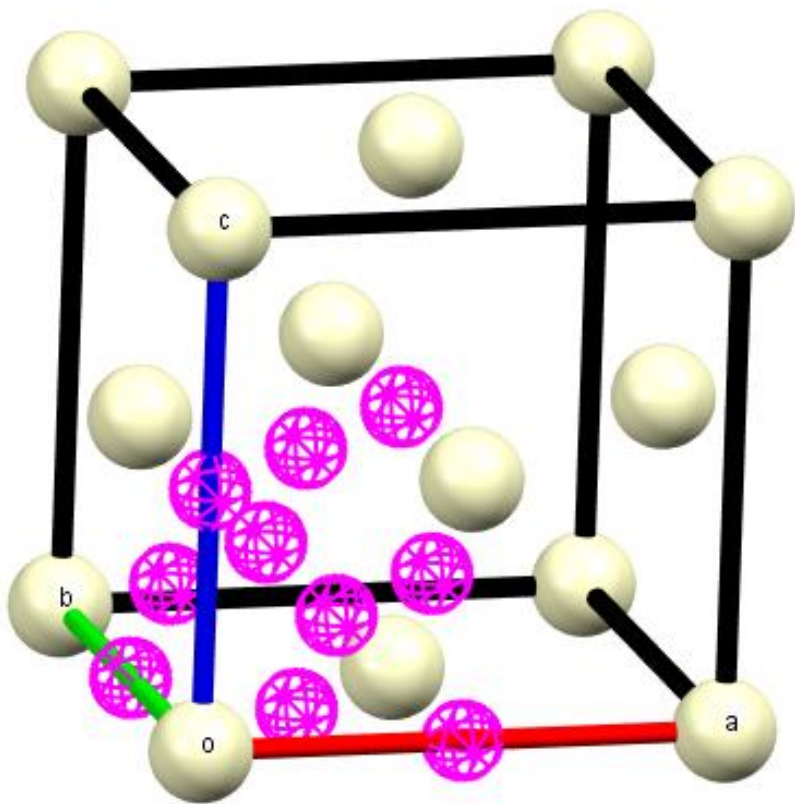


Ce (roh): 12

Ce (stěna): 12

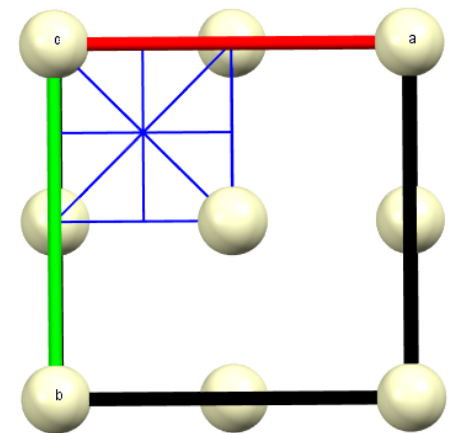
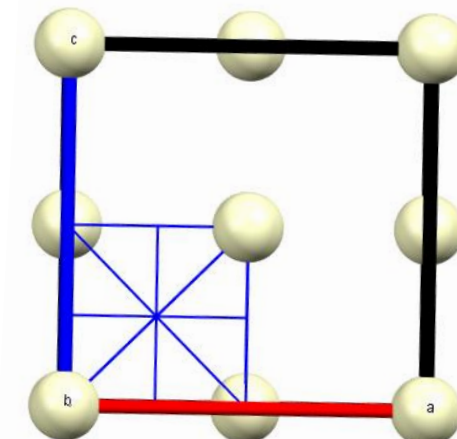
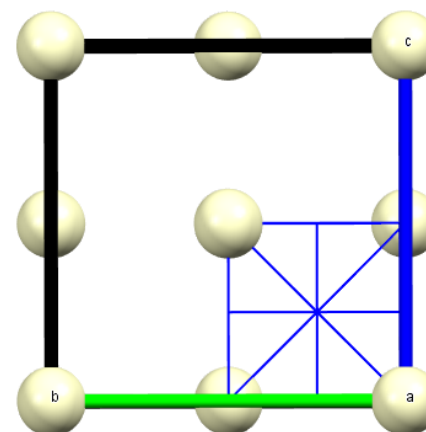
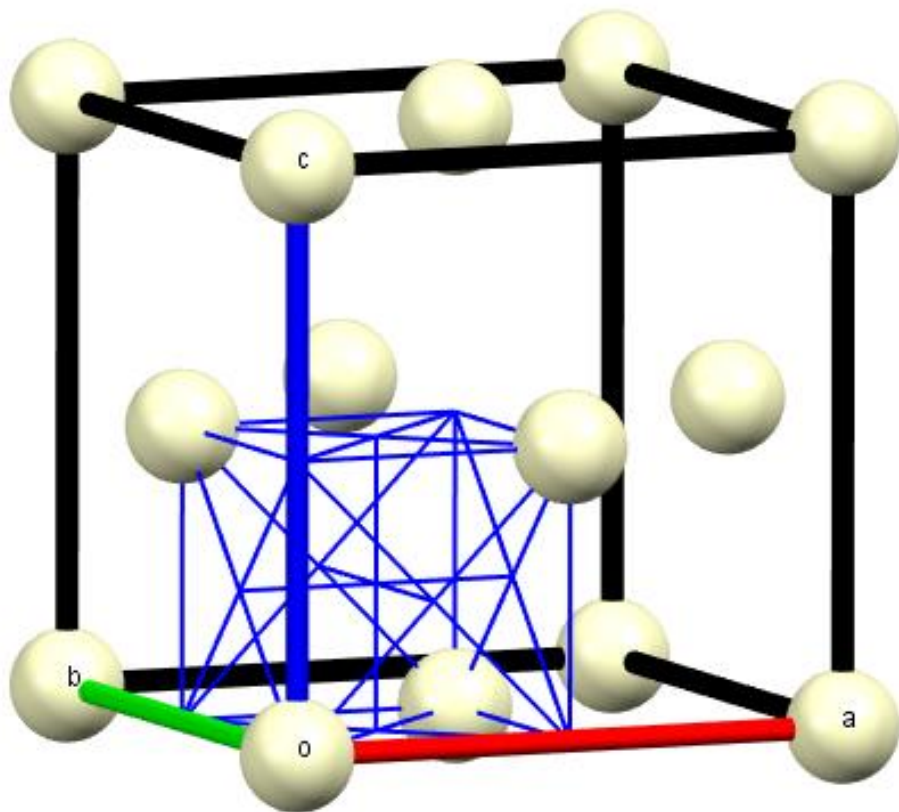
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Body inverze



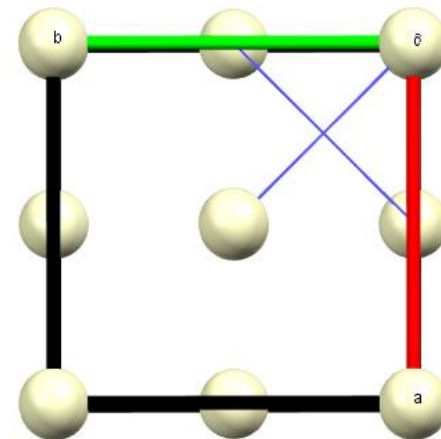
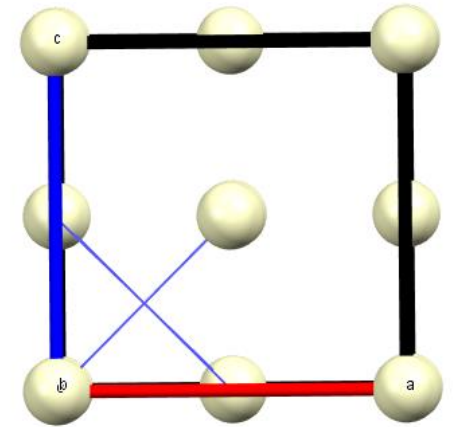
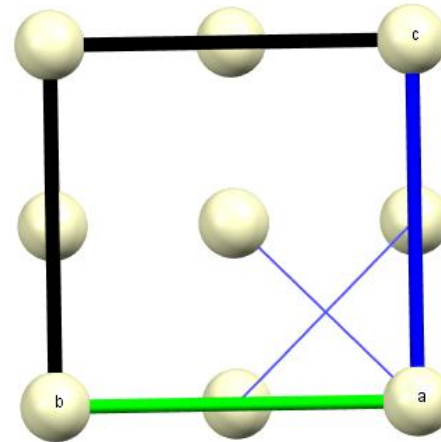
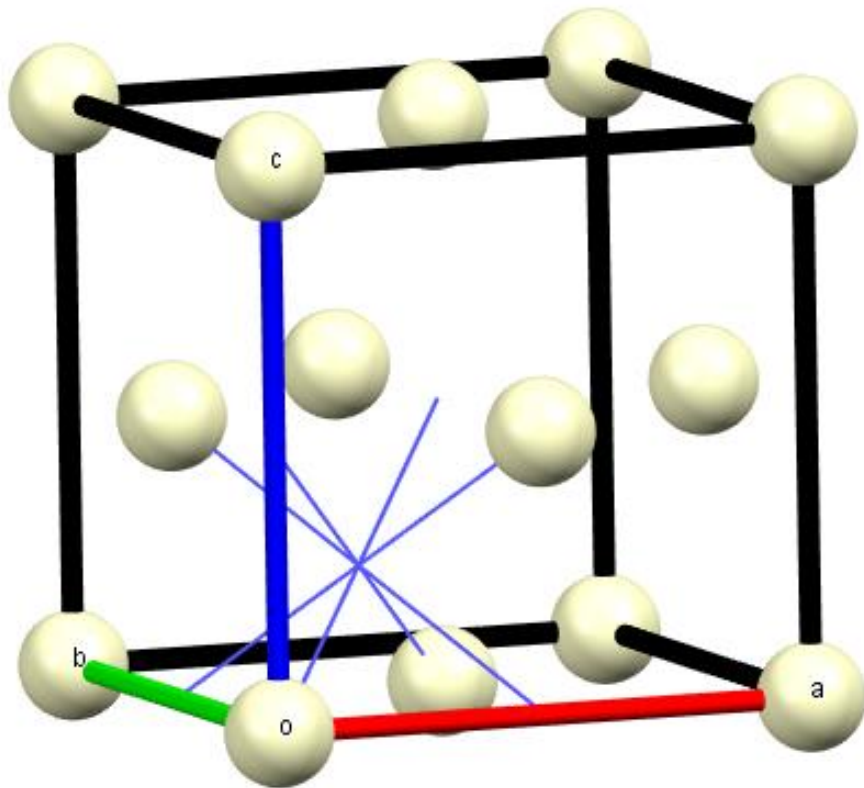
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Dvoučetné rotační osy (2-fold proper rotation axes)



