SUPPORTING INFORMATION

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Revised M11 Exchange–Correlation Functional for Electronic Excitation Energies and Ground–State Properties

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[a]The calculated values are reported using the PBE, B3LYP, M11, and revM11 density functionals.

[b]Most of the tables report MUE or MUEPB. MUE denotes mean unsigned error. MUEPB denotes mean unsigned error per bond.

Table S1. Atomization energies (kcal/mol) of the SR-MGM-BE8 database

System	PBE	B3LYP	M11	revM11	Ref.
$AlCl_3$	303.9	291.9	308.6	301.9	309.9
AlF_3	425.8	415.8	438.6	426.8	429.6
KOH	84.3	80.0	92.4	86.0	85.0
NaO	68.5	64.8	70.2	66.1	65.2
LiCl	109.4	109.0	110.8	109.2	113.9
AlCl	119.8	116.2	118.5	116.6	121.6
ZnSe	30.5	22.6	39.8	20.6	25.2
ZnCl	52.5	46.9	64.3	54.7	53.5
MUEPB[a]	2.5	4.4	5.9	2.6	0.0

[a]MUEPB denotes mean unsigned error per bond. It was computed as follows. First, each entry is used to compute the average bond energy in the given molecule by dividing the atomization energy by the number of bonds (for this purpose single, double, and triple bonds all count as just one bond). Then we compute the error in the average bond energy of the molecule by subtracting the reference value from the density functional value. Then we calculate the MUEPB by averaging the absolute values of these errors over all the rows of the table. Thus the MUEPB is the MUE of the average bond energies.

Table S2. Atomization energies (kcal/mol) of the SR-MGN-BE107 database

System	PBE	B3LYP	M11	revM11	Ref.
C_2H_6	96.9	91.7	97.8	96.8	97.4
iPr-CH_3	89.6	85.0	92.6	92.7	95.0
C_2H_6O	86.8	82.1	90.3	91.8	89.8
iPr-OCH_3	83.7	79.7	89.3	91.3	91.5
Et-H	104.9	106.4	108.6	108.0	108.9
Et-CH_3	93.1	88.2	94.9	94.5	95.9
Et-OCH_3	86.3	82.1	90.6	92.5	95.3
Et-OH	99.6	93.3	99.7	101.3	100.3
tBu-H	97.3	99.6	102.2	102.7	103.9
tBu-CH_3	86.2	81.6	90.9	91.2	93.7
tBu-OCH_3	80.1	76.2	87.9	89.7	89.3
tBu-OH	97.0	91.1	99.2	101.2	115.0
CH ($^2\prod$)	84.5	85.3	82.9	84.4	84.2
CH_2 ($^3B_1$)	194.4	192.0	187.7	192.4	190.7
CH_2 ($^1A_1$)	178.6	180.5	179.9	183.3	181.4
CH_3 ($^2A"_2$)	309.9	309.8	307.4	309.5	307.8
CH_4	420.1	420.9	420.8	421.5	420.3
NH	88.3	87.9	83.3	88.0	83.1
NH_2	188.2	187.6	186.2	187.3	182.6
NH_3	301.7	300.7	303.6	303.0	298.0
OH	109.5	107.9	107.4	107.9	107.2
H_2O	233.5	230.3	233.6	233.5	232.8
HF	141.2	138.5	142.1	142.2	141.3
SiH_2 ($^1A_1$)	147.4	153.3	152.8	153.6	151.8
SiH_2 ($^3B_1$)	131.2	132.7	133.2	134.7	131.1
SiH_3	222.0	228.1	228.0	231.8	227.6
SiH_4	313.0	323.3	323.2	329.2	324.5
PH_2	154.4	158.6	155.4	156.2	153.2
PH_3	239.1	244.7	242.3	243.0	242.3
H_2S	181.5	181.5	183.3	180.9	183.4
HCl	105.4	104.1	106.3	104.6	106.7
C_2H_2	414.7	403.0	402.1	403.8	405.4
CH_2CH_2	571.4	563.0	562.1	563.7	563.5
CH_3CH_3	716.8	711.4	712.6	715.7	712.8
HCN	326.0	313.1	313.8	315.5	313.3
HCO	294.7	279.9	278.7	282.9	279.1
H_2CO	385.6	373.2	373.7	377.4	374.4
CH_3OH	519.5	511.1	514.6	518.2	513.2
NH_2NH_2	452.6	443.6	450.0	452.8	438.6
HOOH	281.0	266.1	269.2	273.1	268.6
Si_2 (multiplicity = 3)	79.3	70.5	68.2	67.7	75.7
P_2	121.5	115.8	110.8	105.7	117.6
S_2	113.6	101.8	103.0	99.5	103.1
Cl_2	63.2	53.1	57.6	56.3	58.1

SC	178.8	165.5	165.2	162.6	171.1
ClF	69.6	58.2	61.6	63.3	61.6
Si_2H_6	519.2	529.7	533.0	537.3	535.0
CH_3Cl	398.9	391.6	395.2	396.3	395.5
CH_3SH	477.5	471.1	474.6	474.7	473.8
HOCl	173.3	161.0	165.1	166.3	165.2
BCl_3	332.7	310.9	316.7	318.8	322.9
BF_3	479.9	463.4	469.8	473.4	469.8
C_2Cl_4	496.5	448.1	463.2	467.0	466.3
C_2F_4	628.8	582.2	592.8	606.4	589.4
C_3H_4 (propyne)	720.8	702.4	702.7	706.2	704.8
C_4H_4O	1030.9	987.2	992.9	1001.8	993.7
C_4H_4S	995.6	952.9	958.4	961.8	962.7
C_4H_5N	1110.7	1068.6	1076.5	1083.6	1071.6
C_4H_6 (*trans*-1,3-butadiene)	1034.4	1009.3	1007.9	1011.8	1012.4
C_4H_6 (2-butyne)	1025.6	1000.4	1002.0	1007.6	1004.1
C_5H_5N	1285.0	1235.0	1237.9	1244.9	1237.7
CCH	276.8	262.5	261.4	262.7	265.1
CCl_4	329.1	291.8	307.1	310.5	312.7
CF_3CN	679.1	632.3	641.6	653.5	639.9
CF_4	500.4	466.0	478.8	490.6	476.3
CH_2OH	421.1	410.4	411.8	416.4	409.8
CH_3CN	635.4	616.0	617.7	621.2	615.8
CH_3NH_2	590.8	584.0	587.8	590.9	582.2
CH_3NO_2	641.5	602.0	606.5	616.0	601.3
$CHCl_3$	355.8	329.2	340.0	342.6	343.2
CHF_3	476.7	451.5	460.6	470.1	457.5
ClF_3	159.3	122.7	128.0	132.6	125.3
H_2	104.7	110.3	109.3	112.5	109.5
CH_2CH	457.7	447.1	444.8	446.5	445.9
$HCOOCH_3$	810.8	781.8	787.5	797.1	785.3
HCOOH	521.6	498.0	502.0	508.5	501.0
PF_3	370.4	354.2	362.4	366.2	363.9
SH	87.9	88.1	88.3	87.3	87.0
$SiCl_4$	381.2	358.8	378.2	376.1	384.9
SiF_4	567.6	553.5	577.6	569.1	574.4
C_2H_5	611.9	605.0	604.1	607.7	603.8
C_4H_6 (bicylobutane)	1011.3	977.8	989.8	999.3	987.2
C_4H_6 (cyclobutene)	1023.8	993.8	997.4	1005.3	1001.6
HCOCOH	662.7	630.3	631.7	639.8	633.4
CH_3CHO	694.3	675.1	676.7	682.0	677.0
C_2H_4O	669.5	647.1	653.6	660.6	650.7
C_2H_5O	710.3	694.8	695.3	704.3	698.6
CH_3OCH_3	809.7	795.6	799.9	807.5	798.1
CH_3CH_2OH	821.0	806.2	811.3	817.0	810.4
C_3H_4 (allene)	723.9	704.2	702.7	704.8	703.2

