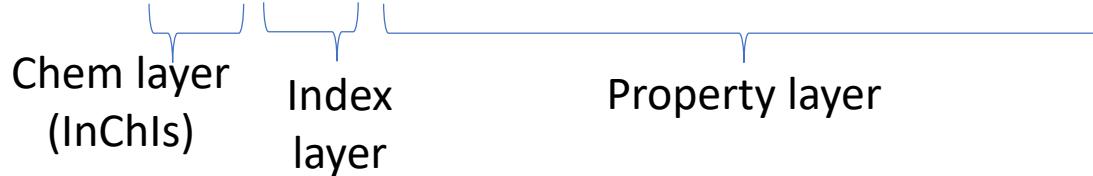


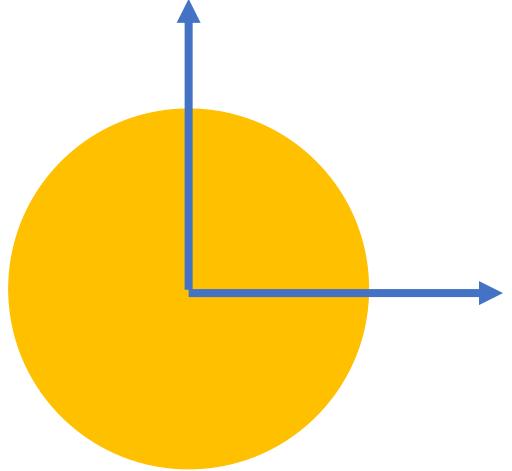
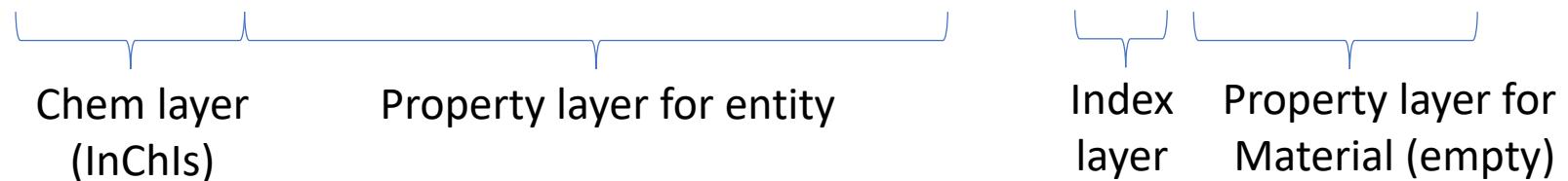
# 30nm gold nanoparticles (with citric acid stabilisation from synthesis)

NInChI=0.00.1A/Au/Nmsp/Ns0:15rxyz-9/Nk225/Ny1

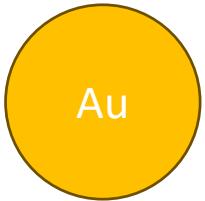
NInChI=0.00.2A/Au/**Nn1**/Nmsp/Ns0:15rxyz-9/Nk225



NInChI=0.00.3A/**InChI=1S**/Au/Nmsp/Ns0:15rxyz-9/Nk225/**Nn1**



# 30nm gold nanoparticles (with citric acid stabilisation from synthesis)



NInChI=0.00.1A/**Au**/*Nmsp/Ns0:15rxyz-9/Nk225!*

C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)  
*/Nmmol/No100*  
*/Ny1>2*

NInChI=0.00.2A/**Au**&

C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)  
*/Nn1>2/Nmsp&mol/Ns0:15rxyz-9&/Nk225&/No &100*

---

NInChI=0.00.3A/**InChI=1S/Au/Nmsp/Ns0:15rxyz-9/Nk225&**

**InChI=1S/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)**  
*/Nmmol*  
*/Ny1>2/No &100*

Morphology, size and crystallinity are properties of an entity (e.g. core)  
Occupation is properties of multiple entities (e.g ligands on surface of core)

# 30nm gold nanoparticles with citric acid and glycine stabilisation

NInChI=0.00.1A/**Au**/*Nmsp/Ns0:15rxyz-9/Nk225!*

C2H5NO2/c3-1-2(4)5/h1,3H2,(H,4,5)/*Nmmol/No50!*

C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)  
*/Nmmol/No50*

*/Ny1>{2&3}*

NInChI=0.00.2A/**Au**&

C2H5NO2/c3-1-2(4)5/h1,3H2,(H,4,5)&

C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)  
*/Nn1>{2&3}/Nm&sp&mol&mol/Ns0:15rxyz-9& &*  
*/Nk225& & /No &50&50*

