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

Reliability of the interacting quantum atom (IQA) data computed in AIMAll from the HF, B3LYP and MP2 wavefunctions

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Supplementary Information

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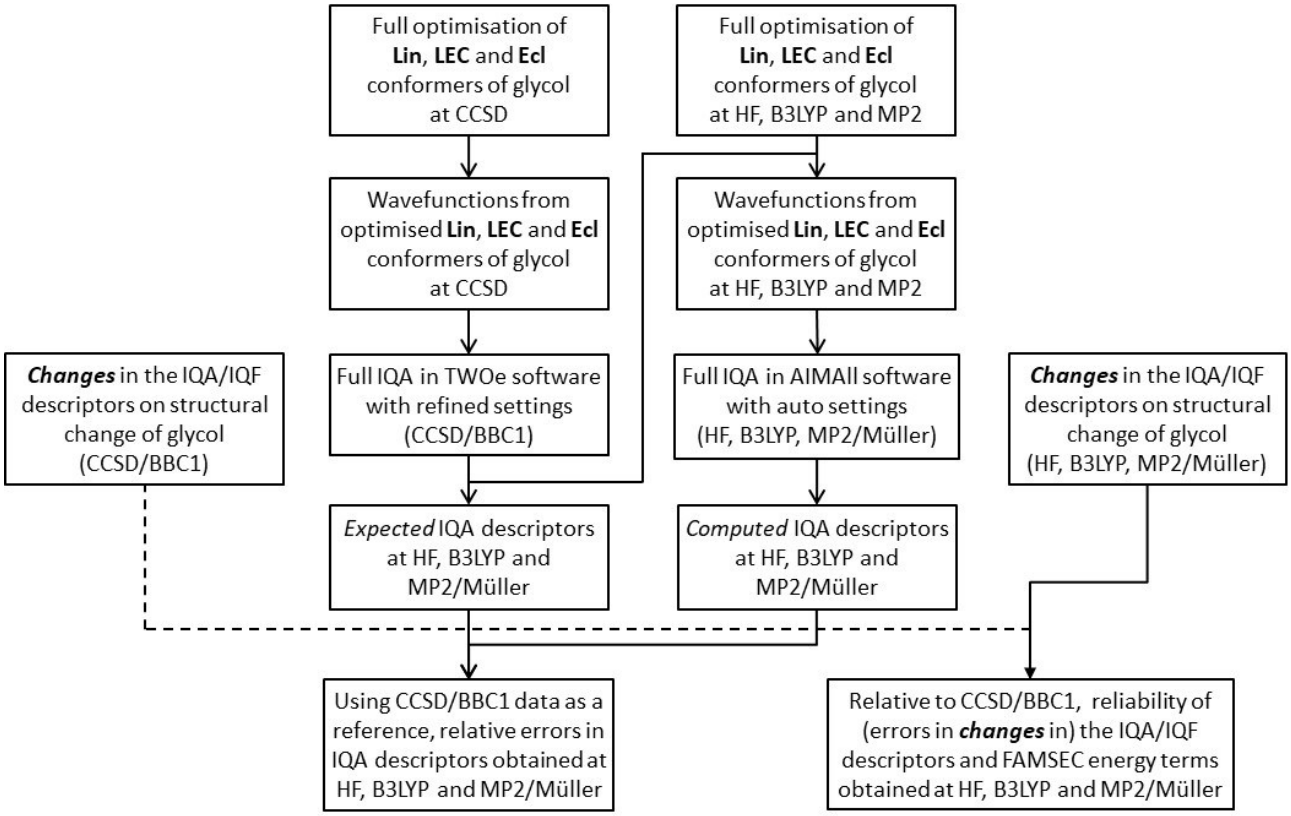

Scheme S1. Protocol used to assess, relative to the CCSD/BBC1/TWOe/refined settings level, reliability of IQA descriptors as well as changes (occurring on a structural change of glycol) in the IQA/IQF and FAMSEC energy terms computed from wavefunctions generated at the HF, B3LYP and MP2/Müller levels using AIMAll with default (auto) settings.

Coordinates of optimised structures

The linear conformer of glycol (**Lin**) optimised at the CCSD level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.553816	-0.522867	0.000000
2	6	0	-0.553816	0.522867	0.000000
3	8	0	-1.794951	-0.195586	0.000000
4	8	0	1.794951	0.195586	0.000000
5	1	0	2.515495	-0.443387	0.000000
6	1	0	-2.515495	0.443387	0.000000
7	1	0	0.457238	-1.160364	0.898339
8	1	0	-0.457238	1.160364	-0.898339
9	1	0	0.457238	-1.160364	-0.898339
10	1	0	-0.457238	1.160364	0.898339

The lowest energy conformer of glycol (**LEC**) optimised at the CCSD level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.684229	0.597927	-0.277310
2	6	0	-0.731587	0.569266	0.281262
3	8	0	-1.457381	-0.566444	-0.189348
4	8	0	1.334773	-0.588133	0.212492
5	1	0	2.170009	-0.700676	-0.253619
6	1	0	-0.909942	-1.338630	0.005819
7	1	0	0.648667	0.595331	-1.382320
8	1	0	-1.284734	1.461493	-0.054744
9	1	0	1.209453	1.508013	0.070908
10	1	0	-0.687386	0.578554	1.387760

The eclipsed conformer of glycol (**Ecl**) optimised at the CCSD level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.777323	0.643676
2	6	0	0.000000	-0.777323	0.643676
3	8	0	0.000000	-1.269736	-0.698118
4	8	0	0.000000	1.269736	-0.698118
5	1	0	0.000000	2.232281	-0.647206
6	1	0	0.000000	-2.232281	-0.647206
7	1	0	-0.894053	1.140748	1.185046
8	1	0	-0.894053	-1.140748	1.185046
9	1	0	0.894053	1.140748	1.185046
10	1	0	0.894053	-1.140748	1.185046

The linear conformer of glycol (**Lin**) optimised at the HF level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.431932	0.621253	0.000000
2	6	0	-0.431932	-0.621253	0.000000
3	8	0	0.431932	-1.732249	0.000000
4	8	0	-0.431932	1.732249	0.000000
5	1	0	0.066566	2.530922	0.000000
6	1	0	-0.066566	-2.530922	0.000000
7	1	0	1.071225	0.618244	0.885281
8	1	0	-1.071225	-0.618244	-0.885281
9	1	0	1.071225	0.618244	-0.885281
10	1	0	-1.071225	-0.618244	0.885281

The lowest energy conformer of glycol (**LEC**) optimised at the HF level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.684924	0.585216	-0.267024
2	6	0	-0.727497	0.558038	0.273948
3	8	0	-1.449579	-0.549228	-0.191731
4	8	0	1.342241	-0.570774	0.205606
5	1	0	2.185772	-0.662124	-0.202803
6	1	0	-0.968041	-1.333443	0.019024
7	1	0	0.660021	0.592239	-1.358791
8	1	0	-1.260081	1.447511	-0.058407
9	1	0	1.191965	1.488910	0.081708
10	1	0	-0.695493	0.567394	1.366729

The eclipsed conformer of glycol (**Ecl**) optimised at the HF level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.772347	0.627211
2	6	0	0.000000	-0.772347	0.627211
3	8	0	0.000000	-1.274898	-0.680951
4	8	0	0.000000	1.274898	-0.680951
5	1	0	0.000000	2.216245	-0.649319
6	1	0	0.000000	-2.216245	-0.649319
7	1	0	-0.881148	1.128172	1.166831
8	1	0	-0.881148	-1.128172	1.166831
9	1	0	0.881148	1.128172	1.166831
10	1	0	0.881148	-1.128172	1.166831

The linear conformer of glycol (**Lin**) optimised at the B3LYP level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.553540	-0.520315	0.000000
2	6	0	-0.553540	0.520315	0.000000
3	8	0	-1.793898	-0.191688	0.000000
4	8	0	1.793898	0.191688	0.000000
5	1	0	2.518232	-0.443054	0.000000
6	1	0	-2.518232	0.443054	0.000000
7	1	0	0.457620	-1.157542	0.894533
8	1	0	-0.457620	1.157542	-0.894533
9	1	0	0.457620	-1.157542	-0.894533
10	1	0	-0.457620	1.157542	0.894533

The lowest energy conformer of glycol (**LEC**) optimised at the B3LYP level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.682927	0.594582	-0.277391
2	6	0	-0.728424	0.566412	0.279837
3	8	0	-1.464236	-0.559924	-0.185335
4	8	0	1.342506	-0.584376	0.207209
5	1	0	2.184856	-0.690772	-0.247737
6	1	0	-0.931749	-1.344116	0.004378
7	1	0	0.648809	0.594188	-1.378992
8	1	0	-1.275739	1.458550	-0.052956
9	1	0	1.201923	1.505110	0.068908
10	1	0	-0.684673	0.577147	1.383179

The eclipsed conformer of glycol (**Ecl**) optimised at the B3LYP level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.775863	0.641928
2	6	0	0.000000	-0.775863	0.641928
3	8	0	0.000000	-1.274025	-0.692589
4	8	0	0.000000	1.274025	-0.692589
5	1	0	0.000000	2.236775	-0.648827
6	1	0	0.000000	-2.236775	-0.648827
7	1	0	-0.890377	1.137132	1.183966
8	1	0	-0.890377	-1.137132	1.183966
9	1	0	0.890377	1.137132	1.183966
10	1	0	0.890377	-1.137132	1.183966

The linear conformer of glycol (**Lin**) optimised at the B3LYP-GD3 level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.439441	0.619663	0.000000
2	6	0	-0.439441	-0.619663	0.000000
3	8	0	0.439441	-1.748495	0.000000
4	8	0	-0.439441	1.748495	0.000000
5	1	0	0.086363	2.555370	0.000000
6	1	0	-0.086363	-2.555370	0.000000
7	1	0	1.084270	0.609321	0.894734
8	1	0	-1.084270	-0.609321	-0.894734
9	1	0	1.084270	0.609321	-0.894734
10	1	0	-1.084270	-0.609321	0.894734

The lowest energy conformer of glycol (**LEC**) optimised at the B3LYP-GD3 level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.685310	0.598067	-0.276321
2	6	0	-0.726375	0.565952	0.281126
3	8	0	-1.460873	-0.558789	-0.192539
4	8	0	1.347720	-0.577050	0.216224
5	1	0	2.188810	-0.687388	-0.239969
6	1	0	-0.930761	-1.344730	-0.003485
7	1	0	0.647256	0.591350	-1.378194
8	1	0	-1.274439	1.460093	-0.045752
9	1	0	1.200620	1.513316	0.064273
10	1	0	-0.679868	0.569956	1.384816

The eclipsed conformer of glycol (**Ecl**) optimised at the B3LYP-GD3 level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.776602	0.640741
2	6	0	0.000000	-0.776602	0.640741
3	8	0	0.000000	-1.274229	-0.694928
4	8	0	0.000000	1.274229	-0.694928
5	1	0	0.000000	2.237025	-0.653057
6	1	0	0.000000	-2.237025	-0.653057
7	1	0	-0.890554	1.137282	1.184020
8	1	0	-0.890554	-1.137282	1.184020
9	1	0	0.890554	1.137282	1.184020
10	1	0	0.890554	-1.137282	1.184020

The linear conformer of glycol (**Lin**) optimised at the MP2 level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.442789	0.616993	0.000000
2	6	0	-0.442789	-0.616993	0.000000
3	8	0	0.442789	-1.748313	0.000000
4	8	0	-0.442789	1.748313	0.000000
5	1	0	0.094801	2.550529	0.000000
6	1	0	-0.094801	-2.550529	0.000000
7	1	0	1.085147	0.607554	0.897394
8	1	0	-1.085147	-0.607554	-0.897394
9	1	0	1.085147	0.607554	-0.897394
10	1	0	-1.085147	-0.607554	0.897394

The lowest energy conformer of glycol (**LEC**) optimised at the MP2 level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.684080	0.607338	-0.275866
2	6	0	-0.727481	0.572436	0.280082
3	8	0	-1.446569	-0.569208	-0.193396
4	8	0	1.332231	-0.581571	0.219109
5	1	0	2.169067	-0.695310	-0.249601
6	1	0	-0.881671	-1.334054	-0.004482
7	1	0	0.649949	0.602254	-1.378813
8	1	0	-1.285887	1.458594	-0.056480
9	1	0	1.207157	1.515736	0.073672
10	1	0	-0.683507	0.580363	1.384698

The eclipsed conformer of glycol (**Ecl**) optimised at the MP2 level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.775481	0.646945
2	6	0	0.000000	-0.775481	0.646945
3	8	0	0.000000	-1.260277	-0.700256
4	8	0	0.000000	1.260277	-0.700256
5	1	0	0.000000	2.225616	-0.649648
6	1	0	0.000000	-2.225616	-0.649648
7	1	0	-0.892908	1.139710	1.185014
8	1	0	-0.892908	-1.139710	1.185014
9	1	0	0.892908	1.139710	1.185014
10	1	0	0.892908	-1.139710	1.185014

Table S1. Relative to the CCSD/BBC1 data, analysis of additive atomic energies computed for the **LEC** of glycol at the B3LYP level.[a]

	CCSD/BBC1		B3LYP			
Atom A	E^{A}_{add}	E^{A}_{add} / E	$^{Comput}E^{A}_{add}$	$^{Expect}E^{A}_{add}$	ΔE^{A}_{add}	Δ^{A}_{add}
C1	-37.94313	0.16518	-38.0434	-38.0392	-62.9	-2.6
C2	-37.94389	0.16518	-38.0435	-38.0400	-62.5	-2.2
O3	-75.25949	0.32762	-75.4367	-75.4501	-111.2	8.4
O4	-75.27158	0.32768	-75.4464	-75.4622	-109.7	9.9
H5	-0.48480	0.00211	-0.4867	-0.4860	-1.2	-0.4
H6	-0.48892	0.00213	-0.4917	-0.4902	-1.7	-1.0
H7	-0.58017	0.00253	-0.5867	-0.5816	-4.1	-3.2
H8	-0.58022	0.00253	-0.5859	-0.5817	-3.5	-2.6
H9	-0.58095	0.00253	-0.5877	-0.5824	-4.2	-3.3
H10	-0.57971	0.00252	-0.5864	-0.5812	-4.2	-3.3

[a]) Additive atomic energies are in au. Differences $\Delta E^{A}_{add} = (E^{A}_{add})_{B3LYP} - (E^{A}_{add})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{add} = {}^{Comput}E^{A}_{add} - {}^{Expect}E^{A}_{add}$ are in kcal mol^{-1}.

Table S2. Relative to the CCSD/BBC1 data, analysis of additive atomic energies computed for the **LEC** of glycol at the B3LYP-GD3 level.[a]

	CCSD/BBC1		B3LYP-GD3			
Atom A	E^{A}_{add}	E^{A}_{add} / E	$^{Comput}E^{A}_{add}$	$^{Expect}E^{A}_{add}$	ΔE^{A}_{add}	Δ^{A}_{add}
C1	-37.94313	0.16518	-38.0436	-38.0400	-63.0	-2.2
C2	-37.94389	0.16518	-38.0435	-38.0408	-62.5	-1.7
O3	-75.25949	0.32762	-75.4368	-75.4517	-111.3	9.3
O4	-75.27158	0.32768	-75.4463	-75.4638	-109.6	11.0
H5	-0.48480	0.00211	-0.4868	-0.4860	-1.3	-0.5
H6	-0.48892	0.00213	-0.4917	-0.4902	-1.7	-1.0
H7	-0.58017	0.00253	-0.5866	-0.5817	-4.0	-3.1
H8	-0.58022	0.00253	-0.5859	-0.5817	-3.6	-2.6
H9	-0.58095	0.00253	-0.5877	-0.5824	-4.2	-3.3
H10	-0.57971	0.00252	-0.5863	-0.5812	-4.2	-3.2

[a]) Additive atomic energies are in au. Differences $\Delta E^{A}_{add} = (E^{A}_{add})_{B3LYP\text{-}GD3} - (E^{A}_{add})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{add} = {}^{Comput}E^{A}_{add} - {}^{Expect}E^{A}_{add}$ are in kcal mol^{-1}.

Table S3. Relative to the CCSD/BBC1 data, analysis of additive atomic energies computed for the **LEC** of glycol at the MP2/Müller level.[a]

	CCSD/BBC1		MP2/Müller			
Atom A	E^{A}_{add}	E^{A}_{add} / E	$^{Comput}E^{A}_{add}$	$^{Expect}E^{A}_{add}$	ΔE^{A}_{add}	Δ^{A}_{add}
C1	-37.94313	0.16518	-37.9801	-37.9373	-23.2	-26.9
C2	-37.94389	0.16518	-37.9801	-37.9380	-22.7	-26.4
O3	-75.25949	0.32762	-75.3233	-75.2479	-40.1	-47.4
O4	-75.27158	0.32768	-75.3335	-75.2600	-38.9	-46.1
H5	-0.48480	0.00211	-0.4868	-0.4847	-1.3	-1.3
H6	-0.48892	0.00213	-0.4923	-0.4888	-2.1	-2.2
H7	-0.58017	0.00253	-0.5884	-0.5801	-5.1	-5.2
H8	-0.58022	0.00253	-0.5878	-0.5801	-4.8	-4.8
H9	-0.58095	0.00253	-0.5896	-0.5809	-5.4	-5.5
H10	-0.57971	0.00252	-0.5882	-0.5796	-5.3	-5.4

[a]) Additive atomic energies are in au. Differences $\Delta E^{A}_{add} = (E^{A}_{add})_{MP2/Müller} - (E^{A}_{add})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{add} = {}^{Comput}E^{A}_{add} - {}^{Expect}E^{A}_{add}$ are in kcal mol^{-1}.

Table S4. Relative to the CCSD/BBC1 data, analysis of additive atomic energies computed for the **Lin** conformer of glycol at the HF level.[a]

	CCSD/BBC1		HF			
Atom A	E^{A}_{add}	E^{A}_{add} / E	$^{Comput}E^{A}_{add}$	$^{Expect}E^{A}_{add}$	ΔE^{A}_{add}	Δ^{A}_{add}
C1	-37.9415	0.16517	-37.8175	-37.8201	77.9	1.6
C2	-37.9415	0.16517	-37.8175	-37.8201	77.9	1.6
O3	-75.2615	0.32764	-75.0503	-75.0206	132.6	-18.6
O4	-75.2615	0.32764	-75.0503	-75.0206	132.6	-18.6
H5	-0.4863	0.00212	-0.4840	-0.4847	1.4	0.5
H6	-0.4863	0.00212	-0.4840	-0.4847	1.4	0.5
H7	-0.5800	0.00253	-0.5678	-0.5782	7.7	6.5
H8	-0.5800	0.00253	-0.5678	-0.5782	7.7	6.5
H9	-0.5800	0.00253	-0.5678	-0.5782	7.7	6.5
H10	-0.5800	0.00253	-0.5678	-0.5782	7.7	6.5

[a]) Additive atomic energies are in au. Differences $\Delta E^{A}_{add} = (E^{A}_{add})_{HF} - (E^{A}_{add})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{add} = {}^{Comput}E^{A}_{add} - {}^{Expect}E^{A}_{add}$ are in kcal mol^{-1}.

Table S5. Relative to the CCSD/BBC1 data, analysis of additive atomic energies computed for the **Lin** conformer of glycol at the B3LYP level.[a]

	CCSD/BBC1		B3LYP			
Atom A	E^{A}_{add}	E^{A}_{add} / E	$^{Comput}E^{A}_{add}$	$^{Expect}E^{A}_{add}$	ΔE^{A}_{add}	Δ^{A}_{add}
C1	-37.9415	0.16517	-38.0417	-38.0376	-62.9	-2.6
C2	-37.9415	0.16517	-38.0417	-38.0376	-62.9	-2.6
O3	-75.2615	0.32764	-75.4414	-75.4521	-112.9	6.7
O4	-75.2615	0.32764	-75.4414	-75.4521	-112.9	6.7
H5	-0.4863	0.00212	-0.4894	-0.4875	-1.9	-1.2
H6	-0.4863	0.00212	-0.4894	-0.4875	-1.9	-1.2
H7	-0.5800	0.00253	-0.5866	-0.5815	-4.1	-3.2
H8	-0.5800	0.00253	-0.5866	-0.5815	-4.1	-3.2
H9	-0.5800	0.00253	-0.5866	-0.5815	-4.1	-3.2
H10	-0.5800	0.00253	-0.5866	-0.5815	-4.1	-3.2

[a]) Additive atomic energies are in au. Differences $\Delta E^{A}_{add} = (E^{A}_{add})_{B3LYP} - (E^{A}_{add})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{add} = {}^{Comput}E^{A}_{add} - {}^{Expect}E^{A}_{add}$ are in kcal mol^{-1}.

Table S6. Relative to the CCSD/BBC1 data, analysis of additive atomic energies computed for the **Lin** conformer of glycol at the B3LYP-GD3 level.[a]

	CCSD/BBC1		B3LYP-GD3			
Atom A	E^{A}_{add}	E^{A}_{add} / E	$^{Comput}E^{A}_{add}$	$^{Expect}E^{A}_{add}$	ΔE^{A}_{add}	Δ^{A}_{add}
C1	-37.9415	0.16517	-38.0416	-38.0384	-62.8	-2.0
C2	-37.9415	0.16517	-38.0416	-38.0384	-62.8	-2.0
O3	-75.2615	0.32764	-75.4415	-75.4537	-112.9	7.7
O4	-75.2615	0.32764	-75.4415	-75.4537	-112.9	7.7
H5	-0.4863	0.00212	-0.4894	-0.4875	-2.0	-1.2
H6	-0.4863	0.00212	-0.4894	-0.4875	-2.0	-1.2
H7	-0.5800	0.00253	-0.5866	-0.5815	-4.1	-3.2
H8	-0.5800	0.00253	-0.5866	-0.5815	-4.1	-3.2
H9	-0.5800	0.00253	-0.5866	-0.5815	-4.1	-3.2
H10	-0.5800	0.00253	-0.5866	-0.5815	-4.1	-3.2

[a]) Additive atomic energies are in au. Differences $\Delta E^{A}_{add} = (E^{A}_{add})_{BeLYP\text{-}GD3} - (E^{A}_{add})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{add} = {}^{Comput}E^{A}_{add} - {}^{Expect}E^{A}_{add}$ are in kcal mol^{-1}.

Table S7. Relative to the CCSD/BBC1 data, analysis of additive atomic energies computed for the **Lin** conformer of glycol at the MP2/Müller level.[a]

	CCSD/BBC1		MP2/Müller			
Atom A	E^{A}_{add}	E^{A}_{add} / E	$^{Comput}E^{A}_{add}$	$^{Expect}E^{A}_{add}$	ΔE^{A}_{add}	Δ^{A}_{add}
C1	-37.9415	0.16517	-37.9781	-37.9356	-23.0	-26.7
C2	-37.9415	0.16517	-37.9781	-37.9356	-23.0	-26.7
O3	-75.2615	0.32764	-75.3279	-75.2498	-41.7	-49.0
O4	-75.2615	0.32764	-75.3279	-75.2498	-41.7	-49.0
H5	-0.4863	0.00212	-0.4898	-0.4862	-2.2	-2.3
H6	-0.4863	0.00212	-0.4898	-0.4862	-2.2	-2.3
H7	-0.5800	0.00253	-0.5884	-0.5799	-5.3	-5.3
H8	-0.5800	0.00253	-0.5884	-0.5799	-5.3	-5.3
H9	-0.5800	0.00253	-0.5884	-0.5799	-5.3	-5.3
H10	-0.5800	0.00253	-0.5884	-0.5799	-5.3	-5.3

[a]) Additive atomic energies are in au. Differences $\Delta E^{A}_{add} = (E^{A}_{add})_{MP2/Müller} - (E^{A}_{add})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{add} = {}^{Comput}E^{A}_{add} - {}^{Expect}E^{A}_{add}$ are in kcal mol^{-1}.

Table S8. Relative to the CCSD/BBC1 data, analysis of additive atomic energies computed for the **Ecl** conformer of glycol at the HF level.[a]

	CCSD/BBC1		HF			
Atom A	E^{A}_{add}	E^{A}_{add} / E	$^{Comput}E^{A}_{add}$	$^{Expect}E^{A}_{add}$	ΔE^{A}_{add}	Δ^{A}_{add}
C1	-37.9412	0.16518	-37.8166	-37.8195	78.2	1.8
C2	-37.9412	0.16518	-37.8169	-37.8195	78.0	1.6
O3	-75.2510	0.32761	-75.0378	-75.0096	133.8	-17.7
O4	-75.2510	0.32761	-75.0378	-75.0096	133.8	-17.7
H5	-0.4894	0.00213	-0.4871	-0.4878	1.4	0.4
H6	-0.4894	0.00213	-0.4871	-0.4878	1.4	0.4
H7	-0.5812	0.00253	-0.5687	-0.5794	7.8	6.7
H8	-0.5812	0.00253	-0.5687	-0.5794	7.8	6.7
H9	-0.5812	0.00253	-0.5687	-0.5794	7.8	6.7
H10	-0.5812	0.00253	-0.5687	-0.5794	7.8	6.7

[a]) Additive atomic energies are in au. Differences $\Delta E^{A}_{add} = (E^{A}_{add})_{HF} - (E^{A}_{add})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{add} = {}^{Comput}E^{A}_{add} - {}^{Expect}E^{A}_{add}$ are in kcal mol^{-1}.

Table S9. Relative to the CCSD/BBC1 data, analysis of additive atomic energies computed for the **Ecl** conformer of glycol at the B3LYP level.[a]

	CCSD/BBC1		B3LYP			
Atom A	E^{A}_{add}	E^{A}_{add} / E	$^{Comput}E^{A}_{add}$	$^{Expect}E^{A}_{add}$	ΔE^{A}_{add}	Δ^{A}_{add}
C1	-37.9412	0.16518	-38.0412	-38.0373	-62.8	-2.4
C2	-37.9412	0.16518	-38.0413	-38.0373	-62.9	-2.5
O3	-75.2510	0.32761	-75.4290	-75.4418	-111.7	8.0
O4	-75.2510	0.32761	-75.4290	-75.4418	-111.7	8.0
H5	-0.4894	0.00213	-0.4922	-0.4906	-1.8	-1.0
H6	-0.4894	0.00213	-0.4922	-0.4906	-1.8	-1.0
H7	-0.5812	0.00253	-0.5880	-0.5827	-4.3	-3.3
H8	-0.5812	0.00253	-0.5880	-0.5827	-4.3	-3.3
H9	-0.5812	0.00253	-0.5880	-0.5827	-4.3	-3.3
H10	-0.5812	0.00253	-0.5880	-0.5827	-4.3	-3.3

[a]) Additive atomic energies are in au. Differences $\Delta E^{A}_{add} = (E^{A}_{add})_{B3LYP} - (E^{A}_{add})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{add} = {}^{Comput}E^{A}_{add} - {}^{Expect}E^{A}_{add}$ are in kcal mol^{-1}.

Table S10. Relative to the CCSD/BBC1 data, analysis of additive atomic energies computed for the **Ecl** conformer of glycol at the B3LYP-GD3 level.[a]

	CCSD/BBC1		B3LYP-GD3			
Atom A	E^{A}_{add}	E^{A}_{add} / E	$^{Comput}E^{A}_{add}$	$^{Expect}E^{A}_{add}$	ΔE^{A}_{add}	Δ^{A}_{add}
C1	-37.9412	0.16518	-38.0413	-38.0380	-62.8	-2.0
C2	-37.9412	0.16518	-38.0414	-38.0380	-62.9	-2.1
O3	-75.2510	0.32761	-75.4290	-75.4431	-111.7	8.8
O4	-75.2510	0.32761	-75.4290	-75.4431	-111.7	8.8
H5	-0.4894	0.00213	-0.4922	-0.4906	-1.8	-1.0
H6	-0.4894	0.00213	-0.4922	-0.4906	-1.8	-1.0
H7	-0.5812	0.00253	-0.5880	-0.5827	-4.3	-3.3
H8	-0.5812	0.00253	-0.5880	-0.5827	-4.3	-3.3
H9	-0.5812	0.00253	-0.5880	-0.5827	-4.3	-3.3
H10	-0.5812	0.00253	-0.5880	-0.5827	-4.3	-3.3

[a]) Additive atomic energies are in au. Differences $\Delta E^{A}_{add} = (E^{A}_{add})_{B3LYP\text{-}GD3} - (E^{A}_{add})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{add} = {}^{Comput}E^{A}_{add} - {}^{Expect}E^{A}_{add}$ are in kcal mol^{-1}.

Table S11. Relative to the CCSD/BBC1 data, analysis of additive atomic energies computed for the **Ecl** conformer of glycol at the MP2/Müller level.[a]

	CCSD/BBC1		MP2/Müller			
Atom A	E_{add}^{A}	E_{add}^{A} / E	${}^{Comput}E_{add}^{A}$	${}^{Expect}E_{add}^{A}$	ΔE_{add}^{A}	Δ_{add}^{A}
C1	-37.9412	0.16518	-37.9781	-37.9352	-23.2	-26.9
C2	-37.9412	0.16518	-37.9781	-37.9352	-23.2	-26.9
O3	-75.2510	0.32761	-75.3154	-75.2392	-40.4	-47.8
O4	-75.2510	0.32761	-75.3153	-75.2392	-40.4	-47.8
H5	-0.4894	0.00213	-0.4932	-0.4893	-2.4	-2.4
H6	-0.4894	0.00213	-0.4932	-0.4893	-2.4	-2.4
H7	-0.5812	0.00253	-0.5899	-0.5812	-5.4	-5.5
H8	-0.5812	0.00253	-0.5899	-0.5812	-5.4	-5.5
H9	-0.5812	0.00253	-0.5899	-0.5812	-5.4	-5.5
H10	-0.5812	0.00253	-0.5899	-0.5812	-5.4	-5.5

[a]) Additive atomic energies are in au. Differences $\Delta E_{add}^{A} = (E_{add}^{A})_{MP2/Müller} - (E_{add}^{A})_{CCSD/BBC1}$ and relative errors $\Delta_{add}^{A} = {}^{Comput}E_{add}^{A} - {}^{Expect}E_{add}^{A}$ are in kcal mol^{-1}.

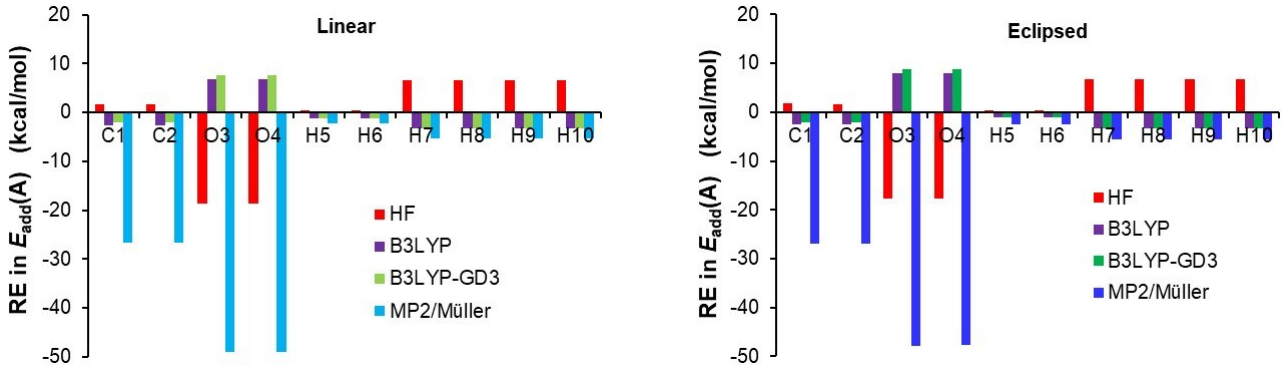

Figure S1. Using the CCSD/BBC1 data as reference, relative errors (RE) in individual additive atomic energies obtained at the indicated levels of theory for the eclipsed and linear conformers of glycol.

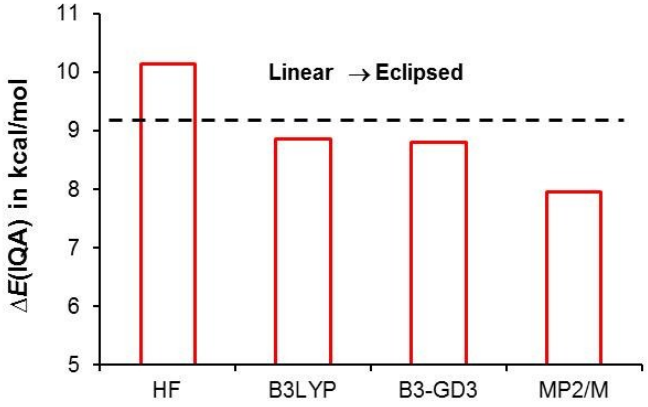

Figure S2. Change in E_{IQA} at the indicated levels of theory for the **Lin** → **Ecl** structural transformation of glycol (dashed line indicates the ΔE value obtained at CCSD. B3-GD3 = B3LYP-GD3 and MP2/M = MP2/Müller.

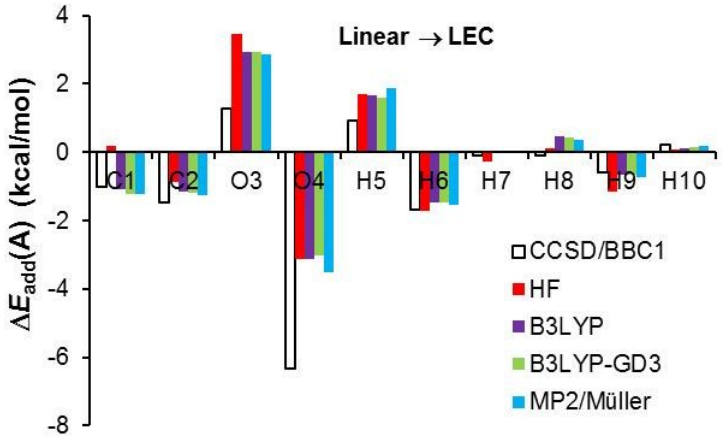

Figure S3. Change in individual additive atomic energies computed at the indicated levels of theory for the **Lin** → **LEC** structural transformation of glycol.

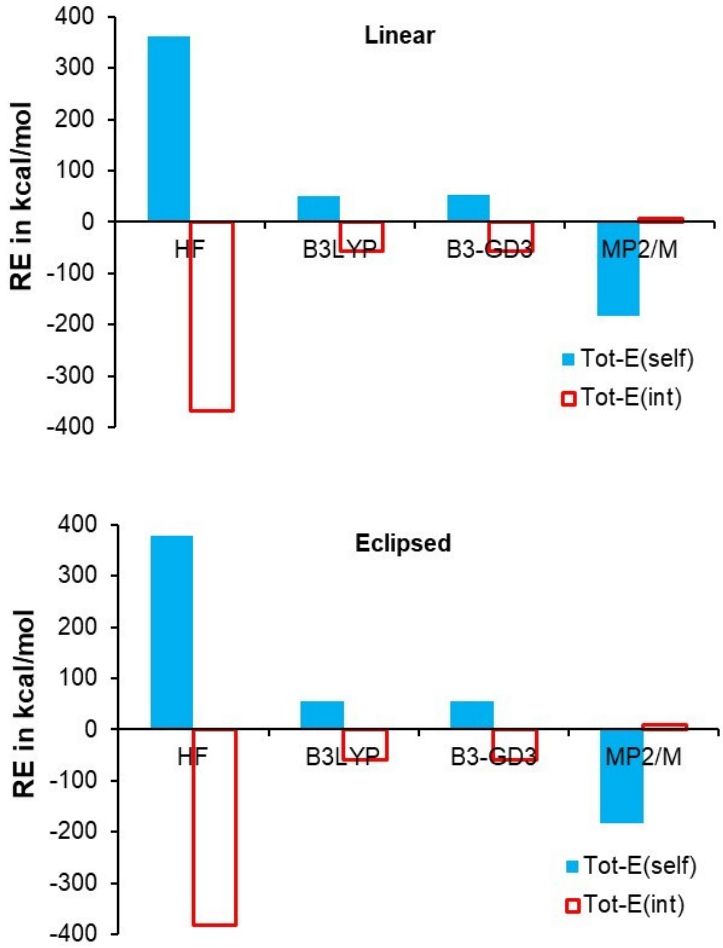

Figure S4. Using the CCSD/BBC1 data as a reference, relative errors (RE) in the total self-molecular and total interaction energies (solid and empty bars, respectively) obtained for the linear and eclipsed conformers of glycol at the indicated levels of theory.

Table S12. Using the CCSD/BBC1 data as a reference, relative errors in the total self-molecular energy (Δ_{self}^{Tot}) and total interaction energy (Δ_{int}^{Tot}) in three conformers of glycol optimized at the specified level of theory. Except CCSD/BBC1, all data are from AIMAll.[a]

***E*-term**	**HF**	**B3LYP**	**B3LYP-GD3**	**MP2/Müller**
	LEC / lowest energy conformer			
${}^{Comput}E_{self}^{Tot}$	-225.2208	-227.0177	-227.0209	-226.7799
${}^{Expect}E_{self}^{Tot}$	-225.8019	-227.1016	-227.1065	-226.4931
Δ_{self}^{Tot}	364.6	52.7	53.7	-180.0
${}^{Comput}E_{int}^{Tot}$	-3.7558	-3.2786	-3.2757	-3.1702
${}^{Expect}E_{int}^{Tot}$	-3.1746	-3.1929	-3.1930	-3.1844
Δ_{int}^{Tot}	-364.7	-53.8	-51.9	8.9
$\Delta_{self}^{Tot} + \Delta_{int}^{Tot}$	-0.1	–1.1	-1.2	-171.1
	Ecl / eclipsed conformer			
${}^{Comput}E_{self}^{Tot}$	-225.1992	-227.0133	-227.0162	-226.7841
${}^{Expect}E_{self}^{Tot}$	-225.8009	-227.1018	-227.1058	-226.4921
Δ_{self}^{Tot}	377.6	55.5	56.3	-183.3
${}^{Comput}E_{int}^{Tot}$	-3.7606	-3.2644	-3.2613	-3.1459
${}^{Expect}E_{int}^{Tot}$	-3.1504	-3.1685	-3.1686	-3.1600
Δ_{int}^{Tot}	-382.9	-60.2	-58.2	8.9
$\Delta_{self}^{Tot} + \Delta_{int}^{Tot}$	-5.3	-4.7	-1.9	-174.4
	Lin / linear conformer			
${}^{Comput}E_{self}^{Tot}$	-225.2322	-227.0256	-227.0267	-226.7905
${}^{Expect}E_{self}^{Tot}$	-225.8071	-227.1060	-227.1106	-226.4969
Δ_{self}^{Tot}	360.8	50.5	52.6	-184.2
${}^{Comput}E_{int}^{Tot}$	-3.7415	-3.2658	-3.2646	-3.1546
${}^{Expect}E_{int}^{Tot}$	-3.1563	-3.1745	-3.1745	-3.1660
Δ_{int}^{Tot}	-367.2	-57.3	-56.5	7.1
$\Delta_{self}^{Tot} + \Delta_{int}^{Tot}$	-6.4	-6.8	-3.8	-177.1

[a] The default settings in AIMAll were used throughout. The expected and computed values (${}^{Expect}E_{self}^{Tot}$, ${}^{Expect}E_{int}^{Tot}$, ${}^{Comput}E_{self}^{Tot}$, ${}^{Comput}E_{int}^{Tot}$) are in au; relative errors (Δ_{self}^{Tot} , Δ_{int}^{Tot}) are in kcal mol^{-1}.

Table S13. Relative to the CCSD/BBC1 data, analysis of self-atomic energies computed for the **LEC** of glycol at the HF level.[a]

	CCSD/BBC1		HF			
Atom A	E^{A}_{self}	E^{A}_{self}/E	${}^{Comput}E^{A}_{self}$	${}^{Expect}E^{A}_{self}$	ΔE^{A}_{self}	Δ^{A}_{self}
C1	-37.37564	0.162706	-37.13622	-37.25584	150.2	75.1
C2	-37.36186	0.162645	-37.11562	-37.24209	154.5	79.4
O3	-74.67762	0.325090	-74.35317	-74.43824	203.6	53.4
O4	-74.68076	0.325104	-74.35866	-74.44138	202.1	51.9
H5	-0.29952	0.001304	-0.27503	-0.29856	15.4	14.8
H6	-0.29375	0.001279	-0.27060	-0.29281	14.5	13.9
H7	-0.45915	0.001999	-0.42755	-0.45768	19.8	18.9
H8	-0.46056	0.002005	-0.42875	-0.45909	20.0	19.0
H9	-0.45985	0.002002	-0.42757	-0.45838	20.3	19.3
H10	-0.45930	0.001999	-0.42767	-0.45783	19.8	18.9

[a]) Self-atomic energies are in au. Differences $\Delta E^{A}_{self} = (E^{A}_{self})_{HF} - (E^{A}_{self})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{self} = {}^{Comput}E^{A}_{self} - {}^{Expect}E^{A}_{self}$ are in kcal mol^{-1}.

Table S14. Relative to the CCSD/BBC1 data, analysis of self-atomic energies computed for the **LEC** of glycol at the B3LYP level.[a]

	CCSD		B3LYP			
Atom A	E^{A}_{self}	E^{A}_{self}/E	${}^{Comput}E^{A}_{self}$	${}^{Expect}E^{A}_{self}$	ΔE^{A}_{self}	Δ^{A}_{self}
C1	-37.37564	0.162706	-37.44785	-37.47029	-45.3	14.1
C2	-37.36186	0.162645	-37.43598	-37.45646	-46.5	12.9
O3	-74.67762	0.325090	-74.86021	-74.86671	-114.6	4.1
O4	-74.68076	0.325104	-74.86238	-74.86987	-114.0	4.7
H5	-0.29952	0.001304	-0.29622	-0.30027	2.1	2.5
H6	-0.29375	0.001279	-0.29243	-0.29449	0.8	1.3
H7	-0.45915	0.001999	-0.45535	-0.46031	2.4	3.1
H8	-0.46056	0.002005	-0.45573	-0.46173	3.0	3.8
H9	-0.45985	0.002002	-0.45600	-0.46101	2.4	3.1
H10	-0.45930	0.001999	-0.45555	-0.46046	2.4	3.1

[a]) Self-atomic energies are in au. Differences $\Delta E^{A}_{self} = (E^{A}_{self})_{B3LYP} - (E^{A}_{self})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{self} = {}^{Comput}E^{A}_{self} - {}^{Expect}E^{A}_{self}$ are in kcal mol^{-1}.

Table S15. Relative to the CCSD/BBC1 data, analysis of self-atomic energies computed for the **LEC** of glycol at the B3LYP-GD3 level.[a]

	CCSD/BBC1		B3LYP-GD3			
Atom A	E^{A}_{self}	E^{A}_{self} / E	$^{Comput}E^{A}_{self}$	$^{Expect}E^{A}_{self}$	ΔE^{A}_{self}	Δ^{A}_{self}
C1	-37.37564	0.162706	-37.44853	-37.47110	-45.7	14.2
C2	-37.36186	0.162645	-37.43679	-37.45727	-47.0	12.9
O3	-74.67762	0.325090	-74.86096	-74.86833	-115.0	4.6
O4	-74.68076	0.325104	-74.86332	-74.87149	-114.6	5.1
H5	-0.29952	0.001304	-0.29626	-0.30028	2.0	2.5
H6	-0.29375	0.001279	-0.29249	-0.29450	0.8	1.3
H7	-0.45915	0.001999	-0.45530	-0.46032	2.4	3.1
H8	-0.46056	0.002005	-0.45576	-0.46174	3.0	3.8
H9	-0.45985	0.002002	-0.45607	-0.46102	2.4	3.1
H10	-0.45930	0.001999	-0.45555	-0.46047	2.4	3.1

[a]) Self-atomic energies are in au. Differences $\Delta E^{A}_{self} = (E^{A}_{self})_{B3LYP\text{-}GD3} - (E^{A}_{self})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{self} = {}^{Comput}E^{A}_{self} - {}^{Expect}E^{A}_{self}$ are in kcal mol^{-1}.

Table S16. Relative to the CCSD/BBC1 data, analysis of self-atomic energies computed for the **LEC** of glycol at the MP2/Müller level.[a]

	CCSD/BBC1		MP2/Müller			
Atom A	E^{A}_{self}	E^{A}_{self} / E	$^{Comput}E^{A}_{self}$	$^{Expect}E^{A}_{self}$	ΔE^{A}_{self}	Δ^{A}_{self}
C1	-37.37564	0.162706	-37.41773	-37.36988	-26.4	-30.0
C2	-37.36186	0.162645	-37.40381	-37.35609	-26.3	-29.9
O3	-74.67762	0.325090	-74.74816	-74.66610	-44.3	-51.5
O4	-74.68076	0.325104	-74.74964	-74.66925	-43.2	-50.4
H5	-0.29952	0.001304	-0.29816	-0.29947	0.9	0.8
H6	-0.29375	0.001279	-0.29313	-0.29370	0.4	0.4
H7	-0.45915	0.001999	-0.46683	-0.45908	-4.8	-4.9
H8	-0.46056	0.002005	-0.46752	-0.46049	-4.4	-4.4
H9	-0.45985	0.002002	-0.46779	-0.45978	-5.0	-5.0
H10	-0.45930	0.001999	-0.46711	-0.45923	-4.9	-4.9

[a]) Self-atomic energies are in au. Differences $\Delta E^{A}_{self} = (E^{A}_{self})_{MP2/Müller} - (E^{A}_{self})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{self} = {}^{Comput}E^{A}_{self} - {}^{Expect}E^{A}_{self}$ are in kcal mol^{-1}.

Table S17. Relative to the CCSD/BBC1 data, analysis of self-atomic energies computed for the **Lin** conformer of glycol at the HF level.[a]

	CCSD/BBC1		HF			
Atom A	E^{A}_{self}	E^{A}_{self} / E	$^{Comput}E^{A}_{self}$	$^{Expect}E^{A}_{self}$	ΔE^{A}_{self}	Δ^{A}_{self}
C1	-37.36617	0.162667	-37.12468	-37.24656	150.2	76.5
C2	-37.36617	0.162667	-37.12468	-37.24656	154.5	76.5
O3	-74.68168	0.325113	-74.36059	-74.44263	203.6	51.5
O4	-74.68168	0.325113	-74.36058	-74.44263	202.1	51.5
H5	-0.29995	0.001306	-0.27593	-0.29899	15.4	14.5
H6	-0.29995	0.001306	-0.27593	-0.29899	14.5	14.5
H7	-0.45916	0.001999	-0.42745	-0.45769	19.8	19.0
H8	-0.45916	0.001999	-0.42745	-0.45769	20.0	19.0
H9	-0.45916	0.001999	-0.42745	-0.45769	20.3	19.0
H10	-0.45916	0.001999	-0.42745	-0.45769	19.8	19.0

[a]) Self-atomic energies are in au. Differences $\Delta E^{A}_{self} = (E^{A}_{self})_{HF} - (E^{A}_{self})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{self} = {}^{Comput}E^{A}_{self} - {}^{Expect}E^{A}_{self}$ are in kcal mol^{-1}.