C_3H_4 (cyclopropene)	701.4	678.3	684.0	688.6	682.7
CH_3COOH	827.6	797.8	803.9	811.6	803.0
CH_3COCH_3	1000.0	974.3	978.1	984.9	978.0
C_3H_6 (cyclopropane)	867.9	849.1	855.9	862.4	853.4
CH_3CHCH_2	873.5	858.3	859.1	862.6	860.6
C_3H_8	1014.9	1003.1	1006.4	1011.8	1006.9
$C_2H_5OCH_3$	1111.1	1090.6	1096.6	1106.2	1095.1
C_4H_{10} (isobutane)	1313.8	1295.2	1301.5	1309.1	1303.0
C_4H_{10} (antiperiplanar butane)	1313.0	1294.7	1300.2	1307.9	1301.3
C_4H_8 (cyclobutane)	1167.1	1141.2	1147.6	1157.1	1149.0
C_4H_8 (isobutene)	1175.3	1153.3	1156.4	1162.0	1158.6
C_5H_8 (spiropentane)	1315.2	1275.9	1289.2	1301.3	1284.3
C_6H_6	1409.2	1360.8	1362.4	1367.4	1367.6
CH_3CO	603.4	582.0	582.5	588.2	581.6
$(CH_3)_2CH$	914.2	900.4	901.5	906.8	900.8
$(CH_3)_3C$	1216.4	1195.6	1199.3	1206.4	1199.3
H_2CCO	557.9	533.5	534.2	537.6	532.3
MUEPB[a]	3.4	2.2	0.9	1.5	0.0

[a]MUEPB denotes mean unsigned error per bond. It is the MUE of the average bond energies as explained in the footnote to Table S1.

Table S3. Atomization energies (kcal/mol) of the SR-TM-BE15 database

System	PBE	B3LYP	M11	revM11	Ref.
$CrCl_2$	176.5	169.5	175.1	172.0	181.1
MnF_2	254.4	233.6	261.0	243.9	232.3
$FeCl_2$	197.4	184.9	204.3	192.8	190.3
$CoCl_2$	186.4	170.4	189.8	180.2	182.9
Ag_2	40.7	35.4	30.2	30.9	38.3
AgH	55.9	54.4	57.2	54.6	54.0
$CrCH_3^+$	43.9	35.0	30.5	31.3	28.8
Cu_2	48.0	41.0	33.5	35.8	47.2
CuAg	44.3	38.2	32.6	31.1	40.7
CuH_2O^+	43.1	38.8	33.0	39.5	38.8
VCO^+	38.2	29.6	41.6	27.9	28.2
Zr_2	85.0	56.6	60.3	40.5	70.8
$Pd(PH_3)_2$–C_6H_8	13.3	3.8	14.5	15.9	16.2
$Pd(PH_3)_2$–$C_{10}H_{12}$-b	9.1	-1.5	14.9	16.1	17.3
FeCl	84.8	78.9	95.3	85.4	80.5
MUEPB[a]	5.4	4.4	7.3	5.4	0.0

[a]MUEPB denotes mean unsigned error per bond. It is the MUE of the average bond energies as explained in the footnote to Table S1.

Table S4. Atomization energies (kcal/mol) of the MR-MGM-BE4 database

System	PBE	B3LYP	M11	revM11	Ref.
CaO	124.2	104.5	110.6	101.6	96.2
LiO^-	61.8	53.4	48.8	58.3	57.6
KO^-	37.7	23.4	17.5	41.9	33.1
MgS	55.3	46.9	49.9	44.0	55.7
MUEPB[a]	9.3	7.8	11.2	6.7	0.0

[a]MUEPB denotes mean unsigned error per bond. It is the MUE of the average bond energies as explained in the footnote to Table S1.

Table S5. Reaction energies (kcal/mol) of the MR-MGN-BE17 database[a]

System	PBE	B3LYP	M11	revM11	Ref.
NF_3	242.6	205.8	212.6	223.0	204.5
CO_2	415.6	387.3	389.2	394.2	389.6
SiO (multiplicity = 1)	195.7	187.4	187.7	186.7	192.4
SO_2	277.1	249.1	250.8	254.9	259.6
CO	268.3	254.7	257.6	260.1	259.4
SO (multiplicity = 1)	139.6	125.4	125.1	127.1	125.7
ClO	79.9	64.9	64.3	65.8	64.8
F_2	51.2	35.6	34.7	39.9	38.3
N_2	243.0	229.0	232.0	234.5	228.5
O_2	142.8	123.0	118.8	127.7	120.4
NO	171.8	154.7	155.1	161.2	152.7
CN	197.0	179.0	176.0	177.0	181.3
B_2	76.9	60.0	48.3	58.1	67.4
C_2	93.6	119.2	109.5	127.6	146.9
$O_3 \rightarrow O_2 + O$	41.2	16.3	14.8	19.2	26.6
$S_4 \rightarrow 2S_2$	28.4	12.9	8.1	16.2	25.8
$Cl_2O \rightarrow Cl_2 + O$	53.0	40.4	40.5	43.9	41.7
MUEPB[b]	14.8	5.1	7.0	5.6	0.0

[a]For the first 14 rows, the reaction is atomization. For the last three rows, the reaction is as shown.

[b]MUEPB denotes mean unsigned error per bond. For the first 14 rows the error is computed from the average bond energy of the molecule as described in the footnote to Table S1. For the last three rows it is the error in the reaction as indicated; note that S_4 is a chain molecule (pictured below), not a four-membered ring, and therefore these three reactions each break one bond.

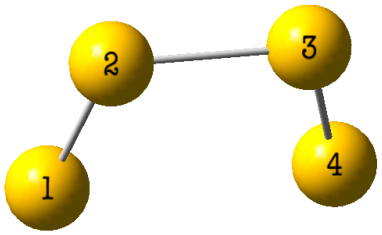

Figure S1. Structure of S_4.

Table S6. Reaction energies (kcal/mol) of the MR-TM-BE12 database[a]

System	PBE	B3LYP	M11	revM11	Ref.
TiCl	115.6	102.9	110.8	104.8	101.7
VF_5	629.8	556.2	563.6	549.2	564.2
CrCl	88.9	85.8	90.3	89.2	90.2
CrOF	254.9	226.7	219.4	221.7	247.6
$(FeBr_2)_2$	369.4	340.4	395.7	359.5	366.8
$Co(CO)_4H$	1309.7	1189.7	1185.3	1217.2	1230.1
CuCl	86.4	80.1	89.4	85.4	90.2
VO	182.1	151.1	158.5	151.3	151.0
NiCl	89.5	81.1	90.6	86.6	88.7
VS	128.3	102.4	111.1	98.4	106.9
$NiCH_2^+ \rightarrow Ni^+ + CH_2$	90.8	73.0	50.3	64.7	76.3
$Fe(CO)_5 \rightarrow Fe + 5CO$	193.0	122.2	100.8	115.2	147.4
MUEPB[b]	10.2	4.8	6.9	4.7	0.0

[a]For the first 14 rows, the reaction is atomization. For the last three rows, the reaction is as shown.

[b]MUEPB denotes mean unsigned error per bond. For the first ten rows the error is computed from the average bond energy of the molecule as described in the footnote to Table S1. For the eleventh row, it is the error in the reaction as indicated; this reaction breaks one bond. For the final row, the error is divided by five so that it corresponds to the average bond energy of the five metal–ligand bonds that are broken.

Table S7. Atomization energies (kcal/mol) of the MR-TMD-BE3 database

System	PBE	B3LYP	M11	revM11	Ref.
Fe_2	41.2	9.4	20.9	1.5	26.6
Cr_2	32.4	-3.3	-136.6	-29.8	36.0
V_2	102.2	37.4	-7.1	9.0	64.2
MUEPB[a]	18.7	27.8	83.2	48.7	0.0

[a]MUEPB denotes mean unsigned error per bond. It is the MUE of the average bond energies as explained in the footnote to Table S1.

