Universität Bielefeld

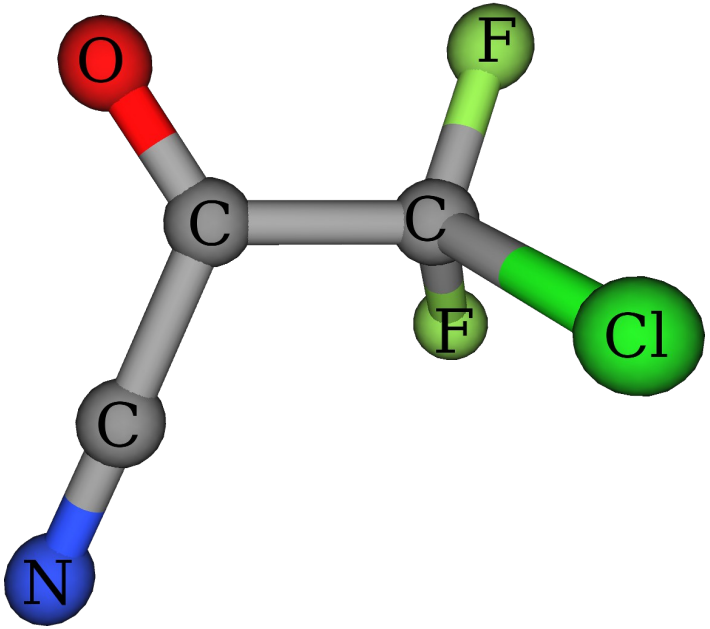
Conformational Properties of $ClF_2CC(O)$-X Molecules, X = -CN, -NCO, -NCS

UNEX Project

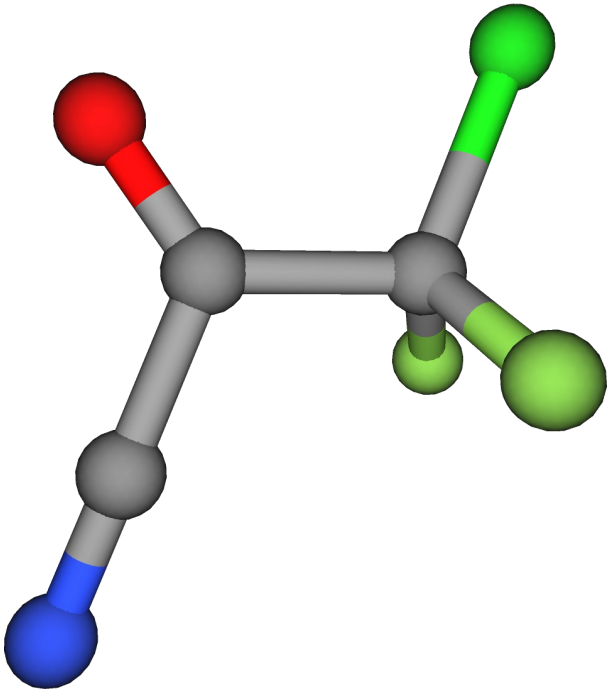
Yury V. Vishnevskiy

Skilizium-2012

$ClF_2CC(O)CN$



Gauche

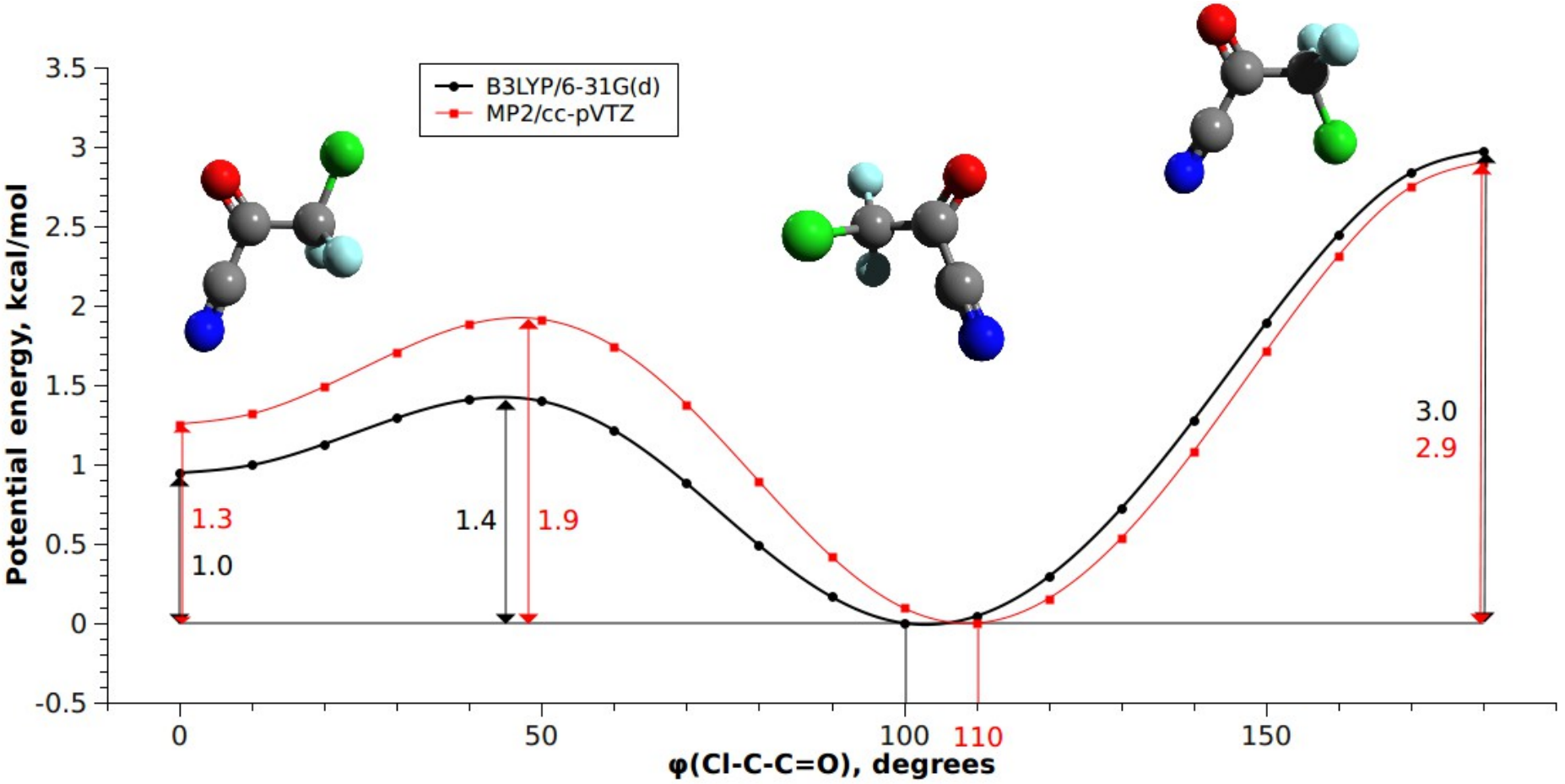


Syn

<u>GED</u>, PIMS, PES, UV-vis, IR/Raman, NMR, QCC:

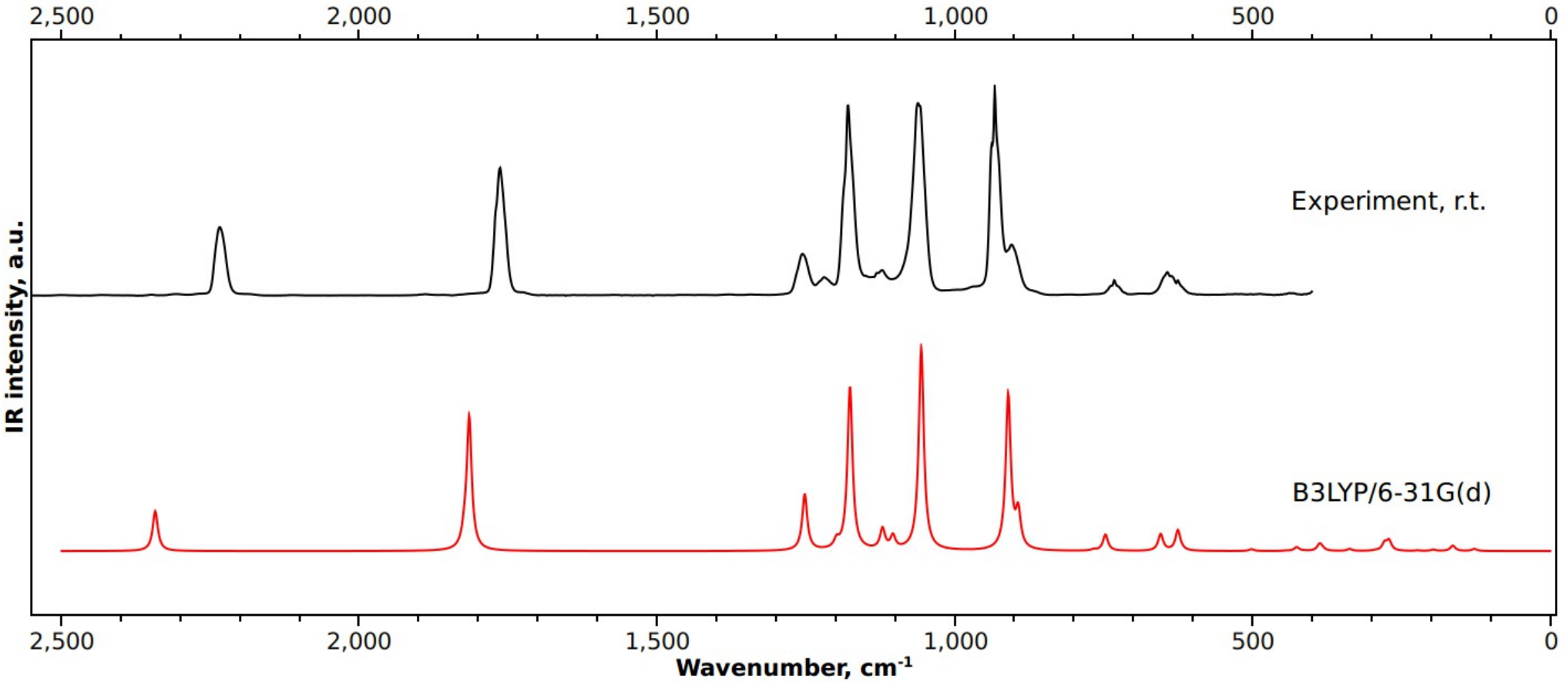
L.A. Ramos, S.E. Ulic, R.M. Romano, S. Tong, M. Ge, Yu.V. Vishnevskiy, R.J. Berger, N.W. Mitzel, H. Beckers, H. Willner and C.O. Della Védova, *Inorganic Chemistry*, 2011, **50**, 9650.

