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

Supporting Information

Energy Components in Energy Decomposition Analysis (EDA) Are Path Functions; Why Does It Matter?

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Table S1. Energy decomposition analysis (EDA) of H_2 at the equilibrium distance (R_e in Å). Energy values are given in kcal.mol^{-1}.[a]

	PBE	TPSS	M06-L	PBE0	TPSSH	M06-2X
ΔE_{int}	-106.0	-114.7	-106.5	-108.2	-115.2	-113.3
ΔE_{Pauli}	-12.8	-21.0	-10.4	-13.2	-21.1	-9.9
$\Delta E_{Pauli\ kinetics}$	0.0	0.0	0.0	0.0	0.0	0.0
$\Delta E_{Pauli\ Coulomb}$	0.0	0.0	0.0	0.0	0.0	0.0
ΔE_{elstat}	6.1	6.1	5.0	9.7	7.5	13.9
ΔE_{orb}	-99.3	-99.7	-98.1	-104.6	-101.1	-109.7
$\Delta E_{orb\ meta}$	---	-0.3	-3.0	---	-0.5	-7.6
$\Delta E_{orb\ kinetic}$	148.8	159.5	160.3	178.6	170.2	202.8
$\Delta E_{orb\ Coulomb}$	-195.3	-203.2	-204.0	-219.6	-212.0	-240.2
$\Delta E_{orb\ xc+hf}$	---	---	---	-63.6	---	---
$\Delta E_{orb\ xc}$	-52.9	-56.0	-57.4	-49.3	-59.9	-80.0
$\Delta E_{orb\ hf}$	---	---	---	-14.3	---	---
R_e	0.7504	0.7422	0.7425	0.7446	0.7409	0.7388

[a] the basis sets were TZ2P.

Table S2. Energy decomposition analysis (EDA) of C_2H_6 at the equilibrium distance (R_e in Å). Energy values are given in kcal.mol^{-1}.[a]

	PBE	TPSS	M06-L	PBE0	TPSSH	M06-2X
ΔE_{int}	-117.8	-112.5	-117.7	-118.7	-120.1	-113.5
ΔE_{Pauli}	200.7	202.3	206.3	212.1	222.4	206.9
$\Delta E_{Pauli\ kinetics}$	509.1	502.2	491.0	520.3	535.5	507.7
$\Delta E_{Pauli\ Coulomb}$	-189.7	-183.7	-172.7	-186.3	-190.1	-183.1
ΔE_{elstat}	-131.3	-132.4	-130.6	-138.8	-144.6	-135.3
ΔE_{orb}	-187.3	-192.5	-196.1	-192.1	-200.5	-194.4
$\Delta E_{orb\ meta}$	---	10.0	2.8	0.0	2.6	9.4
$\Delta E_{orb\ kinetic}$	-374.9	-365.7	-344.1	-355.8	-347.3	-358.9
$\Delta E_{orb\ Coulomb}$	166.7	161.1	140.9	149.5	140.7	154.8
$\Delta E_{orb\ xc+hf}$	---	---	---	14.2	---	---
$\Delta E_{orb\ xc}$	20.9	22.1	9.9	9.5	8.7	19.2
$\Delta E_{orb\ hf}$	---	---	---	4.8	---	---
R_e	1.5297	1.5319	1.5141	1.5204	1.5219	1.5275

[a] the basis sets were TZ2P.

