Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for

Matrix effects in MI-VCD spectra of two chiral oxiranes and their potential microscopic origin

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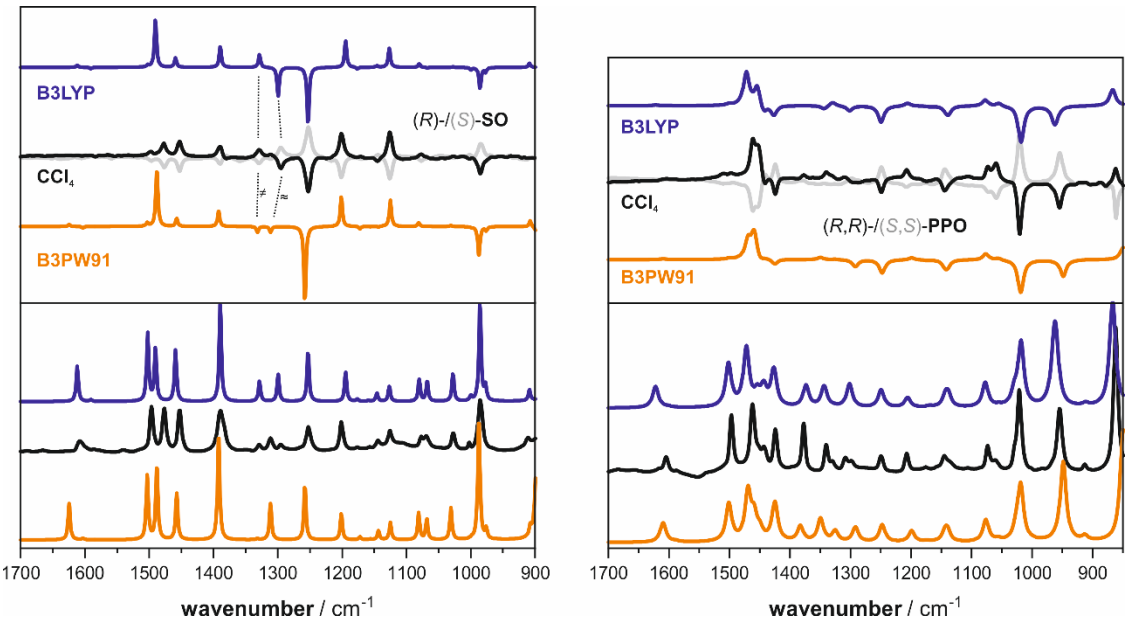

Figure S1. Comparison of the experimental solution phase spectra of **SO** (left) and **PPO** (right) with the corresponding computed spectra obtained with the B3LYP and B3PW91 functionals, the 6-311G++(2d,p) basis set, and the IEFPCM(carbon tetrachloride).