Table S8. Barrier heights (kcal/mol) of the HTBH38/18 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
$H + HCl \rightarrow H_2 + Cl$	0.3	-0.9	4.2	1.8	6.1
	-1.2	4.4	6.4	8.9	8.0
$OH + H_2 \rightarrow H_2O + H$	-5.9	0.9	3.8	5.9	5.2
	13.5	13.2	20.9	19.1	21.6
$CH_3 + H_2 \rightarrow CH_4 + H$	4.0	8.9	10.1	13.5	11.9
	9.5	9.7	14.2	13.0	15.0
$OH + CH_4 \rightarrow H_2O + CH_3$	-5.2	2.3	5.0	4.2	6.3
	8.8	13.9	18.0	18.0	19.5
$H + H_2 \rightarrow H_2 + H$	3.8	4.3	8.7	11.1	9.7
	3.8	4.3	8.7	11.1	9.7
$OH + NH_3 \rightarrow H_2O + NH_2$	-11.6	-2.3	4.2	2.5	3.4
	-0.9	7.2	13.2	12.5	13.7
$HCl + CH_3 \rightarrow CH_4 + Cl$	-5.7	-1.3	-0.9	-0.9	1.8
	-1.8	4.8	5.3	5.7	6.8
$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	-8.6	-0.7	2.4	1.9	3.5
	10.6	15.5	20.2	19.6	20.4
$F + H_2 \rightarrow HF + H$	-12.4	-5.6	-0.9	-1.5	1.6
	24.5	23.1	32.3	28.6	33.8
$O + CH_4 \rightarrow OH + CH_3$	-0.1	7.5	11.6	10.4	14.4
	-0.6	4.4	5.7	6.4	8.9
$H + PH_3 \rightarrow H_2 + PH_2$	-1.7	-0.9	2.0	2.4	2.9
	18.4	23.2	24.4	28.1	24.7
$H + HO \rightarrow H_2 + O$	3.6	4.0	8.5	8.2	10.9
	-1.3	6.3	10.4	12.8	13.2
$H + H_2S \rightarrow H_2 + HS$	-1.1	-0.5	2.8	2.1	3.9
	9.5	15.9	16.5	20.6	17.2
$O + HCl \rightarrow OH + Cl$	-10.1	1.4	9.2	7.5	10.4
	-6.8	4.4	9.5	10.0	9.9
$CH_3 + NH_2 \rightarrow CH_4 + NH$	0.7	6.1	8.3	7.5	8.9
	10.8	17.4	18.7	20.2	22.0
$C_2H_5 + NH_2 \rightarrow C_2H_6 + NH$	2.9	8.2	10.1	8.7	9.8
	7.8	14.8	15.7	17.5	19.4
$NH_2 + C_2H_6 \rightarrow NH_3 + C_2H_5$	1.5	8.8	9.9	9.9	11.3
	10.1	15.6	18.7	17.6	17.8
$NH_2 + CH_4 \rightarrow NH_3 + CH_3$	4.5	11.4	12.7	12.4	13.9
	7.8	13.5	16.7	16.1	16.9
s-trans cis-$C_5H_8 \rightarrow$ *s-trans cis*-C_5H_8	31.4	39.0	38.3	40.1	39.7
	31.4	39.0	38.3	40.1	39.7
MUE	9.7	4.5	1.4	1.8	0.0

Table S9. Barrier heights (kcal/mol) of the NHTBH38/18 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
$H + N_2O \rightarrow OH + N_2$	10.5	11.8	17.2	16.4	17.7
	52.8	73.1	80.2	77.5	82.6
$H + FH \rightarrow HF + H$	28.0	31.8	39.3	39.7	42.1
	28.0	31.8	39.3	39.7	42.1
$H + ClH \rightarrow HCl + H$	10.4	13.1	17.7	16.7	17.8
	10.4	13.1	17.7	16.7	17.8
$H + FCH_3 \rightarrow HF + CH_3$	18.7	22.0	28.8	31.3	30.5
	41.1	48.7	53.9	54.9	56.9
$H + F_2 \rightarrow HF + F$	-9.6	-7.3	0.2	-0.1	1.5
	80.0	95.2	107.2	101.8	104.8
$CH_3 + FCl \rightarrow CH_3F + Cl$	-6.4	-1.5	6.0	7.9	7.1
	42.0	51.2	60.6	62.4	59.8
$F^- + CH_3F \rightarrow FCH_3 + F^-$	-8.3	-3.9	-1.9	-0.4	-0.6
	-8.3	-3.9	-1.9	-0.4	-0.6
$F^-\cdots CH_3F \rightarrow FCH_3\cdots F^-$	6.7	10.0	13.7	14.8	13.4
	6.7	10.0	13.7	14.8	13.4
$Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$	-3.7	-0.5	4.1	6.0	2.5
	-3.7	-0.5	4.1	6.0	2.5
$Cl^-\cdots CH_3Cl \rightarrow ClCH_3\cdots Cl^-$	6.9	9.0	15.3	17.0	13.5
	6.9	9.0	15.3	17.0	13.5
$F^- + CH_3Cl \rightarrow FCH_3 + Cl^-$	-19.5	-16.5	-12.8	-10.9	-12.3
	12.1	18.0	18.5	20.2	19.8
$F^-\cdots CH_3Cl \rightarrow FCH_3\cdots Cl^-$	-1.0	0.1	4.4	5.5	3.5
	21.0	26.2	28.9	30.6	29.6
$OH^- + CH_3F \rightarrow HOCH_3 + F^-$	-10.7	-5.9	-4.2	-2.8	-2.7
	9.6	14.5	18.3	20.8	17.6
$OH^-\cdots CH_3F \rightarrow HOCH_3\cdots F^-$	3.4	7.4	11.5	12.6	11.0
	42.7	45.1	49.4	51.9	47.7
$H + N_2 \rightarrow HN_2$	5.6	7.8	12.2	11.9	14.6
	9.2	11.0	12.0	13.0	10.9
$H + CO \rightarrow HCO$	-1.7	-0.6	2.2	1.9	3.2
	24.7	24.7	23.3	24.6	22.8
$H + C_2H_4 \rightarrow CH_3CH_2$	0.0	-0.1	1.8	1.6	2.0
	40.4	41.9	43.7	45.6	42.0
$CH_3 + C_2H_4 \rightarrow CH_3CH_2CH_2$	1.6	6.1	5.6	6.9	6.4
	29.7	29.4	33.2	36.9	33.0
$HCN \rightarrow HNC$	46.0	47.7	45.6	45.9	48.1
	31.0	33.8	33.8	34.1	33.0
MUE	8.4	4.5	1.3	2.0	0.0

Table S10. Noncovalent complexation energies (kcal/mol) of the NCCE30/18 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
$(NH_3)_2$	3.34	2.67	3.04	3.48	3.09
$(HF)_2$	5.00	4.72	4.85	5.30	4.49
$(H_2O)_2$	5.44	4.96	5.41	5.79	4.91
$NH_3\cdots H_2O$	7.15	6.32	6.56	7.11	6.38
$(HCONH_2)_2$	14.24	13.06	14.97	14.76	15.41
$(HCOOH)_2$	16.33	15.17	17.34	17.32	17.60
$C_2H_4\cdots F_2$	3.17	1.50	1.17	1.39	1.06
$NH_3\cdots F_2$	5.45	2.90	1.57	2.01	1.80
$C_2H_2\cdots ClF$	6.18	3.79	3.80	4.01	3.79
$HCN\cdots ClF$	5.93	4.57	4.68	5.15	4.80
$NH_3\cdots Cl_2$	7.95	5.48	4.22	4.50	4.85
$H_2O\cdots ClF$	7.41	5.69	5.62	5.94	5.20
$NH_3\cdots ClF$	17.09	12.83	9.97	10.58	11.17
$(H_2S)_2$	1.80	0.90	1.26	1.59	1.62
$(HCl)_2$	2.11	1.32	1.57	1.98	1.91
$HCl\cdots H_2S$	4.16	2.87	2.94	3.33	3.26
$CH_3Cl\cdots HCl$	3.39	2.21	3.29	3.62	3.39
$HCN\cdots CH_3SH$	3.52	2.57	3.64	3.77	3.58
$CH_3SH\cdots HCl$	5.61	3.77	4.58	4.93	4.74
$CH_4\cdots Ne$	0.27	0.02	0.23	0.26	0.18
$C_6H_6\cdots Ne$	0.35	-0.11	0.96	0.98	0.41
$(CH_4)_2$	0.01	-0.50	0.41	0.79	0.53
$CO_2\cdots Ar$	0.26	-0.26	0.35	0.66	0.57
$(C_2H_2)_2$	1.00	0.44	1.33	1.58	1.36
$(C_2H_4)_2$	0.36	-0.48	1.73	2.17	1.44
sandwich $(C_6H_6)_2$	-1.56	-2.26	1.57	1.98	1.65
T-shaped $(C_6H_6)_2$	0.11	-0.21	2.89	3.17	2.63
parallel-displaced $(C_6H_6)_2$	-0.96	-1.82	3.18	3.46	2.59
parallel-displaced $(CO_2)_2$	0.71	0.20	1.23	1.70	1.49
sandwich $(C_5H_5N)_2$	-0.19	-1.69	2.74	2.99	2.89
MUE	1.43	1.25	0.28	0.38	0.0