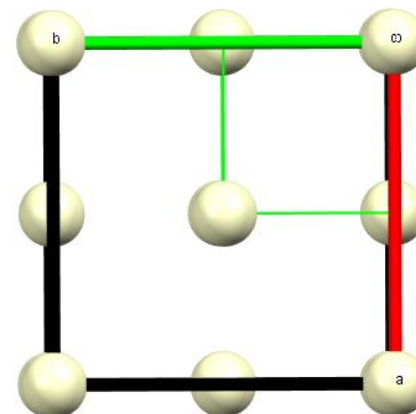
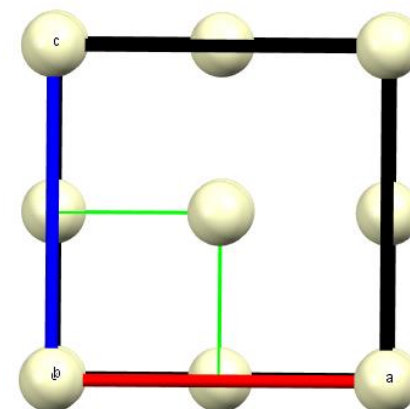
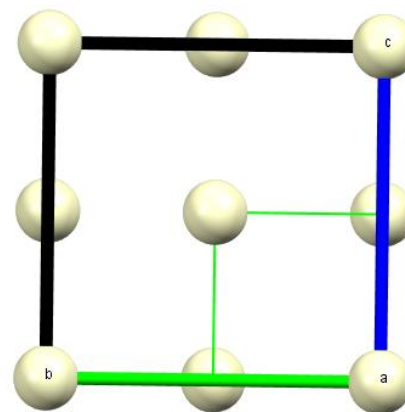
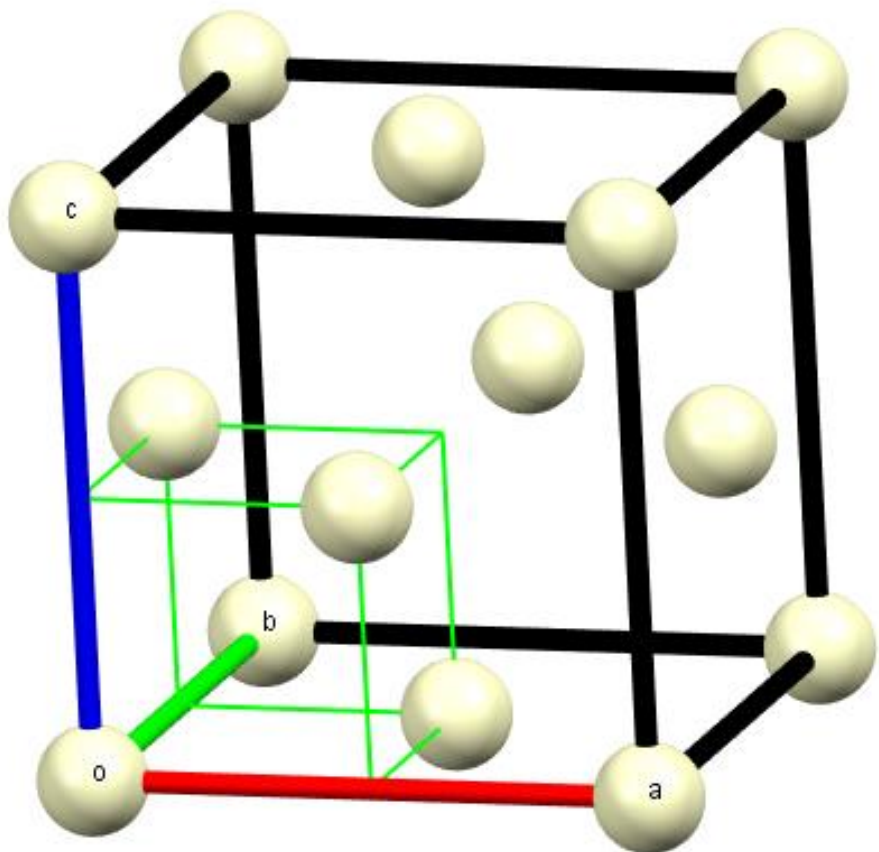
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Trojčetné rotační osy (3-fold proper rotation axes)



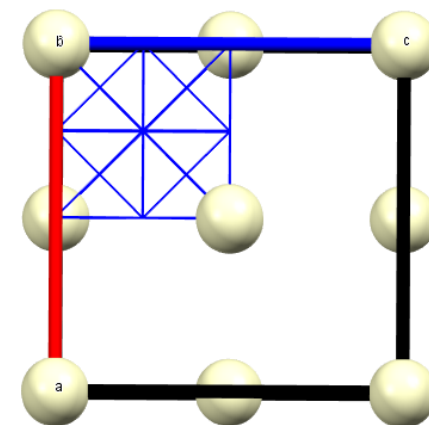
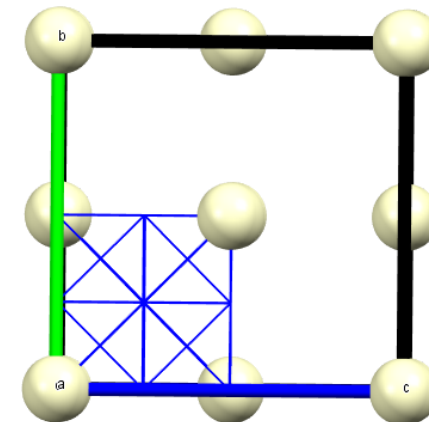
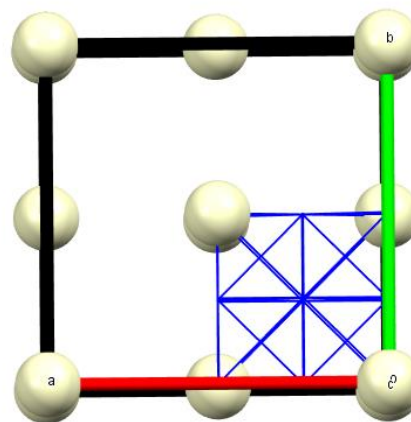
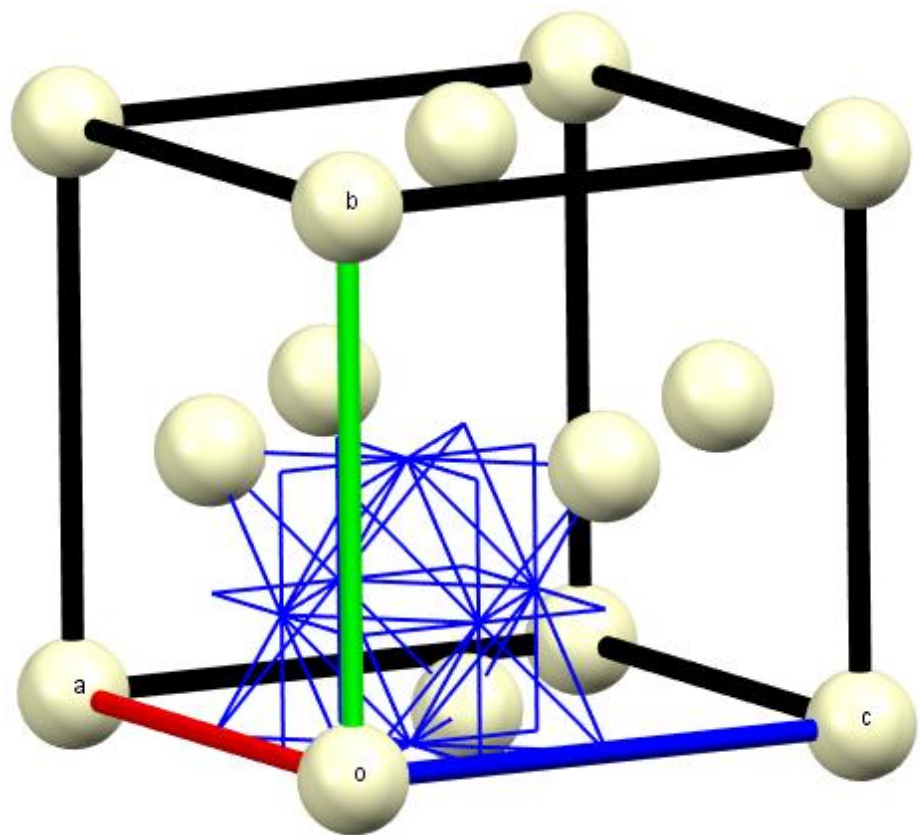
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Čtyřčetné rotační osy (4-fold proper rotation axes)



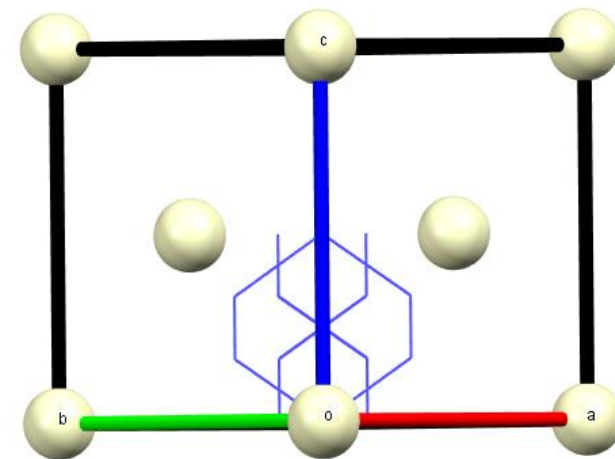
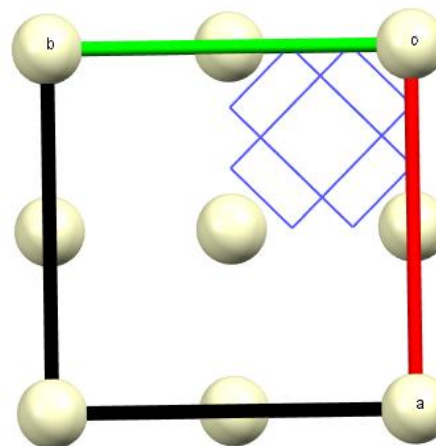
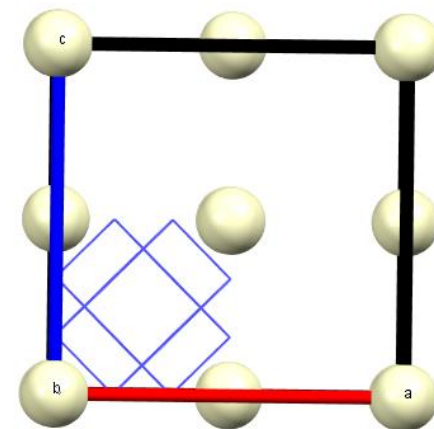
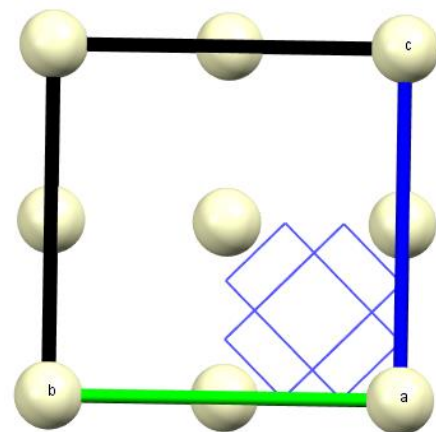
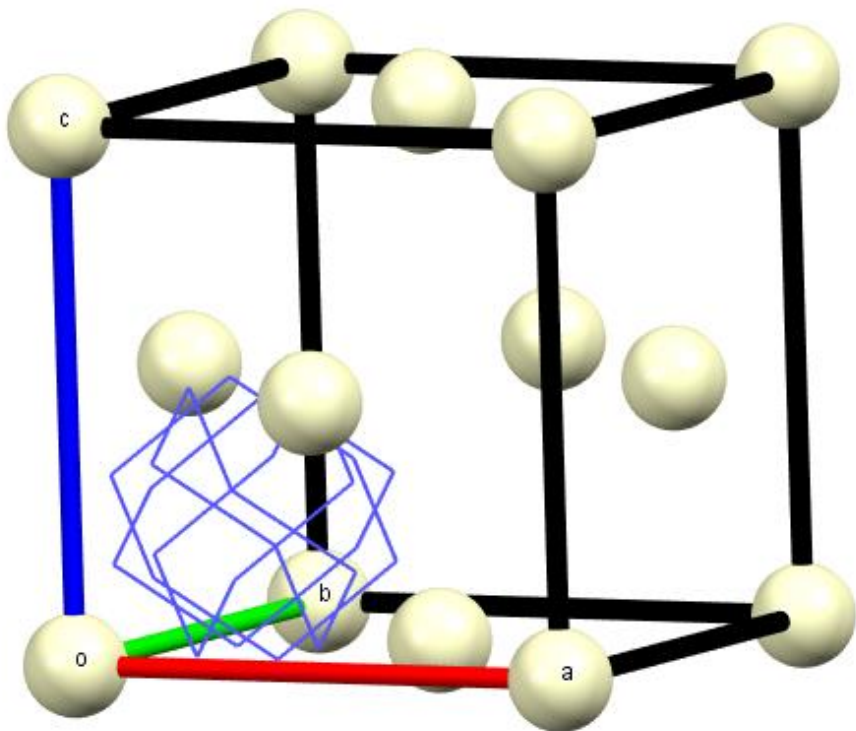
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Dvoučetné šroubové osy (2-fold screw axes)