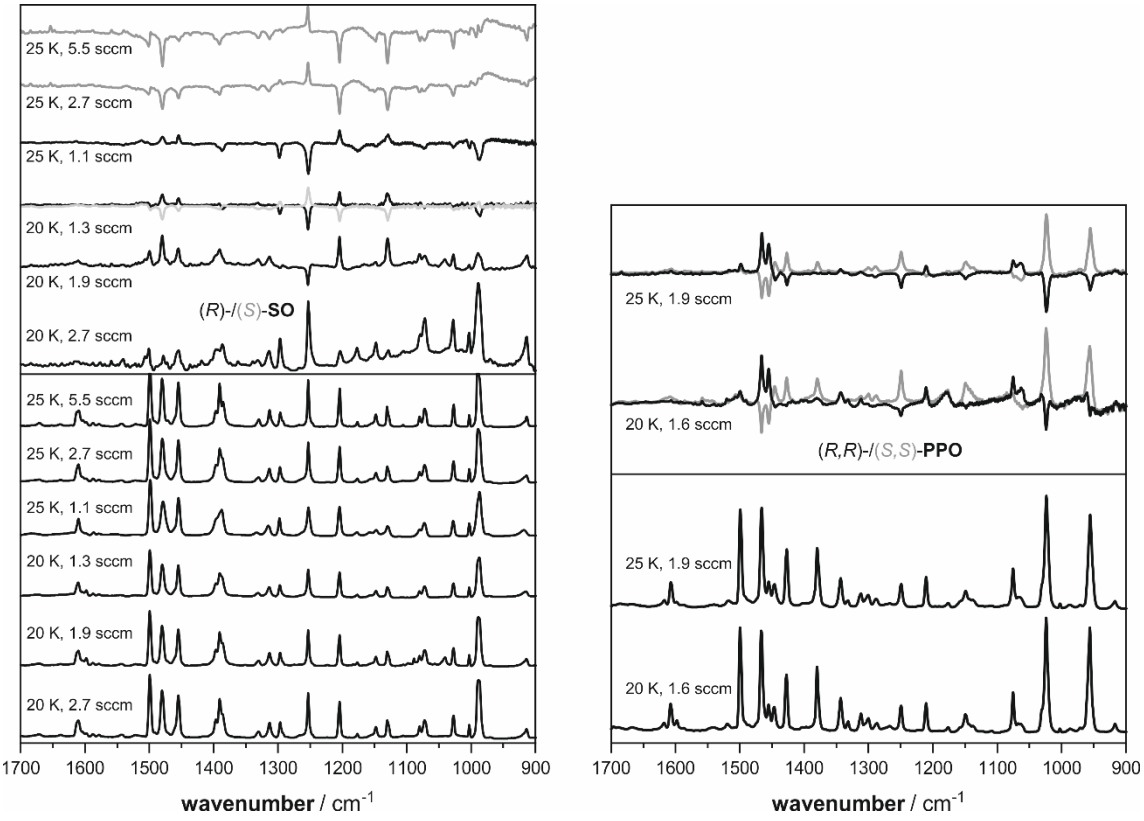

Figure S2. Experimental spectra of **SO** and **PPO** in N_2-matrix

Cartesian coordinates of SO and PPO

(R)-SO

C	1.59730700	0.57761100	0.19120400
C	2.58870300	0.00899200	-0.73890300
O	2.49081900	-0.46483000	0.60747400
H	1.82945400	1.54921500	0.62210700
H	3.49343400	0.56475800	-0.96976000
H	2.25065700	-0.68943900	-1.49920500
C	0.14560300	0.25831300	0.10751200
C	-0.78468600	1.29717800	0.05421800
C	-0.30730600	-1.06144300	0.07266700
C	-2.14401800	1.02414600	-0.05239900
H	-0.44341800	2.32615400	0.09745700
C	-1.66638700	-1.33384100	-0.02864000
H	0.41127000	-1.86863000	0.14504100
C	-2.58862100	-0.29316900	-0.09556200
H	-2.85587200	1.84006700	-0.09444800
H	-2.00786900	-2.36216100	-0.04902500
H	-3.64777300	-0.50804600	-0.17254500

(R,R)-PPO

C	2.49439600	-1.14873600	-0.06956200
C	1.13770200	-1.28678400	0.19026000
C	0.30712100	-0.16839100	0.23160700
C	0.85960500	1.09448600	0.02820800
C	2.21689800	1.23242900	-0.22663400
C	3.03785300	0.11221600	-0.28052200
H	3.12990500	-2.02730300	-0.10042700
H	0.71883800	-2.27371900	0.36401200
H	0.21732900	1.96596000	0.09117600
H	2.63791300	2.22076200	-0.37790100
H	4.09862200	0.22234700	-0.47783800
C	-1.14660700	-0.34139500	0.47752500
H	-1.41590000	-1.23581100	1.03912700
C	-2.17578800	0.20383800	-0.42403400
H	-1.80894900	0.78536200	-1.27024000
C	-3.52131800	-0.43135700	-0.59791100
H	-3.52022100	-1.09547900	-1.46685200
H	-3.79454900	-1.01053400	0.28614500
H	-4.28826000	0.33136200	-0.75842600
O	-1.90423800	0.81490100	0.83720000