$ClF_2CC(O)CN$, QC calculations



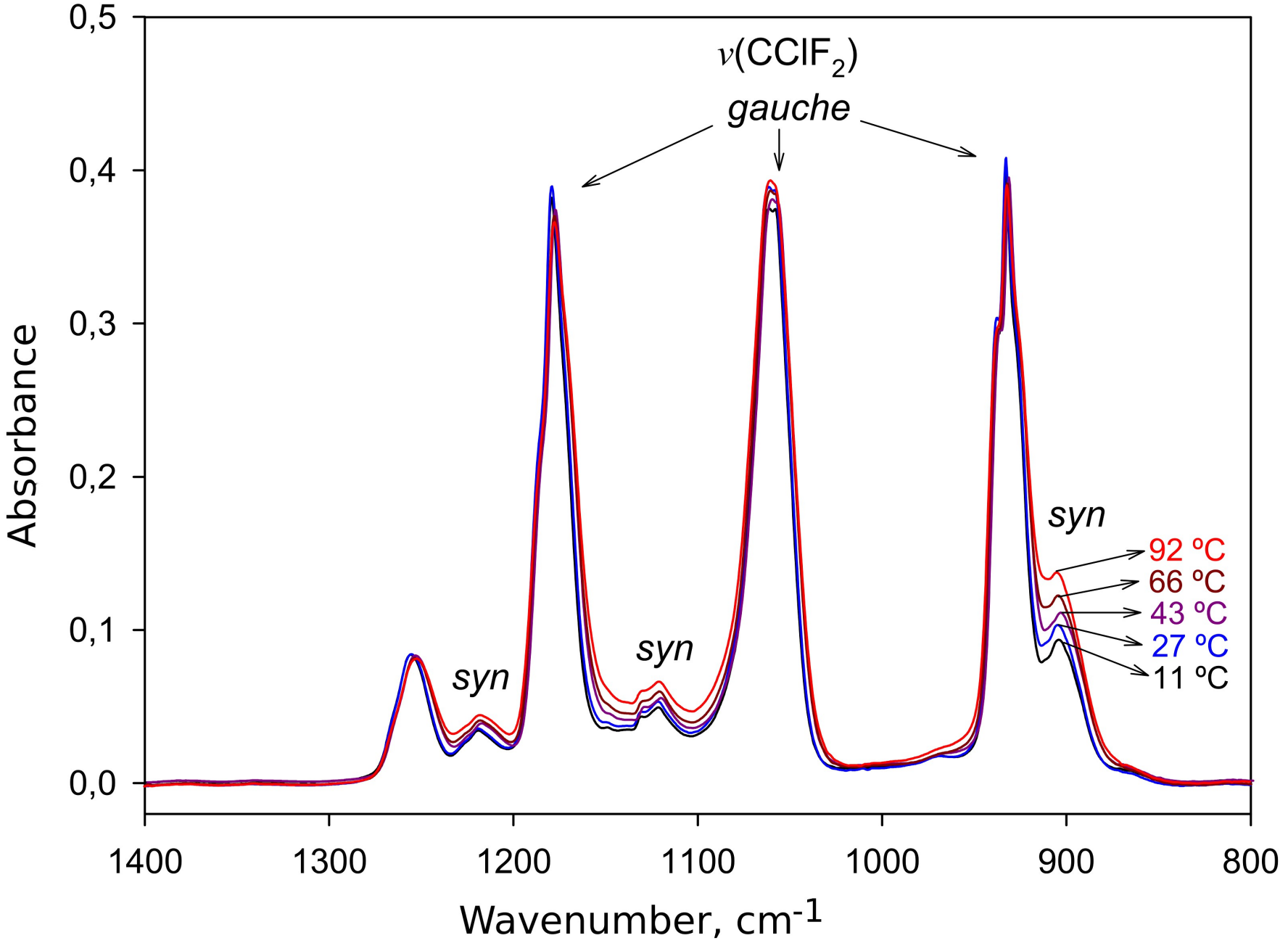
Method	ΔG_{298}	Gauche (%)
B3LYP/6-31G(d)	1.02	92
MP2/cc-pVTZ	1.04	92
CBS-QB3	0.61	85

$ClF_2CC(O)CN$, Gas-phase IR

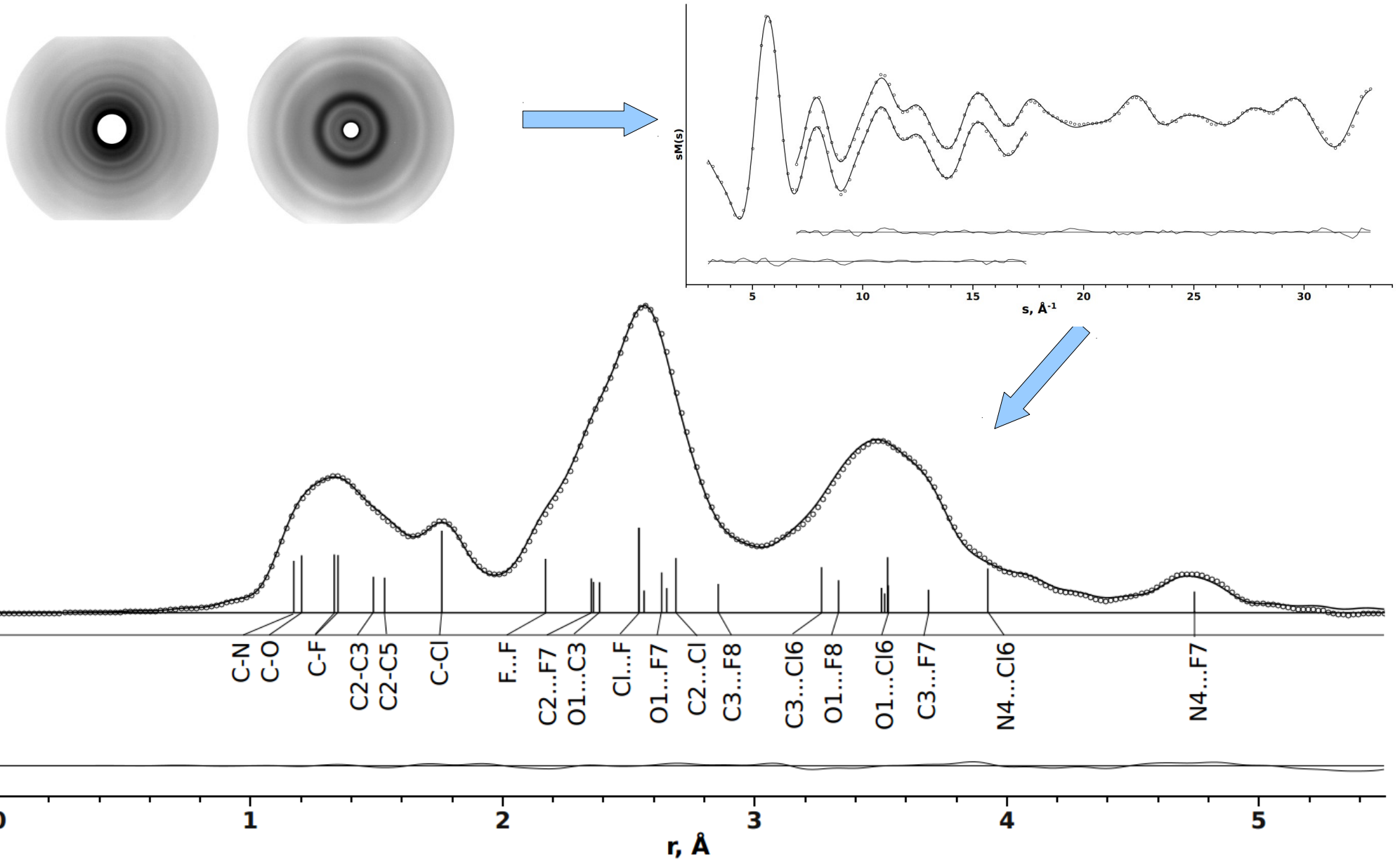


88% of gauche conformer according to IR spectrum.
85-95% according to QC calculations.

