Pt$_2$
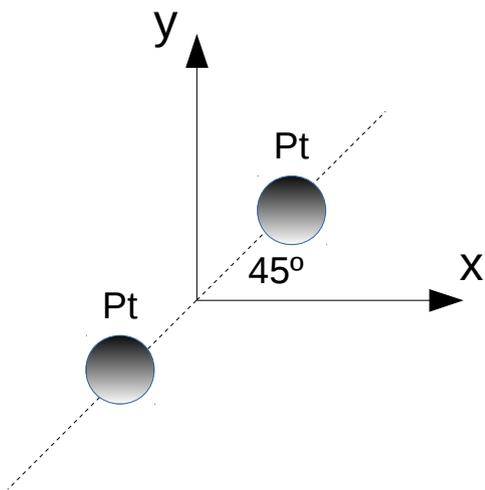

In order to test if the direction of the magnetic moments is correct we prepare the following system:

A Pt dimer is aligned forming 45º with the x axis. We know that the easy axis will be along the easy axis direction. So we perform two calculations: one forming 45º (m$_y$ positive) and -45º (m$_y$ negative). The first one should be the lowest in energy.

We show the results below:

DM.InitSpin	m$_T$	m$_x$	m$_y$	m$_z$	E (eV)	ΔE (eV)
0.9 90 45	1.65	1.16	1.16	0.00	-1530.990	0.141
0.9 90 -45	1.89	1.33	-1.33	0.00	-1531.131	0.000

It is clear that the lowest energy is achieved with the input φ=-45º, instead of the expected value 45º. The subroutine *moments.F* gives the right value (m$_y$>0) for the lowest energy case. The wrong routines are *fill_dscf_from_atom_info* (in *m_new_dm.F90*) and *spnvec* in (*mulliken.F*)