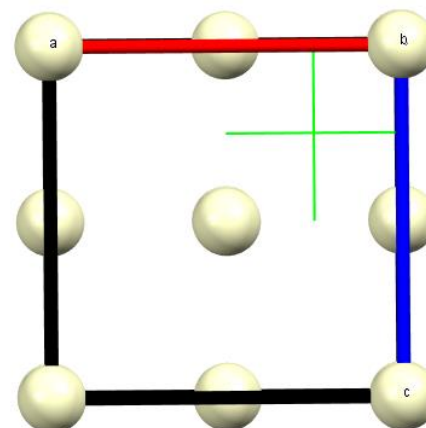
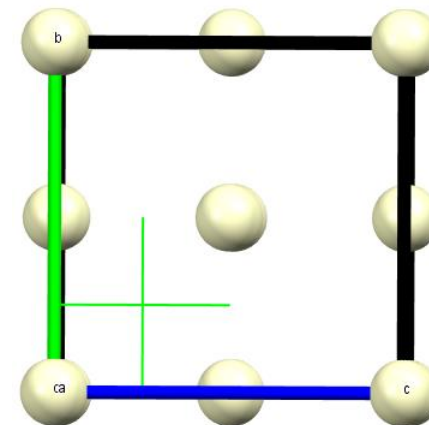
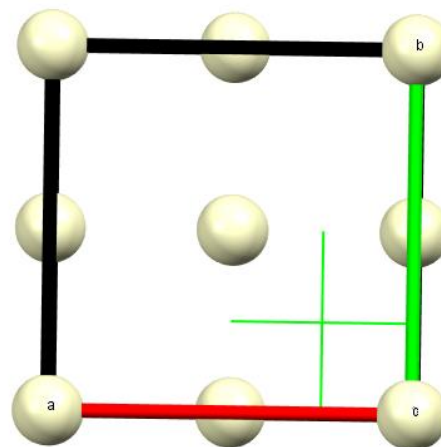
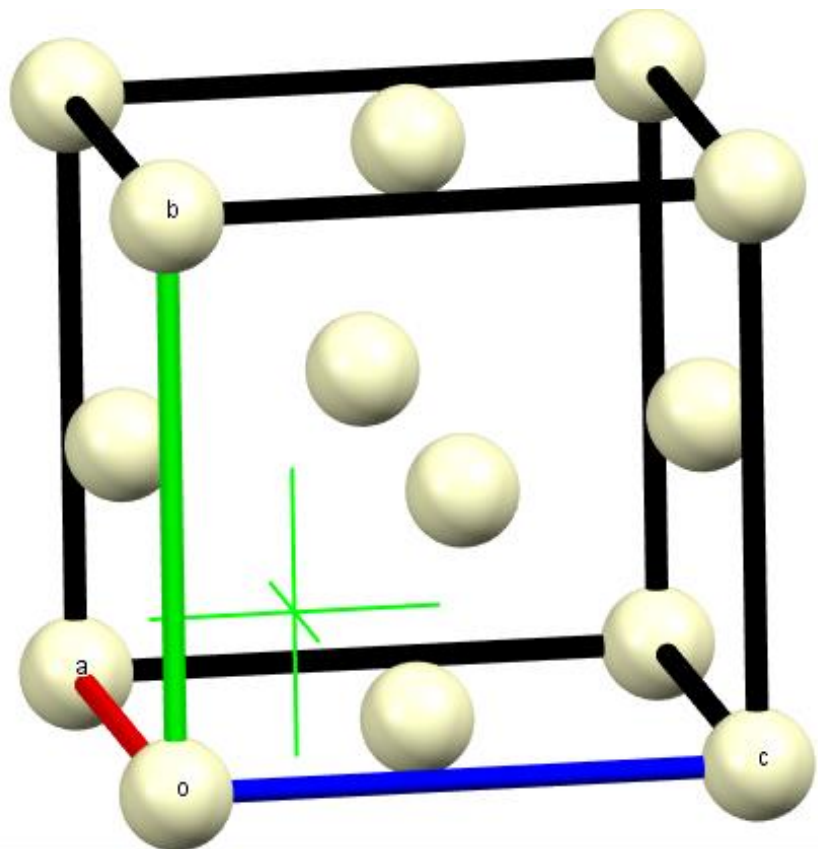
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Trojčetné šroubové osy (3-fold screw axes)



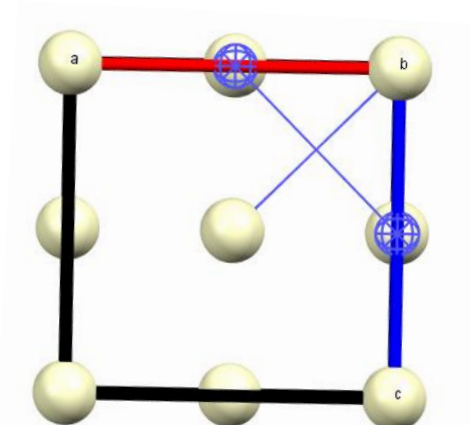
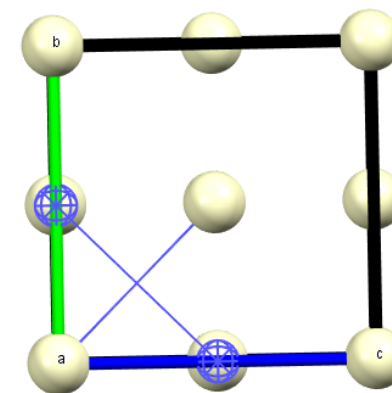
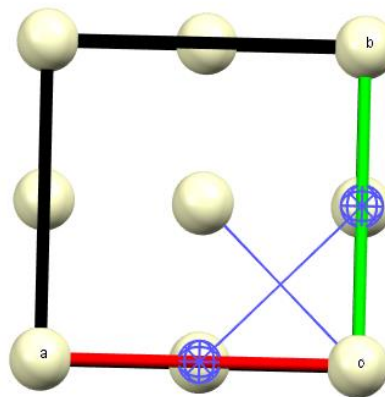
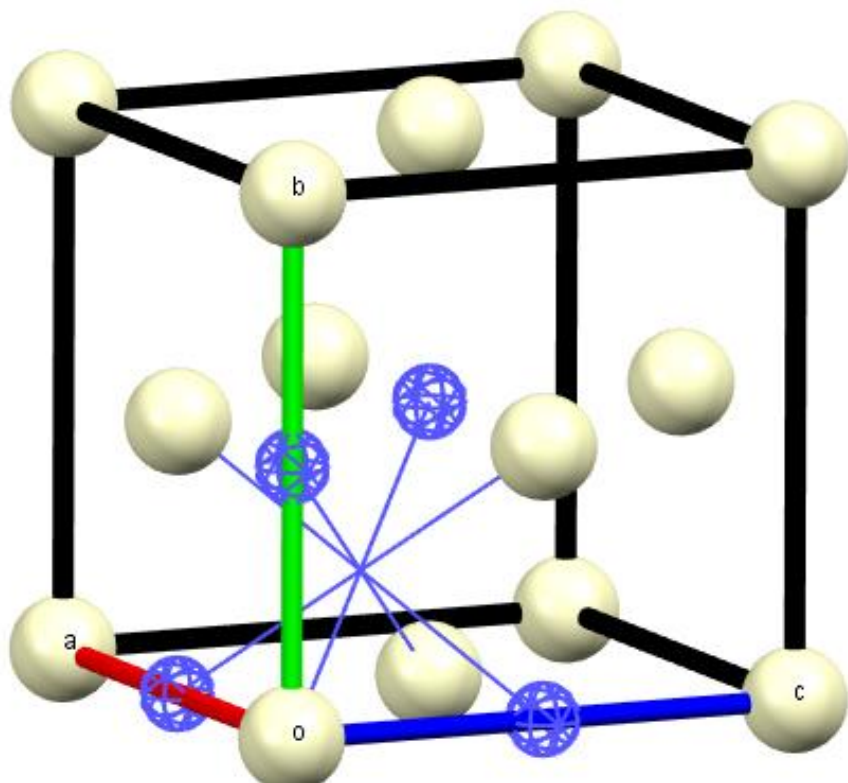
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Čtyřčetné šroubové osy (4-fold screw axes)



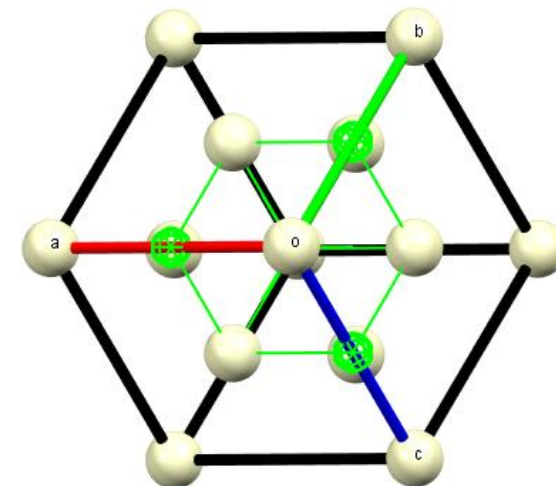
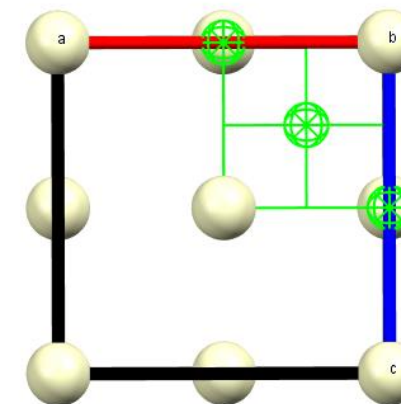
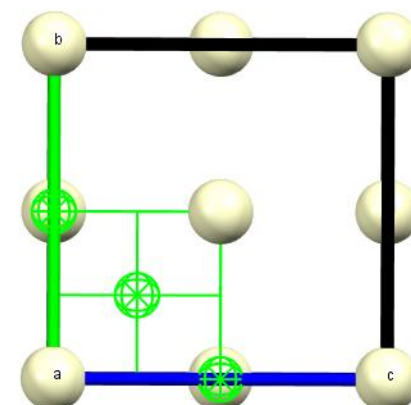
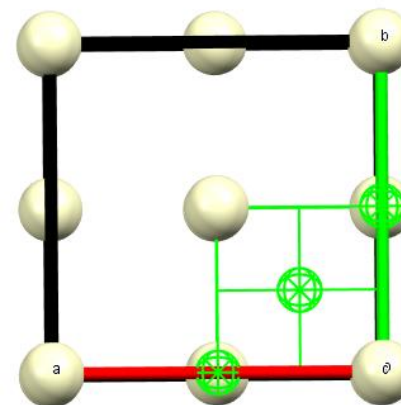
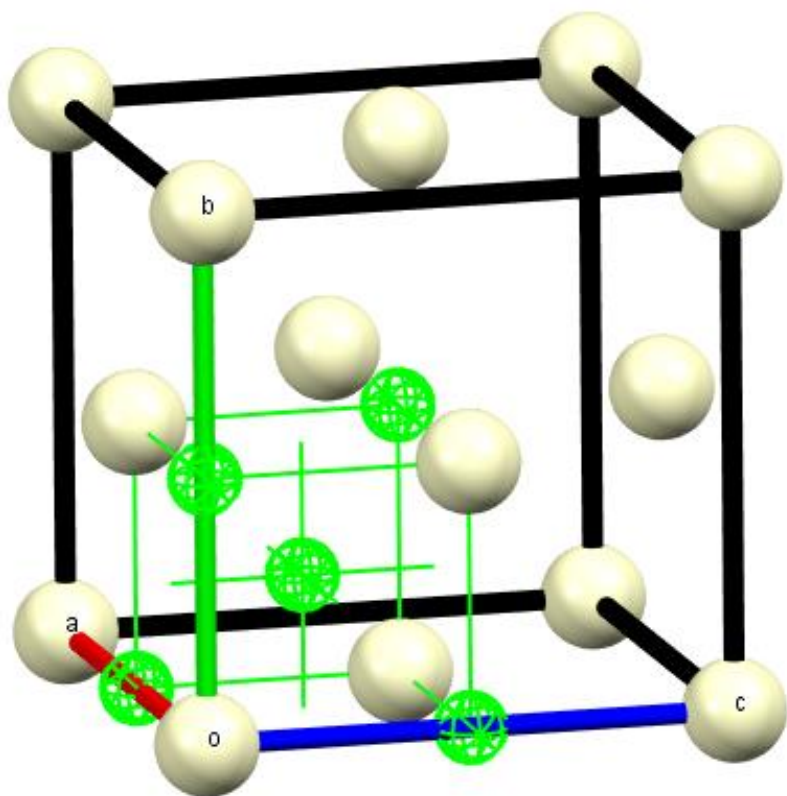
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Trojčetné rotačně inverzní osy (3-fold rotoinversion axes)