Table S18. Relative to the CCSD/BBC1 data, analysis of self-atomic energies computed for the **Lin** conformer of glycol B3LYP level.[a]

	CCSD/BBC1		B3LYP			
Atom A	E^{A}_{self}	E^{A}_{self} / E	$^{Comput}E^{A}_{self}$	$^{Expect}E^{A}_{self}$	ΔE^{A}_{self}	Δ^{A}_{self}
C1	-37.36617	0.162667	-37.43913	-37.46081	-45.8	13.6
C2	-37.36617	0.162667	-37.43912	-37.46081	-45.8	13.6
O3	-74.68168	0.325113	-74.86574	-74.87083	-115.5	3.2
O4	-74.68168	0.325113	-74.86573	-74.87083	-115.5	3.2
H5	-0.29995	0.001306	-0.29720	-0.30071	1.7	2.2
H6	-0.29995	0.001306	-0.29720	-0.30071	1.7	2.2
H7	-0.45916	0.001999	-0.45536	-0.46032	2.4	3.1
H8	-0.45916	0.001999	-0.45536	-0.46032	2.4	3.1
H9	-0.45916	0.001999	-0.45536	-0.46032	2.4	3.1
H10	-0.45916	0.001999	-0.45536	-0.46032	2.4	3.1

[a]) Self-atomic energies are in au. Differences $\Delta E^{A}_{self} = (E^{A}_{self})_{B3LYP} - (E^{A}_{self})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{self} = {}^{Comput}E^{A}_{self} - {}^{Expect}E^{A}_{self}$ are in kcal mol^{-1}.

Table S19. Relative to the CCSD/BBC1 data, analysis of self-atomic energies computed for the **Lin** conformer of glycol B3LYP-GD3 level.[a]

	CCSD		B3LYP-GD3			
Atom A	$E_{\text{self}}^{\text{A}}$	$E_{\text{self}}^{\text{A}} / E$	${}^{\text{Comput}}E_{\text{self}}^{\text{A}}$	${}^{\text{Expect}}E_{\text{self}}^{\text{A}}$	$\Delta E_{\text{self}}^{\text{A}}$	$\Delta_{\text{self}}^{\text{A}}$
C1	-37.36617	0.162667	-37.43910	-37.46157	-45.8	14.1
C2	-37.36617	0.162667	-37.43910	-37.46157	-45.8	14.1
O3	-74.68168	0.325113	-74.86644	-74.87236	-115.9	3.7
O4	-74.68168	0.325113	-74.86645	-74.87236	-115.9	3.7
H5	-0.29995	0.001306	-0.29719	-0.30072	1.7	2.2
H6	-0.29995	0.001306	-0.29719	-0.30072	1.7	2.2
H7	-0.45916	0.001999	-0.45535	-0.46033	2.4	3.1
H8	-0.45916	0.001999	-0.45535	-0.46033	2.4	3.1
H9	-0.45916	0.001999	-0.45535	-0.46033	2.4	3.1
H10	-0.45916	0.001999	-0.45535	-0.46033	2.4	3.1

[a]) Self-atomic energies are in au. Differences $\Delta E_{\text{self}}^{\text{A}} = (E_{\text{self}}^{\text{A}})_{\text{B3LYP-GD3}} - (E_{\text{self}}^{\text{A}})_{\text{CCSD/BBC1}}$ and relative errors $\Delta_{\text{self}}^{\text{A}} = {}^{\text{Comput}}E_{\text{self}}^{\text{A}} - {}^{\text{Expect}}E_{\text{self}}^{\text{A}}$ are in kcal mol^{-1}.

Table S20. Relative to the CCSD/BBC1 data, analysis of self-atomic energies computed for the **Lin** conformer of glycol MP2/Müller level.[a]

	CCSD/BBC1		MP2/Müller			
Atom A	$E_{\text{self}}^{\text{A}}$	$E_{\text{self}}^{\text{A}} / E$	${}^{\text{Comput}}E_{\text{self}}^{\text{A}}$	${}^{\text{Expect}}E_{\text{self}}^{\text{A}}$	$\Delta E_{\text{self}}^{\text{A}}$	$\Delta_{\text{self}}^{\text{A}}$
C1	-37.36617	0.162667	-37.40817	-37.36035	-26.4	-30.0
C2	-37.36617	0.162667	-37.40816	-37.36035	-26.4	-30.0
O3	-74.68168	0.325113	-74.75378	-74.67004	-45.2	-52.5
O4	-74.68168	0.325113	-74.75380	-74.67004	-45.3	-52.6
H5	-0.29995	0.001306	-0.29941	-0.29990	0.3	0.3
H6	-0.29995	0.001306	-0.29941	-0.29990	0.3	0.3
H7	-0.45916	0.001999	-0.46693	-0.45909	-4.9	-4.9
H8	-0.45916	0.001999	-0.46693	-0.45909	-4.9	-4.9
H9	-0.45916	0.001999	-0.46693	-0.45909	-4.9	-4.9
H10	-0.45916	0.001999	-0.46693	-0.45909	-4.9	-4.9

[a]) Self-atomic energies are in au. Differences $\Delta E_{\text{self}}^{\text{A}} = (E_{\text{self}}^{\text{A}})_{\text{MP2/Müller}} - (E_{\text{self}}^{\text{A}})_{\text{CCSD/BBC1}}$ and relative errors $\Delta_{\text{self}}^{\text{A}} = {}^{\text{Comput}}E_{\text{self}}^{\text{A}} - {}^{\text{Expect}}E_{\text{self}}^{\text{A}}$ are in kcal mol^{-1}.

Table S21. Relative to the CCSD/BBC1 data, analysis of self-atomic energies computed for the **Ecl** conformer of glycol at the HF level.[a]

	CCSD/BBC1		HF			
Atom A	E^{A}_{self}	E^{A}_{self}/E	${}^{Comput}E^{A}_{self}$	${}^{Expect}E^{A}_{self}$	ΔE^{A}_{self}	Δ^{A}_{self}
C1	-37.36288	0.162663	-37.11291	-37.24302	156.9	81.6
C2	-37.36288	0.162663	-37.11452	-37.24302	155.8	80.6
O3	-74.68303	0.325140	-74.35874	-74.44345	203.5	53.2
O4	-74.68303	0.325140	-74.35885	-74.44345	203.4	53.1
H5	-0.30250	0.001317	-0.27817	-0.30153	15.3	14.7
H6	-0.30250	0.001317	-0.27817	-0.30153	15.3	14.7
H7	-0.45770	0.001993	-0.42447	-0.45623	20.9	19.9
H8	-0.45770	0.001993	-0.42447	-0.45623	20.9	19.9
H9	-0.45770	0.001993	-0.42447	-0.45623	20.9	19.9
H10	-0.45770	0.001993	-0.42447	-0.45623	20.9	19.9

[a]) Self-atomic energies are in au. Differences $\Delta E^{A}_{self} = (E^{A}_{self})_{HF} - (E^{A}_{self})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{self} = {}^{Comput}E^{A}_{self} - {}^{Expect}E^{A}_{self}$ are in kcal mol^{-1}.

Table S22. Relative to the CCSD/BBC1 data, analysis of self-atomic energies computed for the **Ecl** conformer of glycol at the B3LYP level.[a]

	CCSD/BBC1		B3LYP			
Atom A	E^{A}_{self}	E^{A}_{self}/E	${}^{Comput}E^{A}_{self}$	${}^{Expect}E^{A}_{self}$	ΔE^{A}_{self}	Δ^{A}_{self}
C1	-37.36288	0.162663	-37.43459	-37.45758	-45.0	14.4
C2	-37.36288	0.162663	-37.43510	-37.45758	-45.3	14.1
O3	-74.68303	0.325140	-74.86393	-74.87233	-113.5	5.3
O4	-74.68303	0.325140	-74.86403	-74.87233	-113.6	5.2
H5	-0.30250	0.001317	-0.29928	-0.30326	2.0	2.5
H6	-0.30250	0.001317	-0.29928	-0.30326	2.0	2.5
H7	-0.45770	0.001993	-0.45428	-0.45886	2.1	2.9
H8	-0.45770	0.001993	-0.45428	-0.45886	2.1	2.9
H9	-0.45770	0.001993	-0.45428	-0.45886	2.1	2.9
H10	-0.45770	0.001993	-0.45428	-0.45886	2.1	2.9

[a]) Self-atomic energies are in au. Differences $\Delta E^{A}_{self} = (E^{A}_{self})_{B3LYP} - (E^{A}_{self})_{CCSD/BBC1}$ and relative errors $\Delta^{A}_{self} = {}^{Comput}E^{A}_{self} - {}^{Expect}E^{A}_{self}$ are in kcal mol^{-1}.

Table S23. Relative to the CCSD/BBC1 data, analysis of self-atomic energies computed for the **Ecl** conformer of glycol at the B3LYP-GD3 level.[a]

	CCSD/BBC1		B3LYP-GD3			
Atom A	$E_{\text{self}}^{\text{A}}$	$E_{\text{self}}^{\text{A}} / E$	${}^{\text{Comput}}E_{\text{self}}^{\text{A}}$	${}^{\text{Expect}}E_{\text{self}}^{\text{A}}$	$\Delta E_{\text{self}}^{\text{A}}$	$\Delta_{\text{self}}^{\text{A}}$
C1	-37.36288	0.162663	-37.43546	-37.45825	-45.5	14.3
C2	-37.36288	0.162663	-37.43603	-37.45825	-45.9	13.9
O3	-74.68303	0.325140	-74.86451	-74.87366	-113.9	5.7
O4	-74.68303	0.325140	-74.86454	-74.87366	-113.9	5.7
H5	-0.30250	0.001317	-0.29924	-0.30327	2.0	2.5
H6	-0.30250	0.001317	-0.29924	-0.30327	2.0	2.5
H7	-0.45770	0.001993	-0.45432	-0.45887	2.1	2.9
H8	-0.45770	0.001993	-0.45432	-0.45887	2.1	2.9
H9	-0.45770	0.001993	-0.45432	-0.45887	2.1	2.9
H10	-0.45770	0.001993	-0.45432	-0.45887	2.1	2.9

[a]) Self-atomic energies are in au. Differences $\Delta E_{\text{self}}^{\text{A}} = (E_{\text{self}}^{\text{A}})_{\text{B3LYP-GD3}} - (E_{\text{self}}^{\text{A}})_{\text{CCSD/BBC1}}$ and relative errors $\Delta_{\text{self}}^{\text{A}} = {}^{\text{Comput}}E_{\text{self}}^{\text{A}} - {}^{\text{Expect}}E_{\text{self}}^{\text{A}}$ are in kcal mol^{-1}.

Table S24. Relative to the CCSD/BBC1 data, analysis of self-atomic energies computed for the **Ecl** conformer of glycol at the MP2/Müller level.[a]

	CCSD/BBC1		MP2/Müller			
Atom A	$E_{\text{self}}^{\text{A}}$	$E_{\text{self}}^{\text{A}} / E$	${}^{\text{Comput}}E_{\text{self}}^{\text{A}}$	${}^{\text{Expect}}E_{\text{self}}^{\text{A}}$	$\Delta E_{\text{self}}^{\text{A}}$	$\Delta_{\text{self}}^{\text{A}}$
C1	-37.36288	0.162663	-37.40361	-37.35702	-25.6	-29.2
C2	-37.36288	0.162663	-37.40376	-37.35702	-25.7	-29.3
O3	-74.68303	0.325140	-74.75437	-74.67132	-44.8	-52.1
O4	-74.68303	0.325140	-74.75416	-74.67132	-44.6	-52.0
H5	-0.30250	0.001317	-0.30231	-0.30245	0.1	0.1
H6	-0.30250	0.001317	-0.30230	-0.30245	0.1	0.1
H7	-0.45770	0.001993	-0.46590	-0.45763	-5.1	-5.2
H8	-0.45770	0.001993	-0.46590	-0.45763	-5.1	-5.2
H9	-0.45770	0.001993	-0.46590	-0.45763	-5.1	-5.2
H10	-0.45770	0.001993	-0.46591	-0.45763	-5.1	-5.2

[a]) Self-atomic energies are in au. Differences $\Delta E_{\text{self}}^{\text{A}} = (E_{\text{self}}^{\text{A}})_{\text{MP2/Müller}} - (E_{\text{self}}^{\text{A}})_{\text{CCSD/BBC1}}$ and relative errors $\Delta_{\text{self}}^{\text{A}} = {}^{\text{Comput}}E_{\text{self}}^{\text{A}} - {}^{\text{Expect}}E_{\text{self}}^{\text{A}}$ are in kcal mol^{-1}.

From data in Tables S13-S24, several general trends are observed, namely:

(1) Considering absolute values of differences in the computed self-atomic energies, $\Delta E^{\mathrm{A}}_{\mathrm{self}} = \left(E^{\mathrm{A}}_{\mathrm{self}}\right)_{\mathrm{LoT}} - \left(E^{\mathrm{A}}_{\mathrm{self}}\right)_{\mathrm{CCSD/BBC1}}$, we found the following trend $\left|\Delta E^{\mathrm{O}}_{\mathrm{self}}\right| > \left|\Delta E^{\mathrm{C}}_{\mathrm{self}}\right| >> \left|\Delta E^{\mathrm{H}}_{\mathrm{self}}\right|$. Typically, $\left|\Delta E^{\mathrm{A}}_{\mathrm{self}}\right| >> \left|\Delta^{\mathrm{A}}_{\mathrm{self}}\right|$ for O- and C-atoms, but differences and relative errors computed for H-atoms are comparable.

(2) The self-atomic energies computed at B3LYP and B3LYP/GD3 for O- and C-atoms are systematically larger (more negative) than the CCSD/BBC1 values; hence $\Delta E^{\mathrm{A}}_{\mathrm{self}} < 0$. In reality, however, B3LYP generates underestimated self-atomic energies of O- and C-atoms resulting in $\Delta^{\mathrm{A}}_{\mathrm{self}} > 0$. Self-atomic energies of H-atoms are slightly underestimated ($\Delta E^{\mathrm{A}}_{\mathrm{self}}$ and $\Delta^{\mathrm{A}}_{\mathrm{self}}$ values are small and positive).

(3) There is no change in sign at HF; all $\Delta E^{\mathrm{A}}_{\mathrm{self}}$ and $\Delta^{\mathrm{A}}_{\mathrm{self}}$ values are positive; self-atomic energies of all atoms are being under-estimated.

(4) There is no change in sign at MP2/Müller and, except H3 and H5, all $\Delta E^{\mathrm{A}}_{\mathrm{self}}$ and $\Delta^{\mathrm{A}}_{\mathrm{self}}$ values are negative hence they were overestimated.

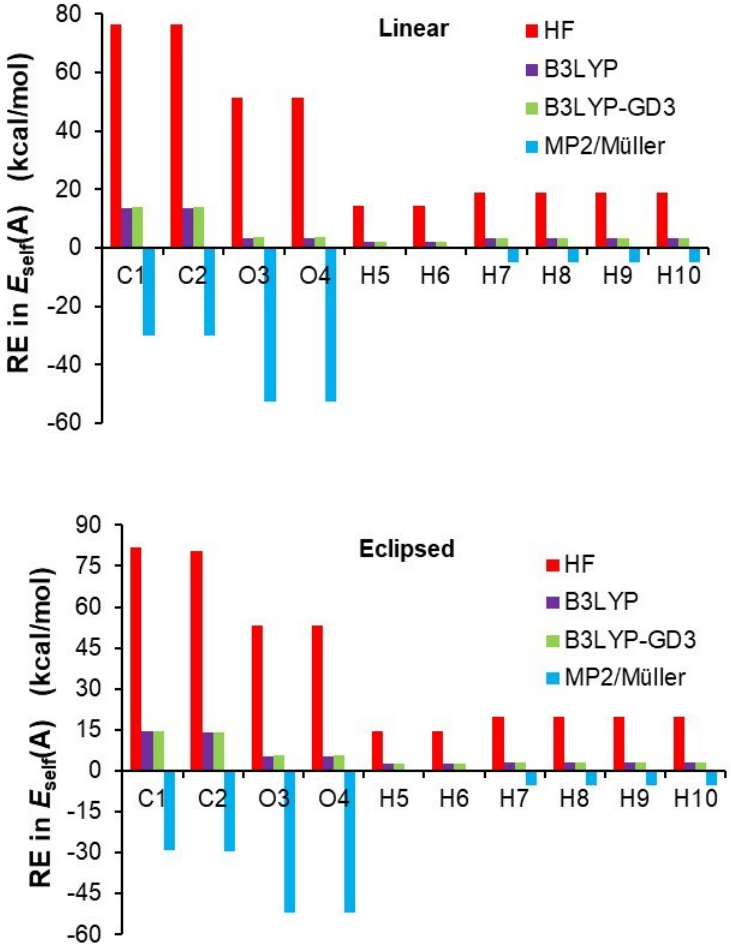

Figure S5. Using CCSD/BBC1 data as a reference, relative errors (RE) in computed self-atomic energies of the eclipsed and linear conformers of glycol at the indicated levels of theory.

Table S25. Part (a) shows a full set of interaction energies, $E_{\text{int}}^{\text{A,B}}$, computed for all 45 unique atom-pairs in the **Lin** and **LEC** conformers of glycol and changes in these interaction energies, $\Delta E_{\text{int}}^{\text{A,B}}$, on the **Lin** → **LEC** structural change. In addition and for convenience of interpretation, the atom pairs are also provided in the ascending order of the computed $\Delta E_{\text{int}}^{\text{A,B}}$ values (from most negative to most positive values) in Part (b). All values are in kcal mol^{-1} and were obtained at the CCSD/BBC1 level.

Part (a)

Atom		**LEC**	**Lin**	**Lin → LEC**
A	**B**	$E_{\text{int}}^{\text{A,B}}$		$\Delta E_{\text{int}}^{\text{A,B}}$
C1	C2	-91.19	-89.87	-1.32
C1	O3	-98.68	-91.80	-6.88
C1	O4	-363.14	-370.62	7.49
C1	H5	78.29	80.84	-2.55
C1	H6	47.76	34.65	13.11
C1	H7	-137.40	-137.72	0.32
C1	H8	-3.92	-4.93	1.00
C1	H9	-138.87	-137.72	-1.15
C1	H10	-5.06	-4.93	-0.13
C2	O3	-378.58	-370.62	-7.96
C2	O4	-102.42	-91.80	-10.63
C2	H5	38.67	34.65	4.02
C2	H6	85.16	80.84	4.31
C2	H7	-4.58	-4.93	0.34
C2	H8	-135.62	-137.72	2.10
C2	H9	-5.06	-4.93	-0.14
C2	H10	-136.84	-137.72	0.88
O3	O4	137.08	103.17	33.90
O3	H5	-63.47	-50.37	-13.10
O3	H6	-318.71	-314.35	-4.36
O3	H7	1.53	2.11	-0.58
O3	H8	-6.44	-3.97	-2.48
O3	H9	1.74	2.11	-0.36
O3	H10	-4.72	-3.97	-0.75
O4	H5	-316.44	-314.35	-2.09
O4	H6	-90.89	-50.37	-40.52
O4	H7	-4.46	-3.97	-0.50
O4	H8	0.02	2.11	-2.08
O4	H9	-3.22	-3.97	0.75
O4	H10	1.98	2.11	-0.12

Part (b)

Atom		**Lin → LEC**
A	**B**	$\Delta E_{\text{int}}^{\text{A,B}}$
O4	H6	-40.52
O3	H5	-13.10
C2	O4	-10.63
C2b	O3	-7.96
C1	O3	-6.88
O3b	H6	-4.36
C1	H5	-2.55
O3	H8	-2.48
O4b	H5	-2.09
O4	H8	-2.08
C1	C2	-1.32
C1	H9	-1.15
O3	H10	-0.75
O3	H7	-0.58
O4	H7	-0.50
O3	H9	-0.36
H5	H9	-0.36
C2	H9	-0.14
C1	H10	-0.13
O4	H10	-0.12
H7	H10	-0.09
H5	H7	-0.07
H5	H10	0.03
H6	H7	0.03
H8	H10	0.12
H8	H9	0.14
H7	H8	0.14
H7	H9	0.19
H9	H10	0.31
H6	H10	0.32

Table S25 continues.

Part (a)

Atom		LEC	Lin	Lin → LEC
A	**B**	$E_{int}^{A,B}$		$\Delta E_{int}^{A,B}$
H5	H6	36.97	22.72	14.24
H5	H7	-1.91	-1.84	-0.07
H5	H8	-0.65	-1.82	1.16
H5	H9	-2.20	-1.84	-0.36
H5	H10	-1.79	-1.82	0.03
H6	H7	-1.78	-1.82	0.03
H6	H8	-0.43	-1.84	1.41
H6	H9	-1.50	-1.82	0.32
H6	H10	-1.52	-1.84	0.32
H7	H8	-0.42	-0.57	0.14
H7	H9	-2.32	-2.51	0.19
H7	H10	-0.55	-0.46	-0.09
H8	H9	-0.32	-0.46	0.14
H8	H10	-2.38	-2.51	0.12
H9	H10	-0.25	-0.57	0.31

Part (b)

Atom		Lin → LEC
A	**B**	$\Delta E_{int}^{A,B}$
H6	H9	0.32
C1	H7	0.32
C2	H7	0.34
O4	H9	0.75
C2	H10	0.88
C1	H8	1.00
H5	H8	1.16
H6	H8	1.41
C2b	H8	2.10
C2	H5	4.02
C2	H6	4.31
C1b	O4	7.49
C1	H6	13.11
H5	H6	14.24
O3	O4	33.90

Table S26. Part (a) shows a full set of classical component, $V_{cl}^{A,B}$, of interaction energies computed for all 45 unique atom-pairs in the **Lin** and **LEC** conformers of glycol and changes in the classical component, $\Delta V_{cl}^{A,B}$, on the **Lin** → **LEC** structural change. In addition and for convenience of interpretation, the atom pairs are also provided in the ascending order of the computed $\Delta V_{cl}^{A,B}$ values (from most negative to most positive values) in Part (b). All values are in kcal mol^{-1} and were obtained at the CCSD/BBC1 level.

Part (a)

Atom		LEC	Lin	Lin → LEC
A	**B**	$V_{cl}^{A,B}$		$\Delta V_{cl}^{A,B}$
C1	C2	78.34	78.42	-0.07
C1	O3	-88.27	-80.85	-7.42
C1	O4	-209.58	-215.79	6.21
C1	H5	79.50	82.17	-2.67
C1	H6	48.29	35.15	13.14
C1	H7	19.68	19.26	0.43
C1	H8	0.12	-1.14	1.26
C1	H9	18.41	19.26	-0.85
C1	H10	-1.10	-1.14	0.04
C2	O3	-221.21	-215.79	-5.42
C2	O4	-92.24	-80.85	-11.39
C2	H5	39.11	35.15	3.96
C2	H6	86.47	82.17	4.30
C2	H7	-0.83	-1.14	0.30
C2	H8	21.87	19.26	2.61
C2	H9	-1.27	-1.14	-0.13
C2	H10	19.50	19.26	0.24
O3	O4	146.25	108.94	37.31
O3	H5	-63.12	-49.87	-13.25
O3	H6	-204.52	-196.27	-8.24
O3	H7	3.53	4.07	-0.54
O3	H8	-0.18	2.14	-2.31
O3	H9	2.88	4.07	-1.19
O3	H10	1.70	2.14	-0.43
O4	H5	-198.05	-196.27	-1.78
O4	H6	-87.85	-49.87	-37.99
O4	H7	1.81	2.14	-0.32
O4	H8	0.88	4.07	-3.18
O4	H9	3.29	2.14	1.15
O4	H10	3.97	4.07	-0.10

Part (b)

Atom		Lin → LEC
A	**B**	$\Delta V_{cl}^{A,B}$
O4	H6	-37.99
O3	H5	-13.25
C2	O4	-11.39
O3	H6	-8.24
C1	O3	-7.42
C2	O3	-5.42
O4	H8	-3.18
C1	H5	-2.67
O3	H8	-2.31
O4	H5	-1.78
O3	H9	-1.19
C1	H9	-0.85
O3	H7	-0.54
O3	H10	-0.43
H5	H9	-0.37
O4	H7	-0.32
H7	H10	-0.13
C2	H9	-0.13
O4	H10	-0.10
C1	C2	-0.07
H8	H10	0.00
H5	H7	0.01
H7	H9	0.02
C1	H10	0.04
H8	H9	0.05
H5	H10	0.07
H6	H7	0.09
H7	H8	0.12
H9	H10	0.22
C2	H10	0.24

Table S26 continues.

Part (a)

Atom		LEC	Lin	Lin → LEC
A	**B**	$V_{cl}^{A,B}$		$\Delta V_{cl}^{A,B}$
H5	H6	37.09	22.91	14.18
H5	H7	-1.73	-1.74	0.01
H5	H8	-0.59	-1.78	1.19
H5	H9	-2.11	-1.74	-0.37
H5	H10	-1.71	-1.78	0.07
H6	H7	-1.70	-1.78	0.09
H6	H8	-0.08	-1.74	1.66
H6	H9	-1.41	-1.78	0.38
H6	H10	-1.38	-1.74	0.35
H7	H8	0.20	0.08	0.12
H7	H9	0.69	0.67	0.02
H7	H10	0.08	0.21	-0.13
H8	H9	0.26	0.21	0.05
H8	H10	0.67	0.67	0.00
H9	H10	0.30	0.08	0.22

Part (b)

Atom		Lin → LEC
A	**B**	$\Delta V_{cl}^{A,B}$
C2	H7	0.30
H6	H10	0.35
H6	H9	0.38
C1	H7	0.43
O4	H9	1.15
H5	H8	1.19
C1	H8	1.26
H6	H8	1.66
C2	H8	2.61
C2	H5	3.96
C2	H6	4.30
C1	O4	6.21
C1	H6	13.14
H5	H6	14.18
O3	O4	37.31

Table S27. Part (a) shows a full set of the XC-term, $V_{XC}^{A,B}$, of interaction energies computed for all 45 unique atom-pairs in the **Lin** and **LEC** conformers of glycol and changes in the XC-term, $\Delta V_{XC}^{A,B}$, on the **Lin** → **LEC** structural change. In addition and for convenience of interpretation, the atom pairs are also provided in the ascending order of the computed $\Delta V_{XC}^{A,B}$ values (from most negative to most positive values) in Part (b). All values are in kcal mol^{-1} and were obtained at the CCSD/BBC1 level.

Part (a)

Atom		LEC	Lin	Lin → LEC
A	**B**	$V_{XC}^{A,B}$		$\Delta V_{XC}^{A,B}$
C1	C2	-169.54	-168.29	-1.25
C1	O3	-10.41	-10.95	0.54
C1	O4	-153.56	-154.83	1.27
C1	H5	-1.21	-1.32	0.11
C1	H6	-0.53	-0.50	-0.04
C1	H7	-157.08	-156.98	-0.10
C1	H8	-4.04	-3.79	-0.26
C1	H9	-157.27	-156.98	-0.29
C1	H10	-3.96	-3.79	-0.17
C2	O3	-157.37	-154.83	-2.54
C2	O4	-10.19	-10.95	0.76
C2	H5	-0.44	-0.50	0.05
C2	H6	-1.31	-1.32	0.01
C2	H7	-3.75	-3.79	0.04
C2	H8	-157.49	-156.98	-0.51
C2	H9	-3.79	-3.79	-0.01
C2	H10	-156.34	-156.98	0.64
O3	O4	-9.17	-5.77	-3.41
O3	H5	-0.35	-0.50	0.15
O3	H6	-114.19	-118.07	3.88
O3	H7	-2.00	-1.96	-0.04
O3	H8	-6.27	-6.10	-0.16
O3	H9	-1.14	-1.96	0.82
O3	H10	-6.42	-6.10	-0.32
O4	H5	-118.39	-118.07	-0.32
O4	H6	-3.03	-0.50	-2.53
O4	H7	-6.28	-6.10	-0.17
O4	H8	-0.86	-1.96	1.10
O4	H9	-6.50	-6.10	-0.40
O4	H10	-1.99	-1.96	-0.03

Part (b)

Atom		Lin → LEC
A	**B**	$\Delta V_{XC}^{A,B}$
O3	O4	-3.41
C2	O3	-2.54
O4	H6	-2.53
C1	C2	-1.25
C2	H8	-0.51
O4	H9	-0.40
O3	H10	-0.32
O4	H5	-0.32
C1	H9	-0.29
C1	H8	-0.26
H6	H8	-0.24
O4	H7	-0.17
C1	H10	-0.17
O3	H8	-0.16
C1	H7	-0.10
H5	H7	-0.07
H6	H7	-0.06
H6	H9	-0.06
H5	H10	-0.04
O3	H7	-0.04
C1	H6	-0.04
H6	H10	-0.03
H5	H8	-0.03
O4	H10	-0.03
C2	H9	-0.01
C2	H6	0.01
H5	H9	0.01
H7	H8	0.02
C2	H7	0.04
H7	H10	0.04

Table S27 continues.

Part (a)

Atom		LEC	Lin	Lin → LEC
A	**B**	$V_{XC}^{A,B}$		$\Delta V_{XC}^{A,B}$
H5	H6	-0.12	-0.19	0.07
H5	H7	-0.18	-0.11	-0.07
H5	H8	-0.06	-0.03	-0.03
H5	H9	-0.09	-0.11	0.01
H5	H10	-0.08	-0.03	-0.04
H6	H7	-0.09	-0.03	-0.06
H6	H8	-0.35	-0.11	-0.24
H6	H9	-0.09	-0.03	-0.06
H6	H10	-0.14	-0.11	-0.03
H7	H8	-0.62	-0.64	0.02
H7	H9	-3.01	-3.18	0.17
H7	H10	-0.63	-0.67	0.04
H8	H9	-0.59	-0.67	0.09
H8	H10	-3.05	-3.18	0.12
H9	H10	-0.55	-0.64	0.09

Part (b)

Atom		Lin → LEC
A	**B**	$\Delta V_{XC}^{A,B}$
C2	H5	0.05
H5	H6	0.07
H8	H9	0.09
H9	H10	0.09
C1	H5	0.11
H8	H10	0.12
O3	H5	0.15
H7	H9	0.17
C1	O3	0.54
C2	H10	0.64
C2	O4	0.76
O3	H9	0.82
O4	H8	1.10
C1	O4	1.27
O3	H6	3.88

Table S28. Part (a) shows a full set of interaction energies, $E_{int}^{A,B}$, computed for all 45 unique atom-pairs in the **Lin** and **Ecl** conformers of glycol and changes in these interaction energies, $\Delta E_{int}^{A,B}$, on the **Lin** → **Ecl** structural change. In addition and for convenience of interpretation, the atom pairs are also provided in the ascending order of the computed $\Delta E_{int}^{A,B}$ values (from most negative to most positive values) in Part (b). All values are in kcal mol^{-1} and were obtained at the CCSD/BBC1 level.

Part (a)

Atom		Ecl	Lin	Lin → Ecl
A	**B**	$E_{int}^{A,B}$		$\Delta E_{int}^{A,B}$
C1	C2	-81.00	-89.87	8.88
C1	O3	-97.02	-91.80	-5.23
C1	O4	-372.06	-370.62	-1.43
C1	H5	82.40	80.84	1.56
C1	H6	37.71	34.65	3.06
C1	H7	-141.30	-137.72	-3.58
C1	H8	-6.60	-4.93	-1.68
C1	H9	-141.30	-137.72	-3.58
C1	H10	-6.60	-4.93	-1.68
C2	O3	-372.06	-370.62	-1.43
C2	O4	-97.02	-91.80	-5.23
C2	H5	37.71	34.65	3.06
C2	H6	82.40	80.84	1.56
C2	H7	-6.60	-4.93	-1.68
C2	H8	-141.30	-137.72	-3.58
C2	H9	-6.60	-4.93	-1.68
C2	H10	-141.30	-137.72	-3.58
O3	O4	121.19	103.17	18.02
O3	H5	-59.43	-50.37	-9.06
O3	H6	-309.99	-314.35	4.36
O3	H7	3.69	2.11	1.59
O3	H8	-1.45	-3.97	2.51
O3	H9	3.69	2.11	1.59
O3	H10	-1.45	-3.97	2.51
O4	H5	-309.99	-314.35	4.36
O4	H6	-59.43	-50.37	-9.06
O4	H7	-1.45	-3.97	2.51
O4	H8	3.69	2.11	1.59
O4	H9	-1.45	-3.97	2.51
O4	H10	3.69	2.11	1.59

Part (b)

Atom		Lin → Ecl
A	**B**	$\Delta E_{int}^{A,B}$
O3	H5	-9.06
O4	H6	-9.06
C1	O3	-5.23
C2	O4	-5.23
C1	H7	-3.58
C1	H9	-3.58
C2	H8	-3.58
C2	H10	-3.58
C1	H8	-1.68
C1	H10	-1.68
C2	H7	-1.68
C2	H9	-1.68
H5	H7	-1.53
H5	H9	-1.53
H6	H8	-1.53
H6	H10	-1.53
C1	O4	-1.43
C2	O3	-1.43
H5	H8	-0.41
H5	H10	-0.41
H6	H7	-0.41
H6	H9	-0.41
H7	H8	-0.32
H9	H10	-0.32
H7	H9	-0.14
H8	H10	-0.14
H7	H10	0.21
H8	H9	0.21
C1	H5	1.56
C2	H6	1.56

Table S28 continues.

Part (a)

Atom		Ecl	Lin	Lin → Ecl
A	**B**	$E_{int}^{A,B}$		$\Delta E_{int}^{A,B}$
H5	H6	25.93	22.72	3.21
H5	H7	-3.37	-1.84	-1.53
H5	H8	-2.23	-1.82	-0.41
H5	H9	-3.37	-1.84	-1.53
H5	H10	-2.23	-1.82	-0.41
H6	H7	-2.23	-1.82	-0.41
H6	H8	-3.37	-1.84	-1.53
H6	H9	-2.23	-1.82	-0.41
H6	H10	-3.37	-1.84	-1.53
H7	H8	-0.88	-0.57	-0.32
H7	H9	-2.65	-2.51	-0.14
H7	H10	-0.25	-0.46	0.21
H8	H9	-0.25	-0.46	0.21
H8	H10	-2.65	-2.51	-0.14
H9	H10	-0.88	-0.57	-0.32

Part (b)

Atom		Lin → Ecl
A	**B**	$\Delta E_{int}^{A,B}$
O3	H7	1.59
O3	H9	1.59
O4	H8	1.59
O4	H10	1.59
O3	H8	2.51
O3	H10	2.51
O4	H7	2.51
O4	H9	2.51
C1	H6	3.06
C2	H5	3.06
H5	H6	3.21
O3	H6	4.36
O4	H5	4.36
C1	C2	8.88
O3	O4	18.02

Table S29. Part (a) shows a full set of classical component, $V_{cl}^{A,B}$, of interaction energies computed for all 45 unique atom-pairs in the **Ecl** and **Lin** conformers of glycol and changes in the classical component, $\Delta V_{cl}^{A,B}$, on the **Lin** → **Ecl** structural change. In addition and for convenience of interpretation, the atom pairs are also provided in the ascending order of the computed $\Delta V_{cl}^{A,B}$ values (from most negative to most positive values) in Part (b). All values are in kcal mol^{-1} and were obtained at the CCSD/BBC1 level.

Part (a)

Atom		Ecl	Lin	Lin → Ecl
A	**B**	$V_{cl}^{A,B}$		$\Delta V_{cl}^{A,B}$
C1	C2	81.66	78.42	3.24
C1	O3	-89.13	-80.85	-8.28
C1	O4	-214.54	-215.79	1.25
C1	H5	83.83	82.17	1.66
C1	H6	38.20	35.15	3.05
C1	H7	16.02	19.26	-3.24
C1	H8	-2.54	-1.14	-1.40
C1	H9	16.02	19.26	-3.24
C1	H10	-2.54	-1.14	-1.40
C2	O3	-214.54	-215.79	1.25
C2	O4	-89.13	-80.85	-8.28
C2	H5	38.20	35.15	3.05
C2	H6	83.83	82.17	1.66
C2	H7	-2.54	-1.14	-1.40
C2	H8	16.02	19.26	-3.24
C2	H9	-2.54	-1.14	-1.40
C2	H10	16.02	19.26	-3.24
O3	O4	136.45	108.94	27.51
O3	H5	-58.77	-49.87	-8.90
O3	H6	-191.06	-196.27	5.21
O3	H7	4.39	4.07	0.32
O3	H8	5.13	2.14	2.99
O3	H9	4.39	4.07	0.32
O3	H10	5.13	2.14	2.99
O4	H5	-191.06	-196.27	5.21
O4	H6	-58.77	-49.87	-8.90
O4	H7	5.13	2.14	2.99
O4	H8	4.39	4.07	0.32
O4	H9	5.13	2.14	2.99
O4	H10	4.39	4.07	0.32

Part (b)

Atom		Lin → Ecl
A	**B**	$\Delta V_{cl}^{A,B}$
O3	H5	-8.90
O4	H6	-8.90
C1	O3	-8.28
C2	O4	-8.28
C1	H7	-3.24
C1	H9	-3.24
C2	H8	-3.24
C2	H10	-3.24
H5	H7	-1.49
H5	H9	-1.49
H6	H8	-1.49
H6	H10	-1.49
C1	H8	-1.40
C1	H10	-1.40
C2	H7	-1.40
C2	H9	-1.40
H5	H8	-0.41
H5	H10	-0.41
H6	H7	-0.41
H6	H9	-0.41
H7	H10	0.04
H8	H9	0.04
H7	H9	0.13
H8	H10	0.13
O3	H7	0.32
O3	H9	0.32
O4	H8	0.32
O4	H10	0.32
H7	H8	0.50
H9	H10	0.50

Table S29 continues.

Part (a)

Atom		Ecl	Lin	Lin → Ecl
A	**B**	$V_{cl}^{A,B}$		$\Delta V_{cl}^{A,B}$
H5	H6	26.14	22.91	3.23
H5	H7	-3.23	-1.74	-1.49
H5	H8	-2.19	-1.78	-0.41
H5	H9	-3.23	-1.74	-1.49
H5	H10	-2.19	-1.78	-0.41
H6	H7	-2.19	-1.78	-0.41
H6	H8	-3.23	-1.74	-1.49
H6	H9	-2.19	-1.78	-0.41
H6	H10	-3.23	-1.74	-1.49
H7	H8	0.58	0.08	0.50
H7	H9	0.80	0.67	0.13
H7	H10	0.25	0.21	0.04
H8	H9	0.25	0.21	0.04
H8	H10	0.80	0.67	0.13
H9	H10	0.58	0.08	0.50

Part (b)

Atom		Lin → Ecl
A	**B**	$\Delta V_{cl}^{A,B}$
C1	O4	1.25
C2	O3	1.25
C1	H5	1.66
C2	H6	1.66
O3	H8	2.99
O3	H10	2.99
O4	H7	2.99
O4	H9	2.99
C1	H6	3.05
C2	H5	3.05
H5	H6	3.23
C1	C2	3.24
O3	H6	5.21
O4	H5	5.21
O3	O4	27.51

Table S30. Part (a) shows a full set of the XC-term, $V_{XC}^{A,B}$, of interaction energies computed for all unique 45 atom-pairs in the **Ecl** and **Lin** conformers of glycol and changes in the XC-term, $\Delta V_{XC}^{A,B}$, on the **Lin** → **Ecl** structural change. In addition and for convenience of interpretation, the atom pairs are also provided in the ascending order of the computed $\Delta V_{XC}^{A,B}$ values (from most negative to most positive values) in Part (b). All values are in kcal mol^{-1} and were obtained at the CCSD/BBC1 level.

Part (a)

Atom		Ecl	Lin	Lin → Ecl
A	**B**	$V_{XC}^{A,B}$		$\Delta V_{XC}^{A,B}$
C1	C2	-162.65	-168.29	5.64
C1	O3	-7.90	-10.95	3.05
C1	O4	-157.51	-154.83	-2.68
C1	H5	-1.43	-1.32	-0.10
C1	H6	-0.48	-0.50	0.01
C1	H7	-157.32	-156.98	-0.34
C1	H8	-4.06	-3.79	-0.28
C1	H9	-157.32	-156.98	-0.34
C1	H10	-4.06	-3.79	-0.28
C2	O3	-157.51	-154.83	-2.68
C2	O4	-7.90	-10.95	3.05
C2	H5	-0.48	-0.50	0.01
C2	H6	-1.43	-1.32	-0.10
C2	H7	-4.06	-3.79	-0.28
C2	H8	-157.32	-156.98	-0.34
C2	H9	-4.06	-3.79	-0.28
C2	H10	-157.32	-156.98	-0.34
O3	O4	-15.26	-5.77	-9.49
O3	H5	-0.67	-0.50	-0.16
O3	H6	-118.93	-118.07	-0.86
O3	H7	-0.70	-1.96	1.26
O3	H8	-6.58	-6.10	-0.48
O3	H9	-0.70	-1.96	1.26
O3	H10	-6.58	-6.10	-0.48
O4	H5	-118.93	-118.07	-0.86
O4	H6	-0.67	-0.50	-0.16
O4	H7	-6.58	-6.10	-0.48
O4	H8	-0.70	-1.96	1.26
O4	H9	-6.58	-6.10	-0.48
O4	H10	-0.70	-1.96	1.26

Part (b)

Atom		Lin → Ecl
A	**B**	$\Delta V_{XC}^{A,B}$
O3	O4	-9.49
C1	O4	-2.68
C2	O3	-2.68
O3	H6	-0.86
O4	H5	-0.86
H7	H8	-0.82
H9	H10	-0.82
O3	H8	-0.48
O3	H10	-0.48
O4	H7	-0.48
O4	H9	-0.48
C1	H7	-0.34
C1	H9	-0.34
C2	H8	-0.34
C2	H10	-0.34
C1	H8	-0.28
C1	H10	-0.28
C2	H7	-0.28
C2	H9	-0.28
H7	H9	-0.27
H8	H10	-0.27
O3	H5	-0.16
O4	H6	-0.16
C1	H5	-0.10
C2	H6	-0.10
H5	H7	-0.03
H5	H9	-0.03
H6	H8	-0.03
H6	H10	-0.03
H5	H6	-0.02

Table S30 continues.

Part (a)

Atom		Ecl	Lin	Lin → Ecl
A	**B**	$V_{XC}^{A,B}$		$\Delta V_{XC}^{A,B}$
H5	H6	-0.20	-0.19	-0.02
H5	H7	-0.14	-0.11	-0.03
H5	H8	-0.04	-0.03	0.00
H5	H9	-0.14	-0.11	-0.03
H5	H10	-0.04	-0.03	0.00
H6	H7	-0.04	-0.03	0.00
H6	H8	-0.14	-0.11	-0.03
H6	H9	-0.04	-0.03	0.00
H6	H10	-0.14	-0.11	-0.03
H7	H8	-1.46	-0.64	-0.82
H7	H9	-3.45	-3.18	-0.27
H7	H10	-0.51	-0.67	0.16
H8	H9	-0.51	-0.67	0.16
H8	H10	-3.45	-3.18	-0.27
H9	H10	-1.46	-0.64	-0.82

Part (b)

Atom		Lin → Ecl
A	**B**	$\Delta V_{XC}^{A,B}$
H5	H8	0.00
H5	H10	0.00
H6	H7	0.00
H6	H9	0.00
C1	H6	0.01
C2	H5	0.01
H7	H10	0.16
H8	H9	0.16
O3	H7	1.26
O3	H9	1.26
O4	H8	1.26
O4	H10	1.26
C1	O3	3.05
C2	O4	3.05
C1	C2	5.64

Table S31. Relative to the CCSD/BBC1 data, analysis of interaction energies obtained at the HF level for covalently bonded atom-pairs and intramolecular interaction O4···H6 in the **LEC** of glycol.[a]

		CCSD/BBC1		HF				
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	${}^{Comput}E_{int}^{A,B}$	${}^{Expect}E_{int}^{A,B}$	$\Delta E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-error
C1	C2	-91.2	6.32638E-04	-64.1	-90.9	27.1	26.8	-41.8
C1	O4	-363.1	2.51920E-03	-471.1	-362.0	-108.0	-109.1	23.2
C1	H7	-137.4	9.53175E-04	-165.4	-137.0	-28.0	-28.5	17.2
C1	H9	-138.9	9.63366E-04	-168.2	-138.4	-29.3	-29.7	17.7
C2	O3	-378.6	2.62634E-03	-492.4	-377.4	-113.8	-115.0	23.4
C2	H8	-135.6	9.40822E-04	-162.8	-135.2	-27.1	-27.6	16.9
C2	H10	-136.8	9.49285E-04	-165.2	-136.4	-28.3	-28.8	17.4
O3	H6	-318.7	2.21099E-03	-366.7	-317.7	-48.0	-49.1	13.4
O4	H5	-316.4	2.19526E-03	-362.5	-315.4	-46.0	-47.0	13.0
O4	H6	-90.9	6.30517E-04	-103.9	-90.6	-13.0	-13.3	12.8

[a]) Interaction energies, differences $\Delta E_{int}^{A,B} = (E_{int}^{A,B})_{HF} - (E_{int}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{int}^{A,B} = {}^{Comput}E_{int}^{A,B} - {}^{Expect}E_{int}^{A,B}$ are in kcal mol^{-1}.

Table S32. Relative to the CCSD/BBC1 data, analysis of interaction energies obtained at the B3LYP level for covalently bonded atom-pairs and intramolecular interaction O4···H6 in the **LEC** of glycol.[a]

		CCSD/BBC1		B3LYP				
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	${}^{Comput}E_{int}^{A,B}$	${}^{Expect}E_{int}^{A,B}$	$\Delta E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-error
C1	C2	-91.2	6.32638E-04	-117.1	-91.4	-25.9	-25.7	22.0
C1	O4	-363.1	2.51920E-03	-352.8	-364.1	10.3	11.2	-3.2
C1	H7	-137.4	9.53175E-04	-149.5	-137.7	-12.1	-11.8	7.9
C1	H9	-138.9	9.63366E-04	-150.7	-139.2	-11.9	-11.5	7.6
C2	O3	-378.6	2.62634E-03	-368.6	-379.5	10.0	11.0	-3.0
C2	H8	-135.6	9.40822E-04	-147.2	-136.0	-11.6	-11.2	7.6
C2	H10	-136.8	9.49285E-04	-148.4	-137.2	-11.6	-11.3	7.6
O3	H6	-318.7	2.21099E-03	-322.0	-319.5	-3.2	-2.4	0.8
O4	H5	-316.4	2.19526E-03	-319.7	-317.2	-3.3	-2.5	0.8
O4	H6	-90.9	6.30517E-04	-86.1	-91.1	4.8	5.0	-5.8

[a]) Interaction energies, differences $\Delta E_{int}^{A,B} = (E_{int}^{A,B})_{B3LYP} - (E_{int}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{int}^{A,B} = {}^{Comput}E_{int}^{A,B} - {}^{Expect}E_{int}^{A,B}$ are in kcal mol^{-1}.