Table S11. Interaction energies (kcal/mol) of the NGD21/18 database

System[a]	PBE	B3LYP	M11	revM11	Ref.
He_2	0.06	-0.04	0.00	0.02	0.02
Ne_2	0.12	-0.06	0.07	0.12	0.08
Ar_2	0.11	-0.22	-0.04	0.21	0.29
Kr_2	0.09	-0.32	-0.03	0.31	0.40
HeNe	0.09	-0.05	0.03	0.05	0.04
HeAr	0.09	-0.08	-0.01	0.05	0.06
NeAr	0.13	-0.10	0.07	0.15	0.13
HeHe_L_0.3A	0.07	-0.07	-0.07	0.02	0.01
HeHe_R_0.3A	0.04	-0.03	0.02	0.02	0.02
ArAr_L_0.3A	-0.18	-0.57	-0.28	0.13	0.14
ArAr_R_0.3A	0.14	-0.11	0.04	0.14	0.24
NeNe_L_0.3A	0.04	-0.16	-0.03	0.14	0.01
NeNe_R_0.3A	0.10	-0.04	0.08	0.06	0.07
KrKr_L_0.3A	-0.29	-0.79	-0.30	0.19	0.24
KrKr_R_0.3A	0.16	-0.16	0.02	0.22	0.34
HeNe_L_0.3A	0.08	-0.10	-0.04	0.08	0.01
HeNe_R_0.3A	0.06	-0.03	0.04	0.03	0.03
HeAr_L_0.3A	0.06	-0.15	-0.10	0.06	0.02
HeAr_R_0.3A	0.07	-0.05	0.02	0.03	0.05
NeAr_L_0.3A	0.02	-0.25	-0.04	0.17	0.05
NeAr_R_0.3A	0.11	-0.06	0.08	0.08	0.11
MUE	0.10	0.28	0.14	0.04	0.0

[a]The notation _L_0.3A indicates 0.3 Å smaller than the equilibrium distance, and the notation _R_0.3A indicates 0.3 Å bigger than the equilibrium distance.

Table S12. Noncovalent interaction energies (kcal/mol) of the S6x6 database

System	PBE	B3LYP	M11	revM11	Ref.
04_Water-Peptide_0.90	-7.03	-6.35	-8.03	-8.53	-7.63
04_Water-Peptide_0.95	-7.44	-6.84	-8.44	-8.91	-8.06
04_Water-Peptide_1.00	-7.48	-6.92	-8.41	-8.90	-8.08
04_Water-Peptide_1.05	-7.27	-6.76	-8.11	-8.63	-7.84
04_Water-Peptide_1.10	-6.93	-6.45	-7.64	-8.20	-7.46
04_Water-Peptide_1.25	-5.61	-5.18	-5.95	-6.54	-5.99
17_Uracil-Uracil_BP_0.90	-14.39	-13.24	-14.47	-14.34	-15.70
17_Uracil-Uracil_BP_0.95	-15.48	-14.55	-15.88	-15.74	-16.90
17_Uracil-Uracil_BP_1.00	-15.72	-14.94	-16.32	-16.22	-17.18
17_Uracil-Uracil_BP_1.05	-15.40	-14.75	-16.09	-16.09	-16.86
17_Uracil-Uracil_BP_1.10	-14.74	-14.17	-15.42	-15.56	-16.17
17_Uracil-Uracil_BP_1.25	-11.95	-11.51	-12.27	-12.85	-13.15
20_AcOH-AcOH_0.90	-17.57	-16.36	-17.99	-18.18	-17.45
20_AcOH-AcOH_0.95	-18.74	-17.69	-19.33	-19.43	-18.79
20_AcOH-AcOH_1.00	-18.91	-18.00	-19.65	-19.70	-19.09
20_AcOH-AcOH_1.05	-18.43	-17.64	-19.27	-19.33	-18.72
20_AcOH-AcOH_1.10	-17.58	-16.86	-18.42	-18.55	-17.94
20_AcOH-AcOH_1.25	-14.12	-13.56	-14.63	-15.17	-14.56
28_Benzene-Uracil_pi-pi_0.90	4.87	7.98	-3.72	-3.05	-3.53
28_Benzene-Uracil_pi-pi_0.95	1.95	4.40	-5.04	-5.15	-5.22
28_Benzene-Uracil_pi-pi_1.00	0.34	2.32	-5.12	-5.75	-5.71
28_Benzene-Uracil_pi-pi_1.05	-0.52	1.14	-4.65	-5.54	-5.55
28_Benzene-Uracil_pi-pi_1.10	-0.92	0.51	-3.96	-4.91	-5.08
28_Benzene-Uracil_pi-pi_1.25	-1.00	-0.03	-1.97	-2.54	-3.29
29_Pyridine-Uracil_pi-pi_0.90	4.92	8.08	-3.94	-3.00	-3.74
29_Pyridine-Uracil_pi-pi_0.95	1.10	3.43	-5.98	-6.04	-6.17
29_Pyridine-Uracil_pi-pi_1.00	-0.81	0.99	-6.16	-6.87	-6.81
29_Pyridine-Uracil_pi-pi_1.05	-1.70	-0.22	-5.60	-6.58	-6.58
29_Pyridine-Uracil_pi-pi_1.10	-2.04	-0.78	-4.79	-5.77	-5.97
29_Pyridine-Uracil_pi-pi_1.25	-1.84	-1.02	-2.58	-3.07	-3.87
47_Benzene-Benzene_TS_0.90	2.17	3.94	-1.17	-1.21	-1.64
47_Benzene-Benzene_TS_0.95	0.66	2.08	-2.01	-2.34	-2.58
47_Benzene-Benzene_TS_1.00	-0.15	1.04	-2.18	-2.71	-2.87
47_Benzene-Benzene_TS_1.05	-0.55	0.46	-2.05	-2.64	-2.82
47_Benzene-Benzene_TS_1.10	-0.72	0.16	-1.80	-2.37	-2.60
47_Benzene-Benzene_TS_1.25	-0.70	-0.09	-1.03	-1.32	-1.77
MUE	2.61	3.78	0.63	0.52	0.00

Table S13. Ionization potentials (kcal/mol) of the IP23 database

System	PBE	B3LYP	M11	revM11	Ref.
C	266.1	266.3	260.2	265.1	259.7
S	240.9	243.8	241.7	243.9	238.9
SH	239.3	241.4	242.4	243.4	238.9
Cl	298.9	301.1	300.3	302.4	299.1
Cl_2	256.0	261.2	263.4	266.3	265.3
OH	304.6	306.3	307.2	306.5	299.1
O	324.7	326.8	328.5	329.8	313.9
O_2	282.5	289.7	284.9	288.1	278.9
P	241.0	238.6	240.9	241.0	241.9
PH	236.0	234.3	234.9	236.8	234.1
PH_2	229.9	228.8	228.1	231.4	226.3
S_2	216.7	219.3	220.0	223.2	216.0
Si	188.9	187.0	188.4	189.5	187.9
Cr	170.5	164.6	148.8	159.9	156.0
Cu	193.1	190.2	165.6	183.0	178.2
FeC	186.8	184.6	170.9	178.9	173.7
Mo	172.1	167.1	152.1	164.6	163.7
Pd	200.2	196.4	191.0	194.3	192.2
Rh	180.4	177.7	159.3	172.7	172.1
Ru	178.9	175.3	135.7	170.9	169.9
Zn	221.2	221.7	197.7	216.9	216.6
Co	187.5	186.9	159.7	179.2	181.1
Sc	146.9	150.8	140.0	149.3	151.3
MUE	6.0	5.3	7.9	4.0	0.0