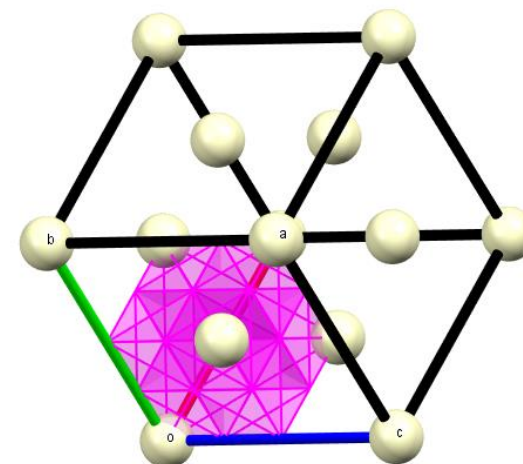
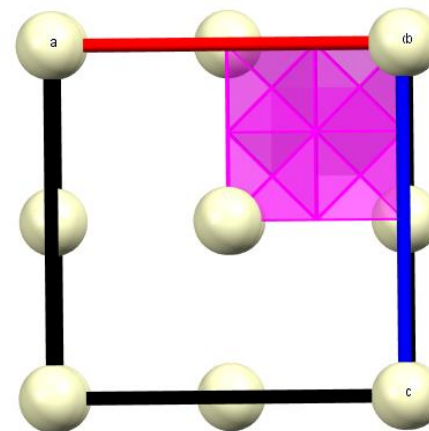
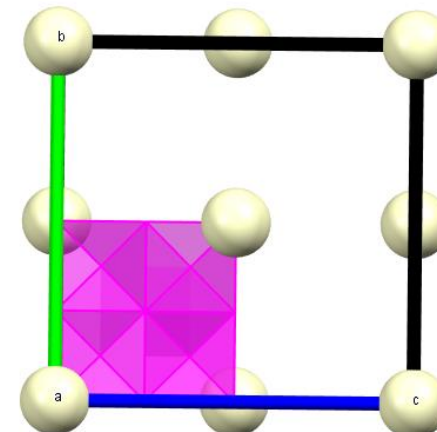
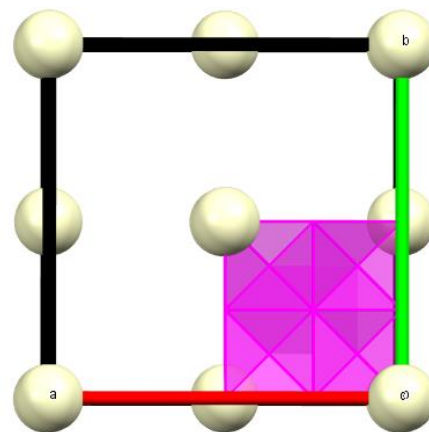
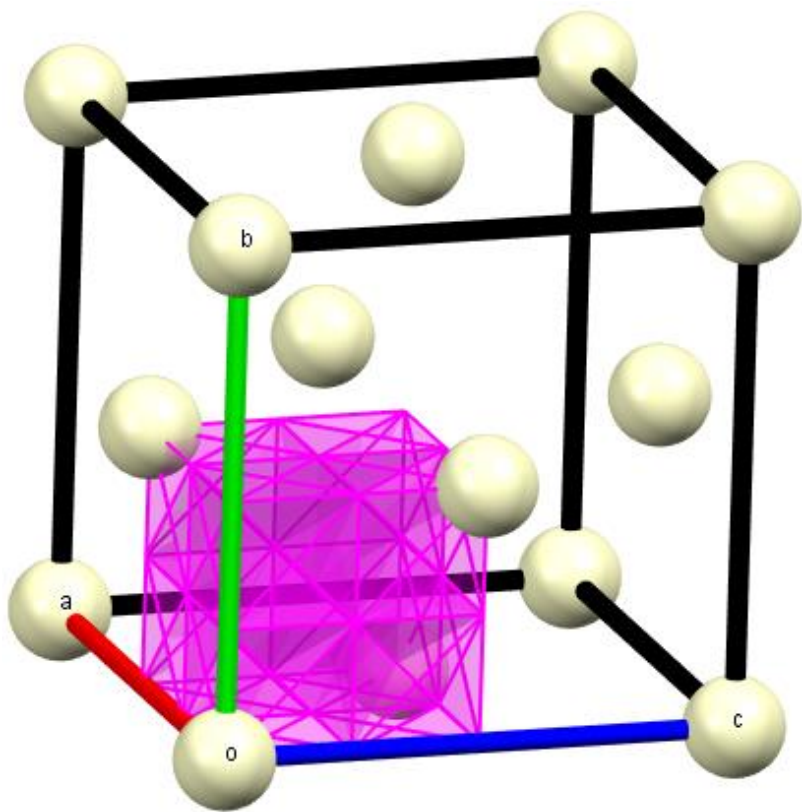
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Čtyřčetné rotačně inverzní osy (4-fold rotoinversion axes)



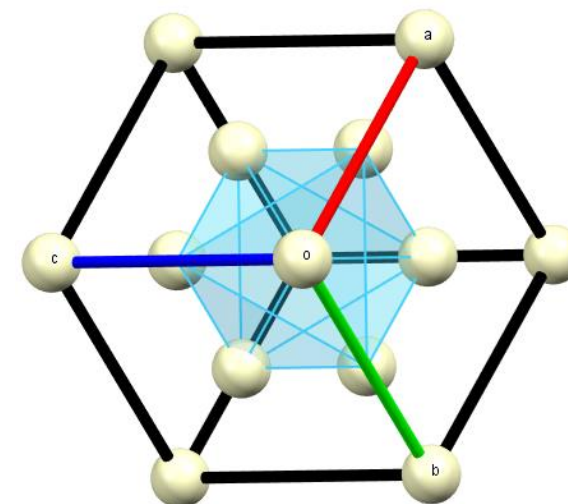
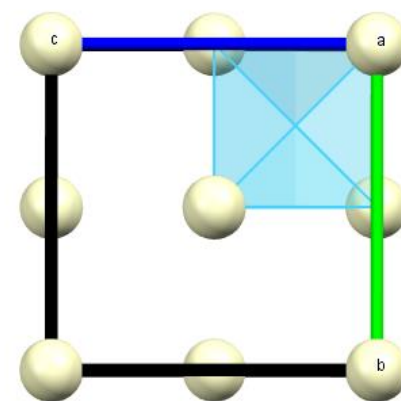
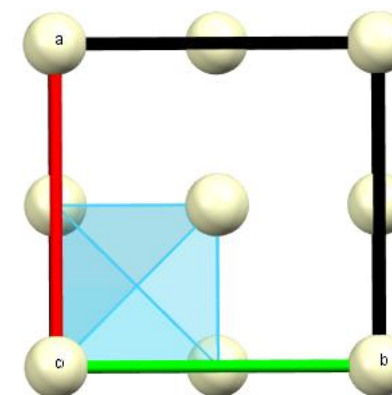
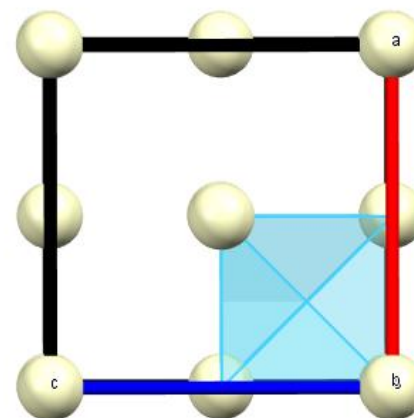
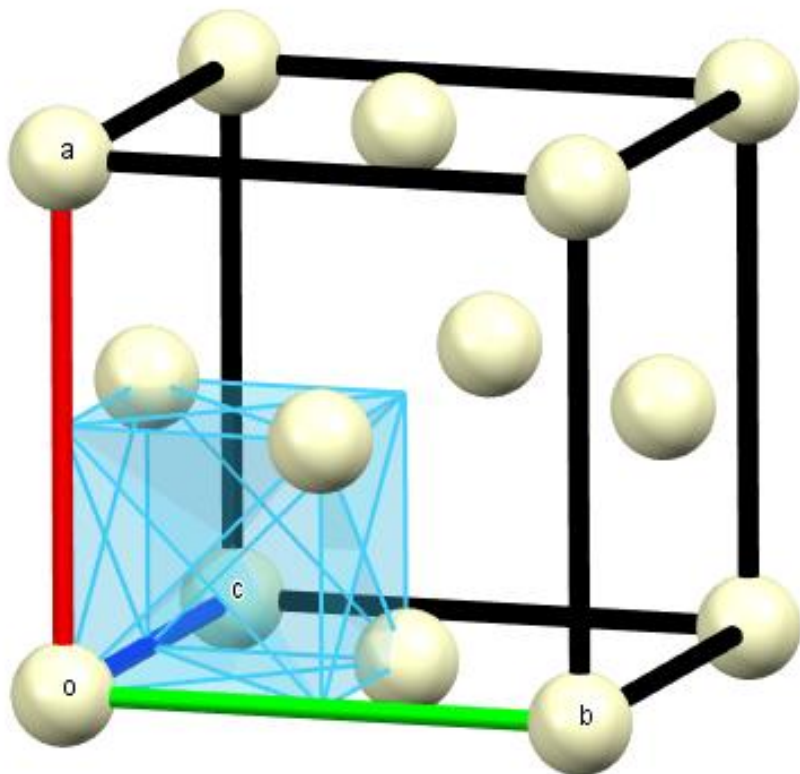
CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Roviny zrcadlení (mirror planes)



CER KUBICKÝ, PLOŠNĚ CENTROVANÝ

Skluzové roviny (glide planes)



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Prvky souměrnosti:

- body inverze

- osy rotace (dvoučetné, trojčetné)

- šroubové osy (dvoučetné)