Table S33. Relative to the CCSD/BBC1 data, analysis of interaction energies obtained at the B3LYP-GD3 level for covalently bonded atom-pairs and intramolecular interaction O4···H6 in the **LEC** of glycol.[a]

		CCSD/BBC1		B3LYP-GD3				
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-error
C1	C2	-91.2	6.32638E-04	-117.4	-91.4	-26.2	-26.0	22.1
C1	O4	-363.1	2.51920E-03	-351.9	-364.1	11.2	12.1	-3.4
C1	H7	-137.4	9.53175E-04	-149.4	-137.7	-12.0	-11.7	7.8
C1	H9	-138.9	9.63366E-04	-150.7	-139.2	-11.8	-11.5	7.6
C2	O3	-378.6	2.62634E-03	-367.7	-379.5	10.9	11.8	-3.2
C2	H8	-135.6	9.40822E-04	-147.2	-136.0	-11.6	-11.2	7.6
C2	H10	-136.8	9.49285E-04	-148.3	-137.2	-11.5	-11.2	7.5
O3	H6	-318.7	2.21099E-03	-321.8	-319.5	-3.1	-2.3	0.7
O4	H5	-316.4	2.19526E-03	-319.6	-317.2	-3.1	-2.3	0.7
O4	H6	-90.9	6.30517E-04	-85.8	-91.1	5.1	5.4	-6.2

[a]) Interaction energies, differences $\Delta E_{int}^{A,B} = (E_{int}^{A,B})_{B3LYP\text{-}GD3} - (E_{int}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{int}^{A,B} = {}^{Comput}E_{int}^{A,B} - {}^{Expect}E_{int}^{A,B}$ are in kcal mol^{-1}.

Table S34. Relative to the CCSD/BBC1 data, analysis of interaction energies obtained at the MP2/Müller level for covalently bonded atom-pairs and intramolecular interaction O4···H6 in the **LEC** of glycol.[a]

		CCSD/BBC1		MP2/Müller				
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-error
C1	C2	-91.2	6.32638E-04	-99.2	-91.2	-8.0	-8.0	8.1
C1	O4	-363.1	2.51920E-03	-352.4	-363.1	10.7	10.7	-3.0
C1	H7	-137.4	9.53175E-04	-139.4	-137.4	-2.0	-2.0	1.4
C1	H9	-138.9	9.63366E-04	-140.8	-138.8	-1.9	-2.0	1.4
C2	O3	-378.6	2.62634E-03	-368.6	-378.5	10.0	9.9	-2.7
C2	H8	-135.6	9.40822E-04	-137.2	-135.6	-1.6	-1.6	1.2
C2	H10	-136.8	9.49285E-04	-138.6	-136.8	-1.7	-1.8	1.3
O3	H6	-318.7	2.21099E-03	-324.9	-318.7	-6.2	-6.2	1.9
O4	H5	-316.4	2.19526E-03	-321.7	-316.4	-5.3	-5.3	1.7
O4	H6	-90.9	6.30517E-04	-93.0	-90.9	-2.1	-2.1	2.2

[a]) Interaction energies, differences $\Delta E_{int}^{A,B} = (E_{int}^{A,B})_{MP2/Müller} - (E_{int}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{int}^{A,B} = {}^{Comput}E_{int}^{A,B} - {}^{Expect}E_{int}^{A,B}$ are in kcal/mol.

Table S35. Relative to the CCSD/BBC1 data, analysis of interaction energies obtained at the HF levels for covalently bonded atom-pairs in the **Lin** conformer of glycol.[a]

		CCSD/BBC1		HF				
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-error
C1	C2	-89.9	6.23500E-04	-62.7	-89.6	27.2	26.9	-43.0
C1	O4	-370.6	2.57119E-03	-481.6	-369.4	-111.0	-112.2	23.3
C1	H7	-137.7	9.55436E-04	-166.1	-137.3	-28.3	-28.8	17.3
C1	H9	-137.7	9.55436E-04	-166.1	-137.3	-28.3	-28.8	17.3
C2	O3	-370.6	2.57119E-03	-481.6	-369.4	-111.0	-112.2	23.3
C2	H8	-137.7	9.55436E-04	-166.1	-137.3	-28.3	-28.8	17.3
C2	H10	-137.7	9.55436E-04	-166.1	-137.3	-28.3	-28.8	17.3
O3	H6	-314.3	2.18078E-03	-361.8	-313.3	-47.4	-48.4	13.4
O4	H5	-314.3	2.18078E-03	-361.8	-313.3	-47.4	-48.4	13.4

[a]) Interaction energies, differences $\Delta E_{int}^{A,B} = (E_{int}^{A,B})_{HF} - (E_{int}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{int}^{A,B} = {}^{Comput}E_{int}^{A,B} - {}^{Expect}E_{int}^{A,B}$ are in kcal mol^{-1}.

Table S36. Relative to the CCSD/BBC1 data, analysis of interaction energies obtained at the B3LYP level for covalently bonded atom-pairs in the **Lin** conformer of glycol.[a]

		CCSD/BBC1		B3LYP				
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-error
C1	C2	-89.9	6.23500E-04	-115.5	-90.1	-25.7	-25.4	22.0
C1	O4	-370.6	2.57119E-03	-361.0	-371.6	9.6	10.5	-2.9
C1	H7	-137.7	9.55436E-04	-149.7	-138.1	-12.0	-11.6	7.8
C1	H9	-137.7	9.55436E-04	-149.7	-138.1	-12.0	-11.6	7.8
C2	O3	-370.6	2.57119E-03	-361.0	-371.6	9.6	10.5	-2.9
C2	H8	-137.7	9.55436E-04	-149.7	-138.1	-12.0	-11.6	7.8
C2	H10	-137.7	9.55436E-04	-149.7	-138.1	-12.0	-11.6	7.8
O3	H6	-314.3	2.18078E-03	-318.9	-315.1	-4.6	-3.8	1.2
O4	H5	-314.3	2.18078E-03	-318.9	-315.1	-4.6	-3.8	1.2

[a]) Interaction energies, differences $\Delta E_{int}^{A,B} = (E_{int}^{A,B})_{B3LYP} - (E_{int}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{int}^{A,B} = {}^{Comput}E_{int}^{A,B} - {}^{Expect}E_{int}^{A,B}$ are in kcal mol^{-1}.

Table S37. Relative to the CCSD/BBC1 data, analysis of interaction energies obtained at the B3LYP-GD3 level for covalently bonded atom-pairs in the **Lin** conformer of glycol.[a]

		CCSD/BBC1		B3LYP-GD3				
Atom A	**Atom B**	$E_{\text{int}}^{\text{A,B}}$	$E_{\text{int}}^{\text{A,B}} / E$	${}^{\text{Comput}}E_{\text{int}}^{\text{A,B}}$	${}^{\text{Expect}}E_{\text{int}}^{\text{A,B}}$	$\Delta E_{\text{int}}^{\text{A,B}}$	$\Delta_{\text{int}}^{\text{A,B}}$	%-error
C1	C2	-89.9	6.23500E-04	-115.6	-90.1	-25.7	-25.5	22.1
C1	O4	-370.6	2.57119E-03	-360.6	-371.6	10.0	10.9	-3.0
C1	H7	-137.7	9.55436E-04	-149.6	-138.1	-11.9	-11.6	7.7
C1	H9	-137.7	9.55436E-04	-149.6	-138.1	-11.9	-11.6	7.7
C2	O3	-370.6	2.57119E-03	-360.6	-371.6	10.0	10.9	-3.0
C2	H8	-137.7	9.55436E-04	-149.6	-138.1	-11.9	-11.6	7.7
C2	H10	-137.7	9.55436E-04	-149.6	-138.1	-11.9	-11.6	7.7
O3	H6	-314.3	2.18078E-03	-318.9	-315.2	-4.5	-3.7	1.2
O4	H5	-314.3	2.18078E-03	-318.9	-315.2	-4.5	-3.7	1.2

[a]) Interaction energies, differences $\Delta E_{\text{int}}^{\text{A,B}} = (E_{\text{int}}^{\text{A,B}})_{\text{B3LYP-GD3}} - (E_{\text{int}}^{\text{A,B}})_{\text{CCSD/BBC1}}$ and relative errors $\Delta_{\text{int}}^{\text{A,B}} = {}^{\text{Comput}}E_{\text{int}}^{\text{A,B}} - {}^{\text{Expect}}E_{\text{int}}^{\text{A,B}}$ are in kcal mol^{-1}.

Table S38. Relative to the CCSD/BBC1 data, analysis of interaction energies obtained at the MP2/Müller level for covalently bonded atom-pairs in the **Lin** conformer of glycol.[a]

		CCSD/BBC1		MP2/Müller				
Atom A	**Atom B**	$E_{\text{int}}^{\text{A,B}}$	$E_{\text{int}}^{\text{A,B}} / E$	${}^{\text{Comput}}E_{\text{int}}^{\text{A,B}}$	${}^{\text{Expect}}E_{\text{int}}^{\text{A,B}}$	$\Delta E_{\text{int}}^{\text{A,B}}$	$\Delta_{\text{int}}^{\text{A,B}}$	%-error
C1	C2	-89.9	6.23500E-04	-97.3	-89.9	-7.4	-7.5	7.7
C1	O4	-370.6	2.57119E-03	-361.0	-370.6	9.6	9.6	-2.7
C1	H7	-137.7	9.55436E-04	-139.7	-137.7	-2.0	-2.0	1.5
C1	H9	-137.7	9.55436E-04	-139.7	-137.7	-2.0	-2.0	1.4
C2	O3	-370.6	2.57119E-03	-361.0	-370.6	9.6	9.6	-2.7
C2	H8	-137.7	9.55436E-04	-139.7	-137.7	-2.0	-2.0	1.5
C2	H10	-137.7	9.55436E-04	-139.7	-137.7	-2.0	-2.0	1.4
O3	H6	-314.3	2.18078E-03	-320.7	-314.3	-6.4	-6.4	2.0
O4	H5	-314.3	2.18078E-03	-320.7	-314.3	-6.4	-6.4	2.0

[a]) Interaction energies, differences $\Delta E_{\text{int}}^{\text{A,B}} = (E_{\text{int}}^{\text{A,B}})_{\text{MP2/Müller}} - (E_{\text{int}}^{\text{A,B}})_{\text{CCSD/BBC1}}$ and relative errors $\Delta_{\text{int}}^{\text{A,B}} = {}^{\text{Comput}}E_{\text{int}}^{\text{A,B}} - {}^{\text{Expect}}E_{\text{int}}^{\text{A,B}}$ are in kcal mol^{-1}.

Table S39. Relative to the CCSD/BBC1 data, analysis of interaction energies obtained at the HF level for covalently bonded atom-pairs and the intramolecular O3···O4 interaction in the **Ecl** conformer of glycol.[a]

		CCSD/BBC1		HF				
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-error
C1	C2	-81.0	5.61947E-04	-51.2	-80.7	29.8	29.6	-57.8
C1	O4	-372.1	2.58130E-03	-489.8	-370.9	-117.7	-118.9	24.3
C1	H7	-141.3	9.80326E-04	-171.8	-140.8	-30.5	-30.9	18.0
C1	H9	-141.3	9.80326E-04	-171.8	-140.8	-30.5	-30.9	18.0
C2	O3	-372.1	2.58130E-03	-489.7	-370.9	-117.7	-118.8	24.3
C2	H8	-141.3	9.80326E-04	-171.8	-140.8	-30.5	-30.9	18.0
C2	H10	-141.3	9.80326E-04	-171.8	-140.8	-30.5	-30.9	18.0
O3	H6	-310.0	2.15069E-03	-358.4	-309.0	-48.4	-49.4	13.8
O4	H5	-310.0	2.15069E-03	-358.4	-309.0	-48.4	-49.4	13.8
O3	O4	121.2	-8.40799E-04	168.1	120.8	46.9	47.3	28.1

[a]) Interaction energies, differences $\Delta E_{int}^{A,B} = (E_{int}^{A,B})_{HF} - (E_{int}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{int}^{A,B} = {}^{Comput}E_{int}^{A,B} - {}^{Expect}E_{int}^{A,B}$ are in kcal mol^{-1}.

Table S40. Relative to the CCSD/BBC1 data, analysis of interaction energies obtained at the B3LYP level for covalently bonded atom-pairs and the intramolecular O3···O4 interaction in the **Ecl** conformer of glycol.[a]

		CCSD/BBC1		B3LYP				
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-error
C1	C2	-81.0	5.61947E-04	-106.2	-81.2	-25.2	-25.0	23.6
C1	O4	-372.1	2.58130E-03	-364.6	-373.0	7.5	8.4	-2.3
C1	H7	-141.3	9.80326E-04	-153.0	-141.7	-11.7	-11.4	7.4
C1	H9	-141.3	9.80326E-04	-153.0	-141.7	-11.7	-11.4	7.4
C2	O3	-372.1	2.58130E-03	-364.6	-373.0	7.5	8.4	-2.3
C2	H8	-141.3	9.80326E-04	-153.0	-141.7	-11.7	-11.4	7.4
C2	H10	-141.3	9.80326E-04	-153.0	-141.7	-11.7	-11.4	7.4
O3	H6	-310.0	2.15069E-03	-315.4	-310.8	-5.4	-4.6	1.5
O4	H5	-310.0	2.15069E-03	-315.4	-310.8	-5.4	-4.6	1.5
O3	O4	121.2	-8.40799E-04	121.4	121.5	0.3	-0.1	0.0

[a]) Interaction energies, differences $\Delta E_{int}^{A,B} = (E_{int}^{A,B})_{B3LYP} - (E_{int}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{int}^{A,B} = {}^{Comput}E_{int}^{A,B} - {}^{Expect}E_{int}^{A,B}$ are in kcal mol^{-1}.

Table S41. Relative to the CCSD/BBC1 data, analysis of interaction energies obtained at the B3LYP-GD3 level for covalently bonded atom-pairs and the intramolecular O3···O4 interaction in the **Ecl** conformer of glycol.[a]

		CCSD/BBC1		B3LYP-GD3				
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-error
C1	C2	-81.0	5.61947E-04	-106.4	-81.2	-25.4	-25.2	23.7
C1	O4	-372.1	2.58130E-03	-363.7	-373.0	8.3	9.3	-2.6
C1	H7	-141.3	9.80326E-04	-153.0	-141.7	-11.7	-11.3	7.4
C1	H9	-141.3	9.80326E-04	-153.0	-141.7	-11.7	-11.3	7.4
C2	O3	-372.1	2.58130E-03	-363.7	-373.0	8.3	9.3	-2.6
C2	H8	-141.3	9.80326E-04	-153.0	-141.7	-11.7	-11.3	7.4
C2	H10	-141.3	9.80326E-04	-153.0	-141.7	-11.7	-11.3	7.4
O3	H6	-310.0	2.15069E-03	-315.2	-310.8	-5.2	-4.5	1.4
O4	H5	-310.0	2.15069E-03	-315.2	-310.8	-5.2	-4.5	1.4
O3	O4	121.2	-8.40799E-04	121.2	121.5	0.1	-0.3	-0.2

[a]) Interaction energies, differences $\Delta E_{int}^{A,B} = (E_{int}^{A,B})_{B3LYP\text{-}GD3} - (E_{int}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{int}^{A,B} = {}^{Comput}E_{int}^{A,B} - {}^{Expect}E_{int}^{A,B}$ are in kcal mol^{-1}.

Table S42. Relative to the CCSD/BBC1 data, analysis of interaction energies obtained at the MP2/Müller level for covalently bonded atom-pairs and the intramolecular O3···O4 interaction in the **Ecl** conformer of glycol.[a]

		CCSD/BBC1		MP2/Müller				
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-error
C1	C2	-81.0	5.61947E-04	-87.9	-81.0	-6.9	-6.9	7.8
C1	O4	-372.1	2.58130E-03	-362.9	-372.0	9.1	9.1	-2.5
C1	H7	-141.3	9.80326E-04	-143.2	-141.3	-1.9	-2.0	1.4
C1	H9	-141.3	9.80326E-04	-143.2	-141.3	-1.9	-2.0	1.4
C2	O3	-372.1	2.58130E-03	-363.0	-372.0	9.1	9.0	-2.5
C2	H8	-141.3	9.80326E-04	-143.2	-141.3	-1.9	-1.9	1.4
C2	H10	-141.3	9.80326E-04	-143.2	-141.3	-1.9	-1.9	1.4
O3	H6	-310.0	2.15069E-03	-316.3	-309.9	-6.3	-6.4	2.0
O4	H5	-310.0	2.15069E-03	-316.3	-309.9	-6.3	-6.3	2.0
O3	O4	121.2	-8.40799E-04	126.8	121.2	5.6	5.6	4.4

[a]) Interaction energies, differences $\Delta E_{int}^{A,B} = (E_{int}^{A,B})_{MP2/Müller} - (E_{int}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{int}^{A,B} = {}^{Comput}E_{int}^{A,B} - {}^{Expect}E_{int}^{A,B}$ are in kcal mol^{-1}.

Table S43. Relative to the CCSD/BBC1 data, analysis of a classical component of interaction energies obtained at the HF level for covalently bonded atom-pairs and the intramolecular O4···H6 interaction in the **LEC** of glycol.[a]

		CCSD/BBC1		HF				
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-error
C1	C2	78.3	-5.43506E-04	118.5	78.1	40.1	40.4	34.1
C1	O4	-209.6	1.45392E-03	-319.3	-208.9	-109.7	-110.4	34.6
C1	H7	19.7	-1.36560E-04	9.6	19.6	-10.1	-10.0	-104.3
C1	H9	18.4	-1.27693E-04	7.0	18.3	-11.5	-11.4	-163.8
C2	O3	-221.2	1.53461E-03	-337.6	-220.5	-116.4	-117.1	34.7
C2	H8	21.9	-1.51739E-04	12.2	21.8	-9.6	-9.6	-78.3
C2	H10	19.5	-1.35299E-04	9.1	19.4	-10.4	-10.4	-114.5
O3	H6	-204.5	1.41879E-03	-250.2	-203.9	-45.7	-46.3	18.5
O4	H5	-198.1	1.37395E-03	-242.4	-197.4	-44.3	-45.0	18.5
O4	H6	-87.9	6.09474E-04	-102.6	-87.6	-14.8	-15.0	14.7

[a]) Classical components of interaction energies, differences $\Delta V_{cl}^{A,B} = (V_{cl}^{A,B})_{HF} - (V_{cl}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{cl}^{A,B} = {}^{Comput}V_{cl}^{A,B} - {}^{Expect}V_{cl}^{A,B}$ are in kcal mol^{-1}.

Table S44. Relative to the CCSD/BBC1 data, analysis of a classical component of interaction energies obtained at the B3LYP level for covalently bonded atom-pairs and the intramolecular O4···H6 interaction in the **LEC** of glycol.[a]

		CCSD/BBC1		B3LYP				
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-error
C1	C2	78.3	-5.43506E-04	66.2	78.5	-12.1	-12.3	-18.6
C1	O4	-209.6	1.45392E-03	-188.2	-210.1	21.4	21.9	-11.7
C1	H7	19.7	-1.36560E-04	22.3	19.7	2.6	2.6	11.6
C1	H9	18.4	-1.27693E-04	21.1	18.5	2.7	2.7	12.6
C2	O3	-221.2	1.53461E-03	-199.8	-221.8	21.4	21.9	-11.0
C2	H8	21.9	-1.51739E-04	24.7	21.9	2.9	2.8	11.3
C2	H10	19.5	-1.35299E-04	22.3	19.6	2.8	2.8	12.4
O3	H6	-204.5	1.41879E-03	-200.1	-205.0	4.4	4.9	-2.5
O4	H5	-198.1	1.37395E-03	-194.1	-198.6	3.9	4.4	-2.3
O4	H6	-87.9	6.09474E-04	-83.8	-88.1	4.0	4.3	-5.1

[a]) Classical components of interaction energies, differences $\Delta V_{cl}^{A,B} = (V_{cl}^{A,B})_{B3LYP} - (V_{cl}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{cl}^{A,B} = {}^{Comput}V_{cl}^{A,B} - {}^{Expect}V_{cl}^{A,B}$ are in kcal mol^{-1}.

Table S45. Relative to the CCSD/BBC1 data, analysis of a classical component of interaction energies obtained at the B3LYP-GD3 level for covalently bonded atom-pairs and the intramolecular O4···H6 interaction in the **LEC** of glycol.[a]

		CCSD/BBC1		B3LYP-GD3				
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-error
C1	C2	78.3	-5.43506E-04	65.9	78.5	-12.5	-12.7	-19.3
C1	O4	-209.6	1.45392E-03	-187.3	-210.1	22.2	22.8	-12.2
C1	H7	19.7	-1.36560E-04	22.4	19.7	2.7	2.6	11.7
C1	H9	18.4	-1.27693E-04	21.1	18.5	2.7	2.7	12.7
C2	O3	-221.2	1.53461E-03	-199.1	-221.8	22.1	22.7	-11.4
C2	H8	21.9	-1.51739E-04	24.7	21.9	2.8	2.8	11.3
C2	H10	19.5	-1.35299E-04	22.4	19.6	2.9	2.8	12.6
O3	H6	-204.5	1.41879E-03	-199.9	-205.0	4.6	5.1	-2.6
O4	H5	-198.1	1.37395E-03	-193.9	-198.6	4.1	4.6	-2.4
O4	H6	-87.9	6.09474E-04	-83.5	-88.1	4.3	4.5	-5.4

[a]) Classical components of interaction energies, differences $\Delta V_{cl}^{A,B} = (V_{cl}^{A,B})_{B3LYP\text{-}GD3} - (V_{cl}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{cl}^{A,B} = {}^{Comput}V_{cl}^{A,B} - {}^{Expect}V_{cl}^{A,B}$ are in kcal mol^{-1}.

Table S46. Relative to the CCSD/BBC1 data, analysis of a classical component of interaction energies obtained at the MP2/Müller level for covalently bonded atom-pairs and the intramolecular O4···H6 interaction in the **LEC** of glycol.[a]

		CCSD/BBC1		MP2/Müller				
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-error
C1	C2	78.3	-5.43506E-04	71.8	78.3	-6.5	-6.5	-9.1
C1	O4	-209.6	1.45392E-03	-196.8	-209.5	12.7	12.7	-6.5
C1	H7	19.7	-1.36560E-04	22.4	19.7	2.7	2.7	12.2
C1	H9	18.4	-1.27693E-04	21.1	18.4	2.7	2.7	12.9
C2	O3	-221.2	1.53461E-03	-209.2	-221.2	12.0	12.0	-5.7
C2	H8	21.9	-1.51739E-04	24.7	21.9	2.8	2.8	11.3
C2	H10	19.5	-1.35299E-04	22.3	19.5	2.8	2.8	12.4
O3	H6	-204.5	1.41879E-03	-210.7	-204.5	-6.2	-6.2	3.0
O4	H5	-198.1	1.37395E-03	-203.9	-198.0	-5.9	-5.9	2.9
O4	H6	-87.9	6.09474E-04	-90.2	-87.8	-2.3	-2.4	2.6

[a]) Classical components of interaction energies, differences $\Delta V_{cl}^{A,B} = (V_{cl}^{A,B})_{B3LYP\text{-}GD3} - (V_{cl}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{cl}^{A,B} = {}^{Comput}V_{cl}^{A,B} - {}^{Expect}V_{cl}^{A,B}$ are in kcal mol^{-1}.

Table S47. Relative to the CCSD/BBC1 data, analysis of a classical component of interaction energies obtained at the HF level for covalently bonded atom-pairs in the **Lin** conformer of glycol.[a]

		CCSD/BBC1		HF				
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-error
C1	C2	78.4	-5.44002E-04	118.5	78.2	40.1	40.4	34.1
C1	O4	-215.8	1.49705E-03	-328.6	-215.1	-112.8	-113.5	34.5
C1	H7	19.3	-1.33604E-04	8.9	19.2	-10.3	-10.3	-115.2
C1	H9	19.3	-1.33604E-04	8.9	19.2	-10.3	-10.3	-115.1
C2	O3	-215.8	1.49705E-03	-328.6	-215.1	-112.8	-113.5	34.5
C2	H8	19.3	-1.33604E-04	8.9	19.2	-10.3	-10.3	-115.2
C2	H10	19.3	-1.33604E-04	8.9	19.2	-10.3	-10.3	-115.1
O3	H6	-196.3	1.36165E-03	-241.1	-195.6	-44.8	-45.4	18.8
O4	H5	-196.3	1.36165E-03	-241.1	-195.6	-44.8	-45.4	18.8

[a]) Classical components of interaction energies, differences $\Delta V_{cl}^{A,B} = (V_{cl}^{A,B})_{HF} - (V_{cl}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{cl}^{A,B} = {}^{Comput}V_{cl}^{A,B} - {}^{Expect}V_{cl}^{A,B}$ are in kcal mol^{-1}.

Table S48. Relative to the CCSD/BBC1 data, analysis of a classical component of interaction energies obtained at the B3LYP level for covalently bonded atom-pairs in the **Lin** conformer of glycol.[a]

		CCSD/BBC1		B3LYP				
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-error
C1	C2	78.4	-5.44002E-04	65.9	78.6	-12.5	-12.7	-19.2
C1	O4	-215.8	1.49705E-03	-194.5	-216.3	21.3	21.8	-11.2
C1	H7	19.3	-1.33604E-04	22.1	19.3	2.8	2.8	12.5
C1	H9	19.3	-1.33604E-04	22.1	19.3	2.8	2.8	12.5
C2	O3	-215.8	1.49705E-03	-194.5	-216.3	21.3	21.8	-11.2
C2	H8	19.3	-1.33604E-04	22.1	19.3	2.8	2.8	12.5
C2	H10	19.3	-1.33604E-04	22.1	19.3	2.8	2.8	12.5
O3	H6	-196.3	1.36165E-03	-192.7	-196.8	3.6	4.1	-2.1
O4	H5	-196.3	1.36165E-03	-192.7	-196.8	3.6	4.1	-2.1

[a]) Classical components of interaction energies, differences $\Delta V_{cl}^{A,B} = (V_{cl}^{A,B})_{B3LYP} - (V_{cl}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{cl}^{A,B} = {}^{Comput}V_{cl}^{A,B} - {}^{Expect}V_{cl}^{A,B}$ are in kcal mol^{-1}.

Table S49. Relative to the CCSD/BBC1 data, analysis of a classical component of interaction energies obtained at the B3LYP-GD3 level for covalently bonded atom-pairs in the **Lin** conformer of glycol.[a]

		CCSD/BBC1		B3LYP-GD3				
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-error
C1	C2	78.4	-5.44002E-04	65.8	78.6	-12.6	-12.8	-19.5
C1	O4	-215.8	1.49705E-03	-194.1	-216.3	21.7	22.2	-11.5
C1	H7	19.3	-1.33604E-04	22.1	19.3	2.8	2.7	12.5
C1	H9	19.3	-1.33604E-04	22.1	19.3	2.8	2.7	12.5
C2	O3	-215.8	1.49705E-03	-194.1	-216.3	21.7	22.2	-11.5
C2	H8	19.3	-1.33604E-04	22.1	19.3	2.8	2.7	12.5
C2	H10	19.3	-1.33604E-04	22.1	19.3	2.8	2.7	12.5
O3	H6	-196.3	1.36165E-03	-192.6	-196.8	3.7	4.2	-2.2
O4	H5	-196.3	1.36165E-03	-192.6	-196.8	3.7	4.2	-2.2

[a]) Classical components of interaction energies, differences $\Delta V_{cl}^{A,B} = (V_{cl}^{A,B})_{B3LYP\text{-}GD3} - (V_{cl}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{cl}^{A,B} = {}^{Comput}V_{cl}^{A,B} - {}^{Expect}V_{cl}^{A,B}$ are in kcal mol^{-1}.

Table S50. Relative to the CCSD/BBC1 data, analysis of a classical component of interaction energies obtained at the MP2/Müller level for covalently bonded atom-pairs in the **Lin** conformer of glycol.[a]

		CCSD/BBC1		MP2/Müller				
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-error
C1	C2	78.4	-5.44002E-04	71.9	78.4	-6.6	-6.5	-9.1
C1	O4	-215.8	1.49705E-03	-203.6	-215.8	12.2	12.2	-6.0
C1	H7	19.3	-1.33604E-04	22.0	19.3	2.8	2.8	12.5
C1	H9	19.3	-1.33604E-04	22.0	19.3	2.8	2.8	12.5
C2	O3	-215.8	1.49705E-03	-203.6	-215.8	12.2	12.2	-6.0
C2	H8	19.3	-1.33604E-04	22.0	19.3	2.8	2.8	12.5
C2	H10	19.3	-1.33604E-04	22.0	19.3	2.8	2.8	12.5
O3	H6	-196.3	1.36165E-03	-202.2	-196.2	-6.0	-6.0	3.0
O4	H5	-196.3	1.36165E-03	-202.2	-196.2	-5.9	-6.0	3.0

[a]) Classical components of interaction energies, differences $\Delta V_{cl}^{A,B} = (V_{cl}^{A,B})_{MP2/Müller} - (V_{cl}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{cl}^{A,B} = {}^{Comput}V_{cl}^{A,B} - {}^{Expect}V_{cl}^{A,B}$ are in kcal mol^{-1}.

Table S51. Relative to the CCSD/BBC1 data, analysis of a classical component of interaction energies obtained at the HF level for covalently bonded atom-pairs and the intramolecular O3···O4 interaction in the **Ecl** conformer of glycol.[a]

		CCSD/BBC1		HF				
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-error
C1	C2	81.7	-5.66525E-04	125.0	81.4	43.3	43.6	34.9
C1	O4	-214.5	1.48848E-03	-333.7	-213.9	-119.1	-119.8	35.9
C1	H7	16.0	-1.11135E-04	3.3	16.0	-12.7	-12.7	-383.6
C1	H9	16.0	-1.11135E-04	3.3	16.0	-12.7	-12.7	-383.9
C2	O3	-214.5	1.48848E-03	-333.5	-213.9	-119.0	-119.7	35.9
C2	H8	16.0	-1.11135E-04	3.3	16.0	-12.7	-12.7	-382.3
C2	H10	16.0	-1.11135E-04	3.3	16.0	-12.7	-12.7	-382.6
O3	H6	-191.1	1.32558E-03	-236.6	-190.5	-45.5	-46.2	19.5
O4	H5	-191.1	1.32558E-03	-236.6	-190.5	-45.5	-46.2	19.5
O3	O4	136.4	-9.46659E-04	175.4	136.0	39.0	39.4	22.5

[a]) Classical components of interaction energies, differences $\Delta V_{cl}^{A,B} = (V_{cl}^{A,B})_{HF} - (V_{cl}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{cl}^{A,B} = {}^{Comput}V_{cl}^{A,B} - {}^{Expect}V_{cl}^{A,B}$ are in kcal mol^{-1}.

Table S52. Relative to the CCSD/BBC1 data, analysis of a classical component of interaction energies obtained at the B3LYP level for covalently bonded atom-pairs and the intramolecular O3···O4 interaction in the **Ecl** conformer of glycol.[a]

		CCSD/BBC1		B3LYP				
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-error
C1	C2	81.7	-5.66525E-04	69.5	81.9	-12.1	-12.3	-17.7
C1	O4	-214.5	1.48848E-03	-194.7	-215.1	19.9	20.4	-10.5
C1	H7	16.0	-1.11135E-04	19.4	16.1	3.3	3.3	17.0
C1	H9	16.0	-1.11135E-04	19.4	16.1	3.3	3.3	17.0
C2	O3	-214.5	1.48848E-03	-194.6	-215.1	19.9	20.5	-10.5
C2	H8	16.0	-1.11135E-04	19.3	16.1	3.3	3.3	17.0
C2	H10	16.0	-1.11135E-04	19.3	16.1	3.3	3.3	17.0
O3	H6	-191.1	1.32558E-03	-188.2	-191.5	2.9	3.3	-1.8
O4	H5	-191.1	1.32558E-03	-188.2	-191.5	2.9	3.3	-1.8
O3	O4	136.4	-9.46659E-04	129.9	136.8	-6.6	-6.9	-5.3

[a]) Classical components of interaction energies, differences $\Delta V_{cl}^{A,B} = (V_{cl}^{A,B})_{B3LYP} - (V_{cl}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{cl}^{A,B} = {}^{Comput}V_{cl}^{A,B} - {}^{Expect}V_{cl}^{A,B}$ are in kcal mol^{-1}.

Table S53. Relative to the CCSD/BBC1 data, analysis of a classical component of interaction energies obtained at the B3LYP-GD3 level for covalently bonded atom-pairs and the intramolecular O3···O4 interaction in the **Ecl** conformer of glycol.[a]

		CCSD/BBC1		B3LYP-GD3				
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-error
C1	C2	81.7	-5.66525E-04	69.1	81.9	-12.5	-12.8	-18.4
C1	O4	-214.5	1.48848E-03	-193.9	-215.1	20.7	21.2	-10.9
C1	H7	16.0	-1.11135E-04	19.4	16.1	3.3	3.3	17.0
C1	H9	16.0	-1.11135E-04	19.4	16.1	3.3	3.3	17.0
C2	O3	-214.5	1.48848E-03	-193.8	-215.1	20.7	21.3	-11.0
C2	H8	16.0	-1.11135E-04	19.4	16.1	3.3	3.3	17.0
C2	H10	16.0	-1.11135E-04	19.4	16.1	3.3	3.3	17.0
O3	H6	-191.1	1.32558E-03	-188.1	-191.6	3.0	3.5	-1.8
O4	H5	-191.1	1.32558E-03	-188.1	-191.6	3.0	3.5	-1.8
O3	O4	136.4	-9.46659E-04	129.7	136.8	-6.8	-7.1	-5.5

[a]) Classical components of interaction energies, differences $\Delta V_{cl}^{A,B} = (V_{cl}^{A,B})_{B3LYP\text{-}GD3} - (V_{cl}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{cl}^{A,B} = {}^{Comput}V_{cl}^{A,B} - {}^{Expect}V_{cl}^{A,B}$ are in kcal mol^{-1}.

Table S54. Relative to the CCSD/BBC1 data, analysis of a classical component of interaction energies obtained at the MP2/Müller level for covalently bonded atom-pairs and the intramolecular O3···O4 interaction in the **Ecl** conformer of glycol.[a]

		CCSD/BBC1		MP2/Müller				
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-error
C1	C2	81.7	-5.66525E-04	75.4	81.6	-6.3	-6.3	-8.3
C1	O4	-214.5	1.48848E-03	-202.8	-214.5	11.7	11.7	-5.8
C1	H7	16.0	-1.11135E-04	19.0	16.0	3.0	3.0	15.9
C1	H9	16.0	-1.11135E-04	19.0	16.0	3.0	3.0	15.9
C2	O3	-214.5	1.48848E-03	-202.8	-214.5	11.7	11.7	-5.8
C2	H8	16.0	-1.11135E-04	19.0	16.0	3.0	3.0	15.9
C2	H10	16.0	-1.11135E-04	19.0	16.0	3.0	3.0	15.9
O3	H6	-191.1	1.32558E-03	-196.8	-191.0	-5.7	-5.8	2.9
O4	H5	-191.1	1.32558E-03	-196.8	-191.0	-5.7	-5.8	2.9
O3	O4	136.4	-9.46659E-04	136.0	136.4	-0.5	-0.5	-0.3

[a]) Classical components of interaction energies, differences $\Delta V_{cl}^{A,B} = (V_{cl}^{A,B})_{MP2/Müller} - (V_{cl}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{cl}^{A,B} = {}^{Comput}V_{cl}^{A,B} - {}^{Expect}V_{cl}^{A,B}$ are in kcal mol^{-1}.

Table S55. Relative to the CCSD/BBC1 data, analysis of an exchange-correlation component of interaction energies obtained at the HF level for covalently bonded atom-pairs and the intramolecular O4···H6 interaction in the **LEC** of glycol.[a]

		CCSD/BBC1		HF				
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-error
C1	C2	-169.5	1.17614E-03	-182.6	-169.0	-13.1	-13.6	7.5
C1	O4	-153.6	1.06528E-03	-151.8	-153.1	1.7	1.3	-0.8
C1	H7	-157.1	1.08973E-03	-175.0	-156.6	-18.0	-18.5	10.5
C1	H9	-157.3	1.09106E-03	-175.1	-156.8	-17.8	-18.3	10.5
C2	O3	-157.4	1.09173E-03	-154.8	-156.9	2.6	2.0	-1.3
C2	H8	-157.5	1.09256E-03	-175.0	-157.0	-17.5	-18.0	10.3
C2	H10	-156.3	1.08458E-03	-174.2	-155.8	-17.9	-18.4	10.6
O3	H6	-114.2	7.92198E-04	-116.6	-113.8	-2.4	-2.8	2.4
O4	H5	-118.4	8.21311E-04	-120.1	-118.0	-1.7	-2.1	1.7
O4	H6	-3.0	2.10430E-05	-1.3	-3.0	1.8	1.8	-139.0

[a]) Exchange-correlation components of interaction energies, differences $\Delta V_{XC}^{A,B} = (V_{XC}^{A,B})_{HF} - (V_{XC}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{XC}^{A,B} = {}^{Comput}V_{XC}^{A,B} - {}^{Expect}V_{XC}^{A,B}$ are in kcal mol^{-1}.

Table S56. Relative to the CCSD/BBC1 data, analysis of an exchange-correlation component of interaction energies obtained at the B3LYP level for covalently bonded atom-pairs and the intramolecular O4···H6 interaction in the **LEC** of glycol.[a]

		CCSD/BBC1		B3LYP				
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-error
C1	C2	-169.5	1.17614E-03	-183.3	-170.0	-13.8	-13.4	7.3
C1	O4	-153.6	1.06528E-03	-164.7	-153.9	-11.1	-10.7	6.5
C1	H7	-157.1	1.08973E-03	-171.8	-157.5	-14.8	-14.4	8.4
C1	H9	-157.3	1.09106E-03	-171.9	-157.7	-14.6	-14.2	8.3
C2	O3	-157.4	1.09173E-03	-168.7	-157.8	-11.4	-11.0	6.5
C2	H8	-157.5	1.09256E-03	-171.9	-157.9	-14.4	-14.0	8.2
C2	H10	-156.3	1.08458E-03	-170.8	-156.7	-14.4	-14.0	8.2
O3	H6	-114.2	7.92198E-04	-121.8	-114.5	-7.6	-7.3	6.0
O4	H5	-118.4	8.21311E-04	-125.6	-118.7	-7.2	-6.9	5.5
O4	H6	-3.0	2.10430E-05	-2.3	-3.0	0.8	0.8	-34.3

[a]) Exchange-correlation components of interaction energies, differences $\Delta V_{XC}^{A,B} = (V_{XC}^{A,B})_{B3LYP} - (V_{XC}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{XC}^{A,B} = {}^{Comput}V_{XC}^{A,B} - {}^{Expect}V_{XC}^{A,B}$ are in kcal mol^{-1}.

Table S57. Relative to the CCSD/BBC1 data, analysis of an exchange-correlation component of interaction energies obtained at the B3LYP-GD3 level for covalently bonded atom-pairs and the intramolecular O4···H6 interaction in the **LEC** of glycol.[a]

		CCSD/BBC1		B3LYP-GD3				
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-error
C1	C2	-169.5	1.17614E-03	-183.3	-170.0	-13.7	-13.3	7.2
C1	O4	-153.6	1.06528E-03	-164.6	-153.9	-11.0	-10.6	6.5
C1	H7	-157.1	1.08973E-03	-171.8	-157.5	-14.7	-14.3	8.3
C1	H9	-157.3	1.09106E-03	-171.8	-157.7	-14.6	-14.2	8.2
C2	O3	-157.4	1.09173E-03	-168.6	-157.8	-11.3	-10.9	6.4
C2	H8	-157.5	1.09256E-03	-171.9	-157.9	-14.4	-14.0	8.2
C2	H10	-156.3	1.08458E-03	-170.7	-156.7	-14.4	-14.0	8.2
O3	H6	-114.2	7.92198E-04	-121.9	-114.5	-7.7	-7.4	6.1
O4	H5	-118.4	8.21311E-04	-125.6	-118.7	-7.2	-6.9	5.5
O4	H6	-3.0	2.10430E-05	-2.2	-3.0	0.8	0.8	-37.2

[a]) Exchange-correlation components of interaction energies, differences $\Delta V_{XC}^{A,B} = (V_{XC}^{A,B})_{B3LYP\text{-}GD3} - (V_{XC}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{XC}^{A,B} = {}^{Comput}V_{XC}^{A,B} - {}^{Expect}V_{XC}^{A,B}$ are in kcal mol^{-1}.

Table S58. Relative to the CCSD/BBC1 data, analysis of an exchange-correlation component of interaction energies obtained at the MP2/Müller level for covalently bonded atom-pairs and the intramolecular O4···H6 interaction in the **LEC** of glycol.[a]

		CCSD/BBC1		MP2/Müller				
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-error
C1	C2	-169.5	1.17614E-03	-171.0	-169.5	-1.5	-1.5	0.9
C1	O4	-153.6	1.06528E-03	-155.6	-153.5	-2.0	-2.0	1.3
C1	H7	-157.1	1.08973E-03	-161.8	-157.1	-4.7	-4.8	2.9
C1	H9	-157.3	1.09106E-03	-161.9	-157.2	-4.7	-4.7	2.9
C2	O3	-157.4	1.09173E-03	-159.4	-157.3	-2.0	-2.1	1.3
C2	H8	-157.5	1.09256E-03	-161.9	-157.5	-4.4	-4.4	2.7
C2	H10	-156.3	1.08458E-03	-160.8	-156.3	-4.5	-4.5	2.8
O3	H6	-114.2	7.92198E-04	-114.2	-114.2	0.0	0.0	0.0
O4	H5	-118.4	8.21311E-04	-117.8	-118.4	0.6	0.5	-0.5
O4	H6	-3.0	2.10430E-05	-2.7	-3.0	0.3	0.3	-10.3

[a]) Exchange-correlation components of interaction energies, differences $\Delta V_{XC}^{A,B} = (V_{XC}^{A,B})_{MP2/Müller} - (V_{XC}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{XC}^{A,B} = {}^{Comput}V_{XC}^{A,B} - {}^{Expect}V_{XC}^{A,B}$ are in kcal mol^{-1}.

Table S59. Relative to the CCSD/BBC1 data, analysis of an exchange-correlation component of interaction energies obtained at the HF level for covalently bonded atom-pairs in the **Lin** conformer of glycol.[a]

		CCSD/BBC1		HF				
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-error
C1	C2	-168.3	1.16750E-03	-181.2	-167.8	-12.9	-13.5	7.4
C1	O4	-154.8	1.07414E-03	-153.0	-154.3	1.8	1.3	-0.9
C1	H7	-157.0	1.08904E-03	-175.0	-156.5	-18.0	-18.5	10.6
C1	H9	-157.0	1.08904E-03	-175.0	-156.5	-18.0	-18.5	10.6
C2	O3	-154.8	1.07414E-03	-153.0	-154.3	1.8	1.3	-0.9
C2	H8	-157.0	1.08904E-03	-175.0	-156.5	-18.0	-18.5	10.6
C2	H10	-157.0	1.08904E-03	-175.0	-156.5	-18.0	-18.5	10.6
O3	H6	-118.1	8.19130E-04	-120.7	-117.7	-2.6	-3.0	2.5
O4	H5	-118.1	8.19130E-04	-120.7	-117.7	-2.6	-3.0	2.5

[a]) Exchange-correlation components of interaction energies, differences $\Delta V_{XC}^{A,B} = (V_{XC}^{A,B})_{HF} - (V_{XC}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{XC}^{A,B} = {}^{Comput}V_{XC}^{A,B} - {}^{Expect}V_{XC}^{A,B}$ are in kcal mol^{-1}.

Table S60. Relative to the CCSD/BBC1 data, analysis of an exchange-correlation component of interaction energies obtained at the B3LYP level for covalently bonded atom-pairs in the **Lin** conformer of glycol.[a]

		CCSD/BBC1		B3LYP				
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-error
C1	C2	-168.3	1.16750E-03	-181.5	-168.7	-13.2	-12.8	7.0
C1	O4	-154.8	1.07414E-03	-166.5	-155.2	-11.7	-11.3	6.8
C1	H7	-157.0	1.08904E-03	-171.8	-157.4	-14.8	-14.4	8.4
C1	H9	-157.0	1.08904E-03	-171.7	-157.4	-14.8	-14.4	8.4
C2	O3	-154.8	1.07414E-03	-166.5	-155.2	-11.7	-11.3	6.8
C2	H8	-157.0	1.08904E-03	-171.8	-157.4	-14.8	-14.4	8.4
C2	H10	-157.0	1.08904E-03	-171.7	-157.4	-14.8	-14.4	8.4
O3	H6	-118.1	8.19130E-04	-126.3	-118.4	-8.2	-7.9	6.3
O4	H5	-118.1	8.19130E-04	-126.3	-118.4	-8.2	-7.9	6.3

[a]) Exchange-correlation components of interaction energies, differences $\Delta V_{XC}^{A,B} = (V_{XC}^{A,B})_{B3LYP} - (V_{XC}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{XC}^{A,B} = {}^{Comput}V_{XC}^{A,B} - {}^{Expect}V_{XC}^{A,B}$ are in kcal mol^{-1}.

Table S61. Relative to the CCSD/BBC1 data, analysis of an exchange-correlation component of interaction energies obtained at the B3LYP-GD3 level for covalently bonded atom-pairs in the **Lin** conformer of glycol.[a]

		CCSD/BBC1		B3LYP-GD3				
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-error
C1	C2	-168.3	1.16750E-03	-181.4	-168.7	-13.1	-12.7	7.0
C1	O4	-154.8	1.07414E-03	-166.5	-155.2	-11.7	-11.3	6.8
C1	H7	-157.0	1.08904E-03	-171.7	-157.4	-14.7	-14.3	8.3
C1	H9	-157.0	1.08904E-03	-171.7	-157.4	-14.7	-14.3	8.3
C2	O3	-154.8	1.07414E-03	-166.5	-155.2	-11.7	-11.3	6.8
C2	H8	-157.0	1.08904E-03	-171.7	-157.4	-14.7	-14.3	8.3
C2	H10	-157.0	1.08904E-03	-171.7	-157.4	-14.7	-14.3	8.3
O3	H6	-118.1	8.19130E-04	-126.3	-118.4	-8.2	-7.9	6.3
O4	H5	-118.1	8.19130E-04	-126.3	-118.4	-8.2	-7.9	6.3

[a]) Exchange-correlation components of interaction energies, differences $\Delta V_{XC}^{A,B} = (V_{XC}^{A,B})_{B3LYP\text{-}GD3} - (V_{XC}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{XC}^{A,B} = {}^{Comput}V_{XC}^{A,B} - {}^{Expect}V_{XC}^{A,B}$ are in kcal mol^{-1}.