Table S14. Electron affinities (kcal/mol) of the EA13/03 database

System	PBE	B3LYP	M11	revM11	Ref.
C	35.8	31.2	31.0	31.8	29.1
S	49.6	50.6	48.9	50.0	47.9
SH	52.7	52.9	53.2	53.6	53.3
Cl	83.1	83.7	83.5	84.1	83.4
Cl_2	59.8	64.6	57.0	58.0	55.6
OH	42.3	40.4	41.6	43.4	42.1
O	38.3	36.9	34.2	38.0	33.7
O_2	8.8	12.0	13.6	13.4	10.8
P	20.2	22.0	18.1	19.7	17.2
PH	24.1	25.1	24.4	24.6	23.2
PH_2	28.2	28.3	28.7	29.0	29.4
S_2	36.2	38.6	39.2	41.3	38.5
Si	33.3	30.0	31.3	30.8	31.9
MUE	2.2	2.3	1.0	1.9	0.0

Table S15. Proton affinities (kcal/mol) of the PA8 database

System	PBE	B3LYP	M11	revM11	Ref.
NH_3	210.9	211.3	211.4	211.0	211.9
H_2O	170.4	170.5	170.6	170.6	171.8
C_2H_2	158.9	158.4	159.2	159.0	156.6
SiH_4	157.0	157.4	154.8	156.9	156.5
PH_3	190.2	193.1	192.0	191.7	193.1
H_2S	174.4	174.8	173.3	171.2	173.7
HCl	138.9	138.0	137.0	135.8	137.1
H_2	106.0	104.5	106.6	107.3	105.9
MUE	1.3	1.0	1.0	1.4	0.0

Table S16. Isomerization energies (kcal/mol) of the 2pIsoE4 database

System	PBE	B3LYP	M11	revM11	Ref.
C	1.5	0.8	3.3	3.2	3.8
N	64.4	69.8	63.7	55.1	57.1
O	9.4	10.8	9.6	10.6	9.9
F	26.1	24.7	26.7	26.5	26.9
MUE	2.7	4.7	1.9	0.9	0.0

Table S17. Isomerization energies (kcal/mol) of the 4pIsoE4 database

System	PBE	B3LYP	M11	revM11	Ref.
As	37.9	44.7	38.4	32.5	33.0
Br	-5.2	-7.7	-7.7	-6.8	-6.3
Ge	22.7	22.9	24.6	20.6	24.6
Se	22.7	23.0	24.2	22.5	20.8
MUE	2.4	4.2	2.5	1.7	0.0

Table S18. Isomerization energies (kcal/mol) of the IsoL6/11 database

System	PBE	B3LYP	M11	revM11	Ref.
10-	5.3	2.5	5.9	4.8	6.8
13-	31.1	30.3	30.8	28.1	33.5
14-	6.2	3.7	4.5	2.6	5.3
20-	4.9	4.3	3.5	4.6	4.7
3-	7.2	7.3	9.1	12.4	9.8
9-	17.6	18.1	21.5	20.5	21.8
MUE	2.0	2.6	1.1	2.3	0.0

Table S19. Reaction energies (kcal/mol) of the πTC13 database[a]

System	PBE	B3LYP	M11	revM11	Ref.
E2-E1	3.1	2.2	0.4	-0.9	-1.4
E4-E3	0.2	-2.4	-7.4	-9.4	-8.8
E6-E5	-1.4	-5.5	-13.4	-16.1	-14.3
P-2	167.9	168.2	169.0	169.3	167.8
P-4	196.4	198.5	194.5	194.0	193.5
P-6	214.3	216.3	210.7	210.1	209.7
P-8	225.7	227.6	220.8	220.0	219.7
P-10	234.0	235.7	227.7	226.7	226.0
SB-2	213.7	215.6	216.5	216.1	214.5
SB-4	228.2	230.0	229.2	228.5	226.2
SB-6	238.3	239.7	237.3	236.3	233.4
SB-8	245.3	246.5	242.7	241.3	238.2
SB-10	250.7	251.5	246.4	244.8	241.0
MUE	5.6	6.0	2.2	1.6	0.0

[a]The first three rows are reaction energies of isomerization reactions, and the next ten rows are proton affinities.

Table S20. Atomic energies (kcal/mol) of the AE17 database

System	PBE	B3LYP	M11	revM11	Ref.
H	-0.5	-0.5	-0.5	-0.5	-0.5
He	-2.9	-2.9	-2.9	-2.9	-2.9
Li	-7.5	-7.5	-7.5	-7.5	-7.5
Be	-14.6	-14.7	-14.7	-14.6	-14.7
B	-24.6	-24.7	-24.7	-24.6	-24.7
C	-37.8	-37.9	-37.8	-37.8	-37.8
N	-54.5	-54.6	-54.6	-54.6	-54.6
O	-75.0	-75.1	-75.1	-75.1	-75.1
F	-99.7	-99.8	-99.8	-99.7	-99.7
Ne	-128.9	-129.0	-129.0	-128.9	-128.9
Na	-162.2	-162.3	-162.3	-162.3	-162.3
Mg	-200.0	-200.1	-200.1	-200.0	-200.1
Al	-242.2	-242.4	-242.4	-242.3	-242.3
Si	-289.2	-289.4	-289.4	-289.4	-289.4
P	-341.1	-341.3	-341.3	-341.3	-341.3
S	-398.0	-398.1	-398.1	-398.1	-398.1
Cl	-460.0	-460.2	-460.2	-460.2	-460.1
MUE	47.3	18.3	9.1	5.0	0.0

Table S21. Energies (kcal/mol) of the HC7/11 database

System	PBE	B3LYP	M11	revM11	Ref.
E22-E1	13.8	-1.1	20.8	32.7	14.3
E31-E1	18.4	1.2	28.9	45.0	25.0
octane iso	-5.2	-8.0	4.5	1.8	1.9
DE (rxn a)	5.8	4.6	7.5	7.3	9.8
DE (rxn b)	8.6	6.8	11.2	10.9	14.8
DE (rxn c)	193.0	163.0	198.8	212.5	194.0
DE (rxn d)	124.9	103.0	129.5	139.9	127.2
MUE	4.0	16.8	3.7	10.9	0.0

Table S22. Atomization energies (kcal/mol) of the SMAE3/19 database

System	PBE	B3LYP	M11	revM11	Ref.
SO_3	370.3	329.2	332.6	339.3	344.2
H_2S_2	244.5	236.6	241.4	238.6	240.8
H_2SO_4	621.7	578.0	590.8	596.2	602.2
MUEPB[a]	4.4	3.5	2.0	1.1	0.0

[a]MUEPB denotes mean unsigned error per bond. It is the MUE of the average bond energies as explained in the footnote to Table S1.

Table S23. Reaction energies (kcal/mol) of the DC9/19 database

Reaction	*n*	PBE	B3LYP	M11	revM11	Ref.
$HCN\cdots BF_3 \rightarrow HCN + BF_3$	1	4.3	3.8	6.8	6.4	5.7
$C_6Cl_6 + 6HCl \rightarrow 6Cl_2 + C_6H_6$	1	136.0	127.0	143.7	143.7	152.6
$P_4 \rightarrow 4P$	6	308.1	278.5	288.7	281.7	289.9
$SF_6 \rightarrow S + 6F$	6	501.9	448.8	472.9	483.9	477.5
$PF_5 \rightarrow P + 5F$	5	562.0	532.8	552.6	556.6	556.4
$P_4O_{10} \rightarrow P_4 + 5O_2$	5	618.6	648.7	702.4	687.1	719.7
$C_6F_6 \rightarrow 6C + 6F$	12	1484.5	1378.4	1395.1	1417.2	1388.1
$Si(OCH_3)_4 \rightarrow Si + 4C + 4O + 12H$	20	2045.6	2003.9	2033.3	2044.6	2023.5
urotropine $\rightarrow$ 6C + 4N + 12H	24	2213.9	2129.1	2167.8	2199.3	2151.1
MUEPB[a]		6.5	6.2	1.9	2.7	0.0

[a]MUEPB denotes mean unsigned error per bond. In computing the MUEPB, the error in each reaction energy was divided by *n* to convert it to per-bond basis. The value of *n* is the net number of bonds broken (the only exception to this is the $C_6Cl_6 + 6HCl$ reaction for which we choose *n* to be 1). For the P_4O_{10} reaction, P_4O_{10} has 16 bonds (four P=O bonds and 12 P–O bonds), P_4 has six bonds, and five O_2 molecules have a total of five bonds; therefore *n* is 5.