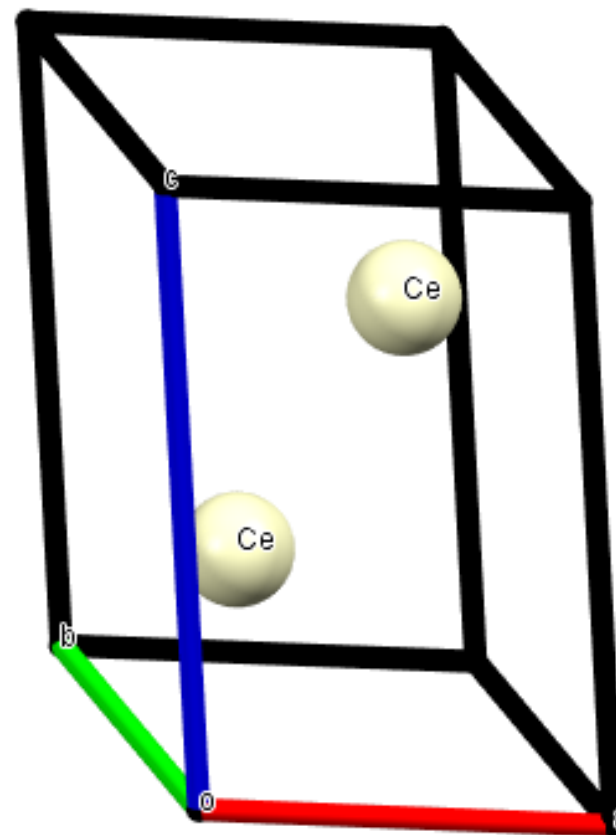
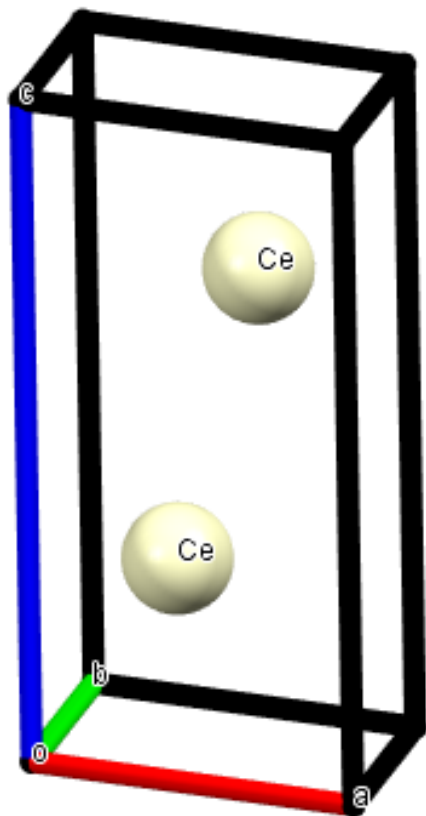
- rotačně inverzní osy (trojčetné, šestičetné)

- skluzové roviny

- roviny zrcadlení

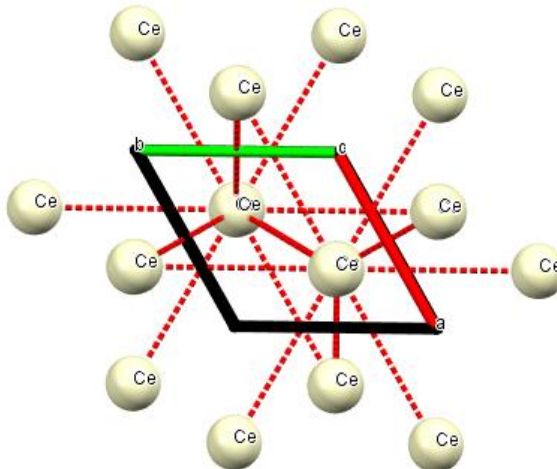
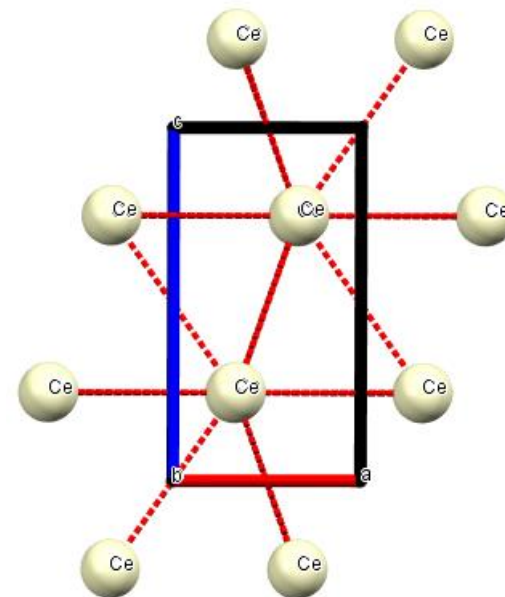
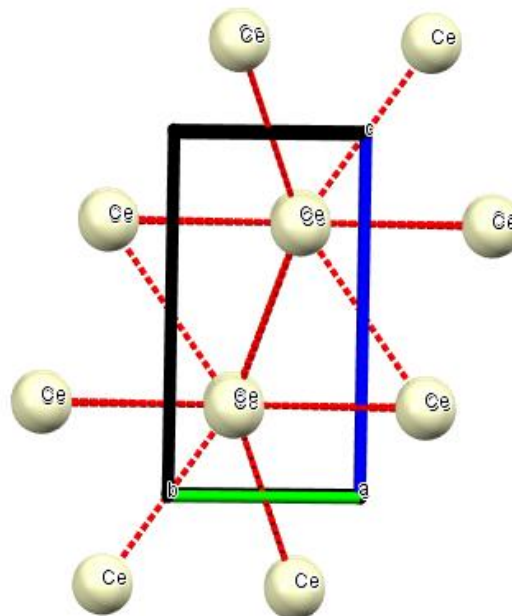
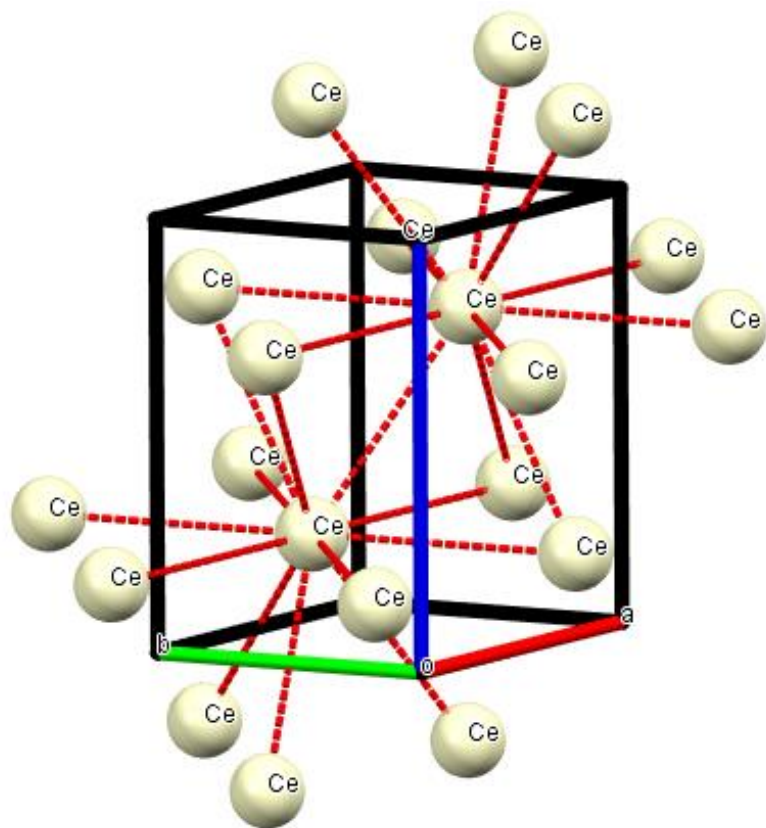
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Základní buňka



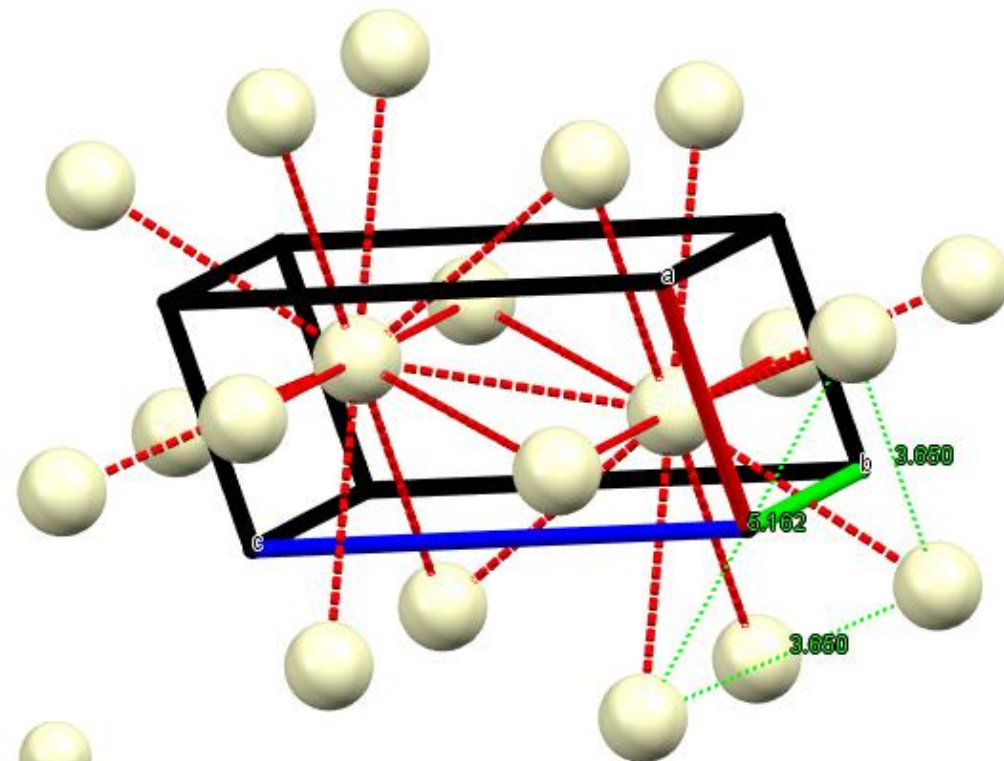
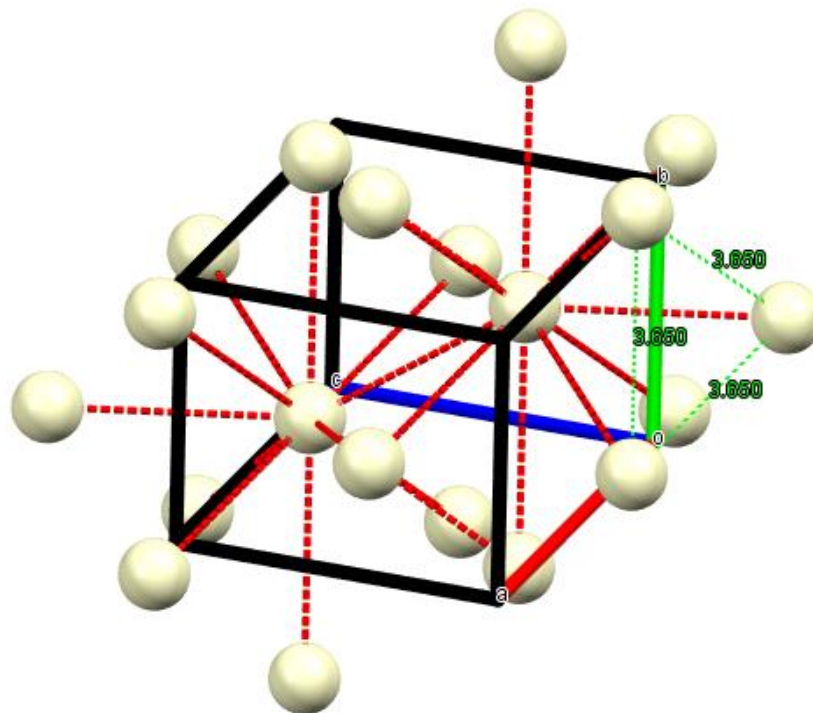
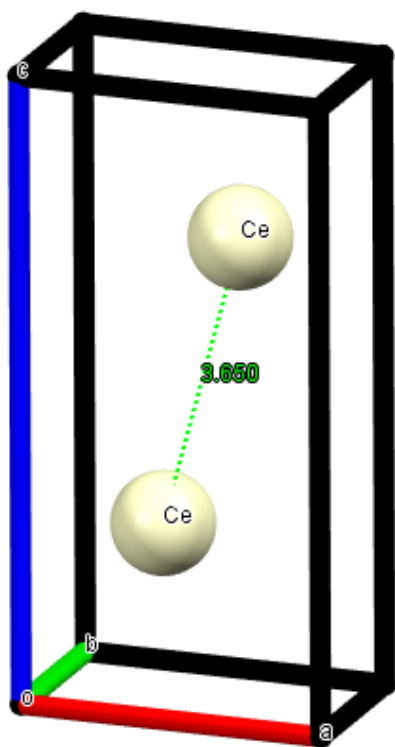
CER „JEDNOKLONNÝ“