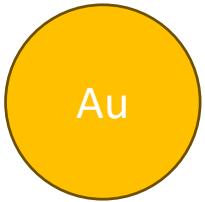
---

NInChI=0.00.3A/**InChI=1S/Au**/*Nmsp/Ns0:15rxyz-9/Nk225&*

*InChI=1S/C2H5NO2/c3-1-2(4)5/h1,3H2,(H,4,5)/Nmmol&*

*InChI=1S/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)*  
*/Nmmol*

*/Ny1>{2&3}/No &50&50*



# 30nm gold nanoparticles with citric acid and glycine stabilisation



Or even as Mixture InChI in a NInChI:

NInChI=0.00.3A/

InChI=1S/Au/Nmsp/Ns0:15rxyz-9/Nk225&

MInChI=0.00.\*S/

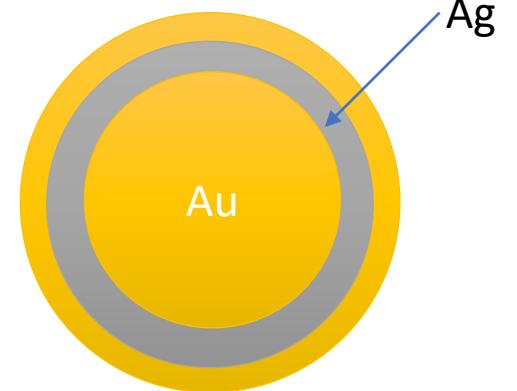
InChI=1S/C2H5NO2/c3-1-2(4)5/h1,3H2,(H,4,5)/Nmmol&

InChI=1S/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)/Nmmol

/Mn1&2/Mg50pp0&

/Nn1>2/No &100

This is not nice since we have NInChI layers in an entity, which can exist outside of a nanomaterial. But since we have the prefix InChI now, we could just remove it, since InChIs are only for molecular entities anyway. For the previous versions, this would mean that *Mm* is empty for entity 2 and 3.



# Gold / silver core shell

NInChI=0.00.1A/Ag/Nm{sp}/Ns{15:20rxyz-9}/No{100}/Nk{225}!

Au/Nm{sp}/Ns{0:15rxyz-9}/Nk{225}!

Au/Nm{sp}/Ns{20:25rxyz-9}/No{100}/Nk{225}!

C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)/Nm{mol}/No{100}  
/Ny{{2>>1}>>3}>4

NInChI=0.00.2A/Ag&

Au&

C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)

/Nn{{2>>1}>>2}>3

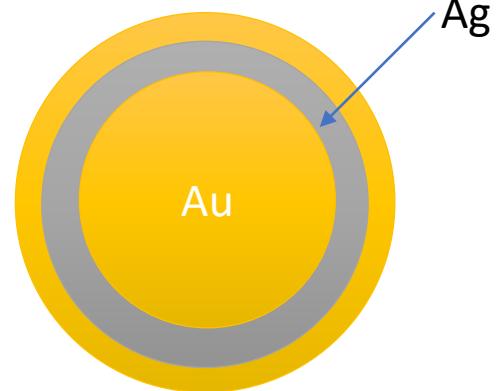
/Nm{sp&sp&sp&mol}

/Ns{0:15rxyz-9}&{15:20rxyz-9}&{20:25rxyz-9}&

/No &{100}&{100}&{100}

/Nk{225}&{225}&{225}&

# Gold / silver core shell



NInChI=0.00.3A/InChI=1S/Ag/Nmsp/Ns15:20rxyz-9/Nk225&

InChI=1S/Au/Nmsp/Ns0:15rxyz-9/Nk225&

InChI=1S/Au/Nmsp/Ns20:25rxyz-9/Nk225&

InChI=1S/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)/Nmmol

/Ny{{2>>1}>>3}>4/No &100&100&100

# Gold nanoparticle in dispersion (NInChI in a MInChI)



MInChI=0.00.\*S/

InChI=1S/H2O/h1H2

NInChI=0.00.3A/

InChI=1S/Au/Nmsp/Ns0:15rxyz-9/Nk225&

InChI=1S/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-  
2H2,(H,7,8)(H,9,10)(H,11,12)

/Nmmol

/Ny1>2/No &100

/Mn1&2/Mg &1mr0