Cartesian coordinates and Bond Energies in kcal/mol

H_2
HF/TZ2P= -262.12 kcal/mol

H	0.000000	0.000000	-0.367253
H	0.000000	0.000000	0.367253

H_2
BP86/TZ2P= -155.28 kcal/mol

H	0.000000	0.000000	-0.374693
H	0.000000	0.000000	0.374693

H_2
PBE/TZ2P= -155.90 kcal/mol

H	0.000000	0.000000	-0.375180
H	0.000000	0.000000	0.375180

H_2
TPSS/TZ2P= -164.65 kcal/mol

H	0.000000	0.000000	-0.371117
H	0.000000	0.000000	0.371117

H_2
M06-L/TZ2P= -167.16 kcal/mol

H	0.000000	0.000000	-0.371231
H	0.000000	0.000000	0.371231

H_2
B3LYP/TZ2P= -177.99 kcal/mol

H	0.000000	0.000000	-0.371228
H	0.000000	0.000000	0.371228

H_2
PBE0/TZ2P= -186.06 kcal/mol

H	0.000000	0.000000	-0.372311
H	0.000000	0.000000	0.372311

H_2
TPSSH/TZ2P= -175.73 kcal/mol

H	0.000000	0.000000	-0.370453
H	0.000000	0.000000	0.370453

H_2
M06-2X/TZ2P= -210.91 kcal/mol

H	0.000000	0.000000	-0.369403
H	0.000000	0.000000	0.369403

C_2H_6
HF/TZ2P= -1524.47 kcal/mol

C	0.000000	0.000000	-0.762043
H	0.000000	1.010598	-1.153961
H	0.875203	-0.505299	-1.153961
H	-0.875203	-0.505299	-1.153961
C	0.000000	0.000000	0.762043
H	-0.875203	0.505299	1.153961
H	0.000000	-1.010598	1.153961
H	0.875203	0.505299	1.153961

C_2H_6
BP86/TZ2P= -923.15 kcal/mol

C	0.000000	0.000000	-0.765514
H	0.000000	1.022622	-1.165753
H	0.885617	-0.511311	-1.165753
H	-0.885617	-0.511311	-1.165753
C	0.000000	0.000000	0.765514
H	-0.885617	0.511311	1.165753
H	0.000000	-1.022622	1.165753
H	0.885617	0.511311	1.165753

C_2H_6
PBE/TZ2P= -933.02 kcal/mol

C	0.000000	0.000000	-0.764859
H	0.000000	1.023780	-1.165562
H	0.886619	-0.511890	-1.165562
H	-0.886619	-0.511890	-1.165562
C	0.000000	0.000000	0.764859
H	-0.886619	0.511890	1.165562
H	0.000000	-1.023780	1.165562
H	0.886619	0.511890	1.165562

C_2H_6
TPSS/TZ2P= -954.17 kcal/mol

C	0.000000	0.000000	-0.765949
H	0.000000	1.020066	-1.161382
H	0.883403	-0.510033	-1.161382
H	-0.883403	-0.510033	-1.161382
C	0.000000	0.000000	0.765949
H	-0.883403	0.510033	1.161382
H	0.000000	-1.020066	1.161382
H	0.883403	0.510033	1.161382

C_2H_6

M06-L/TZ2P= -989.63 kcal/mol

C	0.000000	0.000000	-0.757068
H	0.000000	1.013038	-1.153471
H	0.877316	-0.506519	-1.153471
H	-0.877316	-0.506519	-1.153471
C	0.000000	0.000000	0.757068
H	-0.877316	0.506519	1.153471
H	0.000000	-1.013038	1.153471
H	0.877316	0.506519	1.153471

C_2H_6

B3LYP/TZ2P= -1048.10 kcal/mol

C	0.000000	0.000000	-0.764326
H	0.000000	1.016945	-1.161045
H	0.880700	-0.508472	-1.161045
H	-0.880700	-0.508472	-1.161045
C	0.000000	0.000000	0.764326
H	-0.880700	0.508472	1.161045
H	0.000000	-1.016945	1.161045
H	0.880700	0.508472	1.161045

C_2H_6

PBE0/TZ2P= -1114.34 kcal/mol

C	0.000000	0.000000	-0.760180
H	0.000000	1.016971	-1.157137
H	0.880723	-0.508485	-1.157137
H	-0.880723	-0.508485	-1.157137
C	0.000000	0.000000	0.760180
H	-0.880723	0.508485	1.157137
H	0.000000	-1.016971	1.157137
H	0.880723	0.508485	1.157137

C_2H_6

TPSSH/TZ2P= -1024.07 kcal/mol

C	0.000000	0.000000	-0.763753
H	0.000000	1.017736	-1.158841
H	0.881385	-0.508868	-1.158841
H	-0.881385	-0.508868	-1.158841
C	0.000000	0.000000	0.763753
H	-0.881385	0.508868	1.158841
H	0.000000	-1.017736	1.158841
H	0.881385	0.508868	1.158841

C_2H_6

M06-2X/TZ2P= -1239.52 kcal/mol

C	0.000000	0.000000	-0.760969
H	0.000000	1.016355	-1.152847
H	0.880189	-0.508178	-1.152847
H	-0.880189	-0.508178	-1.152847
C	0.000000	0.000000	0.760969
H	-0.880189	0.508178	1.152847
H	0.000000	-1.016355	1.152847
H	0.880189	0.508178	1.152847