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

ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1: Energies (in au.) for studied conformations of tetrahydrofuran optimized at several levels of theory compared with previous theoretical results. The obtained energies of structures considered in subsequent calculations are presented in bold.

Conformer	Level	This calculation	Cadioli et. al[31]	Rayón et. al.[29]
THF(C_{2v})	HF/6-31G	-230.870470	-230.870468	
	HF/cc-pvDZ	-230.986261		
	MP2/6-31G	-231.349201	-231,351690	
	MP2/cc-pvDZ	-231,728543		-231,728543
	MP2/aug-cc-pvDZ	-231,778524		-231,778524
	B3LYP/6-311++G(d,p)	**-232.366731**		
THF(Cs)	HF/6-31G	-230.873088	-230.873088	
	HF/cc-pvDZ	-231.005821		
	MP2/6-31G	-231.353382	-231.355568	
	MP2/cc-pvDZ	-231.736063		-231.736063
	B3LYP/6-311++G(d,p)	**-232.371765**		

Table S2: Geometrical parameters for studied conformations of tetrahydrofuran optimized at the B3LYP/6-311++G(d,p) level of theory. Distances are given in angstroms and angles in degrees. See Figure S1 for notation.

Distance	THF(C_{2v})	THF(C_s)	Angle	THF(C_{2v})	THF(C_s)
R(O-C1)	1.429	1.426	A(C1-O-C2)	112.3	105.7
R(O-C2)	1.429	1.426	A(O-C1-C4)	108.3	105.6
R(C1-C4)	1.543	1.542	A(O-C1-H2)	108.4	107.8
R(C1-H2)	1.096	1.091	A(O-C1-H1)	108.4	109.8
R(C1-H1)	1.096	1.101	A(O-C2-C3)	108.3	105.6
R(C2-C3)	1.543	1.542	A(O-C2-H3)	108.4	107.8
R(C2-H3)	1.096	1.091	A(O-C2-H4)	108.4	109.8
R(C2-H4)	1.096	1.101	A(C4-C1-H2)	111.8	114.1
R(C4-C3)	1.548	1.554	A(C4-C1-H1)	111.8	110.8
R(C3-H6)	1.092	1.092	A(C1-C4-C3)	105.5	103.5
R(C3-H5)	1.092	1.092	A(C1-C4-H8)	110.9	111.7
R(C4-H7)	1.092	1.092	A(C1-C4-H7)	110.9	110.7
R(C4-H8)	1.092	1.092	A(H2-C1-H1)	107.9	108.6
			A(C3-C2-H3)	111.8	114.1
			A(C3-C2-H4)	111.8	110.8
			A(C2-C3-C4)	105.5	103.5
			A(C2-C3-H6)	110.9	111.7
			A(C2-C3-H5)	110.9	110.7
			A(H3-C2-H4)	107.9	108.6
			A(C3-C4-H8)	111.2	112.6
			A(C3-C4-H7)	111.2	110.7
			A(C4-C3-H6)	111.2	112.6
			A(C4-C3-H5)	111.2	110.7
			A(H8-C4-H7)	107.2	107.6
			A(H6-C3-H5)	107.2	107.6
			D(C4-C3-C2-O)	0	23.4

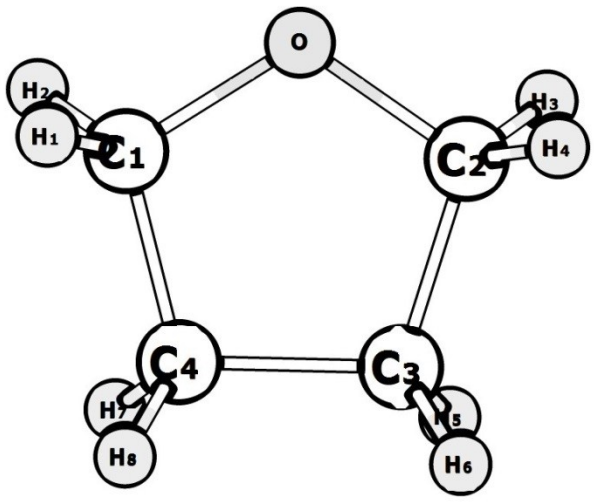

Figure S1. Structure of THF in C_{2v} symmetry

Table S3: Excitation energies (in eV) for C_{2v} conformation of tetrahydrofuran calculated using EOM-CCSD method with 6-311G++(d,p) basis set.

State		Maximum coeficient	Excitation	Excitation energy [eV]	f_{kl} [10^{-2} a.u.]	$< r^2 >$
S_1	$1\ ^1B_2$	-0.79206	$3b_2 \rightarrow 10a_1$	6.221	73.357300	101
S_2	$1\ ^1A_2$	-0.88181	$3b_2 \rightarrow 7b_1$	7.100	0.000000	120
S_3	$2\ ^1A_1$	0.87540	$3b_2 \rightarrow 4b_2$	7.103	0.028366	111
S_4	$2\ ^1B_2$	-0.77624	$3b_2 \rightarrow 11a_1$	7.321	0.048447	117
S_5	$3\ ^1B_2$	-0.79741	$3b_2 \rightarrow 12a_1$	7.610	1.823895	103
S_6	$2\ ^1A_2$	-0.84219	$3b_2 \rightarrow 8b_1$	7.910	0.000000	124
S_7	$1\ ^1B_1$	-0.88523	$3b_2 \rightarrow 3a_1$	7.937	6.326274	125
S_8	$3\ ^1A_1$	0.75428	$9a_1 \rightarrow 10a_1$	8.221	1.656358	104
S_9	$4\ ^1A_1$	-0.82293	$3b_2 \rightarrow 5b_2$	8.320	0.122849	123
S_{10}	$4\ ^1B_2$	-0.88125	$3b_2 \rightarrow 13a_1$	8.414	0.689903	104

Table S4: Excitation energies (in eV) for C_s conformation of tetrahydrofuran calculated using EOM-CCSD method with 6-311G++(d,p) basis set.

State		Maximum coeficient	Excitation	Excitation energy [eV]	f_{kl} [10^{-2} a.u.]	$< r^2 >$
S_1	$2\ ^1A'$	-0.78958	12a'→13a'	6.653	1.590244	104
S_2	$3\ ^1A'$	0.8021	12a'→14a'	7.307	5.029580	111
S_3	$1\ ^1A''$	0.88124	12a'→9a''	7.408	0.332022	120
S_4	$4\ ^1A'$	0.68062	12a'→15a'	7.604	1.057016	115
S_5	$5\ ^1A'$	0.6331	12a'→17a'	7.975	0.730500	108
S_6	$2\ ^1A''$	0.79424	12a'→10a''	8.222	0.397233	125
S_7	$3\ ^1A''$	-0.82628	12a'→11a''	8.279	2.026174	126
S_8	$6\ ^1A'$	0.63567	11a'→13a'	8.500	1.237103	110
S_9	$4\ ^1A''$	0.82835	8a''→13a'	8.809	0.004424	104
S_{10}	$5\ ^1A''$	0.66063	11a'→9a''	9.136	2.638141	113