Table S62. Relative to the CCSD/BBC1 data, analysis of an exchange-correlation component of interaction energies obtained at the MP2/Müller level for covalently bonded atom-pairs in the **Lin** conformer of glycol.[a]

		CCSD/BBC1		MP2/Müller				
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-error
C1	C2	-168.3	1.16750E-03	-168.3	-169.2	-168.3	-0.9	0.5
C1	O4	-154.8	1.07414E-03	-154.8	-157.4	-154.8	-2.6	1.7
C1	H7	-157.0	1.08904E-03	-157.0	-161.7	-157.0	-4.8	3.0
C1	H9	-157.0	1.08904E-03	-157.0	-161.7	-157.0	-4.7	3.0
C2	O3	-154.8	1.07414E-03	-154.8	-157.4	-154.8	-2.6	1.7
C2	H8	-157.0	1.08904E-03	-157.0	-161.7	-157.0	-4.8	3.0
C2	H10	-157.0	1.08904E-03	-157.0	-161.7	-157.0	-4.7	3.0
O3	H6	-118.1	8.19130E-04	-118.1	-118.5	-118.1	-0.4	0.4
O4	H5	-118.1	8.19130E-04	-118.1	-118.5	-118.1	-0.4	0.4

[a]) Exchange-correlation components of interaction energies, differences $\Delta V_{XC}^{A,B} = (V_{XC}^{A,B})_{MP2/Müller} - (V_{XC}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{XC}^{A,B} = {}^{Comput}V_{XC}^{A,B} - {}^{Expect}V_{XC}^{A,B}$ are in kcal mol^{-1}.

Table S63. Relative to the CCSD/BBC1 data, analysis of an exchange-correlation component of interaction energies obtained at the HF level for covalently bonded atom-pairs and the intramolecular O3···O4 interaction in the **Ecl** conformer of glycol.[a]

		CCSD/BBC1		HF				
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}$ / E	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-error
C1	C2	-162.7	1.12847E-03	-176.1	-162.1	-13.5	-14.0	8.0
C1	O4	-157.5	1.09282E-03	-156.1	-157.0	1.4	0.9	-0.6
C1	H7	-157.3	1.09146E-03	-175.1	-156.8	-17.7	-18.2	10.4
C1	H9	-157.3	1.09146E-03	-175.1	-156.8	-17.7	-18.2	10.4
C2	O3	-157.5	1.09282E-03	-156.2	-157.0	1.3	0.8	-0.5
C2	H8	-157.3	1.09146E-03	-175.1	-156.8	-17.8	-18.3	10.4
C2	H10	-157.3	1.09146E-03	-175.1	-156.8	-17.7	-18.2	10.4
O3	H6	-118.9	8.25117E-04	-121.8	-118.5	-2.9	-3.3	2.7
O4	H5	-118.9	8.25117E-04	-121.8	-118.5	-2.9	-3.3	2.7
O3	O4	-15.3	1.05859E-04	-7.3	-15.2	7.9	7.9	-107.7

[a]) Exchange-correlation components of interaction energies, differences $\Delta V_{XC}^{A,B} = (V_{XC}^{A,B})_{HF} - (V_{XC}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{XC}^{A,B} = {}^{Comput}V_{XC}^{A,B} - {}^{Expect}V_{XC}^{A,B}$ are in kcal mol^{-1}.

Table S64. Relative to the CCSD/BBC1 data, analysis of an exchange-correlation component of interaction energies obtained at the B3LYP level for covalently bonded atom-pairs and the intramolecular O3···O4 interaction in the **Ecl** conformer of glycol.[a]

		CCSD/BBC1		B3LYP				
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}$ / E	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-error
C1	C2	-162.7	1.12847E-03	-175.8	-163.1	-13.1	-12.7	7.2
C1	O4	-157.5	1.09282E-03	-169.9	-157.9	-12.4	-12.0	7.0
C1	H7	-157.3	1.09146E-03	-172.4	-157.7	-15.1	-14.7	8.5
C1	H9	-157.3	1.09146E-03	-172.4	-157.7	-15.1	-14.7	8.5
C2	O3	-157.5	1.09282E-03	-169.9	-157.9	-12.4	-12.0	7.1
C2	H8	-157.3	1.09146E-03	-172.4	-157.7	-15.1	-14.7	8.5
C2	H10	-157.3	1.09146E-03	-172.4	-157.7	-15.1	-14.7	8.5
O3	H6	-118.9	8.25117E-04	-127.2	-119.2	-8.2	-7.9	6.2
O4	H5	-118.9	8.25117E-04	-127.2	-119.2	-8.2	-7.9	6.2
O3	O4	-15.3	1.05859E-04	-8.4	-15.3	6.8	6.9	-81.4

[a]) Exchange-correlation components of interaction energies, differences $\Delta V_{XC}^{A,B} = (V_{XC}^{A,B})_{B3LYP} - (V_{XC}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{XC}^{A,B} = {}^{Comput}V_{XC}^{A,B} - {}^{Expect}V_{XC}^{A,B}$ are in kcal mol^{-1}.

Table S65. Relative to the CCSD/BBC1 data, analysis of an exchange-correlation component of interaction energies obtained at the B3LYP-GD3 level for covalently bonded atom-pairs and the intramolecular O3···O4 interaction in the **Ecl** conformer.[a]

		CCSD/BBC1		B3LYP-GD3				
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-error
C1	C2	-162.7	1.12847E-03	-175.5	-163.1	-12.9	-12.5	7.1
C1	O4	-157.5	1.09282E-03	-169.8	-157.9	-12.3	-11.9	7.0
C1	H7	-157.3	1.09146E-03	-172.3	-157.7	-15.0	-14.6	8.5
C1	H9	-157.3	1.09146E-03	-172.3	-157.7	-15.0	-14.6	8.5
C2	O3	-157.5	1.09282E-03	-169.9	-157.9	-12.4	-12.0	7.0
C2	H8	-157.3	1.09146E-03	-172.3	-157.7	-15.0	-14.6	8.5
C2	H10	-157.3	1.09146E-03	-172.3	-157.7	-15.0	-14.6	8.5
O3	H6	-118.9	8.25117E-04	-127.1	-119.2	-8.2	-7.9	6.2
O4	H5	-118.9	8.25117E-04	-127.1	-119.2	-8.2	-7.9	6.2
O3	O4	-15.3	1.05859E-04	-8.4	-15.3	6.8	6.9	-81.4

[a]) Exchange-correlation components of interaction energies, differences $\Delta V_{XC}^{A,B} = (V_{XC}^{A,B})_{B3LYP\text{-}GD3} - (V_{XC}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{XC}^{A,B} = {}^{Comput}V_{XC}^{A,B} - {}^{Expect}V_{XC}^{A,B}$ are in kcal mol^{-1}.

Table S66. Relative to the CCSD/BBC1 data, analysis of an exchange-correlation component of interaction energies obtained at the MP2/Müller level for covalently bonded atom-pairs and the intramolecular O3···O4 interaction in the **Ecl** conformer.[a]

		CCSD/BBC1		MP2/Müller				
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-error
C1	C2	-162.7	1.12847E-03	-163.3	-162.6	-0.6	-0.6	0.4
C1	O4	-157.5	1.09282E-03	-160.1	-157.5	-2.6	-2.6	1.6
C1	H7	-157.3	1.09146E-03	-162.3	-157.3	-5.0	-5.0	3.1
C1	H9	-157.3	1.09146E-03	-162.3	-157.3	-5.0	-5.0	3.1
C2	O3	-157.5	1.09282E-03	-160.1	-157.5	-2.6	-2.7	1.7
C2	H8	-157.3	1.09146E-03	-162.3	-157.3	-4.9	-5.0	3.1
C2	H10	-157.3	1.09146E-03	-162.3	-157.3	-5.0	-5.0	3.1
O3	H6	-118.9	8.25117E-04	-119.5	-118.9	-0.6	-0.6	0.5
O4	H5	-118.9	8.25117E-04	-119.5	-118.9	-0.6	-0.6	0.5
O3	O4	-15.3	1.05859E-04	-9.2	-15.3	6.1	6.1	-66.1

[a]) Exchange-correlation components of interaction energies, differences $\Delta V_{XC}^{A,B} = (V_{XC}^{A,B})_{MP2/Müller} - (V_{XC}^{A,B})_{CCSD/BBC1}$ and relative errors $\Delta_{XC}^{A,B} = {}^{Comput}V_{XC}^{A,B} - {}^{Expect}V_{XC}^{A,B}$ are in kcal/mol.

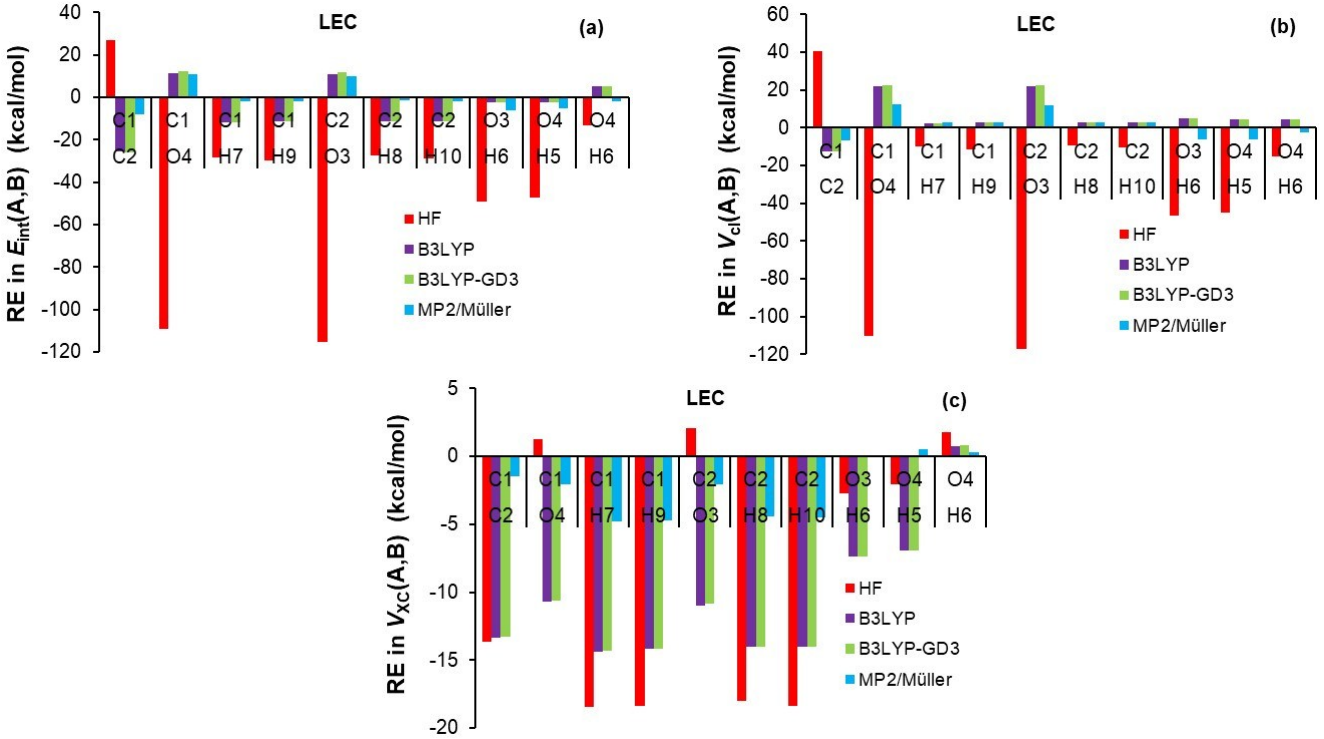

Figure S6. Using CCSD/BBC1 data as a reference, relative errors (RE) obtained at the indicated levels of theory in the interaction energy (Part (a)) as well as its components (classical in Part (b) and XC-term in Part (c)) computed for covalently bonded atoms and the intramolecular O4···H6 interaction in the lowest energy conformer (**LEC**) of glycol.

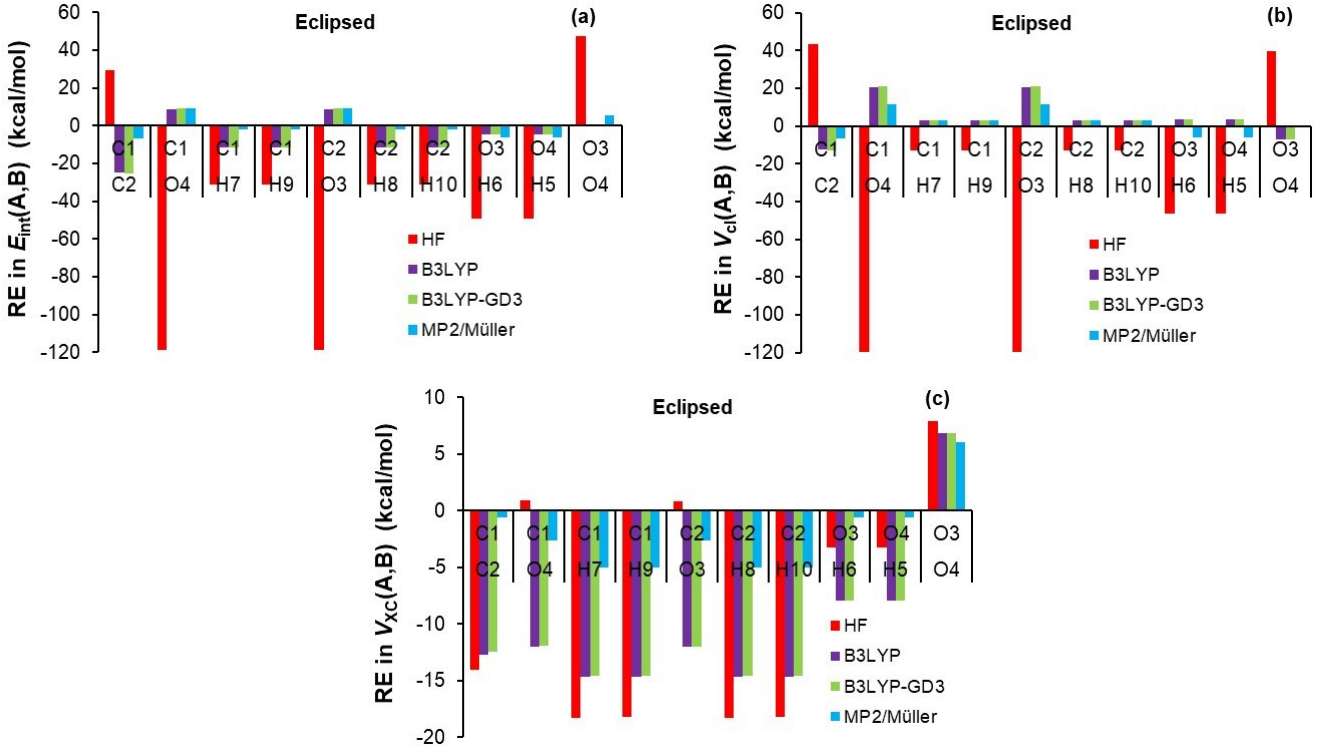

Figure S7. Using CCSD/BBC1 data as a reference, relative errors (RE) obtained at the indicated levels of theory in the interaction energy (Part (a)) as well as its components (classical in Part (b) and XC-term in Part (c)) computed for covalently bonded atoms and the intramolecular O3···O4 interaction in the eclipsed conformer of glycol.

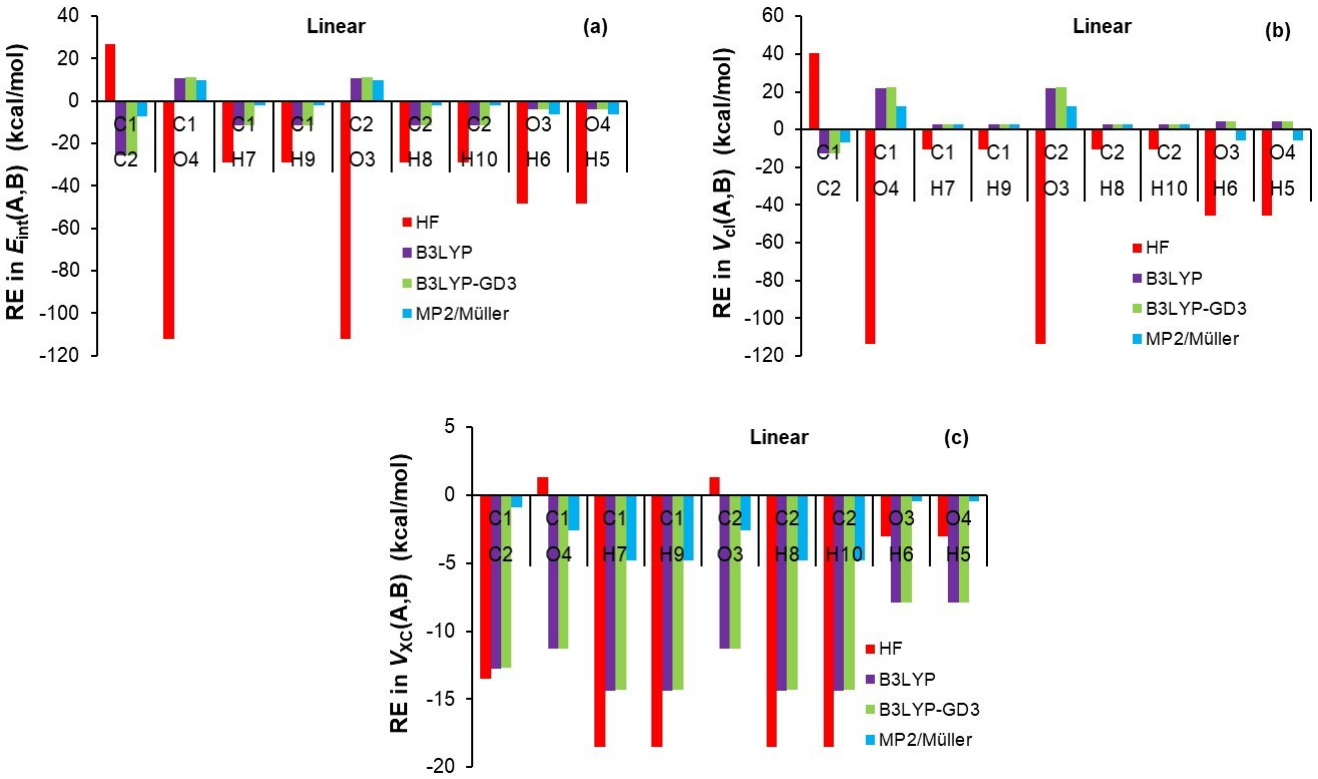

Figure S8. Using CCSD/BBC1 data as a reference, relative errors (RE) obtained at the indicated levels of theory in the interaction energy (Part (a)) as well as its components (classical in Part (b) and XC-term in Part (c)) computed for covalently bonded atoms in the linear conformer of glycol.

Table S67. Combined analysis of relative errors, $\Delta_{int}^{A,B}$, in the computed diatomic interaction energies, ${}^{Comput}E_{int}^{A,B}$, of covalently bonded atoms for each conformer of glycol at the indicated levels of theory. Data for C–C bonds is shown in Part A; for C–O bonds in Part B; for C–H bonds in Part C; for O–H bonds in Part D. All values are in kcal mol^{-1}.

Part A

		HF			B3LYP		
Conformer	**Bond**	${}^{Comput}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-err	${}^{Comput}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-err
LEC	C1–C2	-64.1	26.8	-41.8	-117.1	-25.7	22.0
Lin	C1–C2	-62.7	26.9	-43.0	-115.5	-25.4	22.0
Ecl	C1–C2	-51.2	29.6	-57.8	-106.2	-25.0	23.6
	Average:	-59.3	27.8	-47.5	-113.0	-25.4	22.5
	Standard deviation:	7.1	1.6	8.9	5.9	0.3	0.9

		B3LYP-GD3			MP2/Müller		
Conformer	**Bond**	${}^{Comput}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-err	${}^{Comput}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-err
LEC	C1–C2	-117.4	-26.0	22.1	-99.2	-8.0	8.1
Lin	C1–C2	-115.6	-25.5	22.1	-97.3	-7.5	7.7
Ecl	C1–C2	-106.4	-25.2	23.7	-87.9	-6.9	7.8
	Average:	-113.1	-25.6	22.6	-94.8	-7.4	7.9
	Standard deviation:	5.9	0.4	0.9	6.1	0.5	0.2

Part B

		HF			B3LYP		
Conformer	**Bond**	${}^{Comput}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-err	${}^{Comput}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-err
LEC	C1–O4	-471.1	-109.1	23.2	-352.8	11.2	-3.2
	C2–O3	-492.4	-115.0	23.4	-368.6	11.0	-3.0
Lin	C1–O4	-481.6	-112.2	23.3	-361.0	10.5	-2.9
	C2–O3	-481.6	-112.2	23.3	-361.0	10.5	-2.9
Ecl	C1–O4	-489.8	-118.9	24.3	-364.6	8.4	-2.3
	C2–O3	-489.7	-118.8	24.3	-364.6	8.4	-2.3
	Average:	-484.4	-114.4	23.6	-362.1	10.0	-2.8
	Standard deviation:	7.9	4.0	0.5	5.3	1.3	0.4

		B3LYP-GD3			MP2/Müller		
Conformer	**Bond**	${}^{Comput}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-err	${}^{Comput}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$	%-err
LEC	C1–O4	-351.9	12.1	-3.4	-352.4	10.7	-3.0
	C2–O3	-367.7	11.8	-3.2	-368.6	9.9	-2.7
Lin	C1–O4	-360.6	10.9	-3.0	-361.0	9.6	-2.7
	C2–O3	-360.6	10.9	-3.0	-361.0	9.6	-2.7
Ecl	C1–O4	-363.7	9.3	-2.6	-362.9	9.1	-2.5
	C2–O3	-363.7	9.3	-2.6	-363.0	9.0	-2.5
	Average:	-361.4	10.7	-3.0	-361.5	9.6	-2.7
	Standard deviation:	5.3	1.2	0.4	5.3	0.6	0.2

Part C

		HF			B3LYP		
Conformer	**Bond**	$^{\text{Comput}}E_{\text{int}}^{\text{A,B}}$	$\Delta_{\text{int}}^{\text{A,B}}$	%-err	$^{\text{Comput}}E_{\text{int}}^{\text{A,B}}$	$\Delta_{\text{int}}^{\text{A,B}}$	%-err
LEC	C1–H7	-165.4	-28.5	17.2	-149.5	-11.8	7.9
	C1–H9	-168.2	-29.7	17.7	-150.7	-11.5	7.6
	C2–H8	-162.8	-27.6	16.9	-147.2	-11.2	7.6
	C2–H10	-165.2	-28.8	17.4	-148.4	-11.3	7.6
Lin	C1–H7	-166.1	-28.8	17.3	-149.7	-11.6	7.8
	C1–H9	-166.1	-28.8	17.3	-149.7	-11.6	7.8
	C2–H8	-166.1	-28.8	17.3	-149.7	-11.6	7.8
	C2–H10	-166.1	-28.8	17.3	-149.7	-11.6	7.8
Ecl	C1–H7	-171.8	-30.9	18.0	-153.0	-11.4	7.4
	C1–H9	-171.8	-30.9	18.0	-153.0	-11.4	7.4
	C2–H8	-171.8	-30.9	18.0	-153.0	-11.4	7.4
	C2–H10	-171.8	-30.9	18.0	-153.0	-11.4	7.4
	Average:	-167.7	-29.4	17.5	-150.6	-11.5	7.6
	Standard deviation:	3.2	1.2	0.4	2.0	0.2	0.2

		B3LYP-GD3			MP2/Müller		
Conformer	**Bond**	$^{\text{Comput}}E_{\text{int}}^{\text{A,B}}$	$\Delta_{\text{int}}^{\text{A,B}}$	%-err	$^{\text{Comput}}E_{\text{int}}^{\text{A,B}}$	$\Delta_{\text{int}}^{\text{A,B}}$	%-err
LEC	C1–H7	-149.4	-11.7	7.8	-139.4	-2.0	1.4
	C1–H9	-150.7	-11.5	7.6	-140.8	-2.0	1.4
	C2–H8	-147.2	-11.2	7.6	-137.2	-1.6	1.2
	C2–H10	-148.3	-11.2	7.5	-138.6	-1.8	1.3
Lin	C1–H7	-149.6	-11.6	7.7	-139.7	-2.0	1.5
	C1–H9	-149.6	-11.6	7.7	-139.7	-2.0	1.4
	C2–H8	-149.6	-11.6	7.7	-139.7	-2.0	1.5
	C2–H10	-149.6	-11.6	7.7	-139.7	-2.0	1.4
Ecl	C1–H7	-153.0	-11.3	7.4	-143.2	-2.0	1.4
	C1–H9	-153.0	-11.3	7.4	-143.2	-2.0	1.4
	C2–H8	-153.0	-11.3	7.4	-143.2	-1.9	1.4
	C2–H10	-153.0	-11.3	7.4	-143.2	-1.9	1.4
	Average:	-150.5	-11.4	7.6	-140.7	-1.9	1.4
	Standard deviation:	2.0	0.2	0.2	2.1	0.1	0.1

Part D

		HF			B3LYP		
Conformer	**Bond**	$^{\text{Comput}}E_{\text{int}}^{\text{A,B}}$	$\Delta_{\text{int}}^{\text{A,B}}$	%-err	$^{\text{Comput}}E_{\text{int}}^{\text{A,B}}$	$\Delta_{\text{int}}^{\text{A,B}}$	%-err
LEC	O3–H6	-366.7	-49.1	13.4	-322.0	-2.4	0.8
	O4–H5	-362.5	-47.0	13.0	-319.7	-2.5	0.8
Lin	O3–H6	-361.8	-48.4	13.4	-318.9	-3.8	1.2
	O4–H5	-361.8	-48.4	13.4	-318.9	-3.8	1.2
Ecl	O3–H6	-358.4	-49.4	13.8	-315.4	-4.6	1.5
	O4–H5	-358.4	-49.4	13.8	-315.4	-4.6	1.5
	Average:	-361.6	-48.6	13.5	-318.4	-3.6	1.1
	Standard deviation:	3.1	0.9	0.3	2.6	1.0	0.3

		B3LYP-GD3			MP2/Müller		
Conformer	**Bond**	$^{\text{Comput}}E_{\text{int}}^{\text{A,B}}$	$\Delta_{\text{int}}^{\text{A,B}}$	%-err	$^{\text{Comput}}E_{\text{int}}^{\text{A,B}}$	$\Delta_{\text{int}}^{\text{A,B}}$	%-err
LEC	O3–H6	-321.8	-2.3	0.7	-324.9	-6.2	1.9
	O4–H5	-319.6	-2.3	0.7	-321.7	-5.3	1.7
Lin	O3–H6	-318.9	-3.7	1.2	-320.7	-6.4	2.0
	O4–H5	-318.9	-3.7	1.2	-320.7	-6.4	2.0
Ecl	O3–H6	-315.2	-4.5	1.4	-316.3	-6.4	2.0
	O4–H5	-315.2	-4.5	1.4	-316.3	-6.3	2.0
	Average:	-318.3	-3.5	1.1	-320.1	-6.2	1.9
	Standard deviation:	2.6	1.0	0.3	3.3	0.4	0.1

Table S68. Combined analysis of relative errors, $\Delta_{cl}^{A,B}$, in the computed classical term of diatomic interaction energies, ${}^{Comput}V_{cl}^{A,B}$, of covalently bonded atoms for each conformer of glycol at the indicated levels of theory. Data for C–C bonds is shown in Part A; for C–O bonds in Part B; for C–H bonds in Part C; for O–H bonds in Part D. All values are in kcal mol^{-1}.

Part A

		HF			B3LYP		
Conformer	**Bond**	${}^{Comput}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-err	${}^{Comput}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-err
LEC	C1–C2	118.5	40.4	34.1	66.2	-12.3	-18.6
Lin	C1–C2	118.5	40.4	34.1	65.9	-12.7	-19.2
Ecl	C1–C2	125.0	43.6	34.9	69.5	-12.3	-17.7
	Average:	120.7	41.5	34.3	67.2	-12.5	-18.5
	Standard deviation:	3.7	1.8	0.5	2.0	0.2	0.8

		B3LYP-GD3			MP2/Müller		
Conformer	**Bond**	${}^{Comput}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-err	${}^{Comput}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-err
LEC	C1–C2	65.9	-12.7	-19.3	71.8	-6.5	-9.1
Lin	C1–C2	65.8	-12.8	-19.5	71.9	-6.5	-9.1
Ecl	C1–C2	69.1	-12.8	-18.4	75.4	-6.3	-8.3
	Average:	66.9	-12.7	-19.1	73.0	-6.4	-8.8
	Standard deviation:	1.9	0.1	0.5	2.0	0.2	0.4

Part B

		HF			B3LYP		
Conformer	**Bond**	${}^{Comput}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-err	${}^{Comput}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-err
LEC	C1–O4	-319.3	-110.4	34.6	-188.2	21.9	-11.7
	C2–O3	-337.6	-117.1	34.7	-199.8	21.9	-11.0
Lin	C1–O4	-328.6	-113.5	34.5	-194.5	21.8	-11.2
	C2–O3	-328.6	-113.5	34.5	-194.5	21.8	-11.2
Ecl	C1–O4	-333.7	-119.8	35.9	-194.7	20.4	-10.5
	C2–O3	-333.5	-119.7	35.9	-194.6	20.5	-10.5
	Average:	-330.2	-115.7	35.0	-194.4	21.4	-11.0
	Standard deviation:	6.4	3.8	0.7	3.7	0.8	0.5

		B3LYP-GD3			MP2/Müller		
Conformer	**Bond**	${}^{Comput}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-err	${}^{Comput}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$	%-err
LEC	C1–O4	-187.3	22.8	-12.2	-196.8	12.7	-6.5
	C2–O3	-199.1	22.7	-11.4	-209.2	12.0	-5.7
Lin	C1–O4	-194.1	22.2	-11.5	-203.6	12.2	-6.0
	C2–O3	-194.1	22.2	-11.5	-203.6	12.2	-6.0
Ecl	C1–O4	-193.9	21.2	-10.9	-202.8	11.7	-5.8
	C2–O3	-193.8	21.3	-11.0	-202.8	11.7	-5.8
	Average:	-193.7	22.1	-11.4	-203.1	12.1	-5.9
	Standard deviation:	3.7	0.7	0.4	3.9	0.4	0.3

Part C

		HF			B3LYP		
Conformer	**Bond**	$^{\text{Comput}}V_{\text{cl}}^{\text{A,B}}$	$\Delta_{\text{cl}}^{\text{A,B}}$	%-err	$^{\text{Comput}}V_{\text{cl}}^{\text{A,B}}$	$\Delta_{\text{cl}}^{\text{A,B}}$	%-err
LEC	C1–H7	9.6	-10.0	-104.3	22.3	2.6	11.6
	C1–H9	7.0	-11.4	-163.8	21.1	2.7	12.6
	C2–H8	12.2	-9.6	-78.3	24.7	2.8	11.3
	C2–H10	9.1	-10.4	-114.5	22.3	2.8	12.4
Lin	C1–H7	8.9	-10.3	-115.2	22.1	2.8	12.5
	C1–H9	8.9	-10.3	-115.1	22.1	2.8	12.5
	C2–H8	8.9	-10.3	-115.2	22.1	2.8	12.5
	C2–H10	8.9	-10.3	-115.1	22.1	2.8	12.5
Ecl	C1–H7	3.3	-12.7	-383.6	19.4	3.3	17.0
	C1–H9	3.3	-12.7	-383.9	19.4	3.3	17.0
	C2–H8	3.3	-12.7	-382.3	19.3	3.3	17.0
	C2–H10	3.3	-12.7	-382.6	19.3	3.3	17.0
	Average:	7.2	-11.1	-204.5	21.3	2.9	13.8
	Standard deviation:	3.1	1.2	133.2	1.7	0.3	2.4

		B3LYP-GD3			MP2/Müller		
Conformer	**Bond**	$^{\text{Comput}}V_{\text{cl}}^{\text{A,B}}$	$\Delta_{\text{cl}}^{\text{A,B}}$	%-err	$^{\text{Comput}}V_{\text{cl}}^{\text{A,B}}$	$\Delta_{\text{cl}}^{\text{A,B}}$	%-err
LEC	C1–H7	22.4	2.6	11.7	22.4	2.7	12.2
	C1–H9	21.1	2.7	12.7	21.1	2.7	12.9
	C2–H8	24.7	2.8	11.3	24.7	2.8	11.3
	C2–H10	22.4	2.8	12.6	22.3	2.8	12.4
Lin	C1–H7	22.1	2.7	12.5	22.0	2.8	12.5
	C1–H9	22.1	2.7	12.5	22.0	2.8	12.5
	C2–H8	22.1	2.7	12.5	22.0	2.8	12.5
	C2–H10	22.1	2.7	12.5	22.0	2.8	12.5
Ecl	C1–H7	19.4	3.3	17.0	19.0	3.0	15.9
	C1–H9	19.4	3.3	17.0	19.0	3.0	15.9
	C2–H8	19.4	3.3	17.0	19.0	3.0	15.9
	C2–H10	19.4	3.3	17.0	19.0	3.0	15.9
	Average:	21.4	2.9	13.8	21.2	2.8	13.5
	Standard deviation:	1.7	0.3	2.4	1.8	0.1	1.8

Part D

		HF			B3LYP		
Conformer	**Bond**	$^{\text{Comput}}V_{\text{cl}}^{\text{A,B}}$	$\Delta_{\text{cl}}^{\text{A,B}}$	%-err	$^{\text{Comput}}V_{\text{cl}}^{\text{A,B}}$	$\Delta_{\text{cl}}^{\text{A,B}}$	%-err
LEC	O3–H6	-250.2	-46.3	18.5	-200.1	4.9	-2.5
	O4–H5	-242.4	-45.0	18.5	-194.1	4.4	-2.3
Lin	O3–H6	-241.1	-45.4	18.8	-192.7	4.1	-2.1
	O4–H5	-241.1	-45.4	18.8	-192.7	4.1	-2.1
Ecl	O3–H6	-236.6	-46.2	19.5	-188.2	3.3	-1.8
	O4–H5	-236.6	-46.2	19.5	-188.2	3.3	-1.8
	Average:	-241.3	-45.7	19.0	-192.7	4.0	-2.1
	Standard deviation:	5.0	0.5	0.4	4.4	0.6	0.3

		B3LYP-GD3			MP2/Müller		
Conformer	**Bond**	$^{\text{Comput}}V_{\text{cl}}^{\text{A,B}}$	$\Delta_{\text{cl}}^{\text{A,B}}$	%-err	$^{\text{Comput}}V_{\text{cl}}^{\text{A,B}}$	$\Delta_{\text{cl}}^{\text{A,B}}$	%-err
LEC	O3–H6	-199.9	5.1	-2.6	-210.7	-6.2	3.0
	O4–H5	-193.9	4.6	-2.4	-203.9	-5.9	2.9
Lin	O3–H6	-192.6	4.2	-2.2	-202.2	-6.0	3.0
	O4–H5	-192.6	4.2	-2.2	-202.2	-6.0	3.0
Ecl	O3–H6	-188.1	3.5	-1.8	-196.8	-5.8	2.9
	O4–H5	-188.1	3.5	-1.8	-196.8	-5.8	2.9
	Average:	-192.5	4.2	-2.2	-202.1	-5.9	2.9
	Standard deviation:	4.4	0.6	0.3	5.2	0.2	0.0

Table S69. Combined analysis of relative errors, $\Delta_{XC}^{A,B}$, in the computed XC-term, ${}^{Comput}V_{XC}^{A,B}$, of the diatomic interaction energies of covalently bonded atoms for each conformer of glycol at the indicated levels of theory. Data for C–C bonds is shown in Part A; for C–O bonds in Part B; for C–H bonds in Part C; and for O–H bonds in Part D. All values are in kcal mol^{-1}.

Part A

		HF			B3LYP		
Conformer	**Bond**	${}^{Comput}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-err	${}^{Comput}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-err
LEC	C1–C2	-182.6	-13.6	7.5	-183.3	-13.4	7.3
Lin	C1–C2	-181.2	-13.5	7.4	-181.5	-12.8	7.0
Ecl	C1–C2	-176.1	-14.0	8.0	-175.8	-12.7	7.2
	Average:	-180.0	-13.7	7.6	-180.2	-12.9	7.2
	Standard deviation:	3.4	0.3	0.3	3.9	0.4	0.1

		B3LYP-GD3			MP2/Müller		
Conformer	**Bond**	${}^{Comput}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-err	${}^{Comput}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-err
LEC	C1–C2	-183.3	-13.3	7.2	-171.0	-1.5	0.9
Lin	C1–C2	-181.4	-12.7	7.0	-169.2	-0.9	0.5
Ecl	C1–C2	-175.5	-12.5	7.1	-163.3	-0.6	0.4
	Average:	-180.1	-12.8	7.1	-167.8	-1.0	0.6
	Standard deviation:	4.0	0.4	0.1	4.0	0.4	0.2

Part B

		HF			B3LYP		
Conformer	**Bond**	${}^{Comput}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-err	${}^{Comput}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-err
LEC	C1–O4	-151.8	1.3	-0.8	-164.7	-10.7	6.5
	C2–O3	-154.8	2.0	-1.3	-168.7	-11.0	6.5
Lin	C1–O4	-153.0	1.3	-0.9	-166.5	-11.3	6.8
	C2–O3	-153.0	1.3	-0.9	-166.5	-11.3	6.8
Ecl	C1–O4	-156.1	0.9	-0.6	-169.9	-12.0	7.0
	C2–O3	-156.2	0.8	-0.5	-169.9	-12.0	7.1
	Average:	-154.2	1.3	-0.8	-167.7	-11.4	6.8
	Standard deviation:	1.8	0.4	0.3	2.1	0.5	0.2

		B3LYP-GD3			MP2/Müller		
Conformer	**Bond**	${}^{Comput}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-err	${}^{Comput}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$	%-err
LEC	C1–O4	-164.6	-10.6	6.5	-155.6	-2.0	1.3
	C2–O3	-168.6	-10.9	6.4	-159.4	-2.1	1.3
Lin	C1–O4	-166.5	-11.3	6.8	-157.4	-2.6	1.7
	C2–O3	-166.5	-11.3	6.8	-157.4	-2.6	1.7
Ecl	C1–O4	-169.8	-11.9	7.0	-160.1	-2.6	1.6
	C2–O3	-169.9	-12.0	7.0	-160.1	-2.7	1.7
	Average:	-167.7	-11.3	6.8	-158.3	-2.4	1.5
	Standard deviation:	2.1	0.5	0.3	1.8	0.3	0.2

Part C

		HF			B3LYP		
Conformer	**Bond**	$^{\text{Comput}}V_{\text{XC}}^{\text{A,B}}$	$\Delta_{\text{XC}}^{\text{A,B}}$	%-err	$^{\text{Comput}}V_{\text{XC}}^{\text{A,B}}$	$\Delta_{\text{XC}}^{\text{A,B}}$	%-err
LEC	C1–H7	-175.0	-18.5	10.5	-171.8	-14.4	8.4
	C1–H9	-175.1	-18.3	10.5	-171.9	-14.2	8.3
	C2–H8	-175.0	-18.0	10.3	-171.9	-14.0	8.2
	C2–H10	-174.2	-18.4	10.6	-170.8	-14.0	8.2
Lin	C1–H7	-175.0	-18.5	10.6	-171.8	-14.4	8.4
	C1–H9	-175.0	-18.5	10.6	-171.7	-14.4	8.4
	C2–H8	-175.0	-18.5	10.6	-171.8	-14.4	8.4
	C2–H10	-175.0	-18.5	10.6	-171.7	-14.4	8.4
Ecl	C1–H7	-175.1	-18.2	10.4	-172.4	-14.7	8.5
	C1–H9	-175.1	-18.2	10.4	-172.4	-14.7	8.5
	C2–H8	-175.1	-18.3	10.4	-172.4	-14.7	8.5
	C2–H10	-175.1	-18.2	10.4	-172.4	-14.7	8.5
	Average:	-175.0	-18.4	10.5	-171.9	-14.4	8.4
	Standard deviation:	0.2	0.2	0.1	0.5	0.2	0.1

		B3LYP-GD3			MP2/Müller		
Conformer	**Bond**	$^{\text{Comput}}V_{\text{XC}}^{\text{A,B}}$	$\Delta_{\text{XC}}^{\text{A,B}}$	%-err	$^{\text{Comput}}V_{\text{XC}}^{\text{A,B}}$	$\Delta_{\text{XC}}^{\text{A,B}}$	%-err
LEC	C1–H7	-171.8	-14.3	8.3	-161.8	-4.8	2.9
	C1–H9	-171.8	-14.2	8.2	-161.9	-4.7	2.9
	C2–H8	-171.9	-14.0	8.2	-161.9	-4.4	2.7
	C2–H10	-170.7	-14.0	8.2	-160.8	-4.5	2.8
Lin	C1–H7	-171.7	-14.3	8.3	-161.7	-4.8	3.0
	C1–H9	-171.7	-14.3	8.3	-161.7	-4.8	3.0
	C2–H8	-171.7	-14.3	8.3	-161.7	-4.8	3.0
	C2–H10	-171.7	-14.3	8.3	-161.7	-4.8	3.0
Ecl	C1–H7	-172.3	-14.6	8.5	-162.3	-5.0	3.1
	C1–H9	-172.3	-14.6	8.5	-162.3	-5.0	3.1
	C2–H8	-172.3	-14.6	8.5	-162.3	-5.0	3.1
	C2–H10	-172.3	-14.6	8.5	-162.3	-5.0	3.1
	Average:	-171.9	-14.3	8.3	-161.9	-4.8	3.0
	Standard deviation:	0.5	0.2	0.1	0.4	0.2	0.1

Part D

		HF			B3LYP		
Conformer	**Bond**	$^{\text{Comput}}V_{\text{XC}}^{\text{A,B}}$	$\Delta_{\text{XC}}^{\text{A,B}}$	%-err	$^{\text{Comput}}V_{\text{XC}}^{\text{A,B}}$	$\Delta_{\text{XC}}^{\text{A,B}}$	%-err
LEC	O3–H6	-116.6	-2.8	2.4	-121.8	-7.3	6.0
	O4–H5	-120.1	-2.1	1.7	-125.6	-6.9	5.5
Lin	O3–H6	-120.7	-3.0	2.5	-126.3	-7.9	6.3
	O4–H5	-120.7	-3.0	2.5	-126.3	-7.9	6.3
Ecl	O3–H6	-121.8	-3.3	2.7	-127.2	-7.9	6.2
	O4–H5	-121.8	-3.3	2.7	-127.2	-7.9	6.2
	Average:	-120.3	-2.9	2.4	-125.7	-7.7	6.1
	Standard deviation:	1.9	0.4	0.3	2.0	0.4	0.3

		B3LYP-GD3			MP2/Müller		
Conformer	**Bond**	$^{\text{Comput}}V_{\text{XC}}^{\text{A,B}}$	$\Delta_{\text{XC}}^{\text{A,B}}$	%-err	$^{\text{Comput}}V_{\text{XC}}^{\text{A,B}}$	$\Delta_{\text{XC}}^{\text{A,B}}$	%-err
LEC	O3–H6	-121.9	-7.4	6.1	-114.2	0.0	0.0
	O4–H5	-125.6	-6.9	5.5	-117.8	0.5	-0.5
Lin	O3–H6	-126.3	-7.9	6.3	-118.5	-0.5	0.4
	O4–H5	-126.3	-7.9	6.3	-118.5	-0.5	0.4
Ecl	O3–H6	-127.1	-7.9	6.2	-119.5	-0.6	0.5
	O4–H5	-127.1	-7.9	6.2	-119.5	-0.6	0.5
	Average:	-125.7	-7.7	6.1	-118.0	-0.3	0.2
	Standard deviation:	2.0	0.4	0.3	2.0	0.4	0.4

Table S70. Comparative analysis of computed/expected (for all conformers) interaction energy (part a) and its components (a classical term in part b and an XC-term in part c) for the O4···H6 and O3···O4 intramolecular interactions at the indicated levels of theory. Energies are in kcal mol^{-1}.