Table S24. Bond dissociation energies (kcal/mol) of the ABDE13 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
propene → methyl + vinyl	105.7	101.4	106.9	106.6	107.2
methyl formate → HC(O)O + methyl	87.7	88.6	104.8	104.0	97.0
butane → propyl + methyl	93.5	88.7	95.9	95.2	96.2
butane → 2 ethyl	89.1	84.7	92.0	92.4	94.4
cis-3-hexene → C_2H_5CHCH + ethyl	100.0	95.8	102.3	102.8	104.4
cis-3-hexene → $C_2H_5CHCHCH_2$ + methyl	76.3	71.6	78.4	79.4	80.2
1-pentene → $CH_2CHCH_2CH_2$ + methyl	93.6	88.9	96.1	95.3	96.4
1-pentene → CH_2CHCH_2 + ethyl	73.8	69.2	77.2	78.7	80.0
1-pentene → CH_2CH + propyl	102.2	98.2	104.3	104.8	106.3
methyl butanoate → $CH_3OC(O)CH_2CH_2$ + methyl	94.8	89.9	97.3	96.3	97.4
methyl butanoate → $CH_3OC(O)CH_2$ + ethyl	85.1	80.8	90.0	89.9	91.2
methyl butanoate → $CH_3OC(O)$ + propyl	92.3	89.2	97.4	97.0	98.7
methyl butanoate → CH_3 + $OC(O)CH_2CH_2CH_3$	83.5	84.4	101.3	100.4	94.0
MUE	5.1	8.6	2.3	2.1	0.0

Table S25. Bond distances (Å) of the DGL6 database

System	PBE	B3LYP	M11	revM11	Ref.
Cl_2	2.011	2.016	1.987	1.978	1.988
H_2	0.751	0.743	0.751	0.742	0.741
HF	0.929	0.922	0.923	0.923	0.917
MgS	2.157	2.151	2.134	2.118	2.143
N_2	1.103	1.091	1.084	1.088	1.098
OH	0.983	0.974	0.973	0.974	0.970
MUE	0.013	0.009	0.007	0.009	0.000

Table S26. Bond distances (Å) of the DGH4 database

System	PBE	B3LYP	M11	revM11	Ref.
NaBr	2.522	2.520	2.535	2.501	2.502
HBr	1.432	1.424	1.422	1.419	1.414
ZnS	2.063	2.077	2.043	2.035	2.046
Ag_2	2.559	2.584	2.556	2.554	2.530
MUE	0.021	0.028	0.018	0.010	0.000

Table S27. ΔSCF excitation energies (kcal/mol) of the 3dEE8 database

System	PBE	B3LYP	M11	revM11	Ref.
Sc	13.3	20.1	18.9	25.9	32.9
Mn^+	26.6	21.9	24.0	21.0	27.1
Fe	21.3	22.4	16.0	23.0	34.2
Ni^+	24.2	17.9	35.2	36.6	24.0
Zn	96.8	97.7	79.0	88.8	92.4
Ca^+	24.2	27.4	20.9	27.2	39.0
V	-12.2	-0.5	-13.2	-5.8	6.0
Fe_2	11.3	-3.6	-6.2	1.8	12.2
MUE	9.0	9.4	14.5	9.3	0.0

Table S28. ΔSCF excitation energies (kcal/mol) of the 4dAEE5 database

System	PBE	B3LYP	M11	revM11	Ref.
Mo^+	32.9	27.8	41.5	34.2	43.5
Ru^+	24.0	28.1	30.5	24.3	26.2
Rh^+	16.5	16.5	14.9	12.6	23.3
Pd	15.8	13.8	27.6	17.4	18.8
Y^+	-1.4	0.5	-3.3	3.0	2.4
MUE	5.3	6.3	5.8	4.8	0.0

Table S29. ΔSCF excitation energies (kcal/mol) of the pAEE5 database

System	PBE	B3LYP	M11	revM11	Ref.
F	293.5	295.1	301.1	297.3	292.8
Ar	261.4	262.9	272.4	266.8	266.3
C^+	114.1	122.6	122.7	125.0	123.0
Al	82.9	88.4	78.5	84.8	83.0
Si^+	121.9	127.7	118.9	126.3	126.0
MUE	3.7	2.6	5.3	1.8	0.0

Table S30. Excitation energies (eV) of the EE23 database

Reaction	Transition	PBE	B3LYP	M11	revM11	Ref.
Acetaldehyde	$^1A''$ n → π*	4.1	4.2	3.9	3.9	4.3
Acetone	$^1A_2$ n → π*	4.2	4.4	4.1	4.0	4.4
Formaldehyde	$^1A_2$ n → π*	3.8	3.9	3.5	3.6	4.0
Pyrazine	$^1B_{3u}$ n → π*	3.5	3.9	4.0	4.0	4.0
Pyridazine	$^1B_1$ n → π*	3.1	3.6	3.6	3.7	3.6
Pyridine	$^1B_1$ n → π*	4.3	4.8	4.9	4.9	4.7
Pyrimidine	$^1B_1$ n → π*	3.8	4.2	4.4	4.5	4.2
s-Tetrazine	$^1B_{3u}$ n → π*	1.8	2.3	2.3	2.3	2.3
Ethylene	$^1B_{1u}$ π → π*	7.4	7.3	7.3	7.4	8.0
Butadiene	^1B_u π → π*	5.4	5.5	5.7	5.8	6.2
Benzene	$^1B_{2u}$, π → π*	5.1	5.3	5.5	5.4	4.9
Benzene	$^3B_{1u}$ π → π*	3.9	3.7	3.6	3.5	4.1
Napthalene	$^1B_{3u}$ π → π*	4.0	4.3	4.7	4.8	4.0
Napthalene	$^3B_{2u}$ π → π*	2.8	2.7	2.7	2.6	3.1
Furan	$^1B_2$ π → π*	5.9	5.9	6.0	6.1	6.1
Furan	$^3B_2$ π → π*	3.9	3.7	3.9	3.7	4.2
Hexatriene	^1B_u π → π*	4.4	4.6	4.9	5.0	4.9
Hexatriene	^3B_u π → π*	2.3	2.1	2.0	2.1	2.7
Water	Singlet, $2p_x$ → 3s	6.4	6.9	6.9	7.2	7.4
Water	Triplet, $2p_x$ → 3s	6.0	6.5	6.7	6.8	7.0
*p*NA	Intramolecular CT, $^1A_1$, π → π*	3.6	4.0	4.7	4.8	4.3
DMABN	Intramolecular CT, $^1A_1$, π → π*	4.4	4.7	5.0	5.0	4.6
B-TCNE	Intermolecular CT, ^1A, π → π*	1.4	1.9	3.6	3.9	3.6
	MUE (VEE18)	0.4	0.3	0.3	0.4	0.0
	MUE (REE2)	1.0	0.5	0.4	0.2	0.0
	MUE (CTEE3)	1.1	0.7	0.3	0.4	0.0

Table S31. Charge transfer excitation energies (eV) of the LRCTEE9[a] database

System	PBE	B3LYP	M11	revM11	Ref.
d **($NH_3\cdots HNO_2$)**					
3.6772	2.21	3.56	6.28	6.93	7.10
6.1133	1.85	3.44	7.16	7.86	8.22
8.5632	1.78	3.49	7.69	8.39	8.75
11.0156	1.75	3.53	8.01	8.70	9.13
13.4708	1.74	3.56	8.22	8.92	9.35
15.9272	1.73	3.58	8.37	9.07	9.51
18.3868	1.73	3.60	8.49	9.18	9.62
23.3034	1.72	3.63	8.64	9.33	9.77
25.763	1.72	3.64	8.70	9.39	9.83
MUE	7.23	5.47	1.08	0.39	0.00

[a]The LRCTEE9 database comprises of $\pi \rightarrow \pi^*$ $^1A_1$ excitations of the $NH_3\cdots HNO_2$ complex at nine intermonomer distances (*d* in Å).