$ClF_2CC(O)CN$, Temp.-dep. Gas-phase IR

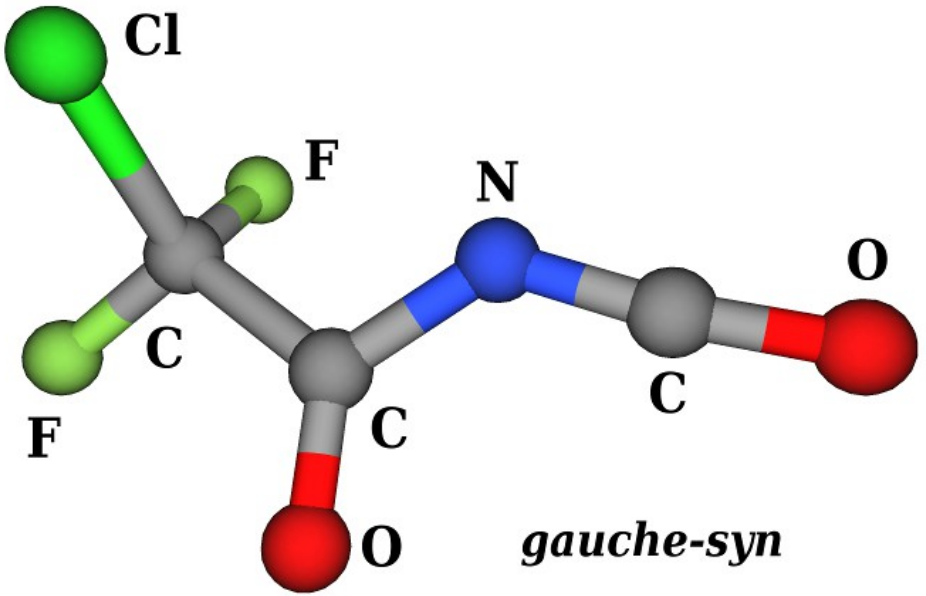


$ClF_2CC(O)CN$, GED

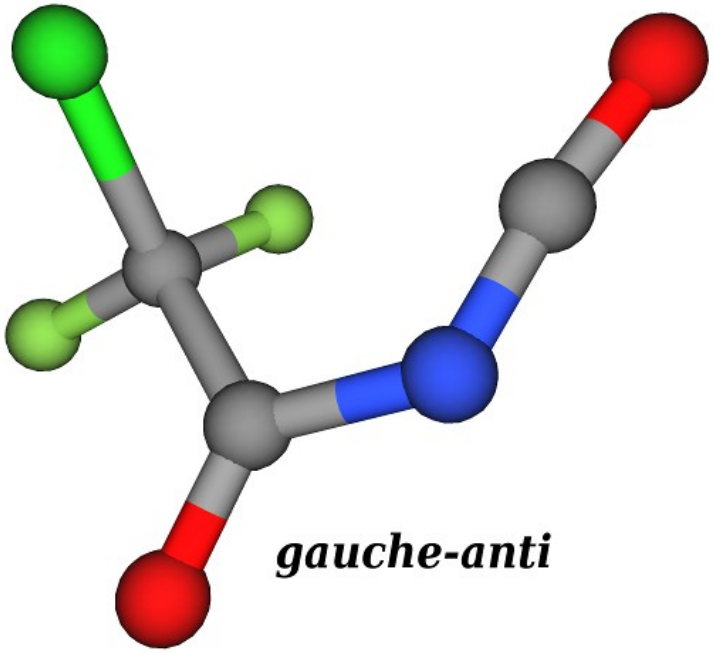


90(5)% of gauche conformer from GED two-conformer model
88% from IR; 85-95% from QC.