Part a	**CCSD/BBC1**	**HF**	**B3LYP**	**B3LYP-GD3**	**MP2/Müller**
Conformer	Computed		Computed/Expected $E_{\text{int}}^{\text{O4,H6}}$		
Lin	–50.4	–60.6/–50.2	–48.4/–50.5	–48.4/–50.5	–50.8/–50.4
LEC	–90.9	–103.9/–90.6	–86.1/–91.1	–85.8/–91.1	–93.0/–90.9
Ecl	–59.4	–71.3/–59.2	–57.2/–59.6	–57.2/–59.6	–60.0/–59.4
	Averaged error	–11.9±1.5	3.2±1.6	3.3±1.8	–1.0±0.9
	Averaged %-error	17.8	–4.8	–4.9	1.5
Conformer	Computed		Computed/Expected $E_{\text{int}}^{\text{O3,O4}}$		
Lin	103.2	140.1/102.8	102.4/103.4	102.4/103.4	107.8/103.2
LEC	137.1	181.0/136.6	133.9/137.4	133.6/137.4	142.3137.1
Ecl	121.2	168.1/120.8	121.4/121.5	121.2/121.5	126.8/121.2
	Averaged error	43.0±5.2	–1.5±1.8	–1.7±1.9	5.2±0.5
	Averaged %-error	35.7	–1.3	–1.4	4.3

Part b	**CCSD/BBC1**	**HF**	**B3LYP**	**B3LYP-GD3**	**MP2/Müller**
Conformer	Computed		Computed/Expected $V_{\text{cl}}^{\text{O4,H6}}$		
Lin	–49.9	–60.5/–49.7	–48.3/–50.0	–48.3/–50.0	–50.7/–49.9
LEC	–87.9	-102.6/–87.6	–83.8/–88.1	–83.5/–88.1	–90.2/–87.8
Ecl	–58.8	–71.2/–58.6	–57.1/–58.9	–57.0/–58.9	–59.9/–58.8
	Averaged error	–12.8±2.1	2.6±1.4	2.7±1.6	–1.4±0.8
	Averaged %-error	19.6	–4.0	–4.1	2.2
Conformer	Computed		Computed/Expected $V_{\text{cl}}^{\text{O3,O4}}$		
Lin	108.9	140.9/108.6	103.4/109.2	103.4/109.2	108.5/108.9
LEC	146.3	184.9/145.8	138.2/146.6	137.9/146.6	146.8/146.2
Ecl	136.4	175.4/136.0	129.9/136.8	129.7/136.8	136.0/136.4
	Averaged error	37.0±4.0	–7.0±1.3	–7.2±1.5	–0.1±0.6
	Averaged %-error	28.3	–5.4	–5.5	–0.1

Part c	**CCSD/BBC1**	**HF**	**B3LYP**	**B3LYP-GD3**	**MP2/Müller**
Conformer	Computed		Computed/Expected $V_{\text{XC}}^{\text{O4,H6}}$		
Lin	–0.50	–0.05/–0.50	–0.07/–0.50	–0.07/–0.50	–0.05/–0.50
LEC	–3.03	–1.26/–3.02	–2.26/–3.04	–2.22/–3.04	–2.75/–3.03
Ecl	–0.67	–0.11/–0.66	–0.15/–0.67	–0.15/–0.67	–0.14/–0.67
	Averaged error	0.92±0.72	0.58±0.18	0.59±0.20	0.42±0.13
	Averaged %-error	–65.9	–41.3	–42.4	–30.1
Conformer	Computed		Computed/Expected $V_{\text{XC}}^{\text{O3,O4}}$		
Lin	–5.8	–0.8/–5.7	–1.0/–5.8	–1.0/–5.8	–0.7/–5.8
LEC	–9.2	–3.8/–9.1	–4.3/–9.2	–4.3/–9.2	–4.6/–9.2
Ecl	–15.3	–7.3/–15.2	–8.4/–15.3	–8.4/–15.3	–9.2/–15.3
	Averaged error	6.1±1.6	5.5±1.2	5.5±1.2	5.2±0.8
	Averaged %-error	–60.1	–54.8	–54.9	–52.1

Table S71. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{int}^{A,B}$ in interaction energies $E_{int}^{A,B}$ computed at HF for distant C,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

C···H in LEC		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
C1	H5	78.29	-5.43115E-04	105.18	78.04	27.14
C1	H6	47.76	-3.31314E-04	64.01	47.61	16.40
C1	H8	-3.92	2.72198E-05	-8.73	-3.91	-4.82
C1	H10	-5.06	3.50861E-05	-10.64	-5.04	-5.59
C2	H5	38.67	-2.68255E-04	52.84	38.54	14.30
C2	H6	85.16	-5.90764E-04	113.38	84.88	28.49
C2	H7	-4.58	3.17769E-05	-10.39	-4.57	-5.82
C2	H9	-5.06	3.51173E-05	-11.38	-5.05	-6.34
				Average for $\lvert\Delta_{int}^{A,B}\rvert$:		13.6
				Standard deviation for $\lvert\Delta_{int}^{A,B}\rvert$:		9.8

C···H in Linear		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
C1	H5	80.84	-5.60847E-04	108.39	80.58	27.80
C1	H6	34.65	-2.40395E-04	47.95	34.54	13.41
C1	H8	-4.93	3.41684E-05	-10.56	-4.91	-5.65
C1	H10	-4.93	3.41684E-05	-10.56	-4.91	-5.65
C2	H5	34.65	-2.40395E-04	47.95	34.54	13.41
C2	H6	80.84	-5.60847E-04	108.39	80.58	27.80
C2	H7	-4.93	3.41684E-05	-10.56	-4.91	-5.65
C2	H9	-4.93	3.41684E-05	-10.56	-4.91	-5.65
				Average for $\lvert\Delta_{int}^{A,B}\rvert$:		13.1
				Standard deviation for $\lvert\Delta_{int}^{A,B}\rvert$:		9.7

C···H in Eclipsed		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
C1	H5	82.40	-5.71696E-04	111.63	82.14	29.49
C1	H6	37.71	-2.61656E-04	51.89	37.59	14.30
C1	H8	-6.60	4.58093E-05	-12.88	-6.58	-6.30
C1	H10	-6.60	4.58093E-05	-12.88	-6.58	-6.29
C2	H5	37.71	-2.61656E-04	51.84	37.59	14.24
C2	H6	82.40	-5.71696E-04	111.57	82.14	29.43
C2	H7	-6.60	4.58093E-05	-12.87	-6.58	-6.29
C2	H9	-6.60	4.58093E-05	-12.87	-6.58	-6.29
				Average for $\lvert\Delta_{int}^{A,B}\rvert$:		14.1
				Standard deviation for $\lvert\Delta_{int}^{A,B}\rvert$:		10.1

Table S72. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{cl}^{A,B}$ in classical term $V_{cl}^{A,B}$ of interaction energies computed at HF for distant C,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

C···H in LEC		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
C1	H5	79.50	-5.51515E-04	106.02	79.24	26.77
C1	H6	48.29	-3.35024E-04	64.12	48.14	15.99
C1	H8	0.12	-8.38500E-07	-4.55	0.12	-4.67
C1	H10	-1.10	7.61256E-06	-6.66	-1.09	-5.57
C2	H5	39.11	-2.71330E-04	53.14	38.99	14.15
C2	H6	86.47	-5.99872E-04	114.17	86.19	27.98
C2	H7	-0.83	5.78789E-06	-6.85	-0.83	-6.02
C2	H9	-1.27	8.79525E-06	-7.48	-1.26	-6.21
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$:		13.4
				Standard deviation for $\lvert\Delta_{cl}^{A,B}\rvert$:		9.6

C···H in Linear		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
C1	H5	82.17	-5.70019E-04	109.23	81.90	27.33
C1	H6	35.15	-2.43847E-04	48.26	35.04	13.22
C1	H8	-1.14	7.88614E-06	-6.95	-1.13	-5.81
C1	H10	-1.14	7.88614E-06	-6.95	-1.13	-5.82
C2	H5	35.15	-2.43847E-04	48.26	35.04	13.22
C2	H6	82.17	-5.70019E-04	109.23	81.90	27.33
C2	H7	-1.14	7.88614E-06	-6.95	-1.13	-5.81
C2	H9	-1.14	7.88614E-06	-6.95	-1.13	-5.82
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$:		13.0
				Standard deviation for $\lvert\Delta_{cl}^{A,B}\rvert$:		9.4

C···H in Eclipsed		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
C1	H5	83.83	-5.81584E-04	112.51	83.56	28.96
C1	H6	38.20	-2.65018E-04	52.18	38.08	14.10
C1	H8	-2.54	1.76089E-05	-8.93	-2.53	-6.40
C1	H10	-2.54	1.76089E-05	-8.94	-2.53	-6.41
C2	H5	38.20	-2.65018E-04	52.12	38.08	14.05
C2	H6	83.83	-5.81584E-04	112.46	83.56	28.90
C2	H7	-2.54	1.76089E-05	-8.93	-2.53	-6.40
C2	H9	-2.54	1.76089E-05	-8.93	-2.53	-6.40
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$:		14.0
				Standard deviation for $\lvert\Delta_{cl}^{A,B}\rvert$:		9.8

Table S73. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{XC}^{A,B}$ in the XC-term $V_{XC}^{A,B}$ of interaction energies computed at HF for distant C,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

C···H in LEC		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
C1	H5	-1.21	8.40036E-06	-0.84	-1.21	0.37
C1	H6	-0.53	3.70975E-06	-0.12	-0.53	0.42
C1	H8	-4.04	2.80583E-05	-4.18	-4.03	-0.15
C1	H10	-3.96	2.74736E-05	-3.97	-3.95	-0.03
C2	H5	-0.44	3.07551E-06	-0.30	-0.44	0.14
C2	H6	-1.31	9.10774E-06	-0.80	-1.31	0.51
C2	H7	-3.75	2.59890E-05	-3.54	-3.73	0.19
C2	H9	-3.79	2.63220E-05	-3.91	-3.78	-0.13
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2
					Standard deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2

C···H in Linear		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
C1	H5	-1.32	9.17191E-06	-0.85	-1.32	0.47
C1	H6	-0.50	3.45234E-06	-0.31	-0.50	0.19
C1	H8	-3.79	2.62822E-05	-3.61	-3.78	0.17
C1	H10	-3.79	2.62822E-05	-3.61	-3.78	0.17
C2	H5	-0.50	3.45234E-06	-0.31	-0.50	0.19
C2	H6	-1.32	9.17191E-06	-0.85	-1.32	0.47
C2	H7	-3.79	2.62822E-05	-3.61	-3.78	0.17
C2	H9	-3.79	2.62822E-05	-3.61	-3.78	0.17
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2
					Standard deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

C···H in Eclipsed		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
C1	H5	-1.43	9.88825E-06	-0.89	-1.42	0.53
C1	H6	-0.48	3.36254E-06	-0.29	-0.48	0.20
C1	H8	-4.06	2.82004E-05	-3.94	-4.05	0.11
C1	H10	-4.06	2.82004E-05	-3.94	-4.05	0.11
C2	H5	-0.48	3.36254E-06	-0.29	-0.48	0.20
C2	H6	-1.43	9.88825E-06	-0.89	-1.42	0.53
C2	H7	-4.06	2.82004E-05	-3.95	-4.05	0.11
C2	H9	-4.06	2.82004E-05	-3.94	-4.05	0.11
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2
					Standard deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2

Table S74. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{int}^{A,B}$ in interaction energies $E_{int}^{A,B}$ computed at HF for distant O,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

O···H in LEC		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
O3	H5	-63.47	4.40340E-04	-75.22	-63.27	-11.95
O3	H7	1.53	-1.05919E-05	9.69	1.52	8.17
O3	H8	-6.44	4.46864E-05	0.42	-6.42	6.84
O3	H9	1.74	-1.20837E-05	8.66	1.74	6.92
O3	H10	-4.72	3.27422E-05	3.02	-4.70	7.73
O4	H6	-90.89	6.30517E-04	-103.88	-90.60	-13.28
O4	H7	-4.46	3.09496E-05	3.38	-4.45	7.83
O4	H8	0.02	-1.51058E-07	5.79	0.02	5.77
O4	H9	-3.22	2.23074E-05	5.50	-3.21	8.71
O4	H10	1.98	-1.37476E-05	9.77	1.98	7.80
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		8.5
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		2.3

O···H in Linear		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
O3	H5	-50.37	3.49449E-04	-60.55	-50.21	-10.34
O3	H7	2.11	-1.46101E-05	9.91	2.10	7.81
O3	H8	-3.97	2.75121E-05	3.68	-3.95	7.63
O3	H9	2.11	-1.46101E-05	9.91	2.10	7.81
O3	H10	-3.97	2.75121E-05	3.68	-3.95	7.63
O4	H6	-50.37	3.49449E-04	-60.55	-50.21	-10.34
O4	H7	-3.97	2.75121E-05	3.68	-3.95	7.63
O4	H8	2.11	-1.46101E-05	9.91	2.10	7.81
O4	H9	-3.97	2.75121E-05	3.68	-3.95	7.63
O4	H10	2.11	-1.46101E-05	9.91	2.10	7.81
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		8.2
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		1.1

O···H in Eclipsed		CCSD/BBC1		HF		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	${}^{Comput}E_{int}^{A,B}$	${}^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
O3	H5	-59.43	4.12334E-04	-71.32	-59.24	-12.08
O3	H7	3.69	-2.56299E-05	10.84	3.68	7.16
O3	H8	-1.45	1.00861E-05	7.17	-1.45	8.62
O3	H9	3.69	-2.56299E-05	10.84	3.68	7.16
O3	H10	-1.45	1.00861E-05	7.17	-1.45	8.62
O4	H6	-59.43	4.12334E-04	-71.32	-59.24	-12.08
O4	H7	-1.45	1.00861E-05	7.17	-1.45	8.62
O4	H8	3.69	-2.56299E-05	10.84	3.68	7.16
O4	H9	-1.45	1.00861E-05	7.17	-1.45	8.62
O4	H10	3.69	-2.56299E-05	10.84	3.68	7.16
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		8.7
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		1.9

Table S75. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{cl}^{A,B}$ of classical term $V_{cl}^{A,B}$ of interaction energies computed at HF for distant O,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

O···H in LEC		CCSD/BBC1		HF		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
O3	H5	79.50	-5.51515E-04	106.02	79.24	26.77
O3	H7	48.29	-3.35024E-04	64.12	48.14	15.99
O3	H8	0.12	-8.38500E-07	-4.55	0.12	-4.67
O3	H9	-1.10	7.61256E-06	-6.66	-1.09	-5.57
O3	H10	39.11	-2.71330E-04	53.14	38.99	14.15
O4	H6	86.47	-5.99872E-04	114.17	86.19	27.98
O4	H7	-0.83	5.78789E-06	-6.85	-0.83	-6.02
O4	H8	-1.27	8.79525E-06	-7.48	-1.26	-6.21
O4	H9	79.50	-5.51515E-04	106.02	79.24	26.77
O4	H10	48.29	-3.35024E-04	64.12	48.14	15.99
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		13.4
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		9.6

O···H in Linear		CCSD/BBC1		HF		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
O3	H5	-49.87	3.45955E-04	-60.51	-49.71	-10.80
O3	H7	4.07	-2.82240E-05	11.27	4.06	7.21
O3	H8	2.14	-1.48185E-05	11.48	2.13	9.35
O3	H9	4.07	-2.82240E-05	11.27	4.06	7.21
O3	H10	2.14	-1.48185E-05	11.48	2.13	9.35
O4	H6	-49.87	3.45955E-04	-60.51	-49.71	-10.80
O4	H7	2.14	-1.48185E-05	11.48	2.13	9.35
O4	H8	4.07	-2.82240E-05	11.27	4.06	7.21
O4	H9	2.14	-1.48185E-05	11.48	2.13	9.35
O4	H10	4.07	-2.82240E-05	11.27	4.06	7.21
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		8.8
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		1.5

O···H in Eclipsed		CCSD/BBC1		HF		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
O3	H5	83.83	-5.81584E-04	112.51	83.56	28.96
O3	H7	38.20	-2.65018E-04	52.18	38.08	14.10
O3	H8	-2.54	1.76089E-05	-8.93	-2.53	-6.40
O3	H9	-2.54	1.76089E-05	-8.94	-2.53	-6.41
O3	H10	38.20	-2.65018E-04	52.12	38.08	14.05
O4	H6	83.83	-5.81584E-04	112.46	83.56	28.90
O4	H7	-2.54	1.76089E-05	-8.93	-2.53	-6.40
O4	H8	-2.54	1.76089E-05	-8.93	-2.53	-6.40
O4	H9	83.83	-5.81584E-04	112.51	83.56	28.96
O4	H10	38.20	-2.65018E-04	52.18	38.08	14.10
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		14.0
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		9.8

Table S76. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{XC}^{A,B}$ of the XC-term $V_{XC}^{A,B}$ of interaction energies computed at HF for distant O,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

O···H in LEC		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
O3	H5	-0.35	2.44852E-06	-0.04	-0.35	0.31
O3	H7	-2.00	1.38900E-05	-1.27	-2.00	0.72
O3	H8	-6.27	4.34686E-05	-7.73	-6.25	-1.48
O3	H9	-1.14	7.90820E-06	-0.66	-1.14	0.48
O3	H10	-6.42	4.45528E-05	-7.91	-6.40	-1.51
O4	H6	-3.03	2.10430E-05	-1.26	-3.02	1.76
O4	H7	-6.28	4.35390E-05	-7.92	-6.26	-1.66
O4	H8	-0.86	5.98068E-06	-0.58	-0.86	0.28
O4	H9	-6.50	4.51269E-05	-7.89	-6.48	-1.40
O4	H10	-1.99	1.38080E-05	-1.30	-1.98	0.69
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	1.0
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.6

O···H in Linear		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
O3	H5	-0.50	3.49384E-06	-0.05	-0.50	0.46
O3	H7	-1.96	1.36138E-05	-1.36	-1.96	0.60
O3	H8	-6.10	4.23306E-05	-7.80	-6.08	-1.72
O3	H9	-1.96	1.36138E-05	-1.36	-1.96	0.60
O3	H10	-6.10	4.23306E-05	-7.80	-6.08	-1.72
O4	H6	-0.50	3.49384E-06	-0.05	-0.50	0.46
O4	H7	-6.10	4.23306E-05	-7.80	-6.08	-1.72
O4	H8	-1.96	1.36138E-05	-1.36	-1.96	0.60
O4	H9	-6.10	4.23306E-05	-7.80	-6.08	-1.72
O4	H10	-1.96	1.36138E-05	-1.36	-1.96	0.60
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	1.0
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.6

O···H in Eclipsed		CCSD/BBC1		HF		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
O3	H5	-0.67	4.62679E-06	-0.11	-0.66	0.56
O3	H7	-0.70	4.84171E-06	-0.26	-0.70	0.44
O3	H8	-6.58	4.56687E-05	-8.41	-6.56	-1.85
O3	H9	-0.70	4.84171E-06	-0.26	-0.70	0.44
O3	H10	-6.58	4.56687E-05	-8.41	-6.56	-1.85
O4	H6	-0.67	4.62679E-06	-0.11	-0.66	0.56
O4	H7	-6.58	4.56687E-05	-8.41	-6.56	-1.85
O4	H8	-0.70	4.84171E-06	-0.26	-0.70	0.44
O4	H9	-6.58	4.56687E-05	-8.41	-6.56	-1.85
O4	H10	-0.70	4.84171E-06	-0.26	-0.70	0.44
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	1.0
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.7

Table S77. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{int}^{A,B}$ in interaction energies $E_{int}^{A,B}$ computed at HF for distant H,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

H···H in LEC		CCSD/BBC1		HF		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
H5	H6	36.97	-2.56444E-04	41.19	36.85	4.34
H5	H7	-1.91	1.32190E-05	-6.20	-1.90	-4.30
H5	H8	-0.65	4.54108E-06	-2.95	-0.65	-2.29
H5	H9	-2.20	1.52426E-05	-6.74	-2.19	-4.54
H5	H10	-1.79	1.23902E-05	-4.51	-1.78	-2.73
H6	H7	-1.78	1.23769E-05	-5.13	-1.78	-3.36
H6	H8	-0.43	2.95773E-06	-3.85	-0.42	-3.42
H6	H9	-1.50	1.03754E-05	-4.44	-1.49	-2.94
H6	H10	-1.52	1.05510E-05	-5.76	-1.52	-4.24
H7	H8	-0.42	2.91928E-06	0.31	-0.42	0.73
H7	H9	-2.32	1.60696E-05	-2.64	-2.31	-0.33
H7	H10	-0.55	3.79630E-06	-0.06	-0.55	0.48
H8	H9	-0.32	2.23740E-06	0.41	-0.32	0.74
H8	H10	-2.38	1.65337E-05	-2.84	-2.38	-0.47
H9	H10	-0.25	1.74888E-06	0.53	-0.25	0.78
					Average for $\lvert\Delta_{int}^{A,B}\rvert$	2.4
					Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$	1.6

H···H in Linear		CCSD/BBC1		HF		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
H5	H6	22.72	-1.57635E-04	26.23	22.65	3.58
H5	H7	-1.84	1.27666E-05	-6.09	-1.83	-4.26
H5	H8	-1.82	1.25965E-05	-4.59	-1.81	-2.78
H5	H9	-1.84	1.27666E-05	-6.09	-1.83	-4.26
H5	H10	-1.82	1.25965E-05	-4.59	-1.81	-2.78
H6	H7	-1.82	1.25965E-05	-4.59	-1.81	-2.78
H6	H8	-1.84	1.27666E-05	-6.09	-1.83	-4.26
H6	H9	-1.82	1.25965E-05	-4.59	-1.81	-2.78
H6	H10	-1.84	1.27666E-05	-6.09	-1.83	-4.26
H7	H8	-0.57	3.92163E-06	-0.03	-0.56	0.54
H7	H9	-2.51	1.73979E-05	-2.75	-2.50	-0.25
H7	H10	-0.46	3.19134E-06	0.38	-0.46	0.84
H8	H9	-0.46	3.19134E-06	0.38	-0.46	0.84
H8	H10	-2.51	1.73979E-05	-2.75	-2.50	-0.25
H9	H10	-0.57	3.92163E-06	-0.03	-0.56	0.54
					Average for $\lvert\Delta_{int}^{A,B}\rvert$	2.3
					Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$	1.6

H···H in Eclipsed		CCSD/BBC1		HF		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
H5	H6	25.93	-1.79929E-04	29.92	25.85	4.07
H5	H7	-3.37	2.33517E-05	-8.03	-3.36	-4.68
H5	H8	-2.23	1.54635E-05	-4.92	-2.22	-2.69
H5	H9	-3.37	2.33517E-05	-8.03	-3.36	-4.68
H5	H10	-2.23	1.54635E-05	-4.92	-2.22	-2.69
H6	H7	-2.23	1.54635E-05	-4.92	-2.22	-2.69
H6	H8	-3.37	2.33517E-05	-8.03	-3.36	-4.68
H6	H9	-2.23	1.54635E-05	-4.92	-2.22	-2.69
H6	H10	-3.37	2.33517E-05	-8.03	-3.36	-4.68
H7	H8	-0.88	6.13093E-06	0.43	-0.88	1.31
H7	H9	-2.65	1.83821E-05	-2.56	-2.64	0.08
H7	H10	-0.25	1.76286E-06	0.70	-0.25	0.95
H8	H9	-0.25	1.76286E-06	0.70	-0.25	0.95
H8	H10	-2.65	1.83821E-05	-2.56	-2.64	0.08
H9	H10	-0.88	6.13093E-06	0.43	-0.88	1.31
					Average for $\lvert\Delta_{int}^{A,B}\rvert$	2.5
					Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$	1.7

Table S78. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{cl}^{A,B}$ of classical term $V_{cl}^{A,B}$ of interaction energies computed at HF for distant H,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

H···H in LEC		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
H5	H6	37.09	-2.57280E-04	41.21	36.97	4.24
H5	H7	-1.73	1.19752E-05	-6.10	-1.72	-4.38
H5	H8	-0.59	4.11552E-06	-2.90	-0.59	-2.31
H5	H9	-2.11	1.46141E-05	-6.68	-2.10	-4.58
H5	H10	-1.71	1.18685E-05	-4.49	-1.71	-2.79
H6	H7	-1.70	1.17605E-05	-5.13	-1.69	-3.44
H6	H8	-0.08	5.40273E-07	-3.51	-0.08	-3.43
H6	H9	-1.41	9.76436E-06	-4.42	-1.40	-3.02
H6	H10	-1.38	9.58579E-06	-5.70	-1.38	-4.32
H7	H8	0.20	-1.38967E-06	0.66	0.20	0.46
H7	H9	0.69	-4.78518E-06	1.16	0.69	0.48
H7	H10	0.08	-5.50299E-07	0.44	0.08	0.36
H8	H9	0.26	-1.82468E-06	0.83	0.26	0.56
H8	H10	0.67	-4.65740E-06	0.93	0.67	0.26
H9	H10	0.30	-2.06546E-06	0.91	0.30	0.61
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	2.4
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	1.7

H···H in Linear		**CCSD/BBC1**		**HF**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
H5	H6	22.91	-1.58934E-04	26.24	22.84	3.40
H5	H7	-1.74	1.20370E-05	-6.02	-1.73	-4.29
H5	H8	-1.78	1.23721E-05	-4.57	-1.78	-2.79
H5	H9	-1.74	1.20370E-05	-6.02	-1.73	-4.29
H5	H10	-1.78	1.23721E-05	-4.57	-1.78	-2.79
H6	H7	-1.78	1.23721E-05	-4.57	-1.78	-2.79
H6	H8	-1.74	1.20370E-05	-6.02	-1.73	-4.29
H6	H9	-1.78	1.23721E-05	-4.57	-1.78	-2.79
H6	H10	-1.74	1.20370E-05	-6.02	-1.73	-4.29
H7	H8	0.08	-5.35901E-07	0.45	0.08	0.37
H7	H9	0.67	-4.65362E-06	1.06	0.67	0.39
H7	H10	0.21	-1.46599E-06	0.74	0.21	0.53
H8	H9	0.21	-1.46599E-06	0.74	0.21	0.53
H8	H10	0.67	-4.65362E-06	1.06	0.67	0.39
H9	H10	0.08	-5.35901E-07	0.45	0.08	0.37
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	2.3
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	1.7

H···H in Eclipsed		CCSD/BBC1		HF		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
H5	H6	26.14	-1.81338E-04	29.92	26.05	3.87
H5	H7	-3.23	2.23898E-05	-7.94	-3.22	-4.73
H5	H8	-2.19	1.52172E-05	-4.90	-2.19	-2.71
H5	H9	-3.23	2.23898E-05	-7.94	-3.22	-4.73
H5	H10	-2.19	1.52172E-05	-4.90	-2.19	-2.71
H6	H7	-2.19	1.52172E-05	-4.90	-2.19	-2.71
H6	H8	-3.23	2.23898E-05	-7.94	-3.22	-4.73
H6	H9	-2.19	1.52172E-05	-4.90	-2.19	-2.71
H6	H10	-3.23	2.23898E-05	-7.94	-3.22	-4.72
H7	H8	0.58	-3.99386E-06	1.54	0.57	0.97
H7	H9	0.80	-5.52134E-06	1.62	0.79	0.82
H7	H10	0.25	-1.76849E-06	0.95	0.25	0.70
H8	H9	0.25	-1.76849E-06	0.95	0.25	0.70
H8	H10	0.80	-5.52134E-06	1.62	0.79	0.82
H9	H10	0.58	-3.99386E-06	1.54	0.57	0.97
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		2.6
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		1.7

Table S79.. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{XC}^{A,B}$ in the XC-term $V_{XC}^{A,B}$ of interaction energies computed at HF for distant H,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

H···H in LEC		CCSD/BBC1		HF		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
H5	H6	-0.12	8.35982E-07	-0.02	-0.12	0.10
H5	H7	-0.18	1.24377E-06	-0.10	-0.18	0.08
H5	H8	-0.06	4.25557E-07	-0.04	-0.06	0.02
H5	H9	-0.09	6.28456E-07	-0.05	-0.09	0.04
H5	H10	-0.08	5.21707E-07	-0.02	-0.07	0.06
H6	H7	-0.09	6.16356E-07	-0.01	-0.09	0.08
H6	H8	-0.35	2.41746E-06	-0.33	-0.35	0.01
H6	H9	-0.09	6.11051E-07	-0.01	-0.09	0.08
H6	H10	-0.14	9.65231E-07	-0.06	-0.14	0.08
H7	H8	-0.62	4.30895E-06	-0.35	-0.62	0.27
H7	H9	-3.01	2.08548E-05	-3.81	-3.00	-0.81
H7	H10	-0.63	4.34660E-06	-0.50	-0.62	0.12
H8	H9	-0.59	4.06207E-06	-0.41	-0.58	0.17
H8	H10	-3.05	2.11911E-05	-3.77	-3.04	-0.73
H9	H10	-0.55	3.81434E-06	-0.38	-0.55	0.16
				Average for $\lvert\Delta_{XC}^{A,B}\rvert$		0.2
				Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$		0.2

H···H in Linear		CCSD/BBC1		HF		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
H5	H6	-0.19	1.29892E-06	0.00	-0.19	0.18
H5	H7	-0.11	7.29610E-07	-0.08	-0.10	0.03
H5	H8	-0.03	2.24489E-07	-0.02	-0.03	0.02
H5	H9	-0.11	7.29610E-07	-0.08	-0.10	0.03
H5	H10	-0.03	2.24489E-07	-0.02	-0.03	0.02
H6	H7	-0.03	2.24489E-07	-0.02	-0.03	0.02
H6	H8	-0.11	7.29610E-07	-0.08	-0.10	0.03
H6	H9	-0.03	2.24489E-07	-0.02	-0.03	0.02
H6	H10	-0.11	7.29610E-07	-0.08	-0.10	0.03
H7	H8	-0.64	4.45753E-06	-0.47	-0.64	0.17
H7	H9	-3.18	2.20515E-05	-3.81	-3.17	-0.65
H7	H10	-0.67	4.65732E-06	-0.35	-0.67	0.32
H8	H9	-0.67	4.65732E-06	-0.35	-0.67	0.32
H8	H10	-3.18	2.20515E-05	-3.81	-3.17	-0.65
H9	H10	-0.64	4.45753E-06	-0.47	-0.64	0.17
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2

H···H in Eclipsed		CCSD/BBC1		HF		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
H5	H6	-0.20	1.40935E-06	0.00	-0.20	0.20
H5	H7	-0.14	9.61846E-07	-0.09	-0.14	0.05
H5	H8	-0.04	2.46282E-07	-0.02	-0.04	0.02
H5	H9	-0.14	9.61846E-07	-0.09	-0.14	0.05
H5	H10	-0.04	2.46282E-07	-0.02	-0.04	0.02
H6	H7	-0.04	2.46282E-07	-0.02	-0.04	0.02
H6	H8	-0.14	9.61846E-07	-0.09	-0.14	0.05
H6	H9	-0.04	2.46282E-07	-0.02	-0.04	0.02
H6	H10	-0.14	9.61846E-07	-0.09	-0.14	0.05
H7	H8	-1.46	1.01248E-05	-1.11	-1.45	0.34
H7	H9	-3.45	2.39035E-05	-4.18	-3.43	-0.74
H7	H10	-0.51	3.53135E-06	-0.25	-0.51	0.25
H8	H9	-0.51	3.53135E-06	-0.25	-0.51	0.25
H8	H10	-3.45	2.39035E-05	-4.18	-3.43	-0.74
H9	H10	-1.46	1.01248E-05	-1.11	-1.45	0.34
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2

Table S80. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{int}^{A,B}$ in interaction energies $E_{int}^{A,B}$ computed at B3LYP for distant C,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

C···H in LEC		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
C1	H5	78.29	-5.43115E-04	71.36	78.49	-7.13
C1	H6	47.76	-3.31314E-04	42.96	47.88	-4.92
C1	H8	-3.92	2.72198E-05	-2.34	-3.93	1.59
C1	H10	-5.06	3.50861E-05	-3.17	-5.07	1.90
C2	H5	38.67	-2.68255E-04	34.76	38.77	-4.00
C2	H6	85.16	-5.90764E-04	78.19	85.37	-7.18
C2	H7	-4.58	3.17769E-05	-2.45	-4.59	2.14
C2	H9	-5.06	3.51173E-05	-3.34	-5.07	1.73
				Average for $\lvert\Delta_{int}^{A,B}\rvert$:		3.8
				Standard deviation for $\lvert\Delta_{int}^{A,B}\rvert$:		2.4

C···H in Linear		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
C1	H5	80.84	-5.60847E-04	74.01	81.05	-7.04
C1	H6	34.65	-2.40395E-04	31.05	34.74	-3.69
C1	H8	-4.93	3.41684E-05	-2.72	-4.94	2.22
C1	H10	-4.93	3.41684E-05	-2.72	-4.94	2.22
C2	H5	34.65	-2.40395E-04	31.05	34.74	-3.69
C2	H6	80.84	-5.60847E-04	74.01	81.05	-7.04
C2	H7	-4.93	3.41684E-05	-2.72	-4.94	2.22
C2	H9	-4.93	3.41684E-05	-2.72	-4.94	2.22
				Average for $\lvert\Delta_{int}^{A,B}\rvert$:		3.8
				Standard deviation for $\lvert\Delta_{int}^{A,B}\rvert$:		2.1

C···H in Eclipsed		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
C1	H5	82.40	-5.71696E-04	75.84	82.61	-6.77
C1	H6	37.71	-2.61656E-04	34.34	37.81	-3.47
C1	H8	-6.60	4.58093E-05	-4.41	-6.62	2.21
C1	H10	-6.60	4.58093E-05	-4.41	-6.62	2.21
C2	H5	37.71	-2.61656E-04	34.31	37.81	-3.49
C2	H6	82.40	-5.71696E-04	75.84	82.61	-6.77
C2	H7	-6.60	4.58093E-05	-4.41	-6.62	2.21
C2	H9	-6.60	4.58093E-05	-4.41	-6.62	2.21
				Average for $\lvert\Delta_{int}^{A,B}\rvert$:		3.7
				Standard deviation for $\lvert\Delta_{int}^{A,B}\rvert$:		2.0

Table S81. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{cl}^{A,B}$ in the classical term $V_{cl}^{A,B}$ of interaction energies computed at B3LYP for distant C,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

C···H in LEC		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
C1	H5	79.50	-5.51515E-04	72.50	79.70	-7.20
C1	H6	48.29	-3.35024E-04	43.15	48.42	-5.27
C1	H8	0.12	-8.38500E-07	1.72	0.12	1.60
C1	H10	-1.10	7.61256E-06	0.70	-1.10	1.80
C2	H5	39.11	-2.71330E-04	35.15	39.21	-4.06
C2	H6	86.47	-5.99872E-04	79.29	86.69	-7.40
C2	H7	-0.83	5.78789E-06	1.07	-0.84	1.90
C2	H9	-1.27	8.79525E-06	0.50	-1.27	1.77
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	3.9
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	2.5

C···H in Linear		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
C1	H5	82.17	-5.70019E-04	75.18	82.37	-7.19
C1	H6	35.15	-2.43847E-04	31.44	35.24	-3.80
C1	H8	-1.14	7.88614E-06	0.79	-1.14	1.93
C1	H10	-1.14	7.88614E-06	0.79	-1.14	1.93
C2	H5	35.15	-2.43847E-04	31.44	35.24	-3.80
C2	H6	82.17	-5.70019E-04	75.18	82.37	-7.19
C2	H7	-1.14	7.88614E-06	0.79	-1.14	1.93
C2	H9	-1.14	7.88614E-06	0.79	-1.14	1.93
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	3.7
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	2.3

C···H in Eclipsed		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
C1	H5	83.83	-5.81584E-04	77.09	84.04	-6.95
C1	H6	38.20	-2.65018E-04	34.71	38.30	-3.58
C1	H8	-2.54	1.76089E-05	-0.60	-2.54	1.94
C1	H10	-2.54	1.76089E-05	-0.60	-2.54	1.94
C2	H5	38.20	-2.65018E-04	34.69	38.30	-3.61
C2	H6	83.83	-5.81584E-04	77.09	84.04	-6.95
C2	H7	-2.54	1.76089E-05	-0.60	-2.54	1.94
C2	H9	-2.54	1.76089E-05	-0.60	-2.54	1.94
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	3.6
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	2.2

Table S82. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{XC}^{A,B}$ in the XC-term $V_{XC}^{A,B}$ of interaction energies computed at B3LYP for distant C,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

C···H in LEC		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
C1	H5	-1.21	8.40036E-06	-1.14	-1.21	0.07
C1	H6	-0.53	3.70975E-06	-0.19	-0.54	0.35
C1	H8	-4.04	2.80583E-05	-4.06	-4.05	-0.01
C1	H10	-3.96	2.74736E-05	-3.87	-3.97	0.10
C2	H5	-0.44	3.07551E-06	-0.39	-0.44	0.06
C2	H6	-1.31	9.10774E-06	-1.10	-1.32	0.22
C2	H7	-3.75	2.59890E-05	-3.51	-3.76	0.24
C2	H9	-3.79	2.63220E-05	-3.85	-3.80	-0.04
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

C···H in Linear		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
C1	H5	-1.32	9.17191E-06	-1.17	-1.33	0.16
C1	H6	-0.50	3.45234E-06	-0.39	-0.50	0.11
C1	H8	-3.79	2.62822E-05	-3.51	-3.80	0.29
C1	H10	-3.79	2.62822E-05	-3.50	-3.80	0.29
C2	H5	-0.50	3.45234E-06	-0.39	-0.50	0.11
C2	H6	-1.32	9.17191E-06	-1.17	-1.33	0.16
C2	H7	-3.79	2.62822E-05	-3.51	-3.80	0.29
C2	H9	-3.79	2.62822E-05	-3.50	-3.80	0.29
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

C···H in Eclipsed		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
C1	H5	-1.43	9.88825E-06	-1.25	-1.43	0.18
C1	H6	-0.48	3.36254E-06	-0.37	-0.49	0.11
C1	H8	-4.06	2.82004E-05	-3.81	-4.07	0.27
C1	H10	-4.06	2.82004E-05	-3.81	-4.07	0.27
C2	H5	-0.48	3.36254E-06	-0.37	-0.49	0.11
C2	H6	-1.43	9.88825E-06	-1.25	-1.43	0.18
C2	H7	-4.06	2.82004E-05	-3.81	-4.07	0.27
C2	H9	-4.06	2.82004E-05	-3.81	-4.07	0.27
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

Table S83. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{int}^{A,B}$ in interaction energies $E_{int}^{A,B}$ computed at B3LYP for distant O,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

O···H in LEC		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
O3	H5	-63.47	4.40340E-04	-60.75	-63.63	2.89
O3	H7	1.53	-1.05919E-05	-0.68	1.53	-2.21
O3	H8	-6.44	4.46864E-05	-10.36	-6.46	-3.90
O3	H9	1.74	-1.20837E-05	-0.24	1.75	-1.98
O3	H10	-4.72	3.27422E-05	-8.94	-4.73	-4.21
O4	H6	-90.89	6.30517E-04	-86.09	-91.12	5.03
O4	H7	-4.46	3.09496E-05	-8.63	-4.47	-4.16
O4	H8	0.02	-1.51058E-07	-2.06	0.02	-2.08
O4	H9	-3.22	2.23074E-05	-7.25	-3.22	-4.02
O4	H10	1.98	-1.37476E-05	-0.31	1.99	-2.29
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		3.3
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		1.1

O···H in Linear		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
O3	H5	-50.37	3.49449E-04	-48.35	-50.50	2.15
O3	H7	2.11	-1.46101E-05	-0.09	2.11	-2.20
O3	H8	-3.97	2.75121E-05	-8.26	-3.98	-4.28
O3	H9	2.11	-1.46101E-05	-0.09	2.11	-2.20
O3	H10	-3.97	2.75121E-05	-8.26	-3.98	-4.28
O4	H6	-50.37	3.49449E-04	-48.35	-50.50	2.15
O4	H7	-3.97	2.75121E-05	-8.26	-3.98	-4.28
O4	H8	2.11	-1.46101E-05	-0.09	2.11	-2.20
O4	H9	-3.97	2.75121E-05	-8.26	-3.98	-4.28
O4	H10	2.11	-1.46101E-05	-0.09	2.11	-2.20
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		3.0
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		1.1

O···H in Eclipsed		CCSD/BBC1		B3LYP		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
O3	H5	-59.43	4.12334E-04	-57.22	-59.58	2.36
O3	H7	3.69	-2.56299E-05	1.90	3.70	-1.81
O3	H8	-1.45	1.00861E-05	-5.81	-1.46	-4.35
O3	H9	3.69	-2.56299E-05	1.90	3.70	-1.81
O3	H10	-1.45	1.00861E-05	-5.81	-1.46	-4.35
O4	H6	-59.43	4.12334E-04	-57.22	-59.58	2.36
O4	H7	-1.45	1.00861E-05	-5.81	-1.46	-4.35
O4	H8	3.69	-2.56299E-05	1.90	3.70	-1.81
O4	H9	-1.45	1.00861E-05	-5.81	-1.46	-4.35
O4	H10	3.69	-2.56299E-05	1.90	3.70	-1.81
					Average for $\lvert\Delta_{int}^{A,B}\rvert$	2.9
					Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$	1.2

Table S84. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{cl}^{A,B}$ in the classical term $V_{cl}^{A,B}$ of the interaction energies computed at B3LYP for distant O,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

O···H in LEC		CCSD/BBC1		B3LYP		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
O3	H5	79.50	-5.51515E-04	72.50	79.70	-7.20
O3	H7	48.29	-3.35024E-04	43.15	48.42	-5.27
O3	H8	0.12	-8.38500E-07	1.72	0.12	1.60
O3	H9	-1.10	7.61256E-06	0.70	-1.10	1.80
O3	H10	39.11	-2.71330E-04	35.15	39.21	-4.06
O4	H6	86.47	-5.99872E-04	79.29	86.69	-7.40
O4	H7	-0.83	5.78789E-06	1.07	-0.84	1.90
O4	H8	-1.27	8.79525E-06	0.50	-1.27	1.77
O4	H9	79.50	-5.51515E-04	72.50	79.70	-7.20
O4	H10	48.29	-3.35024E-04	43.15	48.42	-5.27
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	3.9
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	2.5

O···H in Linear		CCSD/BBC1		B3LYP		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
O3	H5	-49.87	3.45955E-04	-48.28	-49.99	1.71
O3	H7	4.07	-2.82240E-05	1.36	4.08	-2.72
O3	H8	2.14	-1.48185E-05	-1.41	2.14	-3.56
O3	H9	4.07	-2.82240E-05	1.36	4.08	-2.72
O3	H10	2.14	-1.48185E-05	-1.41	2.14	-3.56
O4	H6	-49.87	3.45955E-04	-48.28	-49.99	1.71
O4	H7	2.14	-1.48185E-05	-1.41	2.14	-3.56
O4	H8	4.07	-2.82240E-05	1.36	4.08	-2.72
O4	H9	2.14	-1.48185E-05	-1.41	2.14	-3.56
O4	H10	4.07	-2.82240E-05	1.36	4.08	-2.72
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		2.9
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		0.7

O···H in Eclipsed		CCSD/BBC1		B3LYP		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
O3	H5	83.83	-5.81584E-04	77.09	84.04	-6.95
O3	H7	38.20	-2.65018E-04	34.71	38.30	-3.58
O3	H8	-2.54	1.76089E-05	-0.60	-2.54	1.94
O3	H9	-2.54	1.76089E-05	-0.60	-2.54	1.94
O3	H10	38.20	-2.65018E-04	34.69	38.30	-3.61
O4	H6	83.83	-5.81584E-04	77.09	84.04	-6.95
O4	H7	-2.54	1.76089E-05	-0.60	-2.54	1.94
O4	H8	-2.54	1.76089E-05	-0.60	-2.54	1.94
O4	H9	83.83	-5.81584E-04	77.09	84.04	-6.95
O4	H10	38.20	-2.65018E-04	34.71	38.30	-3.58
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		3.6
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		2.2

Table S85. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{XC}^{A,B}$ in the XC-term $V_{XC}^{A,B}$ of the interaction energies computed at B3LYP for distant O,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

O···H in LEC		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
O3	H5	-0.35	2.44852E-06	-0.06	-0.35	0.30
O3	H7	-2.00	1.38900E-05	-1.44	-2.01	0.57
O3	H8	-6.27	4.34686E-05	-6.63	-6.28	-0.34
O3	H9	-1.14	7.90820E-06	-0.83	-1.14	0.31
O3	H10	-6.42	4.45528E-05	-7.01	-6.44	-0.57
O4	H6	-3.03	2.10430E-05	-2.26	-3.04	0.78
O4	H7	-6.28	4.35390E-05	-6.93	-6.29	-0.64
O4	H8	-0.86	5.98068E-06	-0.69	-0.86	0.18
O4	H9	-6.50	4.51269E-05	-6.91	-6.52	-0.39
O4	H10	-1.99	1.38080E-05	-1.44	-2.00	0.56
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.5
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2

O···H in Linear		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
O3	H5	-0.50	3.49384E-06	-0.07	-0.50	0.44
O3	H7	-1.96	1.36138E-05	-1.45	-1.97	0.52
O3	H8	-6.10	4.23306E-05	-6.84	-6.12	-0.72
O3	H9	-1.96	1.36138E-05	-1.45	-1.97	0.52
O3	H10	-6.10	4.23306E-05	-6.84	-6.12	-0.72
O4	H6	-0.50	3.49384E-06	-0.07	-0.50	0.44
O4	H7	-6.10	4.23306E-05	-6.84	-6.12	-0.72
O4	H8	-1.96	1.36138E-05	-1.45	-1.97	0.52
O4	H9	-6.10	4.23306E-05	-6.84	-6.12	-0.72
O4	H10	-1.96	1.36138E-05	-1.45	-1.97	0.52
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.6
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

O···H in Eclipsed		CCSD/BBC1		B3LYP		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
O3	H5	-0.67	4.62679E-06	-0.15	-0.67	0.52
O3	H7	-0.70	4.84171E-06	-0.28	-0.70	0.42
O3	H8	-6.58	4.56687E-05	-7.39	-6.60	-0.79
O3	H9	-0.70	4.84171E-06	-0.28	-0.70	0.42
O3	H10	-6.58	4.56687E-05	-7.39	-6.60	-0.80
O4	H6	-0.67	4.62679E-06	-0.15	-0.67	0.52
O4	H7	-6.58	4.56687E-05	-7.39	-6.60	-0.80
O4	H8	-0.70	4.84171E-06	-0.28	-0.70	0.42
O4	H9	-6.58	4.56687E-05	-7.39	-6.60	-0.80
O4	H10	-0.70	4.84171E-06	-0.28	-0.70	0.42
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.6
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2

Table S86. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{int}^{A,B}$ in interaction energies $E_{int}^{A,B}$ computed at B3LYP for distant H,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

H···H in LEC		CCSD/BBC1		B3LYP		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
H5	H6	36.97	-2.56444E-04	35.99	37.06	-1.06
H5	H7	-1.91	1.32190E-05	-0.07	-1.91	1.84
H5	H8	-0.65	4.54108E-06	0.37	-0.66	1.02
H5	H9	-2.20	1.52426E-05	-0.48	-2.20	1.72
H5	H10	-1.79	1.23902E-05	-0.58	-1.79	1.21
H6	H7	-1.78	1.23769E-05	-0.30	-1.79	1.49
H6	H8	-0.43	2.95773E-06	1.06	-0.43	1.49
H6	H9	-1.50	1.03754E-05	-0.29	-1.50	1.21
H6	H10	-1.52	1.05510E-05	0.34	-1.52	1.86
H7	H8	-0.42	2.91928E-06	-0.17	-0.42	0.25
H7	H9	-2.32	1.60696E-05	-2.49	-2.32	-0.17
H7	H10	-0.55	3.79630E-06	-0.51	-0.55	0.04
H8	H9	-0.32	2.23740E-06	-0.20	-0.32	0.13
H8	H10	-2.38	1.65337E-05	-2.42	-2.39	-0.03
H9	H10	-0.25	1.74888E-06	-0.18	-0.25	0.07
					Average for $\lvert\Delta_{int}^{A,B}\rvert$	0.9
					Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$	0.7

H···H in Linear		CCSD/BBC1		B3LYP		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
H5	H6	22.72	-1.57635E-04	22.58	22.78	-0.20
H5	H7	-1.84	1.27666E-05	-0.08	-1.84	1.76
H5	H8	-1.82	1.25965E-05	-0.65	-1.82	1.17
H5	H9	-1.84	1.27666E-05	-0.08	-1.84	1.76
H5	H10	-1.82	1.25965E-05	-0.65	-1.82	1.17
H6	H7	-1.82	1.25965E-05	-0.65	-1.82	1.17
H6	H8	-1.84	1.27666E-05	-0.08	-1.84	1.76
H6	H9	-1.82	1.25965E-05	-0.65	-1.82	1.17
H6	H10	-1.84	1.27666E-05	-0.08	-1.84	1.76
H7	H8	-0.57	3.92163E-06	-0.48	-0.57	0.09
H7	H9	-2.51	1.73979E-05	-2.53	-2.51	-0.02
H7	H10	-0.46	3.19134E-06	-0.20	-0.46	0.26
H8	H9	-0.46	3.19134E-06	-0.20	-0.46	0.26
H8	H10	-2.51	1.73979E-05	-2.53	-2.51	-0.02
H9	H10	-0.57	3.92163E-06	-0.48	-0.57	0.09
					Average for $\lvert\Delta_{int}^{A,B}\rvert$	0.8
					Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$	0.7