Základní buňka s nejbližším okolím



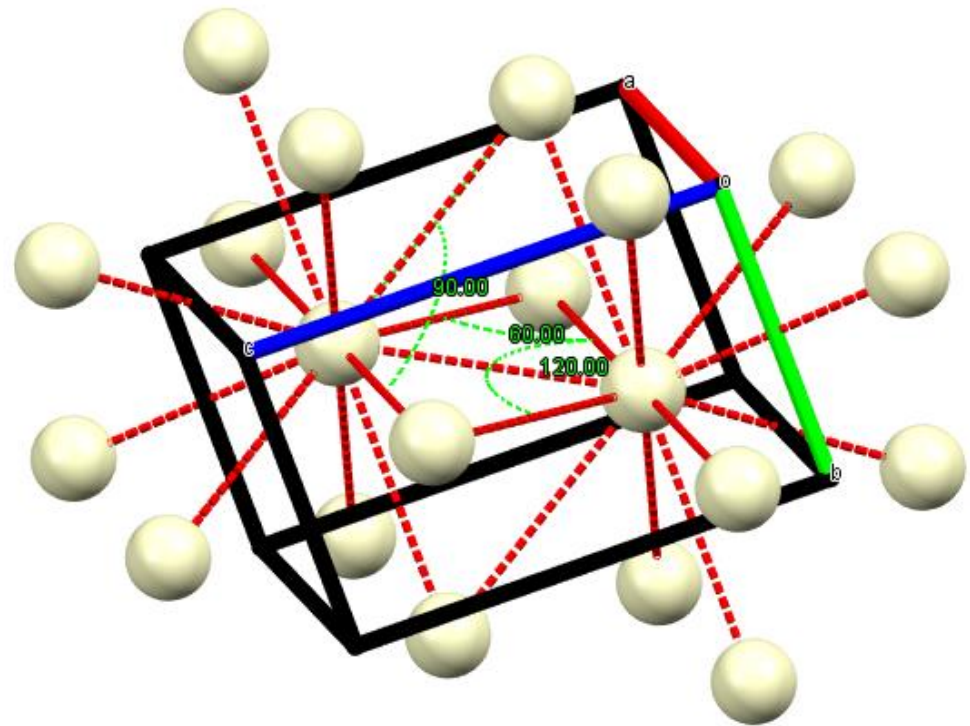
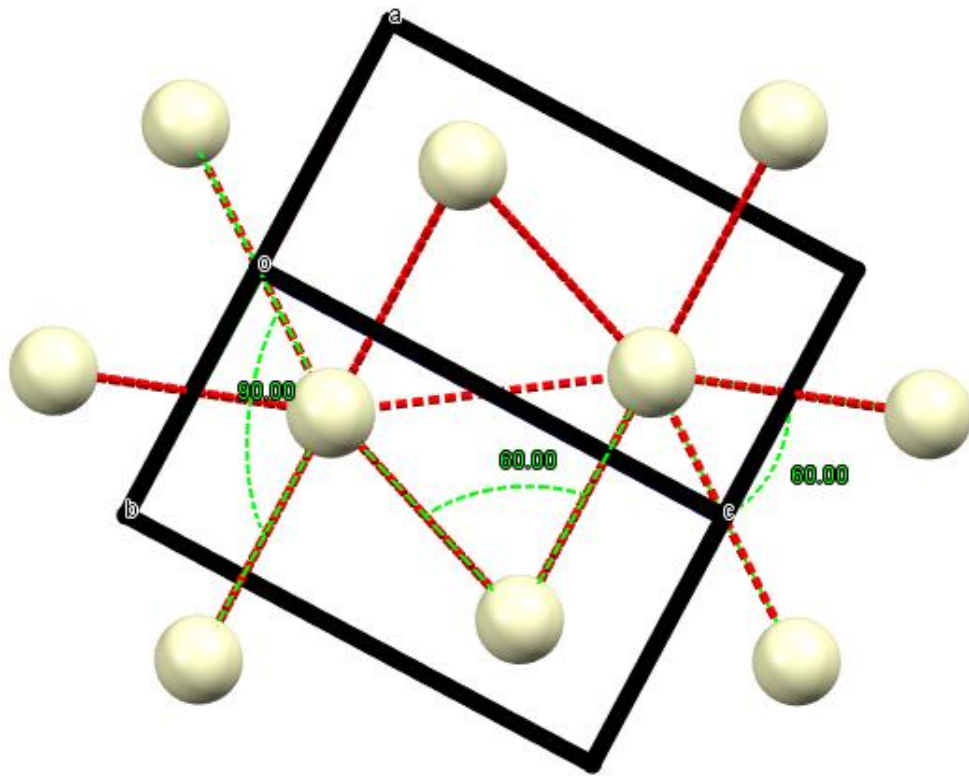
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Délky vazeb



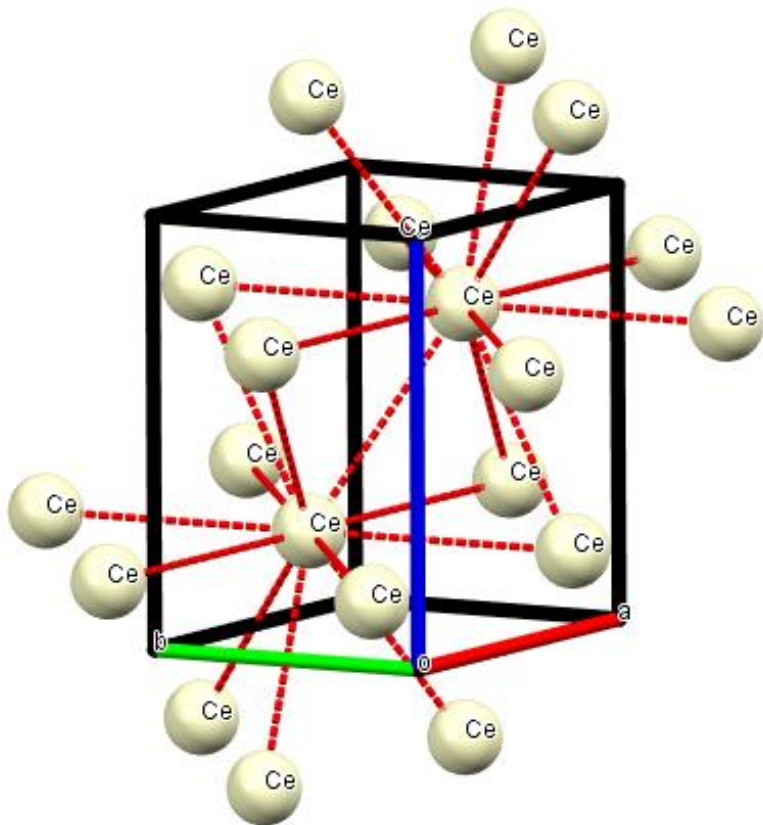
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Vazebné úhly



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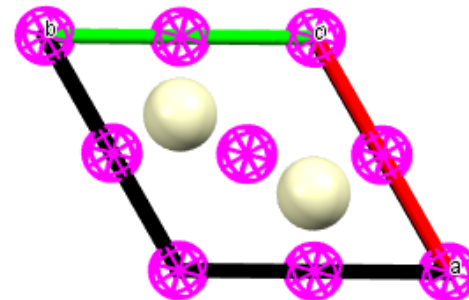
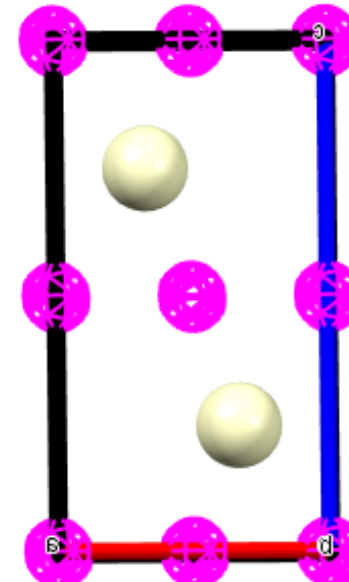
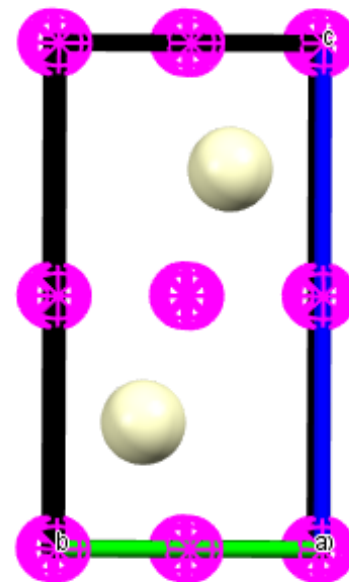
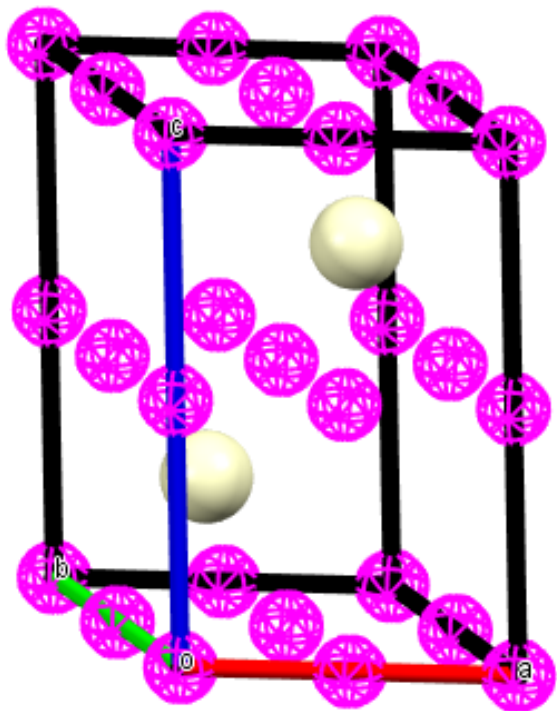
Koordinační čísla