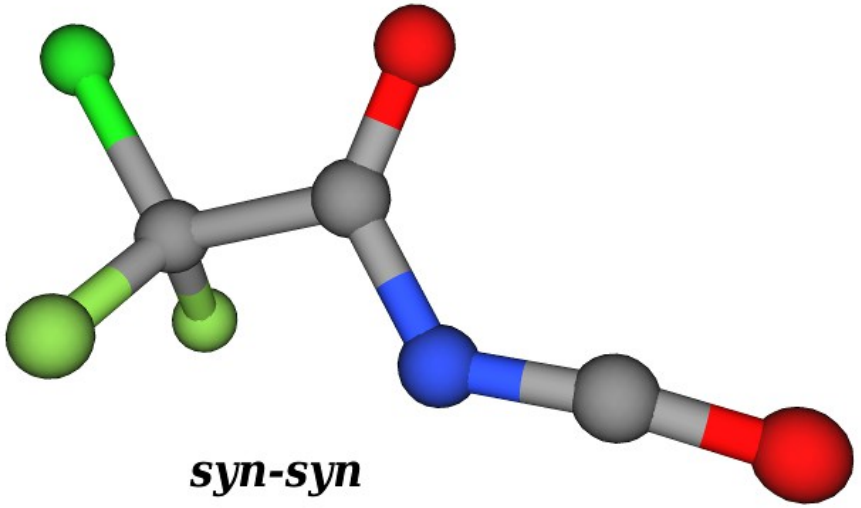
$ClF_2CC(O)NCO$



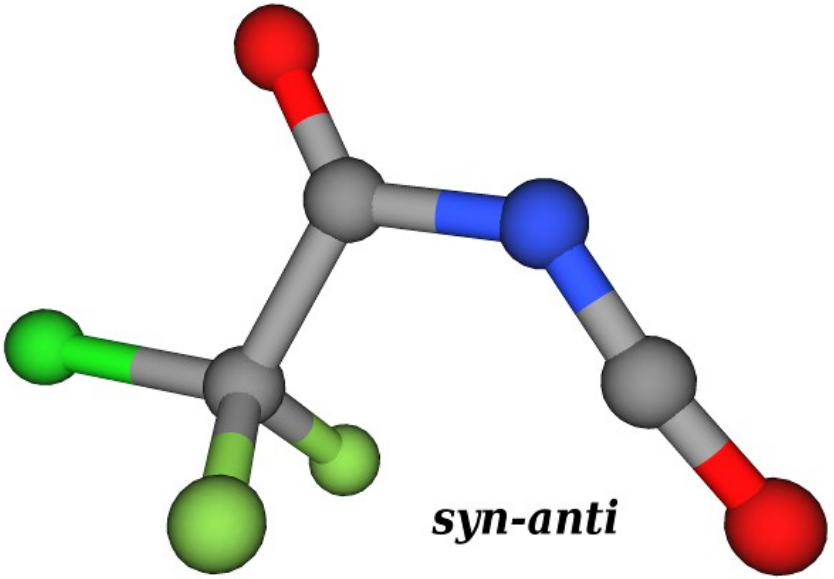
gauche-syn



gauche-anti

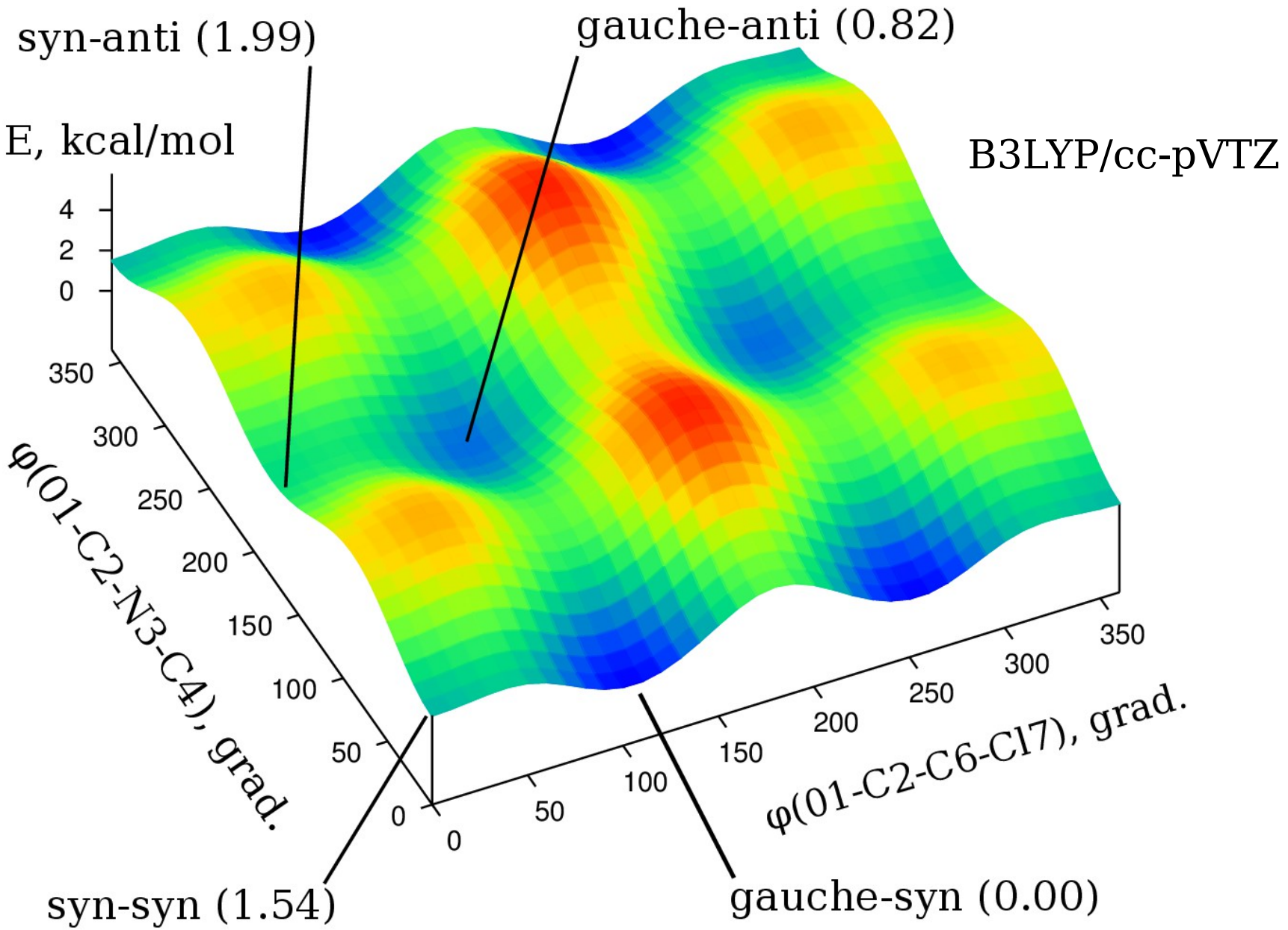


syn-syn

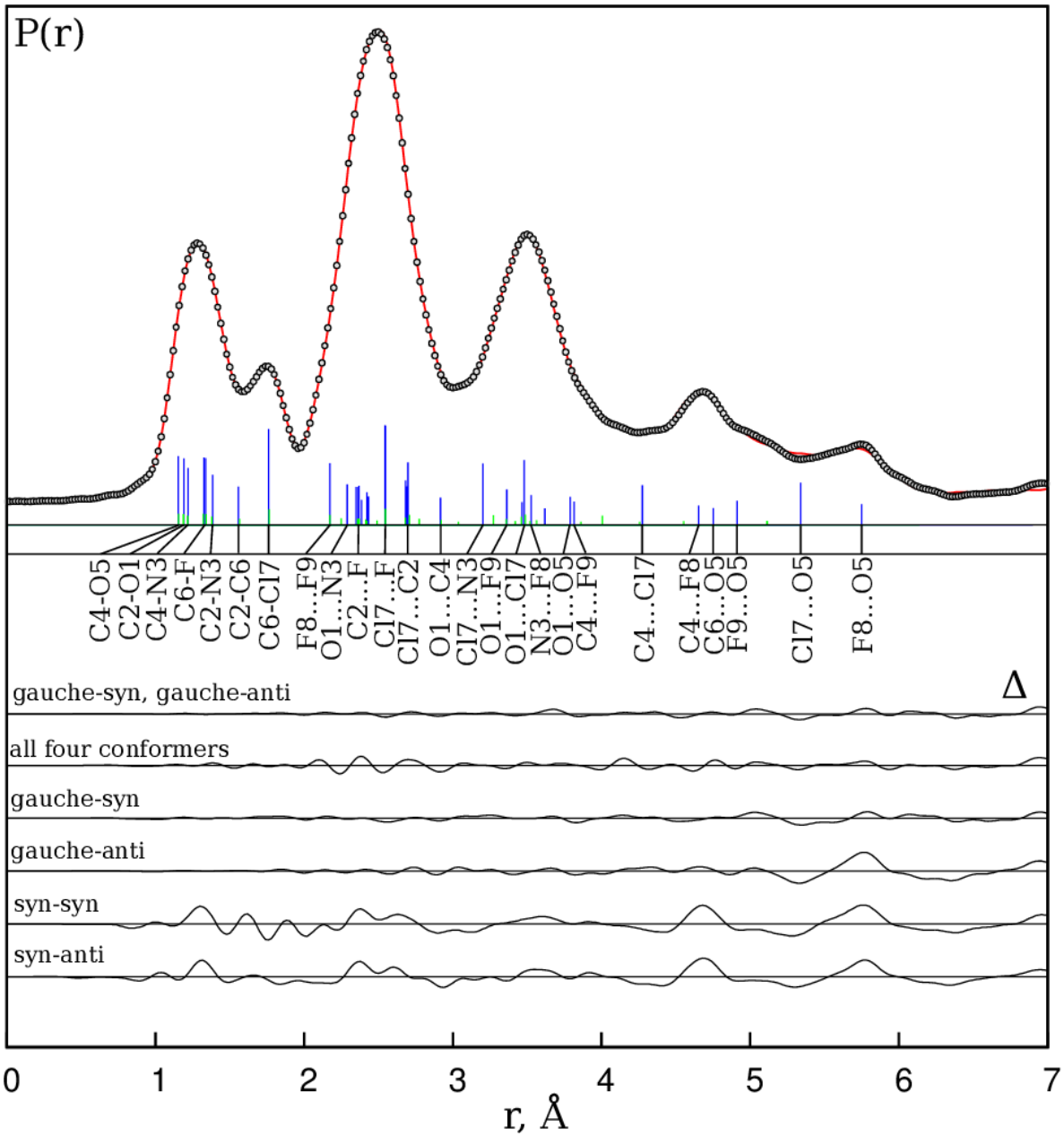


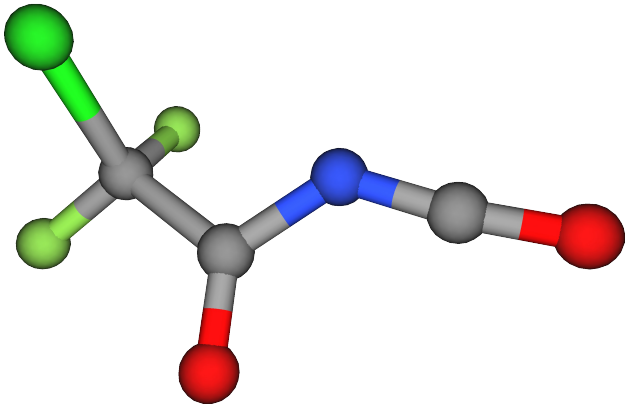
syn-anti

$ClF_2CC(O)NCO$, QC calculations

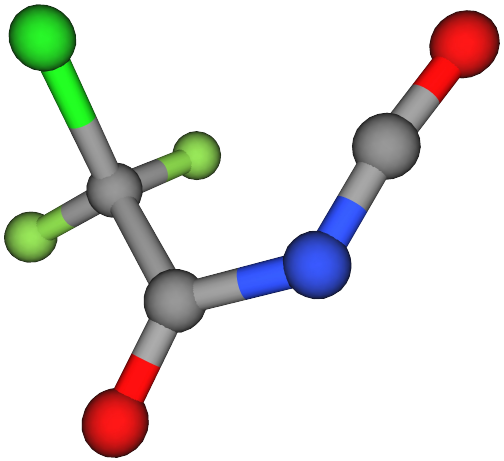