H···H in Eclipsed		CCSD/BBC1		B3LYP		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
H5	H6	25.93	-1.79929E-04	25.84	26.00	-0.16
H5	H7	-3.37	2.33517E-05	-1.59	-3.37	1.79
H5	H8	-2.23	1.54635E-05	-1.21	-2.23	1.02
H5	H9	-3.37	2.33517E-05	-1.59	-3.37	1.79
H5	H10	-2.23	1.54635E-05	-1.21	-2.23	1.02
H6	H7	-2.23	1.54635E-05	-1.21	-2.23	1.02
H6	H8	-3.37	2.33517E-05	-1.59	-3.37	1.79
H6	H9	-2.23	1.54635E-05	-1.21	-2.23	1.02
H6	H10	-3.37	2.33517E-05	-1.59	-3.37	1.79
H7	H8	-0.88	6.13093E-06	-0.70	-0.89	0.18
H7	H9	-2.65	1.83821E-05	-2.84	-2.66	-0.18
H7	H10	-0.25	1.76286E-06	-0.14	-0.25	0.12
H8	H9	-0.25	1.76286E-06	-0.14	-0.25	0.12
H8	H10	-2.65	1.83821E-05	-2.84	-2.66	-0.18
H9	H10	-0.88	6.13093E-06	-0.70	-0.89	0.18
					Average for $\lvert\Delta_{int}^{A,B}\rvert$	0.8
					Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$	0.7

Table S87. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{cl}^{A,B}$ in the classical term $V_{cl}^{A,B}$ of interaction energies computed at B3LYP for distant H,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

H···H in LEC		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
H5	H6	37.09	-2.57280E-04	36.03	37.18	-1.15
H5	H7	-1.73	1.19752E-05	0.06	-1.73	1.79
H5	H8	-0.59	4.11552E-06	0.44	-0.59	1.03
H5	H9	-2.11	1.46141E-05	-0.42	-2.11	1.69
H5	H10	-1.71	1.18685E-05	-0.55	-1.72	1.16
H6	H7	-1.70	1.17605E-05	-0.29	-1.70	1.41
H6	H8	-0.08	5.40273E-07	1.46	-0.08	1.54
H6	H9	-1.41	9.76436E-06	-0.27	-1.41	1.14
H6	H10	-1.38	9.58579E-06	0.41	-1.39	1.79
H7	H8	0.20	-1.38967E-06	0.16	0.20	-0.04
H7	H9	0.69	-4.78518E-06	0.73	0.69	0.04
H7	H10	0.08	-5.50299E-07	0.06	0.08	-0.02
H8	H9	0.26	-1.82468E-06	0.18	0.26	-0.09
H8	H10	0.67	-4.65740E-06	0.79	0.67	0.11
H9	H10	0.30	-2.06546E-06	0.18	0.30	-0.11
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	0.9
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	0.7

H···H in Linear		**CCSD/BBC1**		**B3LYP**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
H5	H6	22.91	-1.58934E-04	22.59	22.97	-0.38
H5	H7	-1.74	1.20370E-05	0.01	-1.74	1.75
H5	H8	-1.78	1.23721E-05	-0.63	-1.79	1.16
H5	H9	-1.74	1.20370E-05	0.01	-1.74	1.75
H5	H10	-1.78	1.23721E-05	-0.63	-1.79	1.16
H6	H7	-1.78	1.23721E-05	-0.63	-1.79	1.16
H6	H8	-1.74	1.20370E-05	0.01	-1.74	1.75
H6	H9	-1.78	1.23721E-05	-0.63	-1.79	1.16
H6	H10	-1.74	1.20370E-05	0.01	-1.74	1.75
H7	H8	0.08	-5.35901E-07	0.06	0.08	-0.02
H7	H9	0.67	-4.65362E-06	0.75	0.67	0.07
H7	H10	0.21	-1.46599E-06	0.15	0.21	-0.06
H8	H9	0.21	-1.46599E-06	0.15	0.21	-0.06
H8	H10	0.67	-4.65362E-06	0.75	0.67	0.07
H9	H10	0.08	-5.35901E-07	0.06	0.08	-0.02
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	0.8
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	0.7

H···H in Eclipsed		CCSD/BBC1		B3LYP		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
H5	H6	26.14	-1.81338E-04	25.84	26.20	-0.36
H5	H7	-3.23	2.23898E-05	-1.47	-3.24	1.76
H5	H8	-2.19	1.52172E-05	-1.19	-2.20	1.01
H5	H9	-3.23	2.23898E-05	-1.47	-3.24	1.76
H5	H10	-2.19	1.52172E-05	-1.19	-2.20	1.01
H6	H7	-2.19	1.52172E-05	-1.19	-2.20	1.01
H6	H8	-3.23	2.23898E-05	-1.47	-3.24	1.76
H6	H9	-2.19	1.52172E-05	-1.19	-2.20	1.01
H6	H10	-3.23	2.23898E-05	-1.47	-3.24	1.76
H7	H8	0.58	-3.99386E-06	0.37	0.58	-0.21
H7	H9	0.80	-5.52134E-06	0.72	0.80	-0.08
H7	H10	0.25	-1.76849E-06	0.13	0.26	-0.13
H8	H9	0.25	-1.76849E-06	0.13	0.26	-0.13
H8	H10	0.80	-5.52134E-06	0.72	0.80	-0.08
H9	H10	0.58	-3.99386E-06	0.37	0.58	-0.21
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		0.8
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		0.7

Table S88. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{XC}^{A,B}$ in the XC-term $V_{XC}^{A,B}$ of interaction energies, computed at B3LYP for distant H,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

H···H in LEC		CCSD/BBC1		B3LYP		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
H5	H6	-0.12	8.35982E-07	-0.03	-0.12	0.09
H5	H7	-0.18	1.24377E-06	-0.13	-0.18	0.05
H5	H8	-0.06	4.25557E-07	-0.07	-0.06	-0.01
H5	H9	-0.09	6.28456E-07	-0.06	-0.09	0.03
H5	H10	-0.08	5.21707E-07	-0.03	-0.08	0.05
H6	H7	-0.09	6.16356E-07	-0.01	-0.09	0.08
H6	H8	-0.35	2.41746E-06	-0.40	-0.35	-0.05
H6	H9	-0.09	6.11051E-07	-0.02	-0.09	0.07
H6	H10	-0.14	9.65231E-07	-0.07	-0.14	0.07
H7	H8	-0.62	4.30895E-06	-0.33	-0.62	0.29
H7	H9	-3.01	2.08548E-05	-3.23	-3.01	-0.21
H7	H10	-0.63	4.34660E-06	-0.57	-0.63	0.05
H8	H9	-0.59	4.06207E-06	-0.37	-0.59	0.21
H8	H10	-3.05	2.11911E-05	-3.21	-3.06	-0.14
H9	H10	-0.55	3.81434E-06	-0.37	-0.55	0.19
				Average for $\lvert\Delta_{XC}^{A,B}\rvert$		0.1
				Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$		0.1

H···H in Linear		CCSD/BBC1		B3LYP		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
H5	H6	-0.19	1.29892E-06	-0.01	-0.19	0.18
H5	H7	-0.11	7.29610E-07	-0.10	-0.11	0.01
H5	H8	-0.03	2.24489E-07	-0.02	-0.03	0.01
H5	H9	-0.11	7.29610E-07	-0.10	-0.11	0.01
H5	H10	-0.03	2.24489E-07	-0.02	-0.03	0.01
H6	H7	-0.03	2.24489E-07	-0.02	-0.03	0.01
H6	H8	-0.11	7.29610E-07	-0.10	-0.11	0.01
H6	H9	-0.03	2.24489E-07	-0.02	-0.03	0.01
H6	H10	-0.11	7.29610E-07	-0.10	-0.11	0.01
H7	H8	-0.64	4.45753E-06	-0.54	-0.64	0.10
H7	H9	-3.18	2.20515E-05	-3.28	-3.19	-0.09
H7	H10	-0.67	4.65732E-06	-0.35	-0.67	0.32
H8	H9	-0.67	4.65732E-06	-0.35	-0.67	0.32
H8	H10	-3.18	2.20515E-05	-3.28	-3.19	-0.09
H9	H10	-0.64	4.45753E-06	-0.54	-0.64	0.10
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

H···H in Eclipsed		CCSD/BBC1		B3LYP		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
H5	H6	-0.20	1.40935E-06	-0.01	-0.20	0.20
H5	H7	-0.14	9.61846E-07	-0.11	-0.14	0.02
H5	H8	-0.04	2.46282E-07	-0.02	-0.04	0.01
H5	H9	-0.14	9.61846E-07	-0.11	-0.14	0.02
H5	H10	-0.04	2.46282E-07	-0.02	-0.04	0.01
H6	H7	-0.04	2.46282E-07	-0.02	-0.04	0.01
H6	H8	-0.14	9.61846E-07	-0.11	-0.14	0.02
H6	H9	-0.04	2.46282E-07	-0.02	-0.04	0.01
H6	H10	-0.14	9.61846E-07	-0.11	-0.14	0.02
H7	H8	-1.46	1.01248E-05	-1.07	-1.46	0.39
H7	H9	-3.45	2.39035E-05	-3.56	-3.45	-0.11
H7	H10	-0.51	3.53135E-06	-0.27	-0.51	0.24
H8	H9	-0.51	3.53135E-06	-0.27	-0.51	0.24
H8	H10	-3.45	2.39035E-05	-3.56	-3.45	-0.11
H9	H10	-1.46	1.01248E-05	-1.07	-1.46	0.39
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

Table S89. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{int}^{A,B}$ of interaction energies $E_{int}^{A,B}$ computed at B3LYP-GD3 for distant C,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

C···H in LEC		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
C1	H5	78.29	-5.43115E-04	71.11	78.49	-7.38
C1	H6	47.76	-3.31314E-04	42.74	47.88	-5.14
C1	H8	-3.92	2.72198E-05	-2.33	-3.93	1.61
C1	H10	-5.06	3.50861E-05	-3.12	-5.07	1.96
C2	H5	38.67	-2.68255E-04	34.68	38.77	-4.09
C2	H6	85.16	-5.90764E-04	77.93	85.37	-7.44
C2	H7	-4.58	3.17769E-05	-2.40	-4.59	2.19
C2	H9	-5.06	3.51173E-05	-3.30	-5.07	1.77
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		3.9
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		2.5

C···H in Linear		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
C1	H5	80.84	-5.60847E-04	73.87	81.05	-7.18
C1	H6	34.65	-2.40395E-04	31.02	34.74	-3.72
C1	H8	-4.93	3.41684E-05	-2.69	-4.94	2.25
C1	H10	-4.93	3.41684E-05	-2.69	-4.94	2.25
C2	H5	34.65	-2.40395E-04	31.02	34.74	-3.72
C2	H6	80.84	-5.60847E-04	73.86	81.05	-7.19
C2	H7	-4.93	3.41684E-05	-2.69	-4.94	2.25
C2	H9	-4.93	3.41684E-05	-2.69	-4.94	2.25
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		3.8
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		2.2

C···H in Eclipsed		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
C1	H5	82.40	-5.71696E-04	75.63	82.61	-6.98
C1	H6	37.71	-2.61656E-04	34.24	37.81	-3.57
C1	H8	-6.60	4.58093E-05	-4.38	-6.62	2.24
C1	H10	-6.60	4.58093E-05	-4.38	-6.62	2.23
C2	H5	37.71	-2.61656E-04	34.22	37.81	-3.60
C2	H6	82.40	-5.71696E-04	75.62	82.61	-6.99
C2	H7	-6.60	4.58093E-05	-4.38	-6.62	2.24
C2	H9	-6.60	4.58093E-05	-4.38	-6.62	2.24
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		3.8
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		2.1

Table S90. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{cl}^{A,B}$ in the classical term $V_{cl}^{A,B}$ of interaction energies computed at B3LYP-GD3 for distant C,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

C···H in LEC		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
C1	H5	79.50	-5.51515E-04	72.25	79.70	-7.45
C1	H6	48.29	-3.35024E-04	42.93	48.42	-5.49
C1	H8	0.12	-8.38500E-07	1.73	0.12	1.61
C1	H10	-1.10	7.61256E-06	0.76	-1.10	1.86
C2	H5	39.11	-2.71330E-04	35.06	39.21	-4.15
C2	H6	86.47	-5.99872E-04	79.03	86.69	-7.66
C2	H7	-0.83	5.78789E-06	1.13	-0.84	1.96
C2	H9	-1.27	8.79525E-06	0.53	-1.27	1.80
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	4.0
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	2.6

C···H in Linear		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
C1	H5	82.17	-5.70019E-04	75.03	82.38	-7.34
C1	H6	35.15	-2.43847E-04	31.41	35.24	-3.83
C1	H8	-1.14	7.88614E-06	0.82	-1.14	1.96
C1	H10	-1.14	7.88614E-06	0.82	-1.14	1.96
C2	H5	35.15	-2.43847E-04	31.41	35.24	-3.83
C2	H6	82.17	-5.70019E-04	75.03	82.38	-7.34
C2	H7	-1.14	7.88614E-06	0.82	-1.14	1.96
C2	H9	-1.14	7.88614E-06	0.82	-1.14	1.96
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	3.8
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	2.4

C···H in Eclipsed		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
C1	H5	83.83	-5.81584E-04	76.88	84.04	-7.16
C1	H6	38.20	-2.65018E-04	34.61	38.30	-3.68
C1	H8	-2.54	1.76089E-05	-0.58	-2.54	1.97
C1	H10	-2.54	1.76089E-05	-0.58	-2.54	1.97
C2	H5	38.20	-2.65018E-04	34.59	38.30	-3.71
C2	H6	83.83	-5.81584E-04	76.87	84.04	-7.17
C2	H7	-2.54	1.76089E-05	-0.58	-2.54	1.97
C2	H9	-2.54	1.76089E-05	-0.58	-2.54	1.97
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	3.7
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	2.3

Table S91. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{XC}^{A,B}$ in the XC-term $V_{XC}^{A,B}$ of interaction energies computed at B3LYP-GD3 for distant C,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

C···H in LEC		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
C1	H5	-1.21	8.40036E-06	-1.14	-1.21	0.07
C1	H6	-0.53	3.70975E-06	-0.19	-0.54	0.35
C1	H8	-4.04	2.80583E-05	-4.06	-4.05	0.00
C1	H10	-3.96	2.74736E-05	-3.87	-3.97	0.10
C2	H5	-0.44	3.07551E-06	-0.39	-0.44	0.06
C2	H6	-1.31	9.10774E-06	-1.10	-1.32	0.22
C2	H7	-3.75	2.59890E-05	-3.53	-3.76	0.23
C2	H9	-3.79	2.63220E-05	-3.84	-3.80	-0.03
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

C···H in Linear		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
C1	H5	-1.32	9.17191E-06	-1.17	-1.33	0.16
C1	H6	-0.50	3.45234E-06	-0.39	-0.50	0.11
C1	H8	-3.79	2.62822E-05	-3.51	-3.80	0.29
C1	H10	-3.79	2.62822E-05	-3.51	-3.80	0.28
C2	H5	-0.50	3.45234E-06	-0.39	-0.50	0.11
C2	H6	-1.32	9.17191E-06	-1.17	-1.33	0.16
C2	H7	-3.79	2.62822E-05	-3.51	-3.80	0.29
C2	H9	-3.79	2.62822E-05	-3.51	-3.80	0.28
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

C···H in Eclipsed		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
C1	H5	-1.43	9.88825E-06	-1.25	-1.43	0.18
C1	H6	-0.48	3.36254E-06	-0.37	-0.49	0.11
C1	H8	-4.06	2.82004E-05	-3.81	-4.08	0.27
C1	H10	-4.06	2.82004E-05	-3.81	-4.08	0.27
C2	H5	-0.48	3.36254E-06	-0.37	-0.49	0.11
C2	H6	-1.43	9.88825E-06	-1.25	-1.43	0.18
C2	H7	-4.06	2.82004E-05	-3.81	-4.08	0.27
C2	H9	-4.06	2.82004E-05	-3.81	-4.08	0.27
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.2
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

Table S92. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{int}^{A,B}$ in interaction energies $E_{int}^{A,B}$ computed at B3LYP-GD3 for distant O,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

O···H in LEC		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
O3	H5	-63.47	4.40340E-04	-60.69	-63.64	2.95
O3	H7	1.53	-1.05919E-05	-0.80	1.53	-2.34
O3	H8	-6.44	4.46864E-05	-10.35	-6.46	-3.89
O3	H9	1.74	-1.20837E-05	-0.28	1.75	-2.02
O3	H10	-4.72	3.27422E-05	-8.98	-4.73	-4.25
O4	H6	-90.89	6.30517E-04	-85.76	-91.12	5.36
O4	H7	-4.46	3.09496E-05	-8.67	-4.47	-4.20
O4	H8	0.02	-1.51058E-07	-2.08	0.02	-2.10
O4	H9	-3.22	2.23074E-05	-7.27	-3.22	-4.05
O4	H10	1.98	-1.37476E-05	-0.43	1.99	-2.42
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		3.4
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		1.1

O···H in Linear		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
O3	H5	-50.37	3.49449E-04	-48.35	-50.50	2.15
O3	H7	2.11	-1.46101E-05	-0.16	2.11	-2.27
O3	H8	-3.97	2.75121E-05	-8.24	-3.98	-4.26
O3	H9	2.11	-1.46101E-05	-0.16	2.11	-2.27
O3	H10	-3.97	2.75121E-05	-8.24	-3.98	-4.26
O4	H6	-50.37	3.49449E-04	-48.35	-50.50	2.15
O4	H7	-3.97	2.75121E-05	-8.24	-3.98	-4.26
O4	H8	2.11	-1.46101E-05	-0.16	2.11	-2.27
O4	H9	-3.97	2.75121E-05	-8.24	-3.98	-4.26
O4	H10	2.11	-1.46101E-05	-0.16	2.11	-2.27
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		3.0
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		1.1

O···H in Eclipsed		CCSD/BBC1		B3LYP-GD3		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
O3	H5	-59.43	4.12334E-04	-57.18	-59.58	2.40
O3	H7	3.69	-2.56299E-05	1.86	3.70	-1.84
O3	H8	-1.45	1.00861E-05	-5.82	-1.46	-4.36
O3	H9	3.69	-2.56299E-05	1.86	3.70	-1.84
O3	H10	-1.45	1.00861E-05	-5.82	-1.46	-4.36
O4	H6	-59.43	4.12334E-04	-57.18	-59.58	2.40
O4	H7	-1.45	1.00861E-05	-5.82	-1.46	-4.36
O4	H8	3.69	-2.56299E-05	1.86	3.70	-1.84
O4	H9	-1.45	1.00861E-05	-5.82	-1.46	-4.36
O4	H10	3.69	-2.56299E-05	1.86	3.70	-1.84
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		3.0
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		1.2

Table S93. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{cl}^{A,B}$ in the classical term $V_{cl}^{A,B}$ of interaction energies computed at B3LYP-GD3 for distant O,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

O···H in LEC		CCSD/BBC1		B3LYP-GD3		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
O3	H5	79.50	-5.51515E-04	72.25	79.70	-7.45
O3	H7	48.29	-3.35024E-04	42.93	48.42	-5.49
O3	H8	0.12	-8.38500E-07	1.73	0.12	1.61
O3	H9	-1.10	7.61256E-06	0.76	-1.10	1.86
O3	H10	39.11	-2.71330E-04	35.06	39.21	-4.15
O4	H6	86.47	-5.99872E-04	79.03	86.69	-7.66
O4	H7	-0.83	5.78789E-06	1.13	-0.84	1.96
O4	H8	-1.27	8.79525E-06	0.53	-1.27	1.80
O4	H9	79.50	-5.51515E-04	72.25	79.70	-7.45
O4	H10	48.29	-3.35024E-04	42.93	48.42	-5.49
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		4.0
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		2.6

O···H in Linear		CCSD/BBC1		B3LYP-GD3		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
O3	H5	-49.87	3.45955E-04	-48.28	-50.00	1.71
O3	H7	4.07	-2.82240E-05	1.31	4.08	-2.77
O3	H8	2.14	-1.48185E-05	-1.44	2.14	-3.59
O3	H9	4.07	-2.82240E-05	1.31	4.08	-2.77
O3	H10	2.14	-1.48185E-05	-1.44	2.14	-3.59
O4	H6	-49.87	3.45955E-04	-48.28	-50.00	1.71
O4	H7	2.14	-1.48185E-05	-1.44	2.14	-3.59
O4	H8	4.07	-2.82240E-05	1.31	4.08	-2.77
O4	H9	2.14	-1.48185E-05	-1.44	2.14	-3.59
O4	H10	4.07	-2.82240E-05	1.31	4.08	-2.77
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		2.9
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		0.7

O···H in Eclipsed		CCSD/BBC1		B3LYP-GD3		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	${}^{Comput}V_{cl}^{A,B}$	${}^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
O3	H5	83.83	-5.81584E-04	76.88	84.04	-7.16
O3	H7	38.20	-2.65018E-04	34.61	38.30	-3.68
O3	H8	-2.54	1.76089E-05	-0.58	-2.54	1.97
O3	H9	-2.54	1.76089E-05	-0.58	-2.54	1.97
O3	H10	38.20	-2.65018E-04	34.59	38.30	-3.71
O4	H6	83.83	-5.81584E-04	76.87	84.04	-7.17
O4	H7	-2.54	1.76089E-05	-0.58	-2.54	1.97
O4	H8	-2.54	1.76089E-05	-0.58	-2.54	1.97
O4	H9	83.83	-5.81584E-04	76.88	84.04	-7.16
O4	H10	38.20	-2.65018E-04	34.61	38.30	-3.68
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		3.7
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		2.3

Table S94. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{XC}^{A,B}$ in the XC_term of interaction energies computed at B3LYP-GD3 for distant O,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

O···H in LEC		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
O3	H5	-0.35	2.44852E-06	-0.06	-0.35	0.30
O3	H7	-2.00	1.38900E-05	-1.49	-2.01	0.52
O3	H8	-6.27	4.34686E-05	-6.60	-6.28	-0.32
O3	H9	-1.14	7.90820E-06	-0.83	-1.14	0.31
O3	H10	-6.42	4.45528E-05	-6.97	-6.44	-0.53
O4	H6	-3.03	2.10430E-05	-2.22	-3.04	0.82
O4	H7	-6.28	4.35390E-05	-6.88	-6.29	-0.59
O4	H8	-0.86	5.98068E-06	-0.69	-0.86	0.18
O4	H9	-6.50	4.51269E-05	-6.88	-6.52	-0.35
O4	H10	-1.99	1.38080E-05	-1.49	-2.00	0.51
				Average for $\lvert\Delta_{XC}^{A,B}\rvert$		0.4
				Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$		0.2

O···H in Linear		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
O3	H5	-0.50	3.49384E-06	-0.07	-0.50	0.43
O3	H7	-1.96	1.36138E-05	-1.47	-1.97	0.50
O3	H8	-6.10	4.23306E-05	-6.80	-6.12	-0.68
O3	H9	-1.96	1.36138E-05	-1.47	-1.97	0.50
O3	H10	-6.10	4.23306E-05	-6.79	-6.12	-0.68
O4	H6	-0.50	3.49384E-06	-0.07	-0.50	0.43
O4	H7	-6.10	4.23306E-05	-6.80	-6.12	-0.68
O4	H8	-1.96	1.36138E-05	-1.47	-1.97	0.50
O4	H9	-6.10	4.23306E-05	-6.80	-6.12	-0.68
O4	H10	-1.96	1.36138E-05	-1.47	-1.97	0.50
				Average for $\lvert\Delta_{XC}^{A,B}\rvert$		0.6
				Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$		0.1

O···H in Eclipsed		CCSD/BBC1		B3LYP-GD3		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
O3	H5	-0.67	4.62679E-06	-0.15	-0.67	0.52
O3	H7	-0.70	4.84171E-06	-0.28	-0.70	0.42
O3	H8	-6.58	4.56687E-05	-7.36	-6.60	-0.76
O3	H9	-0.70	4.84171E-06	-0.28	-0.70	0.42
O3	H10	-6.58	4.56687E-05	-7.36	-6.60	-0.76
O4	H6	-0.67	4.62679E-06	-0.15	-0.67	0.52
O4	H7	-6.58	4.56687E-05	-7.36	-6.60	-0.76
O4	H8	-0.70	4.84171E-06	-0.28	-0.70	0.42
O4	H9	-6.58	4.56687E-05	-7.36	-6.60	-0.76
O4	H10	-0.70	4.84171E-06	-0.28	-0.70	0.42
				Average for $\lvert\Delta_{XC}^{A,B}\rvert$		0.6
				Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$		0.2

Table S95. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{int}^{A,B}$ in interaction energies $E_{int}^{A,B}$ computed at B3LYP-GD3 for distant H,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

H···H in LEC		CCSD/BBC1		B3LYP-GD3		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
H5	H6	36.97	-2.56444E-04	35.95	37.06	-1.11
H5	H7	-1.91	1.32190E-05	-0.02	-1.91	1.89
H5	H8	-0.65	4.54108E-06	0.38	-0.66	1.03
H5	H9	-2.20	1.52426E-05	-0.45	-2.20	1.75
H5	H10	-1.79	1.23902E-05	-0.54	-1.79	1.25
H6	H7	-1.78	1.23769E-05	-0.26	-1.79	1.53
H6	H8	-0.43	2.95773E-06	1.07	-0.43	1.49
H6	H9	-1.50	1.03754E-05	-0.27	-1.50	1.23
H6	H10	-1.52	1.05510E-05	0.38	-1.52	1.91
H7	H8	-0.42	2.91928E-06	-0.16	-0.42	0.26
H7	H9	-2.32	1.60696E-05	-2.48	-2.32	-0.16
H7	H10	-0.55	3.79630E-06	-0.51	-0.55	0.04
H8	H9	-0.32	2.23740E-06	-0.20	-0.32	0.12
H8	H10	-2.38	1.65337E-05	-2.41	-2.39	-0.02
H9	H10	-0.25	1.74888E-06	-0.18	-0.25	0.08
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		0.9
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		0.7

H···H in Linear		CCSD/BBC1		B3LYP-GD3		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	Comput $E_{int}^{A,B}$	Expect $E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
H5	H6	22.72	-1.57635E-04	22.59	22.78	-0.19
H5	H7	-1.84	1.27666E-05	-0.07	-1.84	1.78
H5	H8	-1.82	1.25965E-05	-0.63	-1.82	1.19
H5	H9	-1.84	1.27666E-05	-0.07	-1.84	1.78
H5	H10	-1.82	1.25965E-05	-0.63	-1.82	1.19
H6	H7	-1.82	1.25965E-05	-0.63	-1.82	1.19
H6	H8	-1.84	1.27666E-05	-0.07	-1.84	1.78
H6	H9	-1.82	1.25965E-05	-0.63	-1.82	1.19
H6	H10	-1.84	1.27666E-05	-0.07	-1.84	1.78
H7	H8	-0.57	3.92163E-06	-0.48	-0.57	0.09
H7	H9	-2.51	1.73979E-05	-2.53	-2.51	-0.02
H7	H10	-0.46	3.19134E-06	-0.20	-0.46	0.26
H8	H9	-0.46	3.19134E-06	-0.20	-0.46	0.26
H8	H10	-2.51	1.73979E-05	-2.53	-2.51	-0.02
H9	H10	-0.57	3.92163E-06	-0.48	-0.57	0.09
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		0.9
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		0.7

H···H in Eclipsed		CCSD/BBC1		B3LYP-GD3		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	Comput $E_{int}^{A,B}$	Expect $E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
H5	H6	25.93	-1.79929E-04	25.85	26.00	-0.16
H5	H7	-3.37	2.33517E-05	-1.56	-3.37	1.82
H5	H8	-2.23	1.54635E-05	-1.20	-2.23	1.04
H5	H9	-3.37	2.33517E-05	-1.56	-3.37	1.82
H5	H10	-2.23	1.54635E-05	-1.20	-2.23	1.04
H6	H7	-2.23	1.54635E-05	-1.20	-2.23	1.04
H6	H8	-3.37	2.33517E-05	-1.56	-3.37	1.82
H6	H9	-2.23	1.54635E-05	-1.20	-2.23	1.04
H6	H10	-3.37	2.33517E-05	-1.56	-3.37	1.82
H7	H8	-0.88	6.13093E-06	-0.70	-0.89	0.18
H7	H9	-2.65	1.83821E-05	-2.84	-2.66	-0.18
H7	H10	-0.25	1.76286E-06	-0.14	-0.25	0.12
H8	H9	-0.25	1.76286E-06	-0.14	-0.25	0.12
H8	H10	-2.65	1.83821E-05	-2.84	-2.66	-0.18
H9	H10	-0.88	6.13093E-06	-0.70	-0.89	0.18
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		0.8
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		0.7

Table S96. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{cl}^{A,B}$ in the classical term $V_{cl}^{A,B}$ of interaction energies computed at B3LYP-GD3 for distant H,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

H···H in LEC		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
H5	H6	37.09	-2.57280E-04	35.98	37.18	-1.20
H5	H7	-1.73	1.19752E-05	0.11	-1.73	1.84
H5	H8	-0.59	4.11552E-06	0.44	-0.59	1.04
H5	H9	-2.11	1.46141E-05	-0.39	-2.11	1.72
H5	H10	-1.71	1.18685E-05	-0.52	-1.72	1.20
H6	H7	-1.70	1.17605E-05	-0.25	-1.70	1.45
H6	H8	-0.08	5.40273E-07	1.47	-0.08	1.55
H6	H9	-1.41	9.76436E-06	-0.25	-1.41	1.16
H6	H10	-1.38	9.58579E-06	0.45	-1.39	1.84
H7	H8	0.20	-1.38967E-06	0.16	0.20	-0.04
H7	H9	0.69	-4.78518E-06	0.73	0.69	0.04
H7	H10	0.08	-5.50299E-07	0.06	0.08	-0.02
H8	H9	0.26	-1.82468E-06	0.18	0.26	-0.09
H8	H10	0.67	-4.65740E-06	0.79	0.67	0.11
H9	H10	0.30	-2.06546E-06	0.18	0.30	-0.12
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		0.9
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		0.7

H···H in Linear		**CCSD/BBC1**		**B3LYP-GD3**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
H5	H6	22.91	-1.58934E-04	22.59	22.97	-0.37
H5	H7	-1.74	1.20370E-05	0.03	-1.74	1.77
H5	H8	-1.78	1.23721E-05	-0.61	-1.79	1.18
H5	H9	-1.74	1.20370E-05	0.03	-1.74	1.77
H5	H10	-1.78	1.23721E-05	-0.61	-1.79	1.18
H6	H7	-1.78	1.23721E-05	-0.61	-1.79	1.18
H6	H8	-1.74	1.20370E-05	0.03	-1.74	1.77
H6	H9	-1.78	1.23721E-05	-0.61	-1.79	1.18
H6	H10	-1.74	1.20370E-05	0.03	-1.74	1.77
H7	H8	0.08	-5.35901E-07	0.06	0.08	-0.02
H7	H9	0.67	-4.65362E-06	0.75	0.67	0.08
H7	H10	0.21	-1.46599E-06	0.15	0.21	-0.06
H8	H9	0.21	-1.46599E-06	0.15	0.21	-0.06
H8	H10	0.67	-4.65362E-06	0.75	0.67	0.08
H9	H10	0.08	-5.35901E-07	0.06	0.08	-0.02
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		0.8
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		0.7

H···H in Eclipsed		CCSD/BBC1		B3LYP-GD3		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
H5	H6	26.14	-1.81338E-04	25.85	26.20	-0.35
H5	H7	-3.23	2.23898E-05	-1.45	-3.24	1.79
H5	H8	-2.19	1.52172E-05	-1.17	-2.20	1.03
H5	H9	-3.23	2.23898E-05	-1.45	-3.24	1.79
H5	H10	-2.19	1.52172E-05	-1.17	-2.20	1.03
H6	H7	-2.19	1.52172E-05	-1.17	-2.20	1.03
H6	H8	-3.23	2.23898E-05	-1.45	-3.24	1.79
H6	H9	-2.19	1.52172E-05	-1.17	-2.20	1.03
H6	H10	-3.23	2.23898E-05	-1.45	-3.24	1.79
H7	H8	0.58	-3.99386E-06	0.36	0.58	-0.21
H7	H9	0.80	-5.52134E-06	0.72	0.80	-0.08
H7	H10	0.25	-1.76849E-06	0.13	0.26	-0.13
H8	H9	0.25	-1.76849E-06	0.13	0.26	-0.13
H8	H10	0.80	-5.52134E-06	0.72	0.80	-0.08
H9	H10	0.58	-3.99386E-06	0.36	0.58	-0.21
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		0.8
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		0.7

Table S97. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{XC}^{A,B}$ in the XC-term $V_{XC}^{A,B}$ of interaction energies computed at B3LYP-GD3 for distant H,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

H···H in LEC		CCSD/BBC1		B3LYP-GD3		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
H5	H6	-0.12	8.35982E-07	-0.03	-0.12	0.09
H5	H7	-0.18	1.24377E-06	-0.13	-0.18	0.05
H5	H8	-0.06	4.25557E-07	-0.07	-0.06	-0.01
H5	H9	-0.09	6.28456E-07	-0.06	-0.09	0.03
H5	H10	-0.08	5.21707E-07	-0.03	-0.08	0.05
H6	H7	-0.09	6.16356E-07	-0.01	-0.09	0.08
H6	H8	-0.35	2.41746E-06	-0.40	-0.35	-0.05
H6	H9	-0.09	6.11051E-07	-0.02	-0.09	0.07
H6	H10	-0.14	9.65231E-07	-0.07	-0.14	0.07
H7	H8	-0.62	4.30895E-06	-0.32	-0.62	0.30
H7	H9	-3.01	2.08548E-05	-3.22	-3.01	-0.20
H7	H10	-0.63	4.34660E-06	-0.57	-0.63	0.06
H8	H9	-0.59	4.06207E-06	-0.38	-0.59	0.21
H8	H10	-3.05	2.11911E-05	-3.20	-3.06	-0.14
H9	H10	-0.55	3.81434E-06	-0.36	-0.55	0.20
				Average for $\lvert\Delta_{XC}^{A,B}\rvert$		0.1
				Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$		0.1

H···H in Linear		CCSD/BBC1		B3LYP-GD3		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
H5	H6	-0.19	1.29892E-06	-0.01	-0.19	0.18
H5	H7	-0.11	7.29610E-07	-0.10	-0.11	0.01
H5	H8	-0.03	2.24489E-07	-0.02	-0.03	0.01
H5	H9	-0.11	7.29610E-07	-0.10	-0.11	0.01
H5	H10	-0.03	2.24489E-07	-0.02	-0.03	0.01
H6	H7	-0.03	2.24489E-07	-0.02	-0.03	0.01
H6	H8	-0.11	7.29610E-07	-0.10	-0.11	0.01
H6	H9	-0.03	2.24489E-07	-0.02	-0.03	0.01
H6	H10	-0.11	7.29610E-07	-0.10	-0.11	0.01
H7	H8	-0.64	4.45753E-06	-0.54	-0.64	0.10
H7	H9	-3.18	2.20515E-05	-3.28	-3.19	-0.09
H7	H10	-0.67	4.65732E-06	-0.35	-0.67	0.32
H8	H9	-0.67	4.65732E-06	-0.35	-0.67	0.32
H8	H10	-3.18	2.20515E-05	-3.28	-3.19	-0.09
H9	H10	-0.64	4.45753E-06	-0.54	-0.64	0.10
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

H···H in Eclipsed		CCSD/BBC1		B3LYP-GD3		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
H5	H6	-0.20	1.40935E-06	-0.01	-0.20	0.20
H5	H7	-0.14	9.61846E-07	-0.11	-0.14	0.03
H5	H8	-0.04	2.46282E-07	-0.02	-0.04	0.01
H5	H9	-0.14	9.61846E-07	-0.11	-0.14	0.03
H5	H10	-0.04	2.46282E-07	-0.02	-0.04	0.01
H6	H7	-0.04	2.46282E-07	-0.02	-0.04	0.01
H6	H8	-0.14	9.61846E-07	-0.11	-0.14	0.03
H6	H9	-0.04	2.46282E-07	-0.02	-0.04	0.01
H6	H10	-0.14	9.61846E-07	-0.11	-0.14	0.03
H7	H8	-1.46	1.01248E-05	-1.07	-1.46	0.40
H7	H9	-3.45	2.39035E-05	-3.56	-3.45	-0.11
H7	H10	-0.51	3.53135E-06	-0.27	-0.51	0.24
H8	H9	-0.51	3.53135E-06	-0.27	-0.51	0.24
H8	H10	-3.45	2.39035E-05	-3.56	-3.45	-0.11
H9	H10	-1.46	1.01248E-05	-1.07	-1.46	0.40
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

Table S98. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{int}^{A,B}$ of interaction energies $E_{int}^{A,B}$ computed at MP2/Müller for distant C,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

C···H in LEC		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
C1	H5	80.84	-5.60847E-04	78.56	80.83	-2.28
C1	H6	34.65	-2.40395E-04	33.43	34.65	-1.21
C1	H8	-4.93	3.41684E-05	-2.72	-4.92	2.20
C1	H10	-4.93	3.41684E-05	-2.73	-4.92	2.20
C2	H5	34.65	-2.40395E-04	33.43	34.65	-1.21
C2	H6	80.84	-5.60847E-04	78.56	80.83	-2.28
C2	H7	-4.93	3.41684E-05	-2.72	-4.92	2.20
C2	H9	-4.93	3.41684E-05	-2.73	-4.92	2.20
					Average for $\lvert\Delta_{int}^{A,B}\rvert$	2.0
					Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$	0.5

C···H in Linear		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
C1	H5	78.29	-5.43115E-04	75.67	78.28	-2.61
C1	H6	47.76	-3.31314E-04	46.59	47.75	-1.16
C1	H8	-3.92	2.72198E-05	-2.16	-3.92	1.76
C1	H10	-5.06	3.50861E-05	-3.10	-5.06	1.96
C2	H5	38.67	-2.68255E-04	37.44	38.66	-1.22
C2	H6	85.16	-5.90764E-04	83.19	85.14	-1.96
C2	H7	-4.58	3.17769E-05	-2.34	-4.58	2.24
C2	H9	-5.06	3.51173E-05	-3.20	-5.06	1.86
					Average for $\lvert\Delta_{int}^{A,B}\rvert$	1.8
					Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$	0.5

C···H in Eclipsed		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}$ / E	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
C1	H5	82.40	-5.71696E-04	80.28	82.39	-2.11
C1	H6	37.71	-2.61656E-04	36.74	37.71	-0.97
C1	H8	-6.60	4.58093E-05	-4.44	-6.60	2.16
C1	H10	-6.60	4.58093E-05	-4.44	-6.60	2.16
C2	H5	37.71	-2.61656E-04	36.73	37.71	-0.98
C2	H6	82.40	-5.71696E-04	80.29	82.39	-2.10
C2	H7	-6.60	4.58093E-05	-4.44	-6.60	2.16
C2	H9	-6.60	4.58093E-05	-4.44	-6.60	2.16
					Average for $\lvert\Delta_{int}^{A,B}\rvert$	1.8
					Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$	0.5

Table S99. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{cl}^{A,B}$ in the classical component $V_{cl}^{A,B}$ of interaction energies computed at MP2/Müller for distant C,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

C···H in LEC		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
C1	H5	79.50	-5.51515E-04	76.67	79.49	-2.82
C1	H6	48.29	-3.35024E-04	46.77	48.29	-1.51
C1	H8	0.12	-8.38500E-07	1.38	0.12	1.26
C1	H10	-1.10	7.61256E-06	0.27	-1.10	1.37
C2	H5	39.11	-2.71330E-04	37.72	39.11	-1.39
C2	H6	86.47	-5.99872E-04	84.14	86.46	-2.32
C2	H7	-0.83	5.78789E-06	0.72	-0.83	1.55
C2	H9	-1.27	8.79525E-06	0.12	-1.27	1.39
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	1.7
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	0.6

C···H in Linear		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
C1	H5	82.17	-5.70019E-04	79.58	82.15	-2.57
C1	H6	35.15	-2.43847E-04	33.72	35.14	-1.42
C1	H8	-1.14	7.88614E-06	0.33	-1.14	1.47
C1	H10	-1.14	7.88614E-06	0.33	-1.14	1.47
C2	H5	35.15	-2.43847E-04	33.72	35.14	-1.42
C2	H6	82.17	-5.70019E-04	79.58	82.15	-2.57
C2	H7	-1.14	7.88614E-06	0.33	-1.14	1.47
C2	H9	-1.14	7.88614E-06	0.33	-1.14	1.47
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	1.7
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	0.5

C···H in Eclipsed		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
C1	H5	83.83	-5.81584E-04	81.40	83.81	-2.41
C1	H6	38.20	-2.65018E-04	37.01	38.19	-1.19
C1	H8	-2.54	1.76089E-05	-1.10	-2.54	1.43
C1	H10	-2.54	1.76089E-05	-1.10	-2.54	1.43
C2	H5	38.20	-2.65018E-04	36.99	38.19	-1.20
C2	H6	83.83	-5.81584E-04	81.41	83.81	-2.40
C2	H7	-2.54	1.76089E-05	-1.11	-2.54	1.43
C2	H9	-2.54	1.76089E-05	-1.10	-2.54	1.43
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	1.6
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	0.5

Table S100. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{XC}^{A,B}$ in the XC-term $V_{XC}^{A,B}$ of interaction energies computed at MP2/Müller for distant C,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

C···H in LEC		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
C1	H5	-1.21	8.40036E-06	-1.00	-1.21	0.21
C1	H6	-0.53	3.70975E-06	-0.18	-0.53	0.36
C1	H8	-4.04	2.80583E-05	-3.54	-4.04	0.50
C1	H10	-3.96	2.74736E-05	-3.38	-3.96	0.58
C2	H5	-0.44	3.07551E-06	-0.28	-0.44	0.16
C2	H6	-1.31	9.10774E-06	-0.95	-1.31	0.37
C2	H7	-3.75	2.59890E-05	-3.06	-3.75	0.69
C2	H9	-3.79	2.63220E-05	-3.32	-3.79	0.47
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.42
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.18

C···H in Linear		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
C1	H5	-1.32	9.17191E-06	-1.02	-1.32	0.30
C1	H6	-0.50	3.45234E-06	-0.29	-0.50	0.21
C1	H8	-3.79	2.62822E-05	-3.06	-3.79	0.73
C1	H10	-3.79	2.62822E-05	-3.06	-3.79	0.73
C2	H5	-0.50	3.45234E-06	-0.29	-0.50	0.21
C2	H6	-1.32	9.17191E-06	-1.02	-1.32	0.30
C2	H7	-3.79	2.62822E-05	-3.06	-3.79	0.73
C2	H9	-3.79	2.62822E-05	-3.06	-3.79	0.73
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.5
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.3

C···H in Eclipsed		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
C1	H5	-1.43	9.88825E-06	-1.12	-1.43	0.30
C1	H6	-0.48	3.36254E-06	-0.26	-0.48	0.22
C1	H8	-4.06	2.82004E-05	-3.34	-4.06	0.73
C1	H10	-4.06	2.82004E-05	-3.34	-4.06	0.73
C2	H5	-0.48	3.36254E-06	-0.26	-0.48	0.22
C2	H6	-1.43	9.88825E-06	-1.12	-1.43	0.31
C2	H7	-4.06	2.82004E-05	-3.33	-4.06	0.73
C2	H9	-4.06	2.82004E-05	-3.34	-4.06	0.73
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.5
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.3

Table S101. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{int}^{A,B}$ in interaction energies $E_{int}^{A,B}$ computed at MP2/Müller for distant O,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

O···H in LEC		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
O3	H5	-63.47	4.40340E-04	-64.64	-63.46	-1.17
O3	H7	1.53	-1.05919E-05	-0.07	1.53	-1.60
O3	H8	-6.44	4.46864E-05	-8.69	-6.44	-2.25
O3	H9	1.74	-1.20837E-05	0.56	1.74	-1.18
O3	H10	-4.72	3.27422E-05	-6.95	-4.72	-2.23
O4	H6	-90.89	6.30517E-04	-92.95	-90.87	-2.08
O4	H7	-4.46	3.09496E-05	-6.83	-4.46	-2.37
O4	H8	0.02	-1.51058E-07	-1.28	0.02	-1.30
O4	H9	-3.22	2.23074E-05	-5.36	-3.22	-2.15
O4	H10	1.98	-1.37476E-05	0.44	1.98	-1.54
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		1.8
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		0.5

O···H in Linear		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
O3	H5	-50.37	3.49449E-04	-50.77	-50.36	-0.40
O3	H7	2.11	-1.46101E-05	0.65	2.11	-1.46
O3	H8	-3.97	2.75121E-05	-6.28	-3.97	-2.32
O3	H9	2.11	-1.46101E-05	0.65	2.11	-1.46
O3	H10	-3.97	2.75121E-05	-6.29	-3.97	-2.32
O4	H6	-50.37	3.49449E-04	-50.77	-50.36	-0.40
O4	H7	-3.97	2.75121E-05	-6.28	-3.97	-2.32
O4	H8	2.11	-1.46101E-05	0.65	2.11	-1.46
O4	H9	-3.97	2.75121E-05	-6.29	-3.97	-2.32
O4	H10	2.11	-1.46101E-05	0.65	2.11	-1.46
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		1.6
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		0.7

O···H in Eclipsed		CCSD/BBC1		MP2/Müller		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
O3	H5	-59.43	4.12334E-04	-60.00	-59.42	-0.58
O3	H7	3.69	-2.56299E-05	2.67	3.69	-1.02
O3	H8	-1.45	1.00861E-05	-3.64	-1.45	-2.19
O3	H9	3.69	-2.56299E-05	2.67	3.69	-1.02
O3	H10	-1.45	1.00861E-05	-3.64	-1.45	-2.18
O4	H6	-59.43	4.12334E-04	-60.00	-59.42	-0.57
O4	H7	-1.45	1.00861E-05	-3.64	-1.45	-2.18
O4	H8	3.69	-2.56299E-05	2.67	3.69	-1.02
O4	H9	-1.45	1.00861E-05	-3.64	-1.45	-2.18
O4	H10	3.69	-2.56299E-05	2.67	3.69	-1.02
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		1.4
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		0.7

Table S102. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{cl}^{A,B}$ in the classical term $V_{cl}^{A,B}$ of interaction energies computed at MP2/Müller for distant O,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

O···H in LEC		CCSD/BBC1		MP2/Müller		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
O3	H5	79.50	-5.51515E-04	76.67	79.49	-2.82
O3	H7	48.29	-3.35024E-04	46.77	48.29	-1.51
O3	H8	0.12	-8.38500E-07	1.38	0.12	1.26
O3	H9	-1.10	7.61256E-06	0.27	-1.10	1.37
O3	H10	39.11	-2.71330E-04	37.72	39.11	-1.39
O4	H6	86.47	-5.99872E-04	84.14	86.46	-2.32
O4	H7	-0.83	5.78789E-06	0.72	-0.83	1.55
O4	H8	-1.27	8.79525E-06	0.12	-1.27	1.39
O4	H9	79.50	-5.51515E-04	76.67	79.49	-2.82
O4	H10	48.29	-3.35024E-04	46.77	48.29	-1.51
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		1.7
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		0.6