Ce: 12

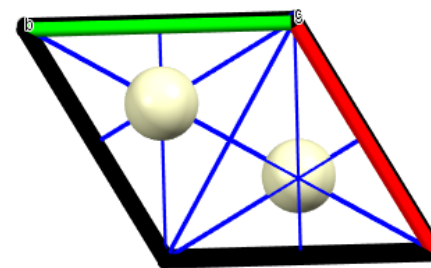
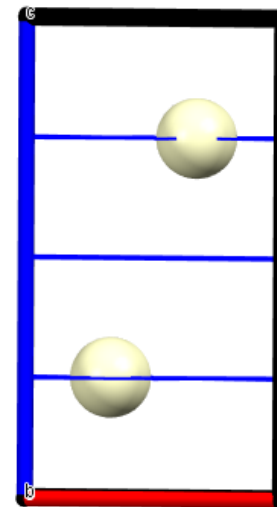
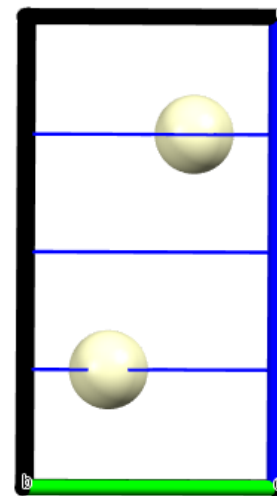
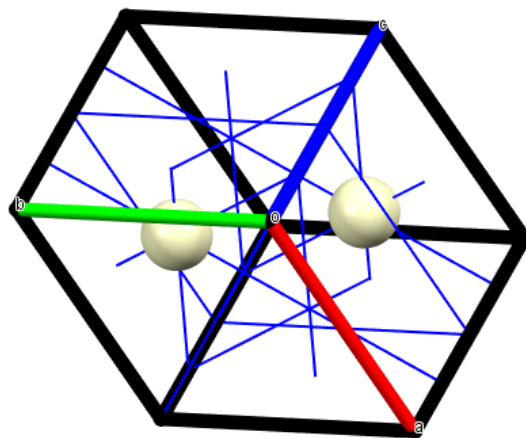
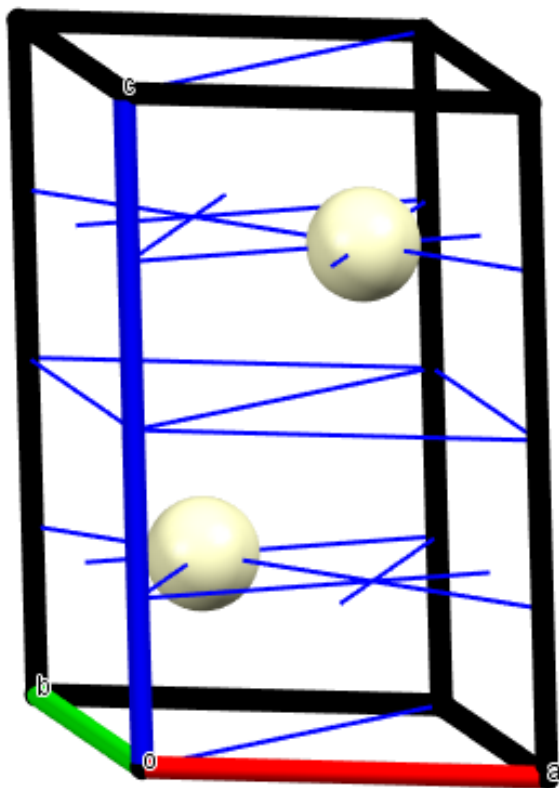
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Body inverze



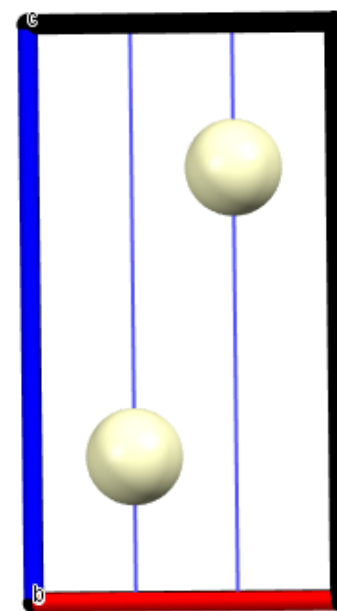
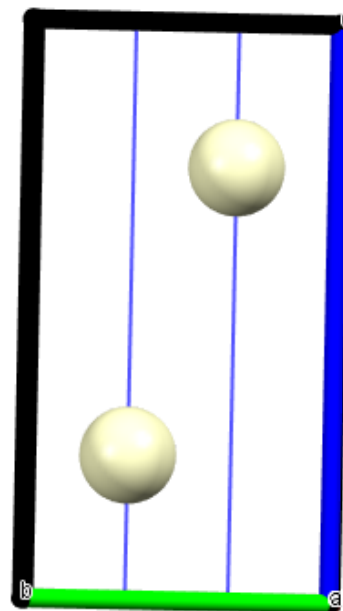
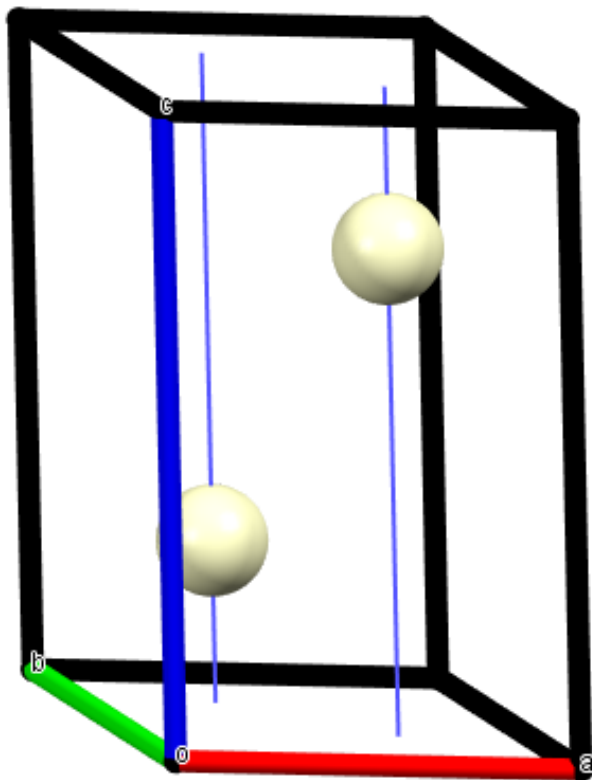
CER „JEDNOKLONNÝ“

Dvoučetné rotační osy (2-fold proper rotation axes)



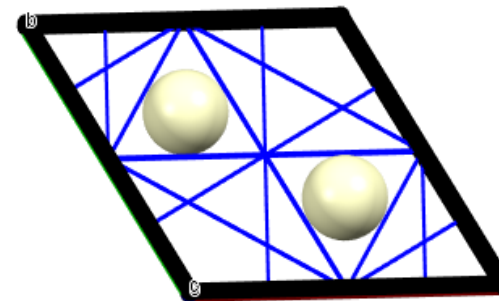
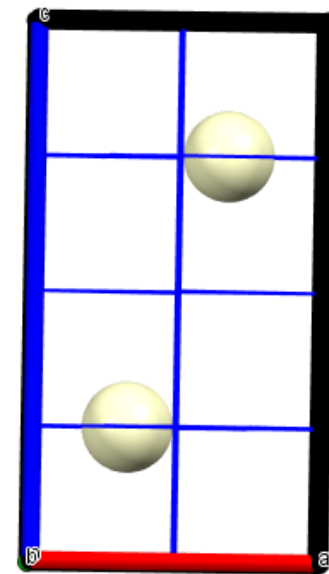
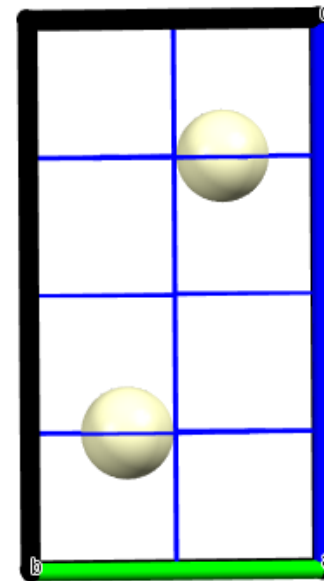
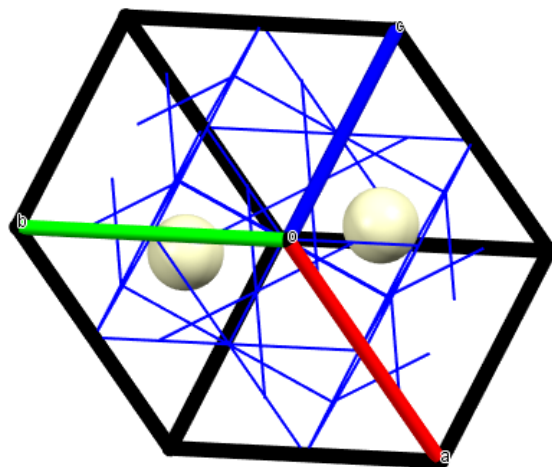
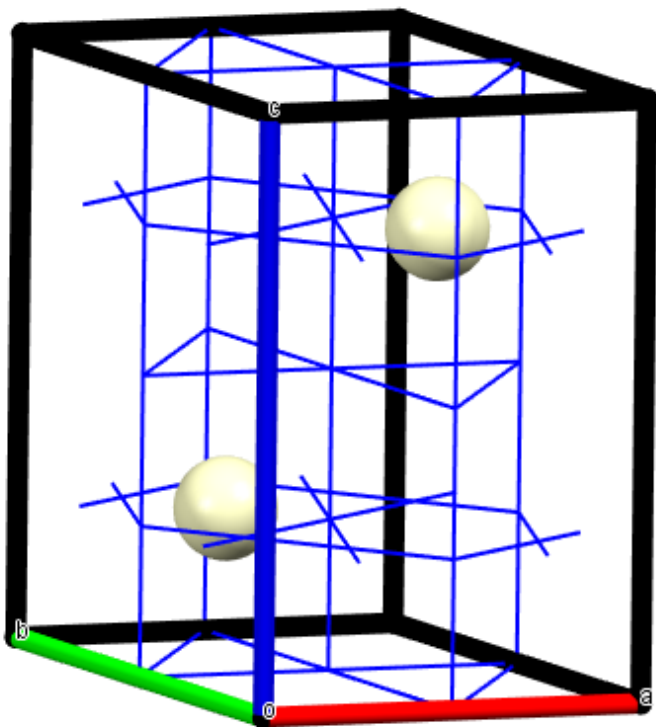
CER „JEDNOKLONNÝ“

Trojčetné rotační osy (3-fold proper rotation axes)



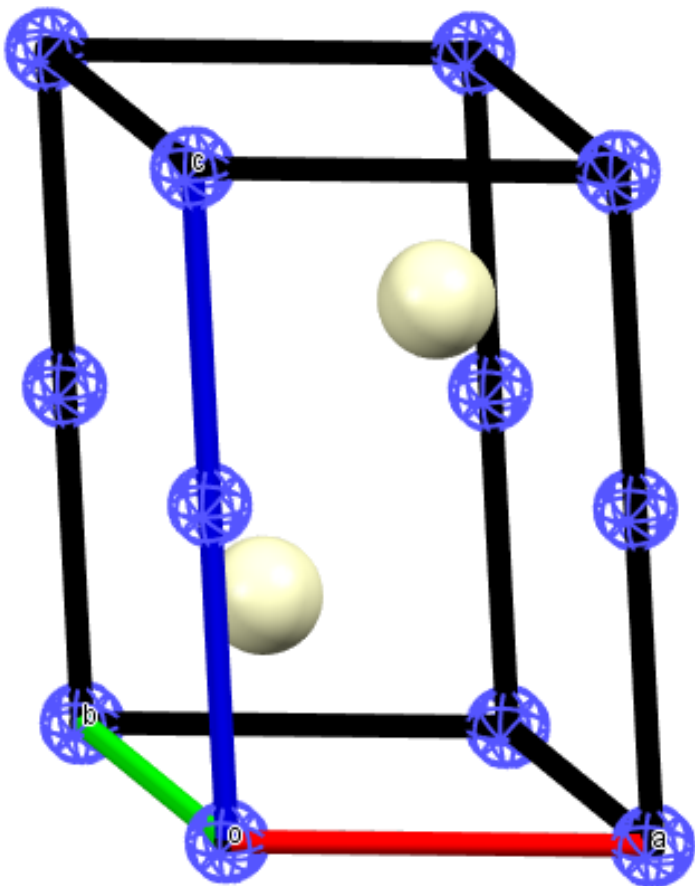
CER „JEDNOKLONNÝ“

Dvoučetné šroubové osy (2-fold screw axes)