$ClF_2CC(O)NCO$, Preliminary GED results



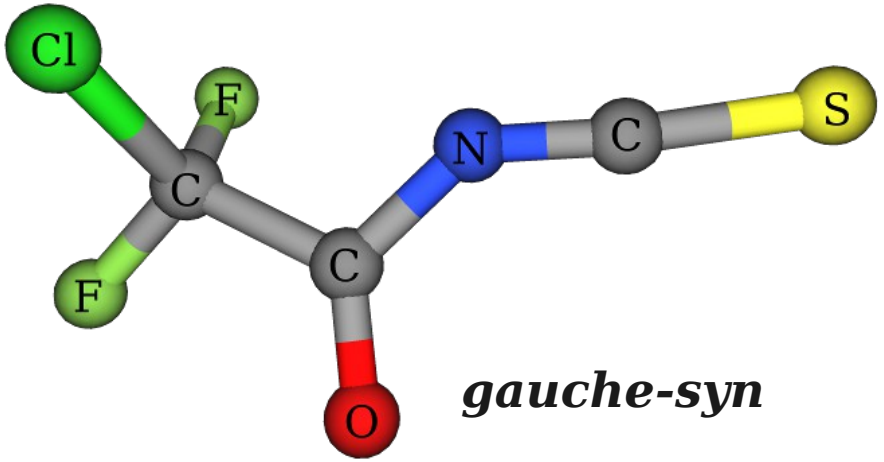


gauche-syn: 86(9)%
QC: 54-81%

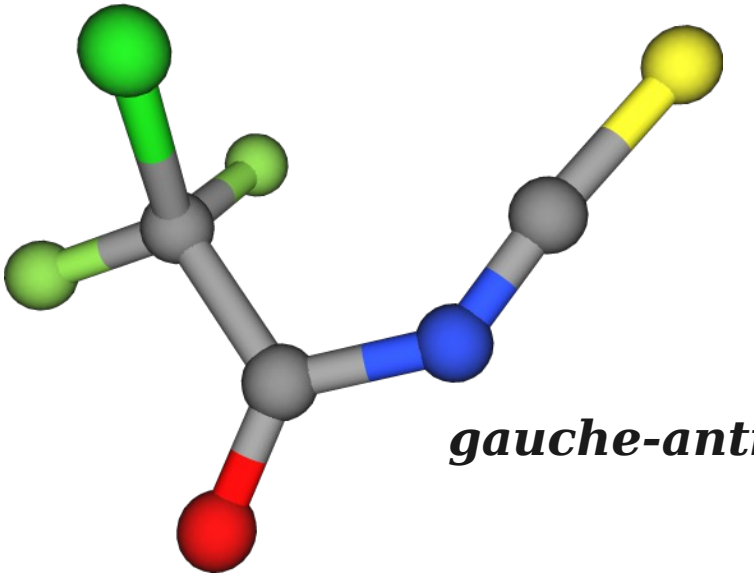


Gauche-anti: 14(9)%
QC: 19-46%

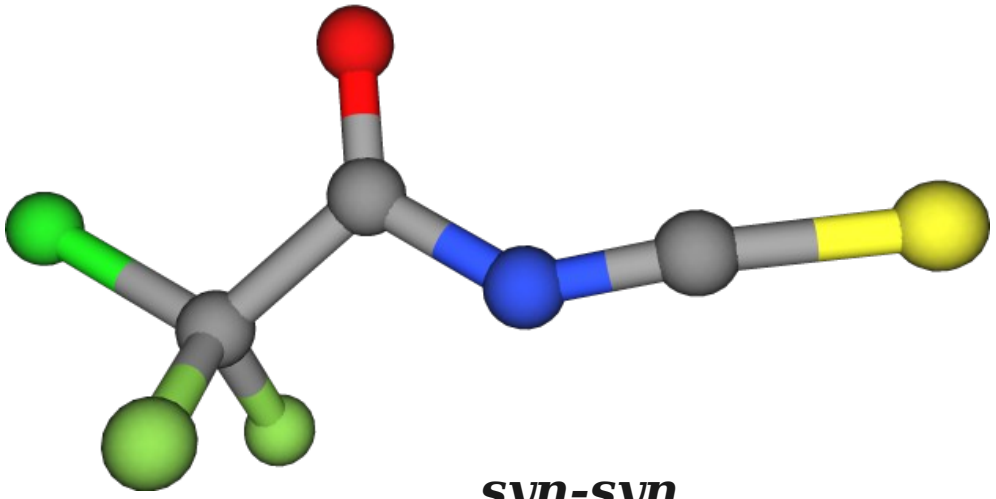
$ClF_2CC(O)NCS$



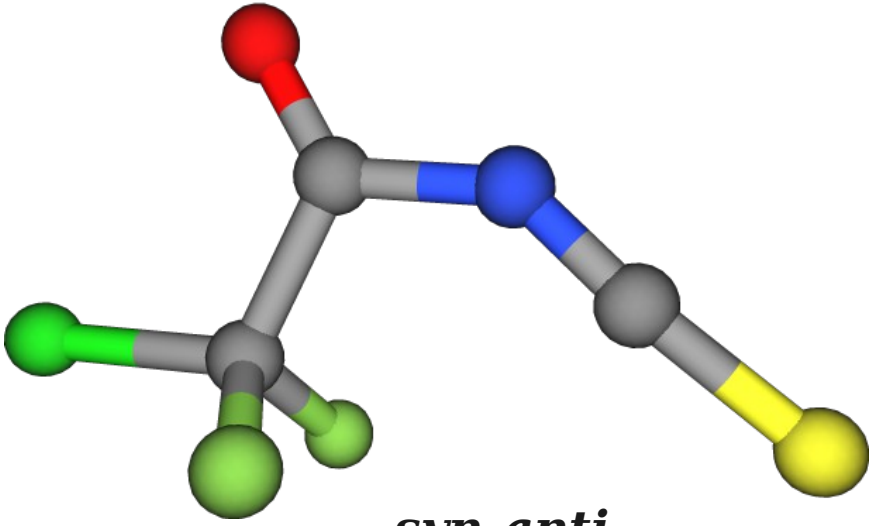
gauche-syn