O···H in Linear		CCSD/BBC1		MP2/Müller		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
O3	H5	-49.87	3.45955E-04	-50.71	-49.86	-0.86
O3	H7	4.07	-2.82240E-05	2.18	4.07	-1.88
O3	H8	2.14	-1.48185E-05	-0.42	2.14	-2.55
O3	H9	4.07	-2.82240E-05	2.18	4.07	-1.89
O3	H10	2.14	-1.48185E-05	-0.42	2.14	-2.56
O4	H6	-49.87	3.45955E-04	-50.71	-49.86	-0.86
O4	H7	2.14	-1.48185E-05	-0.42	2.14	-2.55
O4	H8	4.07	-2.82240E-05	2.18	4.07	-1.88
O4	H9	2.14	-1.48185E-05	-0.42	2.14	-2.56
O4	H10	4.07	-2.82240E-05	2.18	4.07	-1.89
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		1.9
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		0.7

O···H in Eclipsed		CCSD/BBC1		MP2/Müller		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
O3	H5	83.83	-5.81584E-04	81.40	83.81	-2.41
O3	H7	38.20	-2.65018E-04	37.01	38.19	-1.19
O3	H8	-2.54	1.76089E-05	-1.10	-2.54	1.43
O3	H9	-2.54	1.76089E-05	-1.10	-2.54	1.43
O3	H10	38.20	-2.65018E-04	36.99	38.19	-1.20
O4	H6	83.83	-5.81584E-04	81.41	83.81	-2.40
O4	H7	-2.54	1.76089E-05	-1.11	-2.54	1.43
O4	H8	-2.54	1.76089E-05	-1.10	-2.54	1.43
O4	H9	83.83	-5.81584E-04	81.40	83.81	-2.41
O4	H10	38.20	-2.65018E-04	37.01	38.19	-1.19
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		1.6
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		0.5

Table S103. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{XC}^{A,B}$ in the XC-term $V_{XC}^{A,B}$ of interaction energies computed at MP2/Müller for distant O,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

O···H in LEC		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
O3	H5	-0.35	2.44852E-06	-0.05	-0.35	0.30
O3	H7	-2.00	1.38900E-05	-1.49	-2.00	0.51
O3	H8	-6.27	4.34686E-05	-5.88	-6.26	0.38
O3	H9	-1.14	7.90820E-06	-0.59	-1.14	0.55
O3	H10	-6.42	4.45528E-05	-5.99	-6.42	0.43
O4	H6	-3.03	2.10430E-05	-2.75	-3.03	0.28
O4	H7	-6.28	4.35390E-05	-5.97	-6.28	0.30
O4	H8	-0.86	5.98068E-06	-0.50	-0.86	0.37
O4	H9	-6.50	4.51269E-05	-5.92	-6.50	0.58
O4	H10	-1.99	1.38080E-05	-1.49	-1.99	0.50
				Average for $\lvert\Delta_{XC}^{A,B}\rvert$		0.4
				Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$		0.1

O···H in Linear		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
O3	H5	-0.50	3.49384E-06	-0.05	-0.50	0.45
O3	H7	-1.96	1.36138E-05	-1.53	-1.96	0.43
O3	H8	-6.10	4.23306E-05	-5.86	-6.10	0.24
O3	H9	-1.96	1.36138E-05	-1.53	-1.96	0.43
O3	H10	-6.10	4.23306E-05	-5.86	-6.10	0.24
O4	H6	-0.50	3.49384E-06	-0.05	-0.50	0.45
O4	H7	-6.10	4.23306E-05	-5.86	-6.10	0.24
O4	H8	-1.96	1.36138E-05	-1.53	-1.96	0.43
O4	H9	-6.10	4.23306E-05	-5.86	-6.10	0.24
O4	H10	-1.96	1.36138E-05	-1.53	-1.96	0.43
				Average for $\lvert\Delta_{XC}^{A,B}\rvert$		0.4
				Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$		0.1

O···H in Eclipsed		CCSD/BBC1		MP2/Müller		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
O3	H5	-0.67	4.62679E-06	-0.14	-0.67	0.53
O3	H7	-0.70	4.84171E-06	-0.21	-0.70	0.49
O3	H8	-6.58	4.56687E-05	-6.36	-6.58	0.22
O3	H9	-0.70	4.84171E-06	-0.21	-0.70	0.49
O3	H10	-6.58	4.56687E-05	-6.36	-6.58	0.22
O4	H6	-0.67	4.62679E-06	-0.14	-0.67	0.53
O4	H7	-6.58	4.56687E-05	-6.36	-6.58	0.22
O4	H8	-0.70	4.84171E-06	-0.21	-0.70	0.49
O4	H9	-6.58	4.56687E-05	-6.36	-6.58	0.22
O4	H10	-0.70	4.84171E-06	-0.21	-0.70	0.49
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.4
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

Table S104. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{int}^{A,B}$ of interaction energies $E_{int}^{A,B}$ computed at MP2/Müller for distant H,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

H···H in LEC		CCSD/BBC1		MP2/Müller		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B}/E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
H5	H6	36.97	-2.56444E-04	38.74	36.96	1.78
H5	H7	-1.91	1.32190E-05	-0.52	-1.91	1.38
H5	H8	-0.65	4.54108E-06	0.11	-0.65	0.76
H5	H9	-2.20	1.52426E-05	-0.92	-2.20	1.28
H5	H10	-1.79	1.23902E-05	-0.91	-1.79	0.87
H6	H7	-1.78	1.23769E-05	-0.63	-1.78	1.16
H6	H8	-0.43	2.95773E-06	0.77	-0.43	1.19
H6	H9	-1.50	1.03754E-05	-0.57	-1.50	0.93
H6	H10	-1.52	1.05510E-05	-0.13	-1.52	1.39
H7	H8	-0.42	2.91928E-06	-0.16	-0.42	0.26
H7	H9	-2.32	1.60696E-05	-2.17	-2.32	0.15
H7	H10	-0.55	3.79630E-06	-0.38	-0.55	0.17
H8	H9	-0.32	2.23740E-06	-0.17	-0.32	0.15
H8	H10	-2.38	1.65337E-05	-2.14	-2.38	0.25
H9	H10	-0.25	1.74888E-06	-0.16	-0.25	0.09
					Average for $\lvert\Delta_{int}^{A,B}\rvert$	0.8
					Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$	0.6

H···H in Linear		CCSD/BBC1		MP2/Müller		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B} / E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
H5	H6	22.72	-1.57635E-04	23.75	22.72	1.03
H5	H7	-1.84	1.27666E-05	-0.58	-1.84	1.26
H5	H8	-1.82	1.25965E-05	-1.00	-1.82	0.81
H5	H9	-1.84	1.27666E-05	-0.58	-1.84	1.26
H5	H10	-1.82	1.25965E-05	-1.00	-1.82	0.81
H6	H7	-1.82	1.25965E-05	-1.00	-1.82	0.81
H6	H8	-1.84	1.27666E-05	-0.58	-1.84	1.26
H6	H9	-1.82	1.25965E-05	-1.00	-1.82	0.81
H6	H10	-1.84	1.27666E-05	-0.58	-1.84	1.26
H7	H8	-0.57	3.92163E-06	-0.35	-0.57	0.22
H7	H9	-2.51	1.73979E-05	-2.21	-2.51	0.30
H7	H10	-0.46	3.19134E-06	-0.17	-0.46	0.29
H8	H9	-0.46	3.19134E-06	-0.17	-0.46	0.29
H8	H10	-2.51	1.73979E-05	-2.21	-2.51	0.30
H9	H10	-0.57	3.92163E-06	-0.35	-0.57	0.22
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		0.7
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		0.4

H···H in Eclipsed		CCSD/BBC1		MP2/Müller		
Atom A	**Atom B**	$E_{int}^{A,B}$	$E_{int}^{A,B} / E$	$^{Comput}E_{int}^{A,B}$	$^{Expect}E_{int}^{A,B}$	$\Delta_{int}^{A,B}$
H5	H6	25.93	-1.79929E-04	27.13	25.93	1.20
H5	H7	-3.37	2.33517E-05	-2.16	-3.37	1.20
H5	H8	-2.23	1.54635E-05	-1.54	-2.23	0.69
H5	H9	-3.37	2.33517E-05	-2.16	-3.37	1.20
H5	H10	-2.23	1.54635E-05	-1.54	-2.23	0.69
H6	H7	-2.23	1.54635E-05	-1.54	-2.23	0.69
H6	H8	-3.37	2.33517E-05	-2.16	-3.37	1.20
H6	H9	-2.23	1.54635E-05	-1.54	-2.23	0.69
H6	H10	-3.37	2.33517E-05	-2.16	-3.37	1.20
H7	H8	-0.88	6.13093E-06	-0.67	-0.88	0.22
H7	H9	-2.65	1.83821E-05	-2.48	-2.65	0.17
H7	H10	-0.25	1.76286E-06	-0.06	-0.25	0.20
H8	H9	-0.25	1.76286E-06	-0.06	-0.25	0.20
H8	H10	-2.65	1.83821E-05	-2.48	-2.65	0.17
H9	H10	-0.88	6.13093E-06	-0.67	-0.88	0.22
				Average for $\lvert\Delta_{int}^{A,B}\rvert$		0.7
				Std. deviation for $\lvert\Delta_{int}^{A,B}\rvert$		0.4

Table S105. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{cl}^{A,B}$ in the classical term $V_{cl}^{A,B}$ of interaction energies computed at MP2/Müller for distant H,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

H···H in LEC		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
H5	H6	37.09	-2.57280E-04	38.77	37.08	1.69
H5	H7	-1.73	1.19752E-05	-0.38	-1.73	1.34
H5	H8	-0.59	4.11552E-06	0.16	-0.59	0.75
H5	H9	-2.11	1.46141E-05	-0.86	-2.11	1.25
H5	H10	-1.71	1.18685E-05	-0.89	-1.71	0.82
H6	H7	-1.70	1.17605E-05	-0.62	-1.69	1.08
H6	H8	-0.08	5.40273E-07	1.08	-0.08	1.16
H6	H9	-1.41	9.76436E-06	-0.55	-1.41	0.86
H6	H10	-1.38	9.58579E-06	-0.07	-1.38	1.31
H7	H8	0.20	-1.38967E-06	0.16	0.20	-0.04
H7	H9	0.69	-4.78518E-06	0.73	0.69	0.04
H7	H10	0.08	-5.50299E-07	0.06	0.08	-0.02
H8	H9	0.26	-1.82468E-06	0.19	0.26	-0.07
H8	H10	0.67	-4.65740E-06	0.76	0.67	0.09
H9	H10	0.30	-2.06546E-06	0.20	0.30	-0.09
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	0.7
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	0.6

H···H in Linear		**CCSD/BBC1**		**MP2/Müller**		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
H5	H6	22.91	-1.58934E-04	23.75	22.91	0.85
H5	H7	-1.74	1.20370E-05	-0.49	-1.73	1.25
H5	H8	-1.78	1.23721E-05	-0.98	-1.78	0.80
H5	H9	-1.74	1.20370E-05	-0.49	-1.73	1.25
H5	H10	-1.78	1.23721E-05	-0.98	-1.78	0.80
H6	H7	-1.78	1.23721E-05	-0.98	-1.78	0.80
H6	H8	-1.74	1.20370E-05	-0.49	-1.73	1.25
H6	H9	-1.78	1.23721E-05	-0.98	-1.78	0.80
H6	H10	-1.74	1.20370E-05	-0.49	-1.73	1.25
H7	H8	0.08	-5.35901E-07	0.06	0.08	-0.02
H7	H9	0.67	-4.65362E-06	0.73	0.67	0.06
H7	H10	0.21	-1.46599E-06	0.16	0.21	-0.05
H8	H9	0.21	-1.46599E-06	0.16	0.21	-0.05
H8	H10	0.67	-4.65362E-06	0.73	0.67	0.06
H9	H10	0.08	-5.35901E-07	0.06	0.08	-0.02
					Average for $\lvert\Delta_{cl}^{A,B}\rvert$	0.6
					Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$	0.5

H···H in Eclipsed		CCSD/BBC1		MP2/Müller		
Atom A	**Atom B**	$V_{cl}^{A,B}$	$V_{cl}^{A,B}/E$	$^{Comput}V_{cl}^{A,B}$	$^{Expect}V_{cl}^{A,B}$	$\Delta_{cl}^{A,B}$
H5	H6	26.14	-1.81338E-04	27.14	26.13	1.01
H5	H7	-3.23	2.23898E-05	-2.05	-3.23	1.18
H5	H8	-2.19	1.52172E-05	-1.52	-2.19	0.67
H5	H9	-3.23	2.23898E-05	-2.05	-3.23	1.18
H5	H10	-2.19	1.52172E-05	-1.52	-2.19	0.67
H6	H7	-2.19	1.52172E-05	-1.52	-2.19	0.67
H6	H8	-3.23	2.23898E-05	-2.05	-3.23	1.18
H6	H9	-2.19	1.52172E-05	-1.52	-2.19	0.67
H6	H10	-3.23	2.23898E-05	-2.05	-3.23	1.18
H7	H8	0.58	-3.99386E-06	0.42	0.58	-0.15
H7	H9	0.80	-5.52134E-06	0.76	0.80	-0.04
H7	H10	0.25	-1.76849E-06	0.16	0.25	-0.09
H8	H9	0.25	-1.76849E-06	0.16	0.25	-0.09
H8	H10	0.80	-5.52134E-06	0.76	0.80	-0.04
H9	H10	0.58	-3.99386E-06	0.42	0.58	-0.15
				Average for $\lvert\Delta_{cl}^{A,B}\rvert$		0.6
				Std. deviation for $\lvert\Delta_{cl}^{A,B}\rvert$		0.5

Table S106. Using the CCSD/BBC1 data as a reference, analysis of relative errors $\Delta_{XC}^{A,B}$ in the XC-term $V_{XC}^{A,B}$ of interaction energies computed at MP2/Müller for distant H,H atom-pairs in all conformers of glycol (values in kcal mol^{-1}).

H···H in LEC		CCSD/BBC1		MP2/Müller		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B}/E$	$^{Comput}V_{XC}^{A,B}$	$^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
H5	H6	-0.12	8.35982E-07	-0.03	-0.12	0.09
H5	H7	-0.18	1.24377E-06	-0.14	-0.18	0.04
H5	H8	-0.06	4.25557E-07	-0.05	-0.06	0.01
H5	H9	-0.09	6.28456E-07	-0.06	-0.09	0.03
H5	H10	-0.08	5.21707E-07	-0.03	-0.08	0.05
H6	H7	-0.09	6.16356E-07	-0.01	-0.09	0.08
H6	H8	-0.35	2.41746E-06	-0.31	-0.35	0.04
H6	H9	-0.09	6.11051E-07	-0.02	-0.09	0.07
H6	H10	-0.14	9.65231E-07	-0.07	-0.14	0.07
H7	H8	-0.62	4.30895E-06	-0.33	-0.62	0.30
H7	H9	-3.01	2.08548E-05	-2.89	-3.01	0.11
H7	H10	-0.63	4.34660E-06	-0.44	-0.63	0.19
H8	H9	-0.59	4.06207E-06	-0.36	-0.59	0.22
H8	H10	-3.05	2.11911E-05	-2.90	-3.05	0.16
H9	H10	-0.55	3.81434E-06	-0.37	-0.55	0.18
				Average for $\lvert\Delta_{XC}^{A,B}\rvert$		0.1
				Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$		0.1

H···H in Linear		CCSD/BBC1		MP2/Müller		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B} / E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
H5	H6	-0.19	1.29892E-06	-0.01	-0.19	0.18
H5	H7	-0.11	7.29610E-07	-0.09	-0.11	0.01
H5	H8	-0.03	2.24489E-07	-0.02	-0.03	0.01
H5	H9	-0.11	7.29610E-07	-0.09	-0.11	0.01
H5	H10	-0.03	2.24489E-07	-0.02	-0.03	0.01
H6	H7	-0.03	2.24489E-07	-0.02	-0.03	0.01
H6	H8	-0.11	7.29610E-07	-0.09	-0.11	0.01
H6	H9	-0.03	2.24489E-07	-0.02	-0.03	0.01
H6	H10	-0.11	7.29610E-07	-0.09	-0.11	0.01
H7	H8	-0.64	4.45753E-06	-0.41	-0.64	0.23
H7	H9	-3.18	2.20515E-05	-2.94	-3.18	0.23
H7	H10	-0.67	4.65732E-06	-0.33	-0.67	0.34
H8	H9	-0.67	4.65732E-06	-0.33	-0.67	0.34
H8	H10	-3.18	2.20515E-05	-2.94	-3.18	0.23
H9	H10	-0.64	4.45753E-06	-0.41	-0.64	0.23
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

H···H in Eclipsed		CCSD/BBC1		MP2/Müller		
Atom A	**Atom B**	$V_{XC}^{A,B}$	$V_{XC}^{A,B} / E$	${}^{Comput}V_{XC}^{A,B}$	${}^{Expect}V_{XC}^{A,B}$	$\Delta_{XC}^{A,B}$
H5	H6	-0.20	1.40935E-06	-0.01	-0.20	0.20
H5	H7	-0.14	9.61846E-07	-0.12	-0.14	0.02
H5	H8	-0.04	2.46282E-07	-0.02	-0.04	0.02
H5	H9	-0.14	9.61846E-07	-0.12	-0.14	0.02
H5	H10	-0.04	2.46282E-07	-0.02	-0.04	0.02
H6	H7	-0.04	2.46282E-07	-0.02	-0.04	0.02
H6	H8	-0.14	9.61846E-07	-0.12	-0.14	0.02
H6	H9	-0.04	2.46282E-07	-0.02	-0.04	0.02
H6	H10	-0.14	9.61846E-07	-0.12	-0.14	0.02
H7	H8	-1.46	1.01248E-05	-1.09	-1.46	0.37
H7	H9	-3.45	2.39035E-05	-3.23	-3.44	0.21
H7	H10	-0.51	3.53135E-06	-0.22	-0.51	0.29
H8	H9	-0.51	3.53135E-06	-0.22	-0.51	0.29
H8	H10	-3.45	2.39035E-05	-3.23	-3.44	0.21
H9	H10	-1.46	1.01248E-05	-1.09	-1.46	0.37
					Average for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1
					Std. deviation for $\lvert\Delta_{XC}^{A,B}\rvert$	0.1

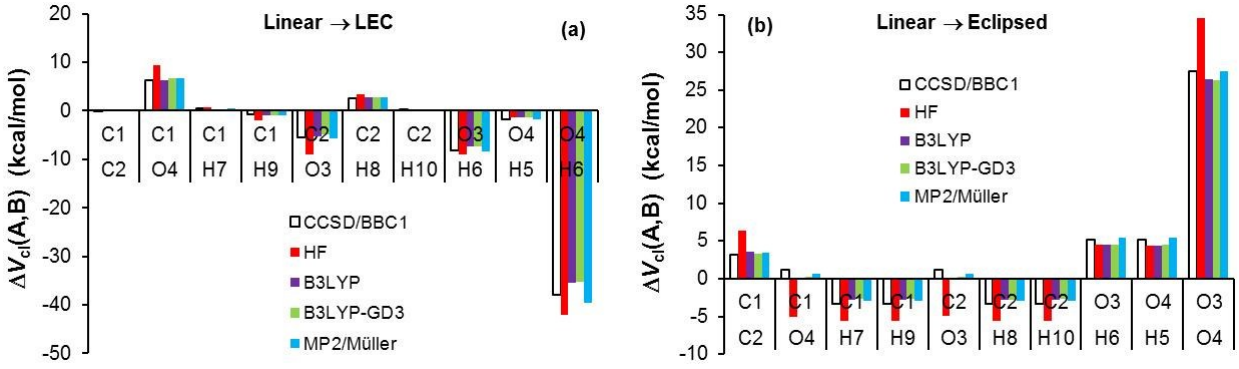

Figure S9. Changes in the classical term of diatomic interaction energies for the indicated atom-pairs on **Lin → LEC** (part a) and **Lin → Ecl** (part b) structural transformations of glycol at specified levels of theory.

Changes in the classical term of interactions are shown in Figure S9. Trends in $\Delta V_{\mathrm{cl}}^{\mathrm{A,B}}$ and their values observed for **Lin → LEC** mimic those for $\Delta E_{\mathrm{int}}^{\mathrm{A,B}}$ seen in Figure 10a in the main body of the text. From that follows that main contributions to $\Delta E_{\mathrm{int}}^{\mathrm{A,B}}$ come from the classical term. For instance, $\Delta V_{\mathrm{cl}}^{\mathrm{O4,H6}} = -38.0$ kcal mol^{-1} is smaller than $\Delta E_{\mathrm{int}}^{\mathrm{O4,H6}}$ by just 2.5 kcal mol^{-1}; this is in full agreement with common knowledge when intramolecular H-bonds are considered. Dominance of classical contributions is also observed for C1–O4 and C2–O3 atom-pairs as they are smaller, relative to their interaction energies, by 1.3 and 2.6 kcal mol^{-1}, respectively). Quite a different picture emerged from the **Lin → Ecl** structural change where $\Delta V_{\mathrm{cl}}^{\mathrm{O3,O4}}$ term is 9.5 kcal mol^{-1} larger than $\Delta E_{\mathrm{int}}^{\mathrm{O3,O4}}$ and this exemplifies a large increase in repulsive forces acting on these two clashing O-atoms in **Ecl**. Interestingly, the change in the interaction energy between C-atoms of the linker ($\Delta E_{\mathrm{int}}^{\mathrm{C1,C2}} = +8.9$ kcal mol^{-1}) is not dominated by the classical term as it became more positive only by +3.2 kcal mol^{-1}, from $V_{\mathrm{cl}}^{\mathrm{C1,C2}}$ of +78.4 (in **Lin**) to +81.6 (in **Ecl**) kcal mol^{-1}.

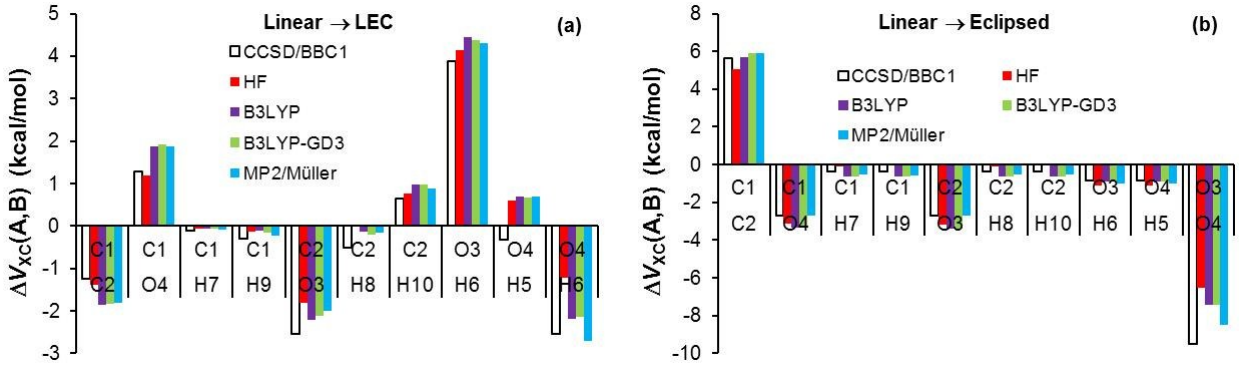

Figure S10. Changes in the XC-term of diatomic interaction energies for the indicated atom-pairs on **Lin → LEC** (part a) and **Lin → Ecl** (part b) structural transformations of glycol at specified levels of theory.

Figure S10 uncovers many atom-pairs for which significant change in covalent component of an interaction took place, the $\Delta V_{\mathrm{XC}}^{\mathrm{A,B}}$ term. There are 3 ({O3,H6}, {O4,H6} and {C2,O3}) and 2 ({C1,C2} and {C1,O4}) atom-pairs in **LEC** for which the XC-term changed at CCSD/BBC1 by more than 2 and 1 kcal mol^{-1}, respectively. Among them, the C1–C2, C2–O3 and O4···H6 atom-pairs experienced an increase in the covalent component of an interaction. On **Lin → LEC** (Figure S10a), the largest change among all possible atom pairs in glycol took place for the O3–H6 atom-pair for which a significant decrease in the XC-term is observed, by +3.9 kcal mol^{-1}. Four significant changes in the XC-term are seen for the **Ecl** conformer in Figure S10b. Note that atoms involved in a steric clash (O3--O4) in the **Ecl** conformer experienced a significant increase in the XC-term as also found for the H-bonding (O4···H6) in **LEC**. Moreover, $\Delta V_{\mathrm{XC}}^{\mathrm{C1,C2}}$ of –9.5 kcal mol^{-1} at CCSD/BBC1 is most significant on **Lin → Ecl**. Recalling that $V_{\mathrm{XC}}^{\mathrm{A,B}} < 0$ always holds (hence, it is always of a stabilizing nature) one could argue that this energy component strengthens the H-bonding (O4···H6) in **LEC** whereas partly counteracts, or compensates for, the increased repulsive classical term in the case of a steric clash (O3--O4) in **Ecl**. Lastly, let us focus on the link for which we observe opposite trends in the two conformers. A significant decrease in the XC-term, by 5.6 kcal mol^{-1}, took place in **Ecl** but a small increase by –1.3 kcal mol^{-1} is observed in **LEC** and in both cases $\Delta V_{\mathrm{XC}}^{\mathrm{C1,C2}}$ is more significant that $\Delta V_{\mathrm{cl}}^{\mathrm{C1,C2}}$. As a consequence, the link became significantly weaker in **Ecl** and somewhat stronger in **LEC**.

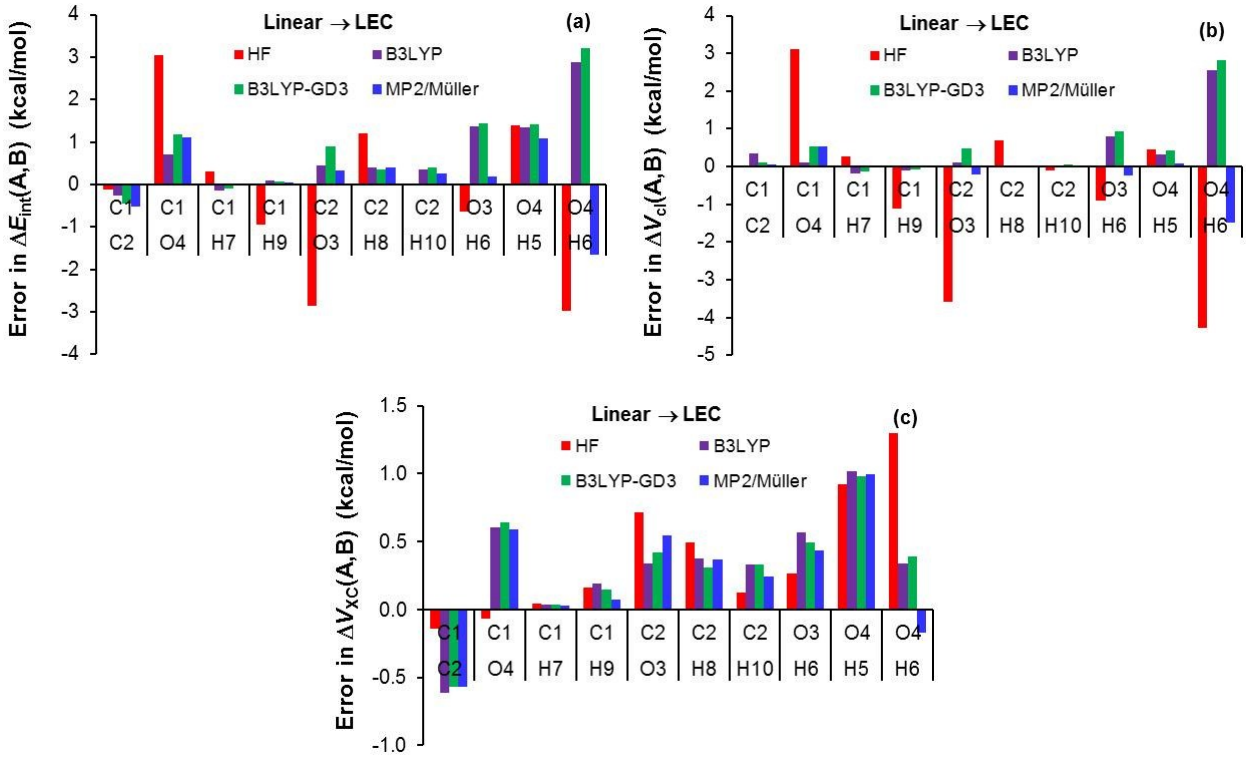

Figure S11. Relative to CCSD/BBC1, errors in $\Delta E_{\text{int}}^{\text{A,B}}$ (part a), $\Delta V_{\text{cl}}^{\text{A,B}}$ (part b) and $\Delta V_{\text{XC}}^{\text{A,B}}$ (part c) obtained for covalently bonded atoms and the intra-molecular O4···H6 interaction on the **Lin → LEC** structural change.

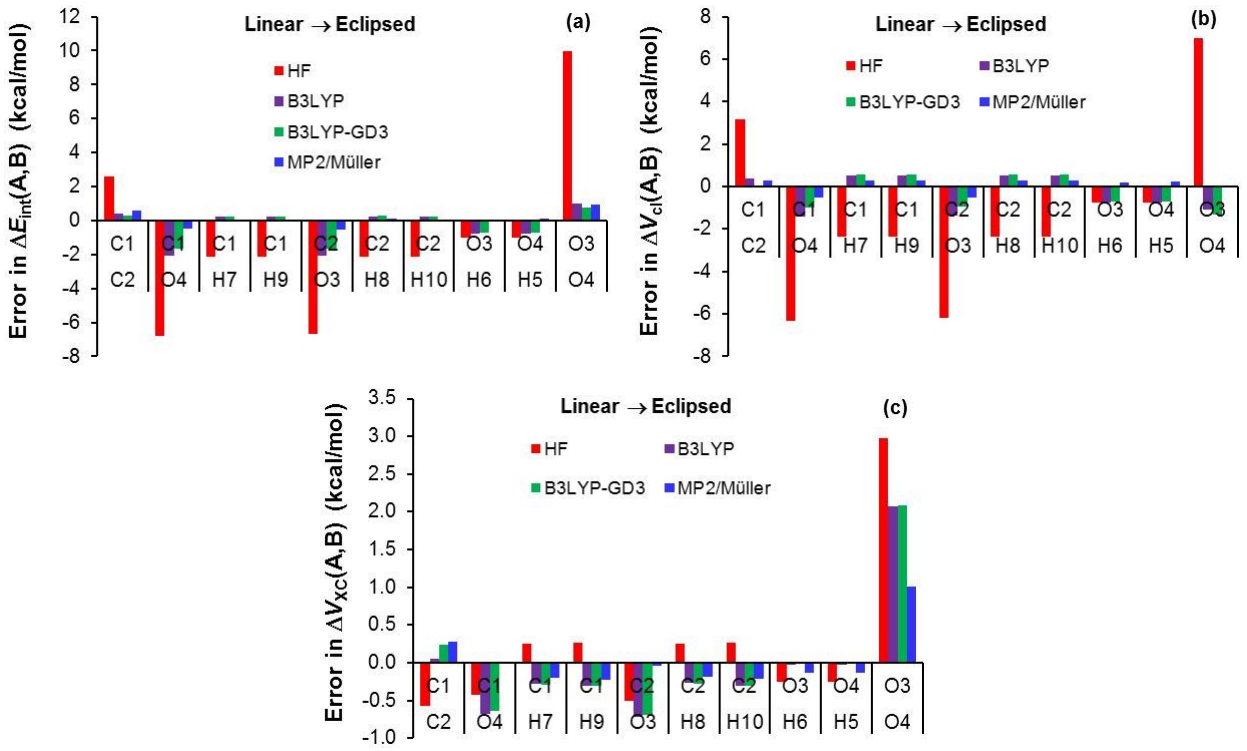

Figure S12. Relative to CCSD/BBC1, errors in $\Delta E_{\text{int}}^{\text{A,B}}$ (part a), $\Delta V_{\text{cl}}^{\text{A,B}}$ (part b) and $\Delta V_{\text{XC}}^{\text{A,B}}$ (part c) obtained for covalently bonded atoms and an intra-molecular interaction O3···O4 on the **Lin → Ecl** structural change.

Table S107. Relative to the CCSD/BBC1 data, errors (part a) and averaged absolute errors (part b) in $\Delta E_{\text{int}}^{\text{A,B}}$ (kcal mol^{-1}) obtained for the **Lin → LEC** structural change at the indicated levels of theory.

Part a		**HF**	**B3LYP**	**B3LYP-GD3**	**MP2/Müller**
Atom A	**Atom B**	Error in $\Delta E_{\text{int}}^{\text{A,B}}$			
C2	C1	-0.13	-0.27	-0.46	-0.53
O4	C1	3.04	0.71	1.19	1.12
H7	C1	0.30	-0.14	-0.09	0.02
H9	C1	-0.96	0.09	0.08	0.05
O3	C2	-2.87	0.44	0.90	0.33
H8	C2	1.20	0.41	0.35	0.41
H10	C2	0.02	0.34	0.40	0.25
H6	O3	-0.63	1.37	1.44	0.19
H5	O4	1.39	1.34	1.42	1.09
H6	O4	-2.97	2.88	3.21	-1.66
	Average:	*-0.16*	*0.72*	*0.84*	*0.13*
	Std. dev.:	*1.85*	*0.94*	*1.05*	*0.80*

Part b		Averaged absolute error in $\Delta E_{\text{int}}^{\text{A,B}}$			
	Average:	*1.35*	*0.80*	*0.95*	*0.56*
	Std. dev.:	*1.19*	*0.86*	*0.95*	*0.55*

Table S108. Relative to the CCSD/BBC1 data, errors (part a) and averaged absolute errors (part b) in $\Delta V_{\text{cl}}^{\text{A,B}}$ (kcal mol^{-1}) obtained for the **Lin → LEC** structural change at the indicated levels of theory.

Part a		**HF**	**B3LYP**	**B3LYP-GD3**	**MP2/Müller**
Atom A	**Atom B**	Error in $\Delta V_{\text{cl}}^{\text{A,B}}$			
C2	C1	0.01	0.34	0.12	0.04
O4	C1	3.11	0.10	0.55	0.53
H7	C1	0.26	-0.18	-0.13	-0.01
H9	C1	-1.12	-0.10	-0.07	-0.03
O3	C2	-3.59	0.11	0.48	-0.22
H8	C2	0.70	0.04	0.04	0.04
H10	C2	-0.10	0.01	0.07	0.00
H6	O3	-0.89	0.80	0.95	-0.24
H5	O4	0.47	0.33	0.44	0.09
H6	O4	-4.27	2.54	2.82	-1.50
	Average:	*-0.54*	*0.40*	*0.53*	*-0.13*
	Std. dev.:	*2.13*	*0.80*	*0.87*	*0.52*

Part b		Averaged absolute error in $\Delta V_{\text{cl}}^{\text{A,B}}$			
	Average:	*1.45*	*0.45*	*0.57*	*0.27*
	Std. dev.:	*1.58*	*0.77*	*0.85*	*0.46*

Table S109. Relative to the CCSD/BBC1 data, errors (part a) and averaged absolute errors (part b) in $\Delta V_{XC}^{A,B}$ (kcal mol^{-1}) obtained for the **Lin → LEC** structural change at the indicated levels of theory.

Part a		**HF**	**B3LYP**	**B3LYP-GD3**	**MP2/Müller**
Atom A	**Atom B**	Error in $\Delta V_{XC}^{A,B}$			
C2	C1	-0.14	-0.61	-0.57	-0.57
O4	C1	-0.07	0.61	0.64	0.59
H7	C1	0.04	0.04	0.03	0.03
H9	C1	0.16	0.19	0.15	0.08
O3	C2	0.72	0.33	0.42	0.55
H8	C2	0.49	0.37	0.31	0.36
H10	C2	0.12	0.33	0.33	0.25
H6	O3	0.26	0.56	0.49	0.43
H5	O4	0.92	1.01	0.98	1.00
H6	O4	1.30	0.34	0.39	-0.17
	Average:	*0.38*	*0.32*	*0.32*	*0.25*
	Std. dev.:	*0.47*	*0.42*	*0.41*	*0.44*

Part b		Averaged absolute error in $\Delta V_{XC}^{A,B}$			
	Average:	*0.42*	*0.44*	*0.43*	*0.40*
	Std. dev.:	*0.43*	*0.27*	*0.27*	*0.29*

Table S110. Relative to the CCSD/BBC1 data, errors (part a) and averaged absolute errors (part b) in $\Delta E_{int}^{A,B}$ (kcal mol^{-1}) obtained for the **Lin → Ecl** structural change at the indicated levels of theory.

Part a		**HF**	**B3LYP**	**B3LYP-GD3**	**MP2/Müller**
Atom A	**Atom B**	Error in $\Delta E_{int}^{A,B}$			
C2	C1	2.61	0.43	0.29	0.56
O4	C1	-6.77	-2.10	-1.66	-0.51
H7	C1	-2.12	0.24	0.25	0.07
H9	C1	-2.11	0.22	0.24	0.06
O3	C2	-6.67	-2.08	-1.65	-0.54
H8	C2	-2.12	0.25	0.26	0.09
H10	C2	-2.11	0.22	0.25	0.07
H6	O3	-1.00	-0.78	-0.73	0.07
H5	O4	-1.00	-0.79	-0.73	0.08
O4	O3	9.97	0.98	0.76	0.96
	Average:	*-1.13*	*-0.34*	*-0.27*	*0.09*
	Std. dev.:	*4.76*	*1.06*	*0.86*	*0.44*

Part b		Averaged absolute error in $\Delta E_{int}^{A,B}$			
	Average:	*3.65*	*0.81*	*0.68*	*0.30*
	Std. dev.:	*3.04*	*0.73*	*0.56*	*0.32*

Table S111. Relative to the CCSD/BBC1 data, errors (part a) and averaged absolute errors (part b) in $\Delta V_{\mathrm{cl}}^{\mathrm{A,B}}$ (kcal mol^{-1}) obtained for the **Lin** → **Ecl** structural change at the indicated levels of theory.

Part a		**HF**	**B3LYP**	**B3LYP-GD3**	**MP2/Müller**
Atom A	**Atom B**	Error in $\Delta V_{\mathrm{cl}}^{\mathrm{A,B}}$			
C2	C1	3.18	0.37	0.05	0.29
O4	C1	-6.34	-1.43	-1.02	-0.51
H7	C1	-2.38	0.52	0.55	0.28
H9	C1	-2.38	0.52	0.55	0.28
O3	C2	-6.17	-1.37	-0.96	-0.51
H8	C2	-2.37	0.52	0.54	0.27
H10	C2	-2.37	0.52	0.55	0.28
H6	O3	-0.75	-0.75	-0.71	0.20
H5	O4	-0.75	-0.76	-0.72	0.21
H6	O4	6.99	-1.09	-1.32	-0.05
	Average:	*-1.34*	*-0.29*	*-0.25*	*0.07*
	Std. dev.:	*3.99*	*0.86*	*0.77*	*0.32*

Part b		Averaged absolute error in $\Delta V_{\mathrm{cl}}^{\mathrm{A,B}}$			
	Average:	*3.37*	*0.78*	*0.70*	*0.29*
	Std. dev.:	*2.30*	*0.38*	*0.35*	*0.14*

Table S112. Relative to the CCSD/BBC1 data, errors (part a) and averaged absolute errors (part b) in $\Delta V_{\mathrm{XC}}^{\mathrm{A,B}}$ (kcal mol^{-1}) obtained for the **Lin** → **Ecl** structural change at the indicated levels of theory.

Part a		**HF**	**B3LYP**	**B3LYP-GD3**	**MP2/Müller**
Atom A	**Atom B**	Error in $\Delta V_{\mathrm{XC}}^{\mathrm{A,B}}$			
C2	C1	-0.57	0.06	0.24	0.28
O4	C1	-0.43	-0.67	-0.64	0.00
H7	C1	0.26	-0.28	-0.30	-0.20
H9	C1	0.27	-0.30	-0.30	-0.22
O3	C2	-0.50	-0.71	-0.68	-0.04
H8	C2	0.25	-0.27	-0.28	-0.19
H10	C2	0.27	-0.30	-0.30	-0.21
H6	O3	-0.25	-0.03	-0.01	-0.13
H5	O4	-0.25	-0.03	-0.02	-0.13
H6	O4	2.98	2.07	2.08	1.01
	Average:	*0.20*	*-0.05*	*-0.02*	*0.02*
	Std. dev.:	*1.03*	*0.78*	*0.79*	*0.38*

Part b		Averaged absolute error in $\Delta V_{\mathrm{XC}}^{\mathrm{A,B}}$			
	Average:	*0.60*	*0.47*	*0.49*	*0.24*
	Std. dev.:	*0.84*	*0.61*	*0.60*	*0.28*

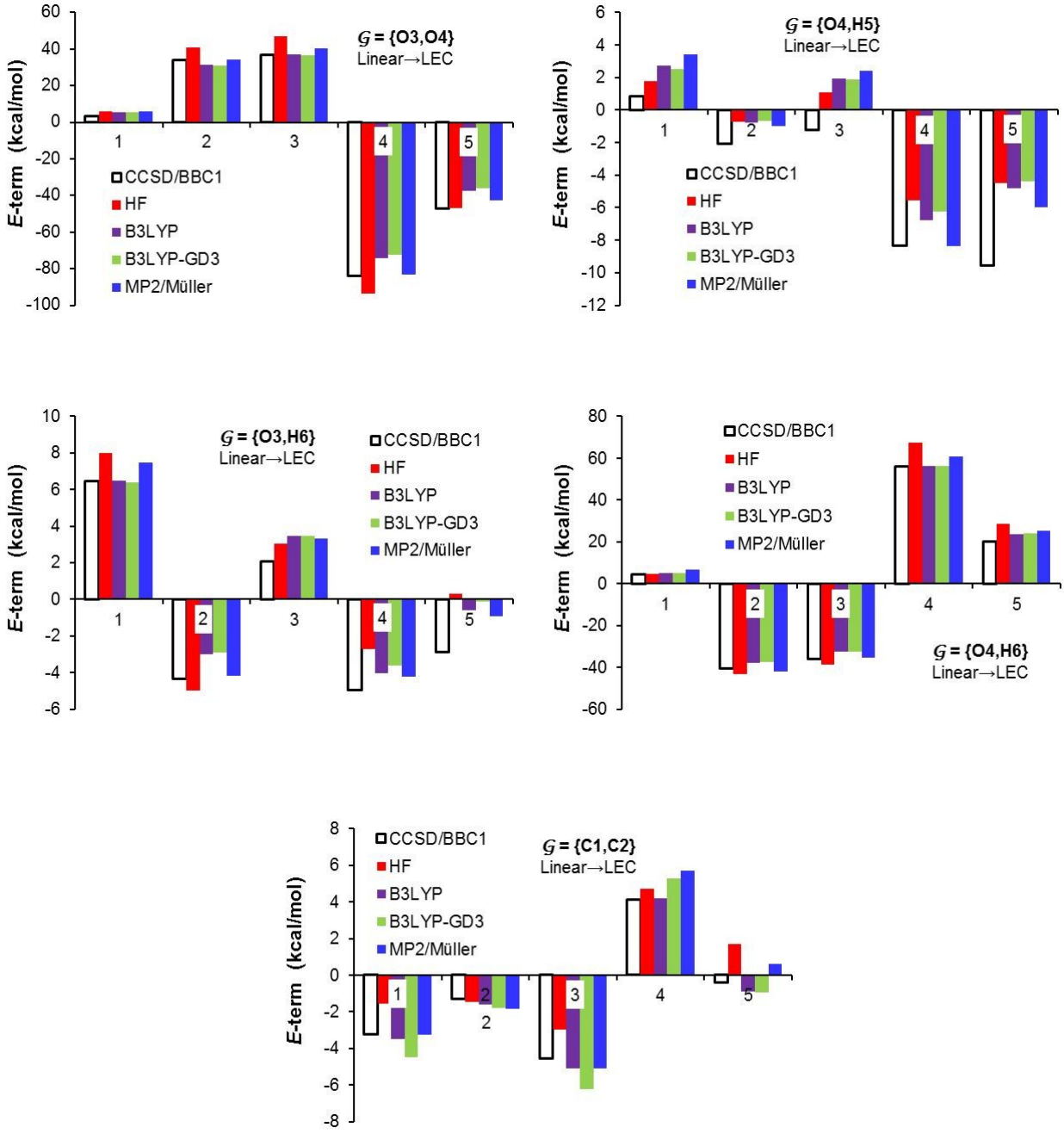

Figure S13. FAMSEC energy terms ΔE^{G}_{self} (**1**), ΔE^{G}_{int} (**2**), $E^{G}_{attr\text{-}loc}$ (**3**), $\Delta E^{G,H}_{int}$ (**4**) and $E^{G}_{attr\text{-}mol}$ (**5**) computed for the specified molecular 2-atom fragments G on the **Lin → LEC** structural change of glycol at the indicated levels of theory. Data obtained at the CCSD/BBC1 level is shown as a reference (for comparison).

