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

Table 1: Optimized geometries of selected molecules

molecule	nucleus	X / bohr	Y / bohr	Z / bohr
(R)-1,3-difluoroallene	F	4.13803287	–0.74903179	0.33807399
	F	–4.13799648	–0.74909816	–0.33801341
	C	–0.00001231	0.61956651	–0.00000894
	C	2.35439015	0.71378522	–0.70236639
	C	–2.35442287	0.71388805	0.70230755
	H	–3.08833039	1.93265986	2.16293668
	H	3.08818066	1.93229645	–2.16327169
(R)-1,3-difluorocyclopropene	C	1.36145473	0.25948420	–0.93993398
	C	–1.22283553	0.28637833	–0.09025310
	C	–0.02712389	2.36771718	0.35656632
	H	1.97231991	0.33956428	–2.89020478
	F	3.13481910	–1.07489898	0.42936236
	H	0.11697583	4.25447692	1.07981123
	F	–3.31607582	–1.00911543	0.09215563
(R)-FOOH	F	–2.05962141	–0.45136819	0.00685795
	O	0.14463284	1.11722666	–0.03047940
	O	2.14971107	–0.51799867	0.12429629
	H	2.41280280	–1.00148896	–1.61822070
FCHO	F	2.00276294	–0.29572027	0.00000000
	O	–2.16266384	–0.40784471	0.00000000
	C	–0.28091357	0.77460428	0.00000000
	H	–0.08603829	2.82430253	0.00000000
cyclopropene	C	0.00000000	0.00000000	–1.66505007
	C	1.21978793	0.00000000	0.90471810
	C	–1.21978793	0.00000000	0.90471810
	H	0.00000000	1.72144844	–2.77938748
	H	0.00000000	–1.72144844	–2.77938748
	H	2.97418735	0.00000000	1.91979697
	H	–2.97418735	0.00000000	1.91979697
fluoroethene	F	2.00670618	0.33194867	0.00000000
	C	–2.38726733	0.41120496	0.00000000
	C	–0.23522599	–0.84813397	0.00000000
	H	–0.03685838	–2.87740062	0.00000000
	H	–2.42692867	2.44880241	0.00000000
	H	–4.13884042	–0.62649231	0.00000000