gauche-anti

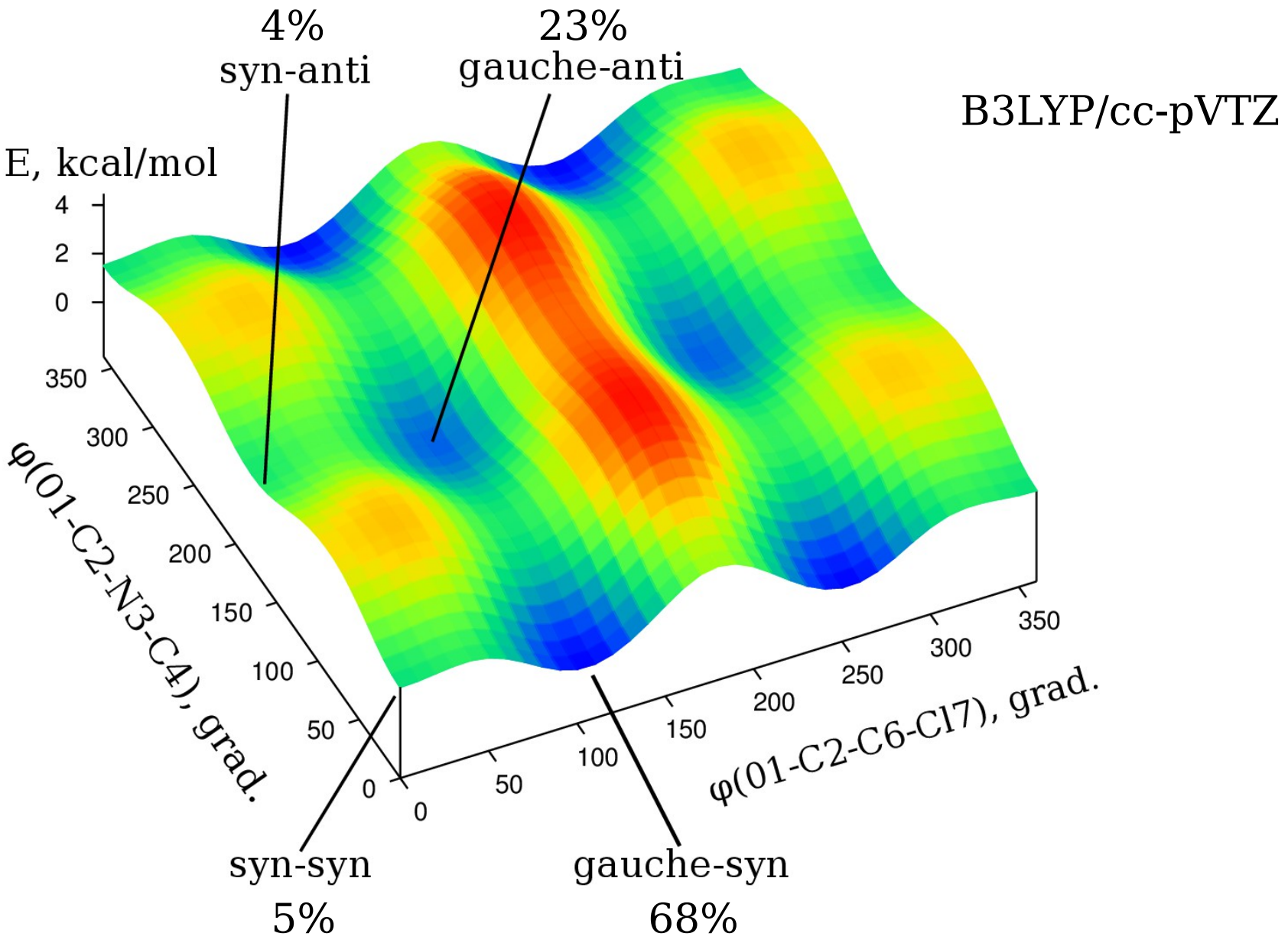


syn-syn



syn-anti

$ClF_2CC(O)NCS$, QC calculations



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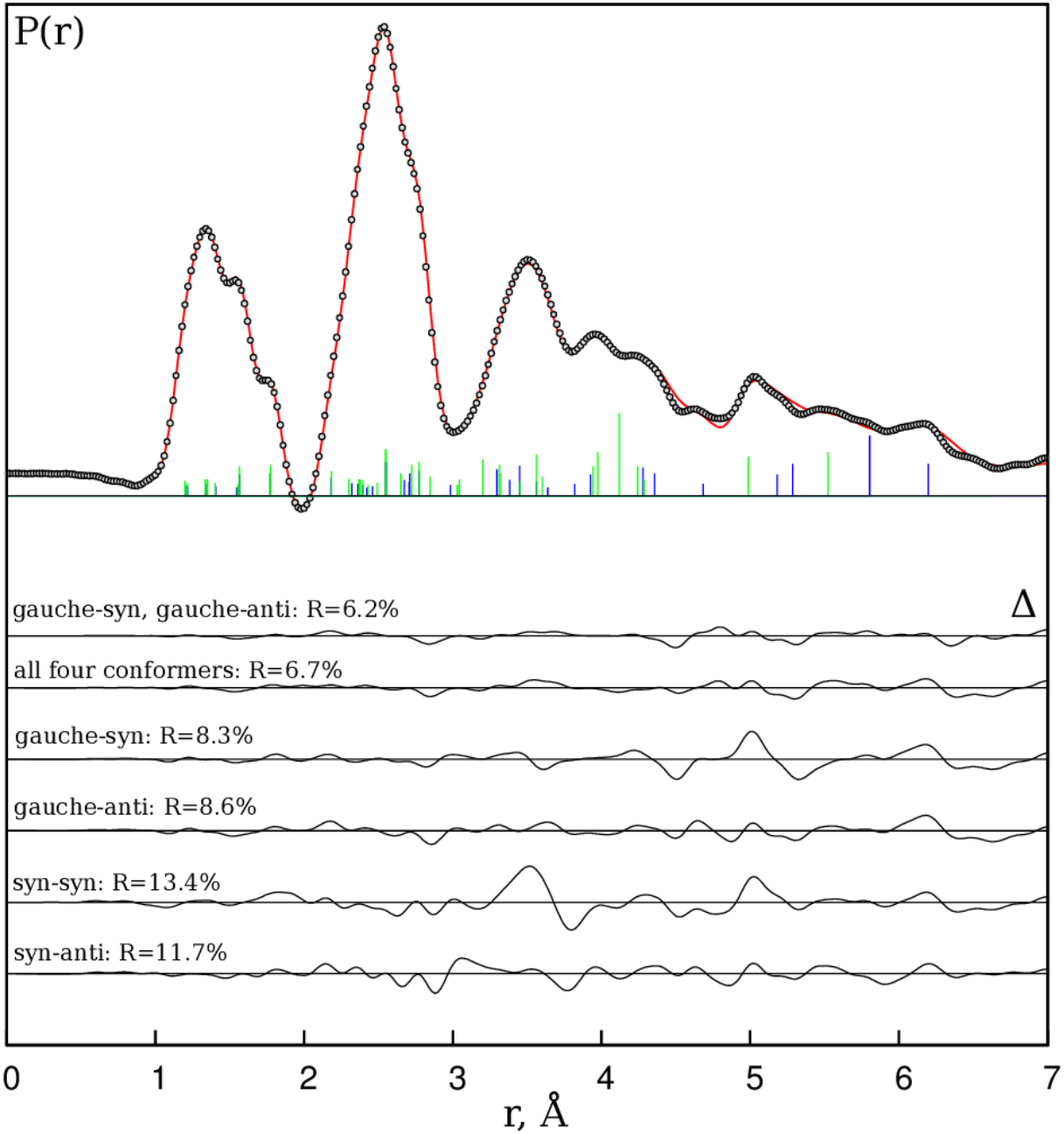
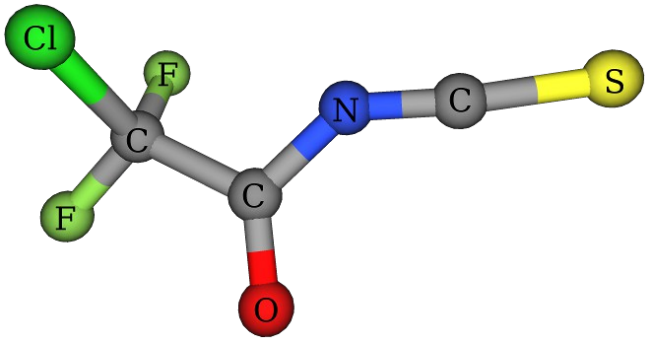
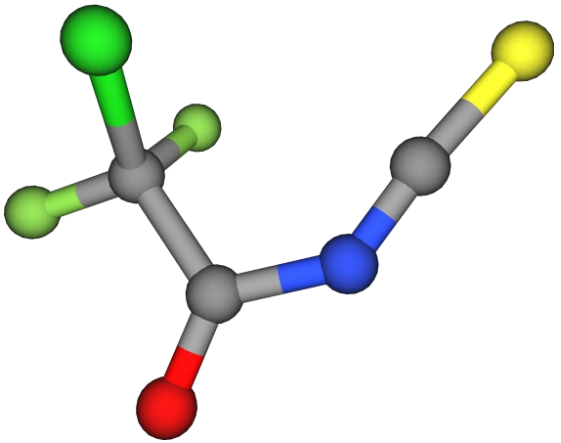
$ClF_2CC(O)NCS$, Preliminary GED results





gauche-syn: **42(10)**%
QC: 29-75%



gauche-anti: **58(9)**%
QC: 25-71%

Summary

In case of conformational problem:

1) GED works as good as IR (and sometimes even better)!
2) Accuracy depends on the object under study (fundamental GED property)!
3) Do not rely on theoretical calculations (unless you do not have any other option)!