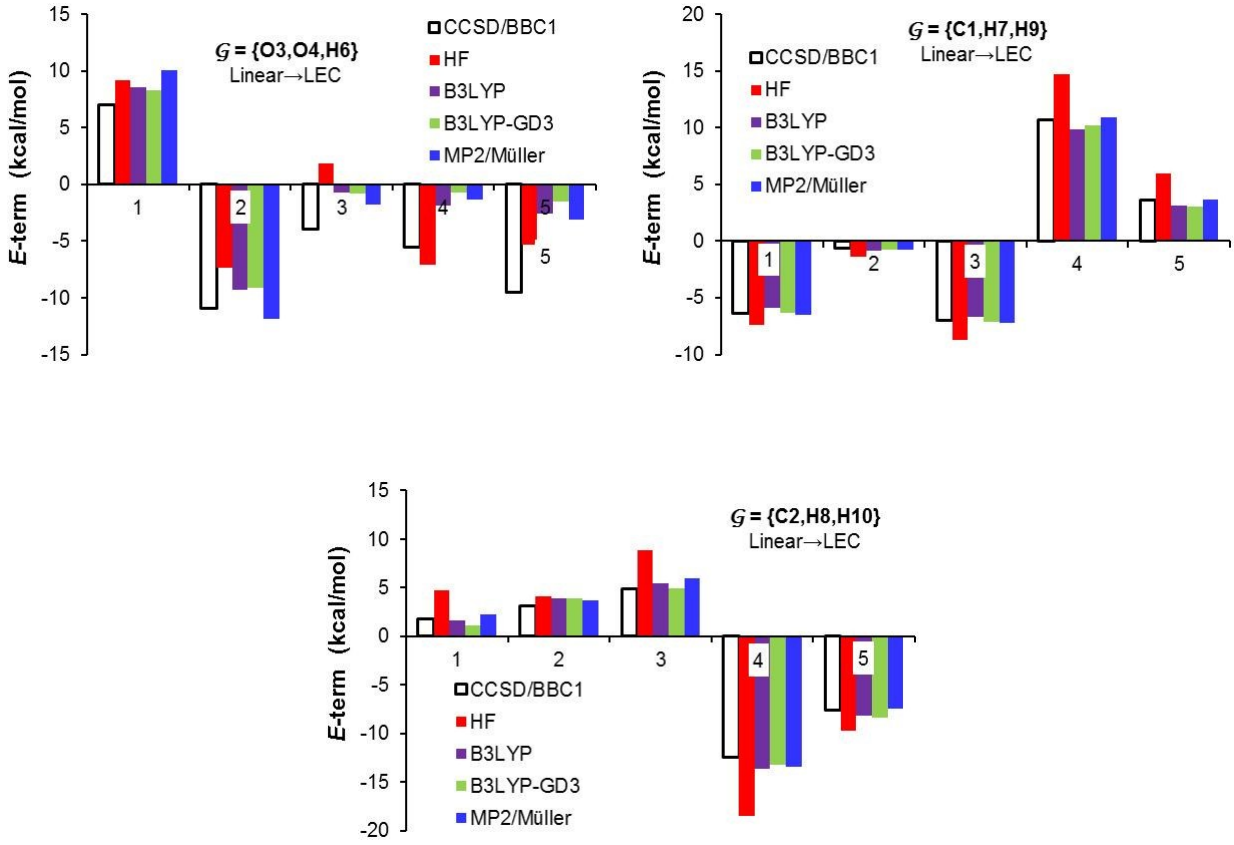

Figure S14. FAMSEC energy terms $\Delta E^{\mathrm{G}}_{\mathrm{self}}$ (**1**), $\Delta E^{\mathrm{G}}_{\mathrm{int}}$ (**2**), $E^{\mathrm{G}}_{\mathrm{attr\text{-}loc}}$ (**3**), $\Delta E^{\mathrm{G,H}}_{\mathrm{int}}$ (**4**) and $E^{\mathrm{G}}_{\mathrm{attr\text{-}mol}}$ (**5**) computed for the specified molecular 3-atom fragments G on the **Lin → LEC** structural change of glycol at the indicated levels of theory. Data obtained at the CCSD/BBC1 level is shown as a reference (for comparison).

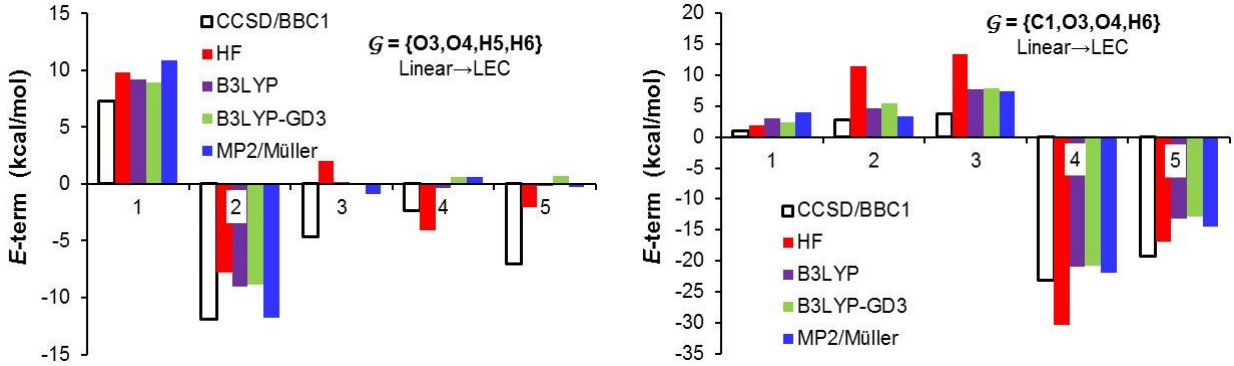

Figure S15. FAMSEC energy terms $\Delta E^{\mathrm{G}}_{\mathrm{self}}$ (**1**), $\Delta E^{\mathrm{G}}_{\mathrm{int}}$ (**2**), $E^{\mathrm{G}}_{\mathrm{attr\text{-}loc}}$ (**3**), $\Delta E^{\mathrm{G,H}}_{\mathrm{int}}$ (**4**) and $E^{\mathrm{G}}_{\mathrm{attr\text{-}mol}}$ (**5**) computed for the specified molecular 4-atom fragments G on the **Lin → LEC** structural change of glycol at the indicated levels of theory. Data obtained at the CCSD/BBC1 level is shown as a reference (for comparison).

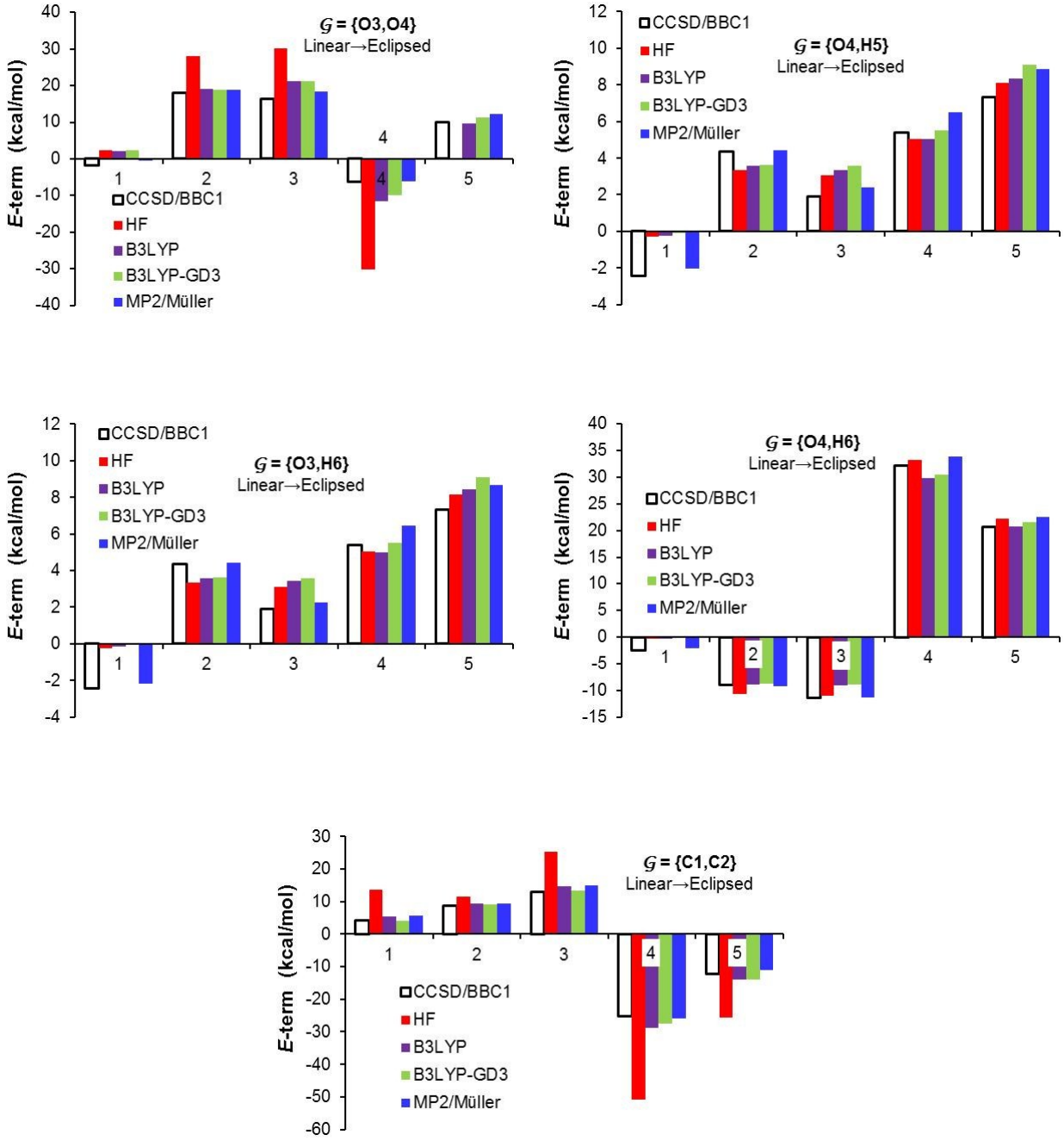

Figure S16. Energy terms $\Delta E^{\mathsf{G}}_{\text{self}}$ (**1**), $\Delta E^{\mathsf{G}}_{\text{int}}$ (**2**), $E^{\mathsf{G}}_{\text{attr-loc}}$ (**3**), $\Delta E^{\mathsf{G,H}}_{\text{int}}$ (**4**) and $E^{\mathsf{G}}_{\text{attr-mol}}$ (**5**) computed for the specified molecular 2-atom fragments G on the **Lin → Ecl** structural change of glycol at the indicated levels of theory. Data obtained at the CCSD/BBC1 level is shown as a reference (for comparison).

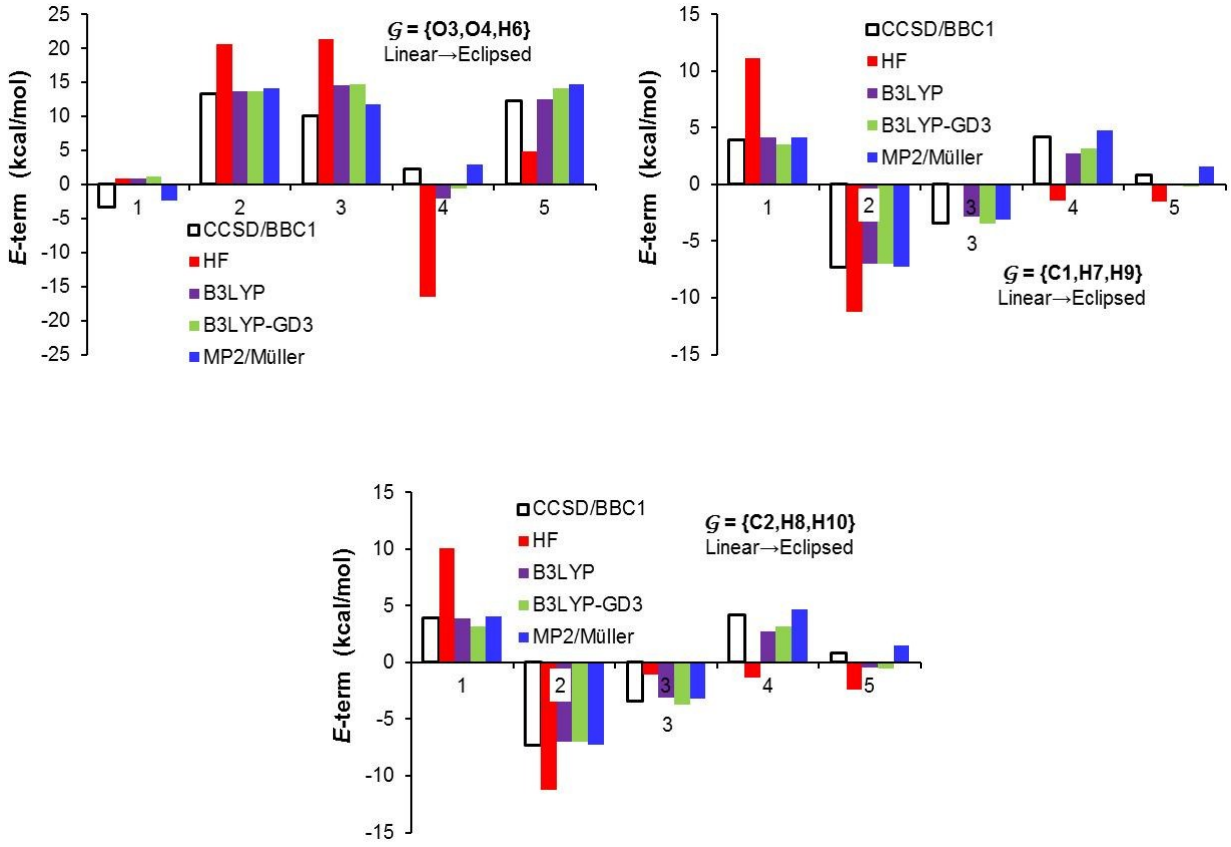

Figure S17. FAMSEC energy terms $\Delta E^{\mathrm{G}}_{\mathrm{self}}$ (**1**), $\Delta E^{\mathrm{G}}_{\mathrm{int}}$ (**2**), $E^{\mathrm{G}}_{\mathrm{attr\text{-}loc}}$ (**3**), $\Delta E^{\mathrm{G,H}}_{\mathrm{int}}$ (**4**) and $E^{\mathrm{G}}_{\mathrm{attr\text{-}mol}}$ (**5**) computed for the specified molecular 3-atom fragments G on the **Lin → Ecl** structural change of glycol at the indicated levels of theory. Data obtained at the CCSD/BBC1 level is shown as a reference (for comparison).

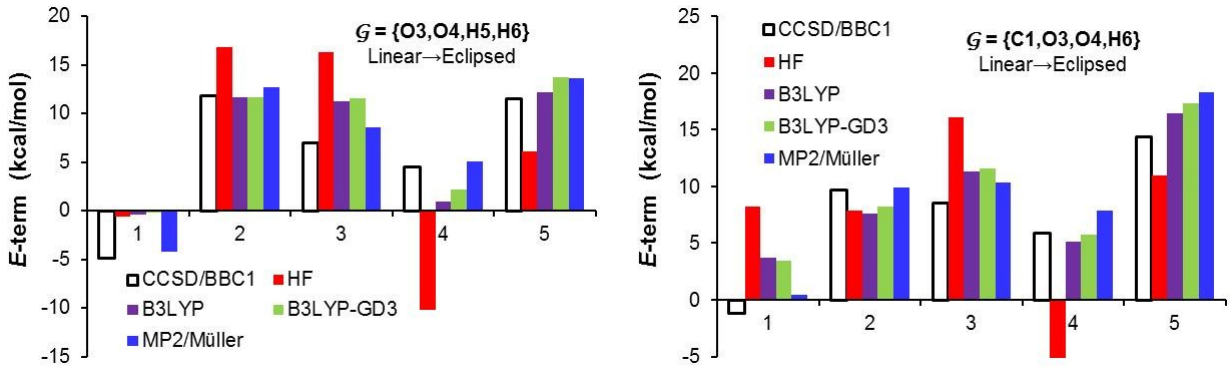

Figure S18. FAMSEC energy terms $\Delta E^{\mathrm{G}}_{\mathrm{self}}$ (**1**), $\Delta E^{\mathrm{G}}_{\mathrm{int}}$ (**2**), $E^{\mathrm{G}}_{\mathrm{attr\text{-}loc}}$ (**3**), $\Delta E^{\mathrm{G,H}}_{\mathrm{int}}$ (**4**) and $E^{\mathrm{G}}_{\mathrm{attr\text{-}mol}}$ (**5**) computed for the specified molecular 4-atom fragments G on the **Lin → Ecl** structural change of glycol at the indicated levels of theory. Data obtained at the CCSD/BBC1 level is shown as a reference (for comparison).

Table S113. FAMSEC descriptors (values in kcal mol^{-1}) computed at the indicated levels of theory for specified and meaningful 2-atom fragments G of glycol (PART 1–5) on the **Lin** → **LEC** structural change.

PART 1	**G = {O3,O4}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	3.13	33.90	37.03	-84.18	-47.14
HF	5.86	40.91	46.77	-93.59	-46.82
B3LYP	5.57	31.46	37.03	-74.35	-37.31
B3LYP-GD3	5.40	31.18	36.59	-72.55	-35.96
MP2/Müller	6.14	34.46	40.60	-83.06	-42.47
Average:	*5.2*	*34.4*	*39.6*	*-81.5*	*-41.9*
Std. dev.:	*1.2*	*3.9*	*4.3*	*8.5*	*5.2*
	Excluding HF data				
Average:	*5.1*	*32.8*	*37.8*	*-78.5*	*-40.7*
Std. dev.:	*1.3*	*1.7*	*1.9*	*5.9*	*5.1*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***4.7***	***32.2***	***36.9***	***-77.0***	***-40.1***
Std. dev.:	***1.4***	***1.5***	***0.3***	***6.3***	***6.1***

PART 2	**G = {O4,H5}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	0.85	-2.09	-1.24	-8.33	-9.58
HF	1.77	-0.70	1.08	-5.57	-4.49
B3LYP	2.72	-0.75	1.96	-6.76	-4.80
B3LYP-GD3	2.54	-0.68	1.87	-6.22	-4.36
MP2/Müller	3.40	-1.01	2.39	-8.37	-5.98
Average:	2.3	-1.0	1.2	-7.1	-5.8
Std. dev.:	1.0	0.6	1.5	1.3	2.2
	Excluding HF data				
Average:	*2.4*	*-1.1*	*1.2*	*-7.4*	*-6.2*
Std. dev.:	*1.1*	*0.7*	*1.7*	*1.1*	*2.4*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***2.0***	***-1.2***	***0.9***	***-7.1***	***-6.2***
Std. dev.:	***1.0***	***0.8***	***1.8***	***1.1***	***2.9***

PART 3	**G = {O3,H6}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	6.44	-4.36	2.08	-4.98	-2.89
HF	8.00	-4.97	3.03	-2.73	0.31
B3LYP	6.47	-3.00	3.47	-4.06	-0.59
B3LYP-GD3	6.39	-2.93	3.46	-3.59	-0.14
MP2/Müller	7.47	-4.17	3.30	-4.23	-0.92
Average:	*7.0*	*-3.9*	*3.1*	*-3.9*	*-0.8*
Std. dev.:	*0.7*	*0.9*	*0.6*	*0.8*	*1.2*
	Excluding HF data				
Average:	*6.7*	*-3.6*	*3.1*	*-4.2*	*-1.1*
Std. dev.:	*0.5*	*0.8*	*0.7*	*0.6*	*1.2*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***6.4***	***-3.4***	***3.0***	***-4.2***	***-1.2***
Std. dev.:	***0.0***	***0.8***	***0.8***	***0.7***	***1.5***

PART 4	**G = {O4,H6}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	4.47	-40.52	-36.05	56.11	20.06
HF	4.56	-43.32	-38.76	67.33	28.57
B3LYP	5.10	-37.73	-32.64	56.22	23.58
B3LYP-GD3	4.91	-37.41	-32.50	56.36	23.87
MP2/Müller	6.56	-42.19	-35.63	60.87	25.24
Average:	*5.1*	*-40.2*	*-35.1*	*59.4*	*24.3*
Std. dev.:	*0.8*	*2.6*	*2.6*	*4.9*	*3.1*
	Excluding HF data				
Average:	*5.3*	*-39.5*	*-34.2*	*57.4*	*23.2*
Std. dev.:	*0.9*	*2.3*	*1.9*	*2.3*	*2.2*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***4.8***	***-38.6***	***-33.7***	***56.2***	***22.5***
Std. dev.:	***0.3***	***1.7***	***2.0***	***0.1***	***2.1***

PART 5	G = {C1,C2}				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	-3.24	-1.32	-4.56	4.15	-0.41
HF	-1.55	-1.44	-3.00	4.70	1.71
B3LYP	-3.50	-1.59	-5.09	4.21	-0.88
B3LYP-GD3	-4.47	-1.78	-6.25	5.30	-0.94
MP2/Müller	-3.27	-1.84	-5.11	5.71	0.60
Average:	*-3.2*	*-1.6*	*-4.8*	*4.8*	*0.0*
Std. dev.:	*1.1*	*0.2*	*1.2*	*0.7*	*1.1*
	Excluding HF data				
Average:	*-3.6*	*-1.6*	*-5.3*	*4.8*	*-0.4*
Std. dev.:	*0.6*	*0.2*	*0.7*	*0.8*	*0.7*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***-3.7***	***-1.6***	***-5.3***	***4.6***	***-0.7***
Std. dev.:	***0.6***	***0.2***	***0.9***	***0.6***	***0.3***

Table S114. FAMSEC descriptors (values in kcal mol^{-1}) computed at the indicated levels of theory for specified and meaningful 3-atom fragments G of glycol (PART 1–3) on the **Lin** → **LEC** structural change.

PART 1	G = {O3,O4,H6}				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	7.02	-10.97	-3.95	-5.55	-9.50
HF	9.21	-7.38	1.83	-7.11	-5.28
B3LYP	8.57	-9.28	-0.71	-1.82	-2.53
B3LYP-GD3	8.35	-9.16	-0.80	-0.73	-1.53
MP2/Müller	10.08	-11.89	-1.81	-1.32	-3.13
Average:	*8.6*	*-9.7*	*-1.1*	*-3.3*	*-4.4*
Std. dev.:	*1.1*	*1.8*	*2.1*	*2.8*	*3.2*
	Excluding HF data				
Average:	*8.5*	*-10.3*	*-1.8*	*-2.4*	*-4.2*
Std. dev.:	*1.3*	*1.3*	*1.5*	*2.2*	*3.6*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***8.0***	***-9.8***	***-1.8***	***-2.7***	***-4.5***
Std. dev.:	***0.8***	***1.0***	***1.8***	***2.5***	***4.3***

PART 2	**G = {C1,H7,H9}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	-6.37	-0.63	-7.00	10.67	3.66
HF	-7.38	-1.36	-8.73	14.71	5.98
B3LYP	-5.87	-0.83	-6.71	9.87	3.16
B3LYP-GD3	-6.34	-0.79	-7.13	10.17	3.05
MP2/Müller	-6.47	-0.71	-7.19	10.89	3.70
Average:	*-6.5*	*-0.9*	*-7.4*	*11.3*	*3.9*
Std. dev.:	*0.5*	*0.3*	*0.8*	*2.0*	*1.2*
	Excluding HF data				
Average:	*-6.3*	*-0.7*	*-7.0*	*10.4*	*3.4*
Std. dev.:	*0.3*	*0.1*	*0.2*	*0.5*	*0.3*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***-6.2***	***-0.8***	***-6.9***	***10.2***	***3.3***
Std. dev.:	***0.3***	***0.1***	***0.2***	***0.4***	***0.3***

PART 3	**G = {C2,H8,H10}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	1.74	3.11	4.85	-12.50	-7.65
HF	4.73	4.10	8.84	-18.55	-9.71
B3LYP	1.61	3.86	5.47	-13.61	-8.14
B3LYP-GD3	1.07	3.87	4.93	-13.27	-8.34
MP2/Müller	2.26	3.72	5.97	-13.43	-7.46
Average:	*2.3*	*3.7*	*6.0*	*-14.3*	*-8.3*
Std. dev.:	*1.4*	*0.4*	*1.6*	*2.4*	*0.9*
	Excluding HF data				
Average:	*1.7*	*3.6*	*5.3*	*-13.2*	*-7.9*
Std. dev.:	*0.5*	*0.4*	*0.5*	*0.5*	*0.4*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***1.5***	***3.6***	***5.1***	***-13.1***	***-8.0***
Std. dev.:	***0.4***	***0.4***	***0.3***	***0.6***	***0.4***

Table S115. FAMSEC descriptors (values in kcal mol^{-1}) computed at the indicated levels of theory for specified and meaningful 4-atom fragments G of glycol (PART 1–2) on the **Lin** → **LEC** structural change.

PART 1	**G = {O3,O4,H5,H6}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	7.29	-11.92	-4.63	-2.37	-7.00
HF	9.78	-7.78	1.99	-4.06	-2.07
B3LYP	9.19	-9.01	0.17	-0.31	-0.14
B3LYP-GD3	8.93	-8.81	0.12	0.58	0.71
MP2/Müller	10.87	-11.78	-0.91	0.62	-0.29
Average:	*9.2*	*-9.9*	*-0.6*	*-1.1*	*-1.8*
Std. dev.:	*1.3*	*1.9*	*2.5*	*2.0*	*3.1*
	Excluding HF data				
Average:	*9.1*	*-10.4*	*-1.3*	*-0.4*	*-1.7*
Std. dev.:	*1.5*	*1.7*	*2.3*	*1.4*	*3.6*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***8.5***	***-9.9***	***-1.4***	***-0.7***	***-2.1***
Std. dev.:	***1.0***	***1.7***	***2.8***	***1.5***	***4.2***

PART 2	**G = {C1,O3,O4,H6}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	1.1	2.7	3.8	-23.1	-19.3
HF	2.0	11.5	13.5	-30.4	-16.9
B3LYP	3.1	4.7	7.8	-21.0	-13.2
B3LYP-GD3	2.4	5.4	7.9	-20.8	-12.9
MP2/Müller	4.1	3.4	7.4	-21.9	-14.4
Average:	*2.5*	*5.6*	*8.1*	*-23.4*	*-15.3*
Std. dev.:	*1.1*	*3.5*	*3.5*	*4.0*	*2.7*
	Excluding HF data				
Average:	*2.7*	*4.1*	*6.7*	*-21.7*	*-14.9*
Std. dev.:	*1.3*	*1.2*	*2.0*	*1.1*	*3.0*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***2.2***	***4.3***	***6.5***	***-21.6***	***-15.1***
Std. dev.:	***1.0***	***1.4***	***2.3***	***1.3***	***3.6***

Table S116. FAMSEC descriptors (values in kcal mol^{-1}) computed at the indicated levels of theory for specified and meaningful 2-atom fragments G of glycol (PART 1–5) on the **Lin** → **Ecl** structural change.

PART 1	**G = {O3,O4}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	-1.68	18.02	16.33	-6.34	10.00
HF	2.25	27.99	30.24	-30.21	0.03
B3LYP	2.20	19.02	21.23	-11.61	9.62
B3LYP-GD3	2.42	18.83	21.24	-9.91	11.34
MP2/Müller	-0.59	18.98	18.39	-6.08	12.31
Average:	*0.9*	*20.6*	*21.5*	*-12.8*	*8.7*
Std. dev.:	*1.9*	*4.2*	*5.3*	*10.0*	*4.9*
	Excluding HF data				
Average:	*0.6*	*18.7*	*19.3*	*-8.5*	*10.8*
Std. dev.:	*2.0*	*0.5*	*2.4*	*2.7*	*1.2*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***1.0***	***18.6***	***19.6***	***-9.3***	***10.3***
Std. dev.:	***2.3***	***0.5***	***2.8***	***2.7***	***0.9***

PART 2	**G = {O4,H5}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	-2.44	4.36	1.92	5.39	7.30
HF	-0.32	3.35	3.04	5.05	8.09
B3LYP	-0.24	3.58	3.34	5.02	8.35
B3LYP-GD3	-0.09	3.64	3.55	5.53	9.08
MP2/Müller	-2.04	4.44	2.40	6.48	8.88
Average:	*-1.0*	*3.9*	*2.8*	*5.5*	*8.3*
Std. dev.:	*1.1*	*0.5*	*0.7*	*0.6*	*0.7*
	Excluding HF data				
Average:	*-1.2*	*4.0*	*2.8*	*5.6*	*8.4*
Std. dev.:	*1.2*	*0.5*	*0.8*	*0.6*	*0.8*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***-0.9***	***3.9***	***2.9***	***5.3***	***8.2***
Std. dev.:	***1.3***	***0.4***	***0.9***	***0.3***	***0.9***

PART 3	**G = {O3,H6}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	-2.44	4.36	1.92	5.39	7.30
HF	-0.24	3.36	3.12	5.02	8.15
B3LYP	-0.17	3.59	3.42	5.01	8.43
B3LYP-GD3	-0.07	3.64	3.57	5.52	9.09
MP2/Müller	-2.18	4.42	2.24	6.45	8.69
Average:	*-1.0*	*3.9*	*2.9*	*5.5*	*8.3*
Std. dev.:	*1.2*	*0.5*	*0.7*	*0.6*	*0.7*
	Excluding HF data				
Average:	*-1.2*	*4.0*	*2.8*	*5.6*	*8.4*
Std. dev.:	*1.3*	*0.4*	*0.8*	*0.6*	*0.8*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***-0.9***	***3.9***	***3.0***	***5.3***	***8.3***
Std. dev.:	***1.3***	***0.4***	***0.9***	***0.3***	***0.9***

PART 4	**G = {O4,H6}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	-2.44	-9.06	-11.50	32.22	20.72
HF	-0.32	-10.77	-11.09	33.30	22.21
B3LYP	-0.24	-8.87	-9.11	29.93	20.82
B3LYP-GD3	-0.09	-8.83	-8.92	30.49	21.57
MP2/Müller	-2.04	-9.23	-11.27	33.84	22.56
Average:	*-1.0*	*-9.4*	*-10.4*	*32.0*	*21.6*
Std. dev.:	*1.1*	*0.8*	*1.3*	*1.7*	*0.8*
	Excluding HF data				
Average:	*-1.2*	*-9.0*	*-10.2*	*31.6*	*21.4*
Std. dev.:	*1.2*	*0.2*	*1.4*	*1.8*	*0.9*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***-0.9***	***-8.9***	***-9.8***	***30.9***	***21.0***
Std. dev.:	***1.3***	***0.1***	***1.4***	***1.2***	***0.5***

PART 5			**G = {C1,C2}**		
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	4.13	8.88	13.01	-25.11	-12.10
HF	13.76	11.49	25.25	-50.92	-25.67
B3LYP	5.37	9.32	14.69	-28.73	-14.04
B3LYP-GD3	4.21	9.20	13.41	-27.48	-14.08
MP2/Müller	5.62	9.44	15.07	-25.97	-10.90
Average:	*6.6*	*9.7*	*16.3*	*-31.6*	*-15.4*
Std. dev.:	*4.0*	*1.0*	*5.1*	*10.9*	*5.9*
			Excluding HF data		
Average:	*4.8*	*9.2*	*14.0*	*-26.8*	*-12.8*
Std. dev.:	*0.8*	*0.2*	*1.0*	*1.6*	*1.6*
			Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data		
Average:	***4.6***	***9.1***	***13.7***	***-27.1***	***-13.4***
Std. dev.:	***0.7***	***0.2***	***0.9***	***1.8***	***1.1***

Table S117. FAMSEC descriptors (values in kcal mol^{-1}) computed at the indicated levels of theory for specified and meaningful 3-atom fragments G of glycol (PART 1–3) on the **Lin** → **Ecl** structural change.

PART 1			**G = {O3,O4,H6}**		
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	-3.28	13.31	10.03	2.32	12.36
HF	0.85	20.59	21.43	-16.53	4.90
B3LYP	0.90	13.74	14.64	-2.07	12.57
B3LYP-GD3	1.13	13.64	14.77	-0.59	14.18
MP2/Müller	-2.41	14.17	11.76	2.93	14.69
Average:	*-0.6*	*15.1*	*14.5*	*-2.8*	*11.7*
Std. dev.:	*2.1*	*3.1*	*4.3*	*8.0*	*4.0*
			Excluding HF data		
Average:	*-0.9*	*13.7*	*12.8*	*0.6*	*13.4*
Std. dev.:	*2.3*	*0.4*	*2.3*	*2.4*	*1.2*
			Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data		
Average:	***-0.4***	***13.6***	***13.1***	***-0.1***	***13.0***
Std. dev.:	***2.5***	***0.2***	***2.7***	***2.2***	***1.0***

PART 2	**G = {C1,H7,H9}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	3.89	-7.30	-3.41	4.22	0.82
HF	11.13	-11.20	-0.07	-1.40	-1.46
B3LYP	4.20	-7.01	-2.81	2.70	-0.12
B3LYP-GD3	3.58	-6.99	-3.42	3.20	-0.21
MP2/Müller	4.16	-7.29	-3.14	4.74	1.60
Average:	*5.4*	*-8.0*	*-2.6*	*2.7*	*0.1*
Std. dev.:	*3.2*	*1.8*	*1.4*	*2.4*	*1.2*
	Excluding HF data				
Average:	*4.0*	*-7.1*	*-3.2*	*3.7*	*0.5*
Std. dev.:	*0.3*	*0.2*	*0.3*	*0.9*	*0.9*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***3.9***	***-7.1***	***-3.2***	***3.4***	***0.2***
Std. dev.:	***0.3***	***0.2***	***0.3***	***0.8***	***0.6***

PART 3	**G = {C2,H8,H10}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	3.89	-7.30	-3.41	4.22	0.82
HF	10.12	-11.20	-1.08	-1.30	-2.38
B3LYP	3.87	-7.00	-3.12	2.71	-0.41
B3LYP-GD3	3.22	-6.98	-3.76	3.22	-0.54
MP2/Müller	4.05	-7.27	-3.22	4.73	1.51
Average:	*5.0*	*-7.9*	*-2.9*	*2.7*	*-0.2*
Std. dev.:	*2.9*	*1.8*	*1.1*	*2.4*	*1.5*
	Excluding HF data				
Average:	*3.8*	*-7.1*	*-3.4*	*3.7*	*0.3*
Std. dev.:	*0.4*	*0.2*	*0.3*	*0.9*	*1.0*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***3.7***	***-7.1***	***-3.4***	***3.4***	***0.0***
Std. dev.:	***0.4***	***0.2***	***0.3***	***0.8***	***0.8***

Table S118. FAMSEC descriptors (values in kcal mol^{-1}) computed at the indicated levels of theory for specified and meaningful 4-atom fragments G of glycol (PART 1–2) on the **Lin** → **Ecl** structural change.

PART 1	**G = {O3,O4,H5,H6}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	-4.9	11.8	6.9	4.6	11.5
HF	-0.6	16.9	16.3	-10.2	6.1
B3LYP	-0.4	11.7	11.3	0.9	12.2
B3LYP-GD3	-0.2	11.7	11.5	2.2	13.7
MP2/Müller	-4.2	12.8	8.5	5.1	13.7
Average:	*-2.0*	*13.0*	*10.9*	*0.5*	*11.4*
Std. dev.:	*2.3*	*2.2*	*3.6*	*6.2*	*3.1*
	Excluding HF data				
Average:	*-2.4*	*12.0*	*9.6*	*3.2*	*12.8*
Std. dev.:	*2.5*	*0.5*	*2.2*	*2.0*	*1.1*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***-1.8***	***11.7***	***9.9***	***2.6***	***12.5***
Std. dev.:	***2.7***	***0.1***	***2.6***	***1.8***	***1.1***

PART 2	**G = {C1,O3,O4,H6}**				
LoT	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
CCSD/BBC1	-1.22	9.71	8.49	5.85	14.34
HF	8.23	7.87	16.10	-5.12	10.98
B3LYP	3.75	7.62	11.37	5.11	16.47
B3LYP-GD3	3.41	8.19	11.60	5.75	17.36
MP2/Müller	0.45	9.91	10.37	7.90	18.27
Average:	*2.9*	*8.7*	*11.6*	*3.9*	*15.5*
Std. dev.:	*3.6*	*1.1*	*2.8*	*5.2*	*2.9*
	Excluding HF data				
Average:	*1.6*	*8.9*	*10.5*	*6.2*	*16.6*
Std. dev.:	*2.4*	*1.1*	*1.4*	*1.2*	*1.7*
	Combined CCSD/BBC1, B3LYP and B3LYP-GD3 data				
Average:	***2.0***	***8.5***	***10.5***	***5.6***	***16.1***
Std. dev.:	***2.8***	***1.1***	***1.7***	***0.4***	***1.5***

Data obtained for the steric clash between O3 and O4 atoms in the **Ecl** conformer is shown in Figures S16-S18 and Tables S116-S118. The data reveals that, except HF, trends and general description obtained at CCSD/BBC1 were reproduced very well. To illustrate this, we combined data obtained at the CCSD/BBC1, B3LYP, B3LYP-GD3 and MP2/Müller levels for 2-atom fragment (G = {O3,O4})

and two 4-atom fragments, G = {C1–O3···O4–H6} and G ={H5–O3···O4–H6}. Former 4-atom fragment resembles the IUPAC recommendation for H-bonds. The steric O3···O4 clash in the **Ecl** conformer consistently resulted in (i) unfavourable change in the inter-fragment interaction energy term, $\Delta E_{\text{int}}^{\text{G}}$, by +18.7±0.5, +8.7±1.1 and +12±0.5 kcal mol^{-1} for 2- and 4-atom fragments, respectively, (ii) locally destabilized fragments with $E_{\text{attr-loc}}^{\text{G}}$ of +19.3±2.4, +10.5±1.4 and +9.6±2.2 kcal mol^{-1} for 2- and 4-atom fragments, respectively, (iii) more favourable environment in the case of 2-atom fragment ($\Delta E_{\text{int}}^{\text{G,H}}$ = –8.5±2.7 kcal mol^{-1}) but less favourable environment in the case of 4-atom fragments with $\Delta E_{\text{int}}^{\text{G,H}}$ of 6.2±1.2 and 3.2±2.0 kcal mol^{-1}, respectively, and (iv) fragments destabilizing the **Ecl** conformer with $E_{\text{attr-mol}}^{\text{G}}$ of +10.8±1.2, 16.6±1.7 and +12.8±1.1 kcal mol^{-1} for 2- and 4-atom fragments, respectively.

Table S119. Relative to the CCSD/BBC1 data, absolute errors in the FAMSEC-defined energy terms ΔE^{G}_{self}, ΔE^{G}_{int}, $E^{G}_{attr\text{-}loc}$, $\Delta E^{G,H}_{int}$, and $E^{G}_{attr\text{-}mol}$ computed for the indicated and meaningful molecular fragments at the HF (part a), B3LYP (part b), B3LYP-GD3 (part c), and MP2/Müller (part d) levels on the **Lin → LEC** and **Lin → Ecl** structural changes of glycol. All values in kcal mol^{-1}.

Part a. Data obtained at the HF level.

Molecular fragment G	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
			Lin → LEC		
{O3,O4}	2.73	7.00	9.74	9.41	0.33
{O4,H5}	0.92	1.40	2.32	2.77	5.09
{O3,H6}	1.56	0.61	0.95	2.25	3.20
{O4,H6}	0.09	2.81	2.72	11.22	8.51
{C1,C2}	1.68	0.12	1.56	0.56	2.12
{O3,O4,H6}	2.19	3.59	5.78	1.55	4.22
{C1,H7,H9}	1.00	0.73	1.73	4.05	2.32
{C2,H8,H10}	2.99	0.99	3.98	6.04	2.06
{O3,O4,H5,H6}	2.48	4.14	6.62	1.69	4.93
{C1,O3,O4,H6}	0.90	8.77	9.67	7.29	2.38
Avr.:	*1.7*	*3.0*	*4.5*	*4.7*	*3.5*
Std. dev.:	*0.9*	*2.9*	*3.3*	*3.6*	*2.3*
			Lin → Ecl		
{O3,O4}	3.93	9.98	13.91	23.87	9.97
{O4,H5}	2.12	1.00	1.12	0.34	0.78
{O3,H6}	2.20	0.99	1.20	0.36	0.84
{O4,H6}	2.12	1.71	0.41	1.08	1.49
{C1,C2}	9.63	2.61	12.24	25.81	13.57
{O3,O4,H6}	4.13	7.27	11.40	18.85	7.45
{C1,H7,H9}	7.24	3.90	3.34	5.62	2.28
{C2,H8,H10}	6.23	3.90	2.33	5.53	3.20
{O3,O4,H5,H6}	4.32	5.04	9.36	14.77	5.41
{C1,O3,O4,H6}	9.45	1.84	7.61	10.97	3.36
Avr.:	*5.1*	*3.8*	*6.3*	*10.7*	*4.8*
Std. dev.:	*2.9*	*2.9*	*5.2*	*9.7*	*4.3*
***Overall Avr.*:**	***3.4***	***3.4***	***5.4***	***7.7***	***4.2***
***Overall Std. dev.*:**	***2.7***	***2.9***	***4.3***	***7.8***	***3.4***
Grand total Avr. for all energy terms:			**4.8**		
Grand total Std. dev. for all energy terms:			**4.8**		

Part b. Data obtained at the B3LYP level.

Molecular fragment G	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
			Lin → LEC		
{O3,O4}	2.45	2.45	0.00	9.83	9.83
{O4,H5}	1.86	1.34	3.20	1.58	4.78
{O3,H6}	0.03	1.36	1.38	0.91	2.30
{O4,H6}	0.63	2.78	3.41	0.11	3.52
{C1,C2}	0.26	0.27	0.54	0.07	0.47
{O3,O4,H6}	1.55	1.70	3.25	3.73	6.98
{C1,H7,H9}	0.50	0.20	0.30	0.80	0.50
{C2,H8,H10}	0.13	0.75	0.62	1.11	0.49
{O3,O4,H5,H6}	1.89	2.91	4.80	2.06	6.86
{C1,O3,O4,H6}	2.02	1.98	4.01	2.08	6.08
Avr.:	*1.1*	*1.6*	*2.2*	*2.2*	*4.2*
Std. dev.:	*0.9*	*1.0*	*1.8*	*2.9*	*3.3*
			Lin → Ecl		
{O3,O4}	3.89	1.00	4.89	5.27	0.38
{O4,H5}	2.20	0.78	1.42	0.37	1.05
{O3,H6}	2.27	0.77	1.50	0.38	1.13
{O4,H6}	2.20	0.19	2.39	2.29	0.10
{C1,C2}	1.24	0.44	1.68	3.61	1.93
{O3,O4,H6}	4.18	0.43	4.61	4.39	0.21
{C1,H7,H9}	0.30	0.29	0.59	1.52	0.93
{C2,H8,H10}	0.02	0.30	0.28	1.51	1.23
{O3,O4,H5,H6}	4.47	0.12	4.36	3.62	0.74
{C1,O3,O4,H6}	4.96	2.09	2.87	0.74	2.13
Avr.:	*2.6*	*0.6*	*2.5*	*2.4*	*1.0*
Std. dev.:	*1.7*	*0.6*	*1.7*	*1.8*	*0.7*
***Overall Avr.*:**	***1.9***	***1.1***	***2.3***	***2.3***	***2.6***
***Overall Std. dev.*:**	***1.5***	***0.9***	***1.7***	***2.3***	***2.8***
Grand total Avr. for all energy terms:			**2.0**		
Grand total Std. dev. for all energy terms:			**2.0**		

Part c. Data obtained at the B3LYP-GD3 level.

Molecular fragment G	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
			Lin → LEC		
{O3,O4}	2.28	2.72	0.45	11.63	11.18
{O4,H5}	1.69	1.41	3.11	2.11	5.22
{O3,H6}	0.05	1.43	1.38	1.38	2.76
{O4,H6}	0.44	3.11	3.55	0.26	3.81
{C1,C2}	1.23	0.46	1.69	1.15	0.53
{O3,O4,H6}	1.33	1.81	3.15	4.82	7.97
{C1,H7,H9}	0.04	0.16	0.12	0.49	0.61
{C2,H8,H10}	0.67	0.75	0.08	0.77	0.69
{O3,O4,H5,H6}	1.64	3.11	4.75	2.95	7.70
{C1,O3,O4,H6}	1.36	2.70	4.06	2.34	6.40
Avr.:	*1.1*	*1.8*	*2.2*	*2.8*	*4.7*
Std. dev.:	*0.7*	*1.1*	*1.7*	*3.4*	*3.6*
			Lin → Ecl		
{O3,O4}	4.10	0.81	4.91	3.57	1.34
{O4,H5}	2.35	0.72	1.63	0.14	1.78
{O3,H6}	2.37	0.72	1.65	0.13	1.78
{O4,H6}	2.35	0.23	2.58	1.73	0.85
{C1,C2}	0.08	0.32	0.40	2.37	1.97
{O3,O4,H6}	4.41	0.33	4.74	2.91	1.82
{C1,H7,H9}	0.32	0.31	0.01	1.02	1.03
{C2,H8,H10}	0.67	0.32	0.36	1.01	1.36
{O3,O4,H5,H6}	4.72	0.11	4.61	2.37	2.24
{C1,O3,O4,H6}	4.63	1.52	3.11	0.10	3.01
Avr.:	*2.6*	*0.5*	*2.4*	*1.5*	*1.7*
Std. dev.:	*1.8*	*0.4*	*1.9*	*1.2*	*0.6*
Overall Avr.:	***1.8***	***1.2***	***2.3***	***2.2***	***3.2***
Overall Std. dev.:	***1.6***	***1.0***	***1.8***	***2.6***	***3.0***
Grand total Avr. for all energy terms:			**2.1**		
Grand total Std. dev. for all energy terms:			**2.2**		

Part d. Data obtained from the MP2/Müller combination.

Molecular fragment G	ΔE^{G}_{self}	ΔE^{G}_{int}	$E^{G}_{attr\text{-}loc}$	$\Delta E^{G,H}_{int}$	$E^{G}_{attr\text{-}mol}$
			Lin → LEC		
{O3,O4}	3.01	0.55	3.57	1.11	4.68
{O4,H5}	2.55	1.09	3.64	0.04	3.60
{O3,H6}	1.03	0.19	1.22	0.75	1.97
{O4,H6}	2.09	1.67	0.42	4.76	5.18
{C1,C2}	0.03	0.53	0.56	1.57	1.01
{O3,O4,H6}	3.06	0.92	2.14	4.23	6.37
{C1,H7,H9}	0.10	0.08	0.18	0.22	0.04
{C2,H8,H10}	0.52	0.60	1.12	0.93	0.19
{O3,O4,H5,H6}	3.58	0.14	3.72	2.99	6.70
{C1,O3,O4,H6}	3.01	0.62	3.63	1.22	4.85
Avr.:	*1.9*	*0.6*	*2.0*	*1.8*	*3.5*
Std. dev.:	*1.4*	*0.5*	*1.5*	*1.6*	*2.5*
			Lin → Ecl		
{O3,O4}	1.09	0.97	2.06	0.26	2.31
{O4,H5}	0.40	0.08	0.48	1.09	1.57
{O3,H6}	0.26	0.07	0.32	1.06	1.39
{O4,H6}	0.40	0.17	0.22	1.62	1.84
{C1,C2}	1.49	0.57	2.06	0.86	1.20
{O3,O4,H6}	0.87	0.86	1.73	0.61	2.34
{C1,H7,H9}	0.26	0.01	0.27	0.52	0.79
{C2,H8,H10}	0.16	0.03	0.19	0.50	0.69
{O3,O4,H5,H6}	0.65	0.95	1.60	0.56	2.16
{C1,O3,O4,H6}	1.67	0.20	1.87	2.05	3.93
Avr.:	*0.7*	*0.4*	*1.1*	*0.9*	*1.8*
Std. dev.:	*0.5*	*0.4*	*0.8*	*0.6*	*0.9*
Overall Avr.:	***1.3***	***0.5***	***1.5***	***1.3***	***2.6***
Overall Std. dev.:	***1.2***	***0.5***	***1.3***	***1.3***	***2.0***
Grand total Avr. for all energy terms:			**1.5**		
Grand total Std. dev. for all energy terms:			**1.5**		