PolyDis Manual ver. 2.6, 05.07.2018

D. Stoiber, R. Niewa: PolyDis: Simple Quantification Tool for Distortion of Polyhedra in Crystalline Solids, *Z. Kristallogr.* Submitted

Installation: Excel Add-in *Solver*

Open Microsoft Office Excel, go to **File → Options** and click on **Add-Ins** in the list on the left side. Next to **Manage** at the bottom is a dropdown box: chose **Excel-Add-Ins** and click **Go**. Check the box next to *Solver* and click OK.

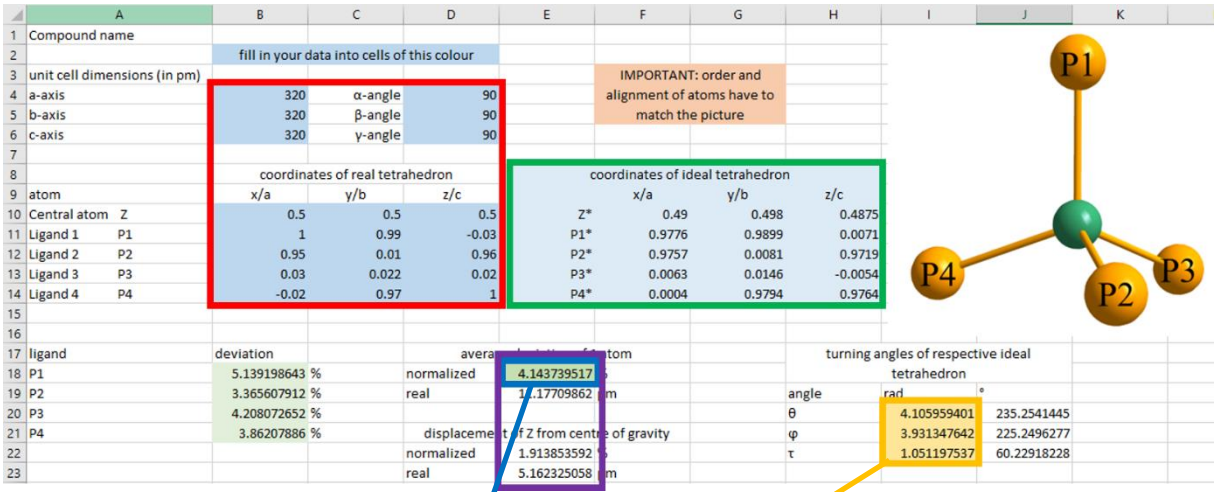
PolyDis

PolyDis provides spreadsheet tabs for the following polyhedra: tetrahedron, hexahedron, octahedron, icosahedron, cuboctahedron, dodecadeltahedron (2 versions), trigonal prism, trigonal antiprism, tetragonal prism, tetragonal antiprism, hexagonal prism. Pick the respective tab at the bottom of the opened excel file.

PolyDis minimizes the deviation between a given and an ideal polyhedron. The data required by the program are the unit cell parameters and atomic positions of the polyhedron. This data has to be filled into the cells within the RED border. It is important to fill in the atomic positions in the exact order shown in the picture of the polyhedron in the top right.

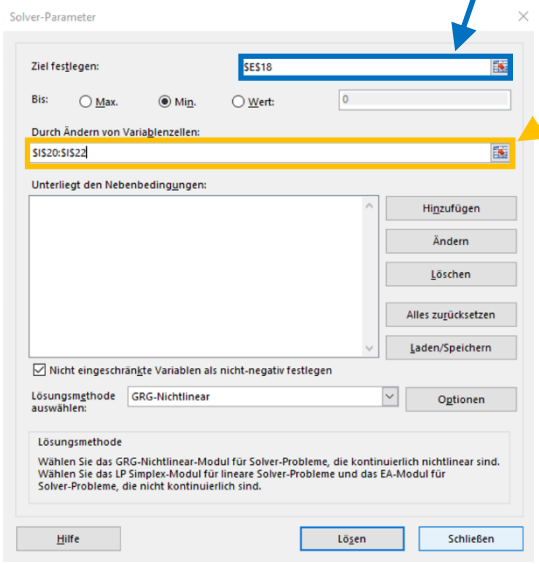
To run the *Solver* add-in go to **Data** and click **Solver** in the analysis group.

Excel spreadsheet



	A	B	C	D	E	F	G	H	I	J	K
1	Compound name										
2		fill in your data into cells of this colour									
3	unit cell dimensions (in pm)					IMPORTANT: order and alignment of atoms have to match the picture					
4	a-axis	320	α-angle	90							
5	b-axis	320	β-angle	90							
6	c-axis	320	γ-angle	90							
7											
8		coordinates of real tetrahedron			coordinates of ideal tetrahedron						
9	atom	x/a	y/b	z/c		x/a	y/b	z/c			
10	Central atom Z	0.5	0.5	0.5	Z*	0.49	0.498	0.4875			
11	Ligand 1 P1	1	0.99	-0.03	P1*	0.9776	0.9899	0.0071			
12	Ligand 2 P2	0.95	0.01	0.96	P2*	0.9757	0.0081	0.9719			
13	Ligand 3 P3	0.03	0.022	0.02	P3*	0.0063	0.0146	-0.0054			
14	Ligand 4 P4	-0.02	0.97	1	P4*	0.0004	0.9794	0.9764			
15											
16											
17	ligand	deviation			average deviation of atom				turning angles of respective ideal tetrahedron		
18	P1	5.139198643	%		normalized	4.143739517	%				
19	P2	3.365607912	%		real	1.17709862	pm		angle	rad	°
20	P3	4.208072652	%						θ	4.105959401	235.2541445
21	P4	3.86207886	%		displacement of Z from center of gravity				φ	3.931347642	225.2496277
22					normalized	1.913853592	%		τ	1.051197537	60.22918228
23					real	5.162325058	pm				

Solver window:



Put the Excel sheet cell address of the cell marked in BLUE into the BLUE target cell of the new window *Solver* and the YELLOW variable cell adresses into the respective YELLOW cell in *Solver*.

Click on Solve.

The coordinates of the scaled and fitted ideal polyhedron are shown within the GREEN border. The deviation of the coordination sphere from ideal conformation and the displacement of the central atom are shown in % and in pm within the PURPLE border.

Troubleshooting:

The *Solver* plugin doesn't change the values within the YELLOW border to negative values. Instead of turning the polyhedron to –10° it stops at 0, which is not the desired result. IF there is a 0 in one of the cells within the YELLOW border replace it with a 5 and run *Solver* again.

The deviations of every single atom are shown in the cells with the green background left of the PURPLE border. IF one of these values is inexplicably very far off the other values check its coordinates and the unit cell parameters for typos.