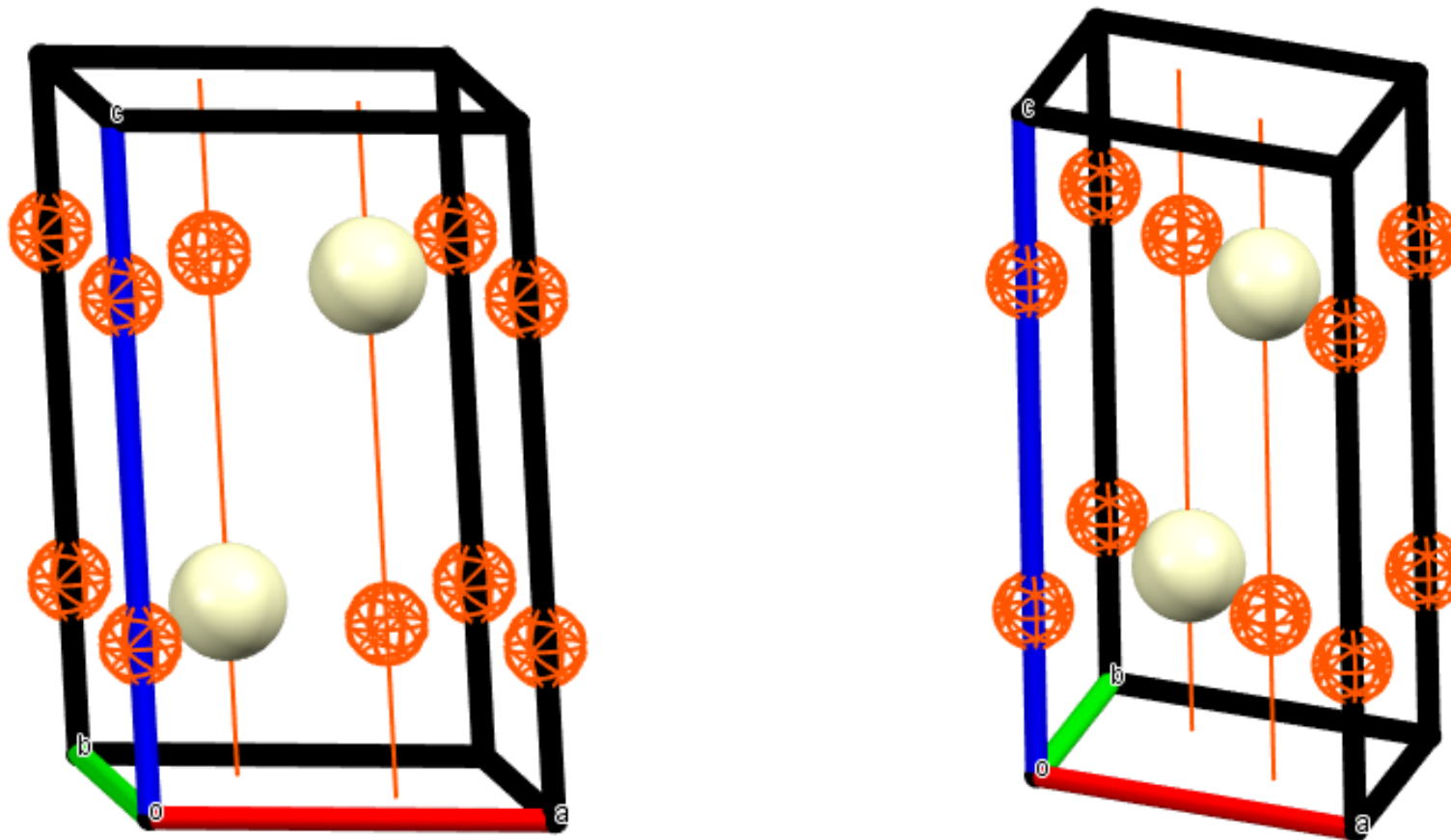
CER „JEDNOKLONNÝ“

Trojčetné rotačně inverzní osy (3-fold rotoinversion axes)



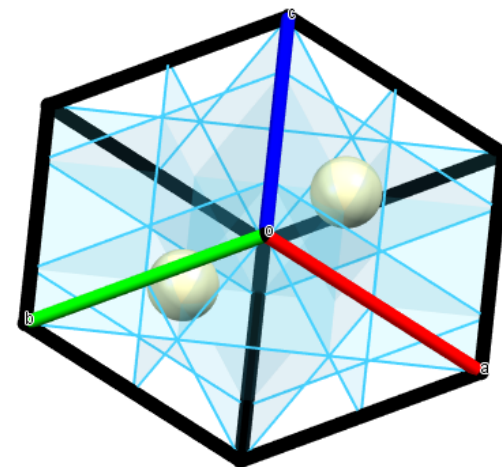
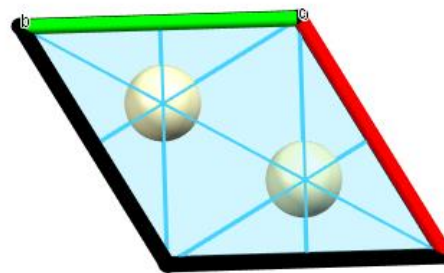
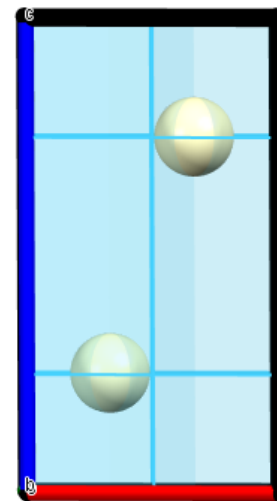
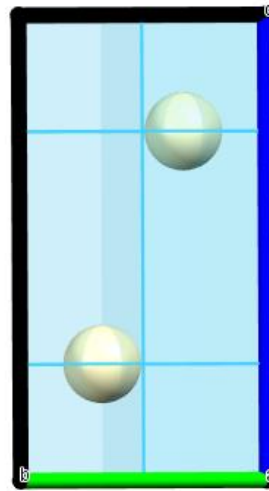
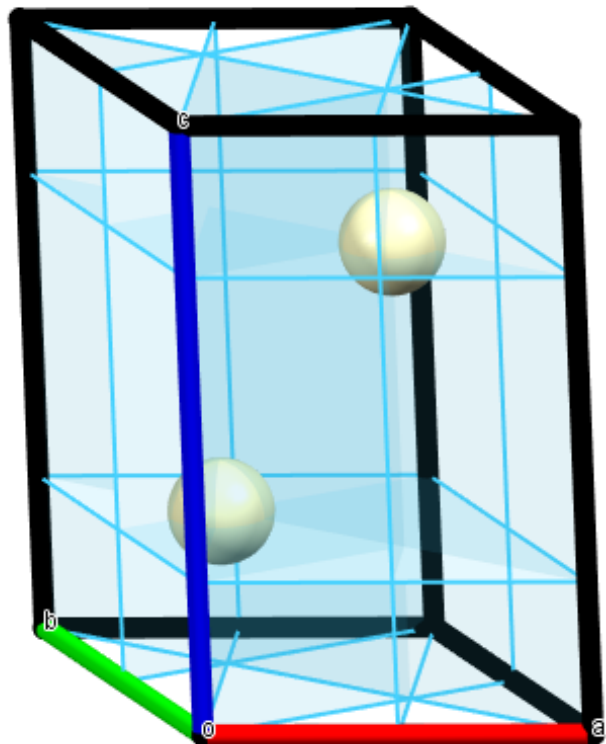
CER „JEDNOKLONNÝ“

Šestičetné rotačně inverzní osy (6-fold rotoinversion axes)



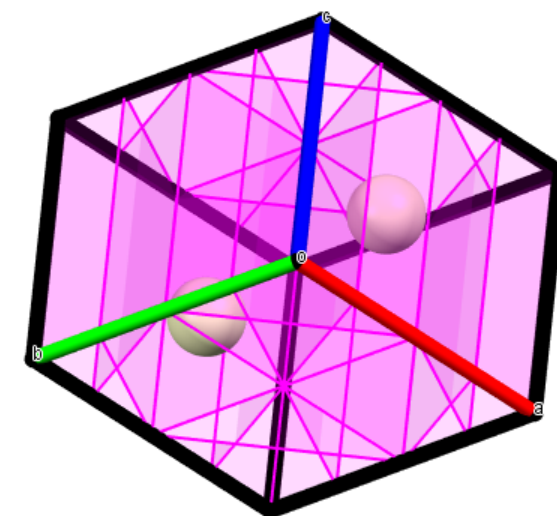
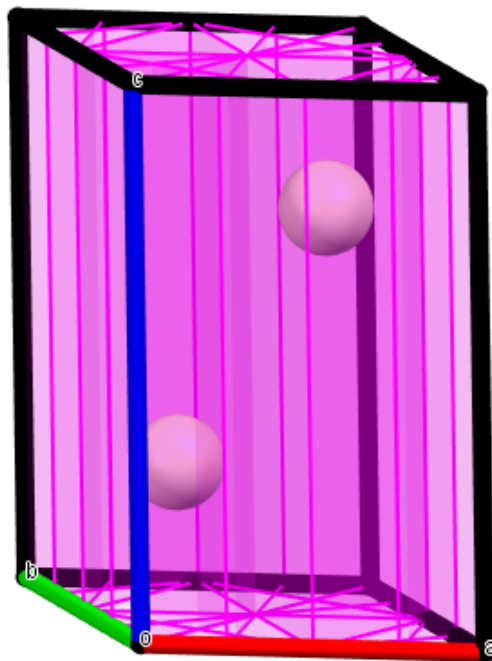
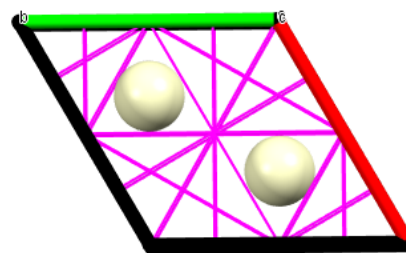
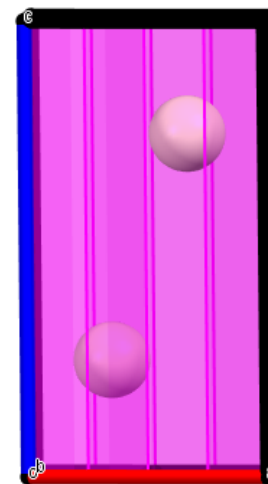
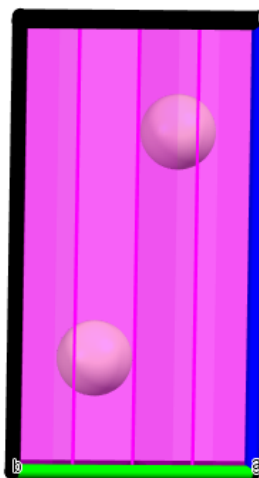
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Skluzové roviny (glide planes)



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Roviny zrcadlení (mirror planes)



POUŽITÁ LITERATURA

- [1] DEGGINGER, Phil. Kieserite, Evaporite. In: *Alamy* [online]. Abingdon, Oxon: Alamy Stock Photo, 2020 [cit. 2020-06-21]. Dostupné z: <https://1url.cz/nzR8I>
- [2] WIKIMEDIA COMMONS PŘÍSPĚVATELÉ. Soubor: Cerium2.jpg. In: *Wikimedia Commons* [online]. Wikimedia Commons, bezplatné úložiště médií., 2016 [cit. 2020-06-21]. Dostupné z: <https://1url.cz/CzR8g>
- [3] BREGEAULT, J., P. HERPIN, J. MANOLI a G. PANNETIER. Kieserite. In: *American Mineralogist Crystal Structure Database* [online]. Bulletin de la Societe Chimique de France, 1970 [cit. 2020-06-21]. Dostupné z: <https://1url.cz/gzR8X>
- [4] PŘÍSPĚVATELÉ WIKIPEDIE. Cer. In: *Wikipedie* [online]. Wikipedie: Otevřená encyklopedie., 2020 [cit. 2020-06-21]. Dostupné z: <https://1url.cz/lzR8S>
- [5] WYCKOFF, RWG. Cerium. In: *American Mineralogist Crystal Structure Database* [online]. New York: Interscience Publishers, 1963 [cit. 2020-06-21]. Dostupné z: <https://1url.cz/2zR8v>
- [6] WYCKOFF, RWG. Cerium. In: *American Mineralogist Crystal Structure Database* [online]. New York: Interscience Publishers, 1963 [cit. 2020-06-21]. Dostupné z: <https://1url.cz/gzR80>