Table S32. Dimerization energies (kcal/mol) of the AL2X6 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
$Al_2H_6 \rightarrow 2AlH_3$	38.6	33.6	39.9	39.2	38.5
$Al_2F_6 \rightarrow 2AlF_3$	44.2	45.0	55.3	50.9	51.6
$Al_2Cl_6 \rightarrow 2AlCl_3$	26.6	21.8	32.2	31.6	32.5
$Al_2Me_4 \rightarrow 2AlMe_2$	35.9	31.2	39.4	38.3	38.4
$Al_2Me_5 \rightarrow AlMe_2 + AlMe_3$	27.1	20.9	32.0	31.4	31.2
$Al_2Me_6 \rightarrow 2AlMe_3$	17.5	9.5	23.9	23.7	23.1
MUE	4.3	8.9	1.3	0.5	0.0

Table S33. Barrier heights (kcal/mol) of the BHDIV10 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
ed1 → ts1	15.9	20.7	24.5	27.6	25.7
ed2 → ts2	59.2	62.2	58.9	54.9	56.9
ed3 → ts3	25.7	30.8	37.8	37.5	36.5
ed4 → ts4	83.1	94.9	94.7	95.1	96.2
ed5 → ts5	5.5	12.9	14.7	17.9	15.9
ed6 → ts6	7.4	13.7	15.2	13.1	13.6
ed7 → ts7	23.0	31.1	28.4	27.3	27.5
ed8 → ts8	36.3	48.2	50.9	55.3	50.2
ed9 → ts9	56.4	64.8	65.2	66.3	65.8
ed10 → ts10	63.2	64.5	61.1	62.1	64.9
MUE	8.2	2.8	1.5	1.7	0.0

Table S34. Barrier heights (kcal/mol) of the BHPERI26 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
Cyclobutene → TS1	32.2	33.1	36.5	40.9	35.3
cis-1,3,5-Hexatriene → TS2	25.5	31.2	30.2	32.8	30.8
ortho-xylylene → TS3	23.2	28.3	29.9	31.5	28.1
1,3-Pentadiene → TS4	31.3	38.9	38.4	40.1	39.7
1,3-Cyclopentadiene → TS5	22.8	27.1	24.2	25.1	28.3
1,5-Hexadiene → TS6	28.2	36.0	34.9	39.3	35.8
1,3-Butadiene + Ethylene → TS7	16.5	26.3	21.6	24.8	22.3
1,3-Cyclopentadiene + Ethylene → TS8	14.6	24.2	18.9	21.2	18.0
1,3-Cyclopentadiene → TS11	13.4	23.8	18.1	20.2	14.5
Cis-triscyclopropacyclohexane → TS9	20.2	21.9	31.1	40.7	26.4
13r_1 + 13_c2h4 → 13ts_1a	20.8	28.9	31.7	31.5	27.6
13r_2 + 13_c2h4 → 13ts_2a	14.6	22.5	24.0	24.1	20.0
13r_3 + 13_c2h4 → 13ts_3a	11.0	18.3	18.0	18.4	13.8
13r_4 + 13_c2h4 → 13ts_4a	7.8	15.5	17.8	18.5	11.8
13r_5 + 13_c2h4 → 13ts_5a	4.2	10.3	9.6	10.1	6.5
13r_6 + 13_c2h4 → 13ts_6a	3.4	9.7	7.6	8.6	4.7
13r_7 + 13_c2h4 → 13ts_7a	9.5	16.5	14.0	14.2	13.1
13r_8 + 13_c2h4 → 13ts_8a	3.5	10.3	6.3	6.9	5.9
13r_9 + 13_c2h4 → 13ts_9a	-0.6	4.8	0.9	1.6	0.5
02r + 00r → 02ts	14.4	24.4	19.0	21.3	18.1
03r + 00r → 03ts	12.0	23.2	17.4	19.8	16.6
04r + 00r → 04ts	19.8	29.6	24.1	25.3	22.9
05r + 00r → 06ts	25.5	35.9	30.8	30.9	27.8
07r + 00r → 07ts	18.7	29.0	22.8	24.6	21.3
07r + 00r → 08ts	18.7	28.9	22.8	24.6	21.6
09r + 00r → 09ts	29.1	39.5	33.2	34.1	31.3
MUE	3.9	4.3	2.2	3.6	0.0

Table S35. Barrier heights (kcal/mol) of the BHROT27 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
ethane_st → ethane_ecl	2.5	2.6	2.5	2.6	2.7
tmethane_60 → tmethane_0	6.8	6.9	7.0	7.1	7.0
tmethane_60 → tmethane_120	3.2	3.2	3.9	3.7	3.5
tmethane_180 → tmethane_120	3.4	3.5	3.9	3.8	3.7
methanol_st → methanol_ecl	1.1	1.0	0.9	0.9	1.0
methylamine_st → methylamine_ecl	2.7	2.4	2.1	2.2	2.3
h2o2 → h2o2_trans	1.0	0.9	1.0	1.1	1.0
h2o2 → h2o2_cis	7.1	7.1	7.3	7.5	7.2
h2s2 → h2s2_trans	6.0	5.8	5.7	5.9	5.8
h2s2 → h2s2_cis	8.3	7.9	7.8	8.1	8.0
n2h4_st1 → n2h4_ecl1	1.8	1.6	1.5	1.5	1.6
n2h4_st1 → n2h4_ecl2	8.4	8.7	9.2	9.5	8.4
nh2oh_st1 → nh2oh_ecl	6.9	6.9	7.1	7.3	6.9
nh2oh_st2 → nh2oh_ecl	2.8	2.8	2.9	3.1	2.7
acetamide_RC → acetamide_TS1	18.8	18.6	18.9	18.3	17.2
acetamide_RC → acetamide_TS2	16.1	15.8	16.0	15.5	14.5
biphenyl → biphenyl_TS	1.7	1.9	2.3	2.5	2.1
bifuran_anti → bifuran_TS	4.7	5.0	4.6	4.0	3.9
bifuran_syn → bifuran_TS	3.2	3.2	3.0	2.3	2.1
bithiophene_anti → bithiophene_TS	2.2	2.0	2.2	1.7	1.8
bithiophene_syn → bithiophene_TS	2.0	1.6	1.7	1.3	1.4
butadiene_strans → butadiene_TS	7.5	7.2	5.9	5.5	6.3
butadiene_scis → butadiene_TS	3.8	3.5	3.5	3.0	3.4
ethylthiourea_180 → ethylthiourea_TS1	10.9	11.2	12.4	12.0	10.4
ethylthiourea_0 → ethylthiourea_TS1	11.0	11.4	12.6	12.3	10.2
ethylthiourea_180 → ethylthiourea_TS2	17.4	17.6	19.1	18.6	17.2
ethylthiourea_0 → ethylthiourea_TS2	17.5	17.8	19.3	18.9	17.1
MUE	0.5	0.4	0.7	0.5	0.0

Table S36. Double ionization potentials (kcal/mol) of the DIPCS10 database

System	PBE	B3LYP	M11	revM11	Ref.
$C_4H_4 \rightarrow C_4H_4^{2+}$	525.3	522.7	525.1	531.5	529.2
$C_2H_6 \rightarrow C_2H_6^{2+}$	654.3	666.7	665.2	676.3	667.1
$C_2H_4 \rightarrow C_2H_4^{2+}$	648.8	650.6	648.5	655.5	655.8
$N_2H_2 \rightarrow N_2H_2^{2+}$	627.1	633.5	628.3	630.6	626.9
$NH_3 \rightarrow NH_3^{2+}$	779.0	779.0	775.1	776.8	776.5
$CH_2O \rightarrow CH_2O^{2+}$	739.2	752.3	751.0	755.0	747.6
$H_2S \rightarrow H_2S^{2+}$	731.2	733.3	733.1	737.4	733.0
$PH_3 \rightarrow PH_3^{2+}$	648.2	649.5	644.9	652.5	649.6
$Mg \rightarrow Mg^{2+}$	529.2	535.1	515.2	531.6	522.1
$Be \rightarrow Be^{2+}$	634.0	639.5	633.3	643.9	634.8
MUE	4.6	4.4	3.3	4.9	0.0

Table S37. Dissociation energies (kcal/mol) of the HeavySB11 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
$Ge_2H_6 \rightarrow 2GeH_3$	70.0	67.6	76.9	70.7	73.8
$Sn_2Me_6 \rightarrow 2SnMe_3$	55.2	52.9	63.6	56.1	61.7
$Pb_2Me_6 \rightarrow 2PbMe_3$	43.7	40.8	50.9	48.0	52.9
$H_2S_2 \rightarrow 2SH$	70.3	61.9	66.1	65.4	67.9
$H_2Se_2 \rightarrow 2SeH$	60.6	53.2	57.8	55.1	58.4
$Te_2Me_2 \rightarrow 2TeMe$	53.7	46.7	50.4	46.2	52.9
$P_2Me_4 \rightarrow 2PMe_2$	54.8	49.0	55.0	55.3	61.9
$As_2Me_4 \rightarrow 2AsMe_2$	47.2	41.7	50.0	48.2	52.2
$Sb_2Me_4 \rightarrow 2SbMe_2$	41.0	35.8	43.9	37.8	43.8
$Cl_2 \rightarrow 2Cl$	65.6	55.4	60.4	58.9	59.7
$Br_2 \rightarrow 2Br$	57.8	49.1	53.1	50.6	53.2
MUE	4.6	7.6	2.0	4.2	0.0

Table S38. Proton-exchange barriers (kcal/mol) of the PX13 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
nh3_2 → nh3_2_ts	50.6	57.5	58.4	56.7	59.3
nh3_3 → nh3_3_ts	34.6	44.2	45.4	42.2	46.9
nh3_4 → nh3_4_ts	36.4	45.8	47.4	45.4	48.4
h2o_2 → h2o_2_ts	38.0	46.0	46.5	44.2	48.6
h2o_3 → h2o_3_ts	18.7	26.7	28.2	25.4	29.8
h2o_4 → h2o_4_ts	14.6	23.0	25.0	20.9	26.6
h2o_5 → h2o_5_ts	15.7	25.6	28.5	23.1	30.1
h2o_6 → h2o_6_ts	18.2	29.7	33.2	26.6	35.1
hf_2 → hf_2_ts	31.6	38.8	37.5	37.2	42.3
hf_3 → hf_3_ts	10.7	16.9	15.0	16.4	20.7
hf_4 → hf_4_ts	5.3	10.8	8.2	9.9	14.7
hf_5 → hf_5_ts	4.3	10.2	7.2	9.1	14.6
hf_6 → hf_6_ts	4.6	11.5	7.9	10.3	16.6
MUE	11.6	3.6	3.5	5.1	0.0

Table S39. Interaction energies (kcal/mol) of the SIE4x4 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
h_2^+_1.0 → h + h^+	68.6	67.6	64.9	70.2	64.4
h_2^+_1.25 → h + h^+	67.0	65.2	63.7	66.5	58.9
h_2^+_1.5 → h + h^+	61.0	58.5	56.9	57.6	48.7
h_2^+_1.75 → h + h^+	54.9	51.6	48.9	48.3	38.3
he_2^+_1.0 → he + he^+	76.4	76.5	69.5	73.6	56.9
he_2^+_1.25 → he + he^+	75.7	73.5	66.2	69.5	46.9
he_2^+_1.5 → he + he^+	69.5	64.9	55.7	59.1	31.3
he_2^+_1.75 → he + he^+	65.6	59.0	47.4	50.4	19.1
$(nh_3)_2^+$_1.0 → nh_3 + nh_3^+	47.2	42.1	39.9	38.7	35.9
$(nh_3)_2^+$_1.25 → nh_3 + nh_3^+	43.9	37.5	31.3	29.3	25.9
$(nh_3)_2^+$_1.5 → nh_3 + nh_3^+	37.8	29.9	19.3	17.0	13.4
$(nh_3)_2^+$_1.75 → nh_3 + nh_3^+	34.7	25.5	11.6	8.4	4.9
$(h_2o)_2^+$_1.0 → h_2o + h_2o^+	57.3	49.6	43.3	44.8	39.7
$(h_2o)_2^+$_1.25 → h_2o + h_2o^+	55.4	45.6	34.1	35.4	29.1
$(h_2o)_2^+$_1.5 → h_2o + h_2o^+	50.6	38.9	23.0	23.6	16.9
$(h_2o)_2^+$_1.75 → h_2o + h_2o^+	48.5	35.5	16.6	16.1	9.3
MUE	23.4	17.6	9.6	10.6	0.0

Table S40. Bond-dissociation energies (kcal/mol) of the YBDE18 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
f2s-cbh22 → f2s + cbh22	51.5	45.2	53.2	54.5	57.2
f2s-ch2 → f2s + ch2	96.3	87.5	90.4	86.8	91.1
h2s-cbh22 → h2s + cbh22	16.3	11.1	19.7	21.0	21.0
h2s-ch2 → h2s + ch2	43.0	35.2	38.8	35.4	36.4
me2s-cbh22 → me2s + cbh22	31.2	25.2	36.4	37.0	39.0
me2s-ch2 → me2s + ch2	55.9	47.9	52.4	48.9	51.7
nf3-cbh22 → nf3 + cbh22	14.2	7.0	11.6	11.9	12.3
nf3-ch2 → nf3 + ch2	63.7	55.0	54.4	50.4	53.7
nh3-cbh22 → nh3 + cbh22	27.2	23.2	31.9	35.7	32.6
nh3-ch2 → nh3 + ch2	31.7	26.9	31.8	31.0	28.9
nme3-cbh22 → nme3 + cbh22	29.4	24.4	41.2	42.6	42.1
nme3-ch2 → nme3 + ch2	40.2	35.1	45.0	42.8	42.8
pf3-cbh22 → pf3 + cbh22	39.7	36.6	48.6	49.3	52.3
pf3-ch2 → pf3 + ch2	74.6	69.5	76.6	72.7	76.4
ph3-cbh22 → ph3 + cbh22	36.1	32.9	41.6	44.3	44.8
ph3-ch2 → ph3 + ch2	62.0	56.7	60.6	58.5	60.1
pme3-cbh22 → pme3 + cbh22	54.8	50.8	62.7	63.2	66.6
pme3-ch2 → pme3 + ch2	77.6	72.2	77.3	73.9	78.0
MUE	5.9	8.2	1.8	2.1	0.0

Table S41. Noncovalent interaction energies (kcal/mol) of the S66x8 database

Complex	0.90	0.95	1.00	1.05	1.10	1.25	1.50	2.00
PBE exchange-correlation functional								
01_Water-Water	-5.00	-5.24	-5.20	-5.00	-4.70	-3.66	-2.25	-0.91
02_Water-MeOH	-5.07	-5.41	-5.42	-5.24	-4.95	-3.86	-2.36	-0.92
03_Water-$MeNH_2$	-7.15	-7.42	-7.34	-7.04	-6.62	-5.15	-3.11	-1.17
04_Water-Peptide	-7.03	-7.44	-7.48	-7.27	-6.93	-5.61	-3.63	-1.36
05_MeOH-MeOH	-4.94	-5.35	-5.41	-5.27	-5.00	-3.96	-2.44	-0.96
06_MeOH-$MeNH_2$	-6.90	-7.38	-7.44	-7.23	-6.87	-5.43	-3.33	-1.26
07_MeOH-Peptide	-6.88	-7.39	-7.49	-7.33	-7.02	-5.71	-3.44	-1.04
08_MeOH-Water	-4.83	-5.14	-5.15	-4.97	-4.70	-3.69	-2.28	-0.93
09_$MeNH_2$-MeOH	-2.02	-2.34	-2.44	-2.39	-2.26	-1.73	-1.00	-0.36
10_$MeNH_2$-$MeNH_2$	-2.62	-3.11	-3.27	-3.23	-3.08	-2.38	-1.17	-0.34
11_$MeNH_2$-Peptide	-2.74	-3.34	-3.60	-3.63	-3.52	-2.48	-1.14	-0.36
12_$MeNH_2$-Water	-6.94	-7.34	-7.33	-7.09	-6.69	-5.23	-3.16	-1.18
13_Peptide-MeOH	-4.08	-4.62	-4.82	-4.80	-4.64	-3.85	-2.56	-1.16
14_Peptide-$MeNH_2$	-5.59	-6.18	-6.37	-6.30	-6.06	-4.97	-3.22	-1.37
15_Peptide-Peptide	-5.67	-6.32	-6.57	-6.55	-6.37	-5.39	-3.70	-1.55
16_Peptide-Water	-4.22	-4.61	-4.70	-4.61	-4.42	-3.60	-2.37	-1.10
17_Uracil-Uracil_BP	-14.39	-15.48	-15.72	-15.40	-14.74	-11.95	-7.61	-3.07
18_Water-Pyridine	-6.78	-7.08	-7.03	-6.76	-6.36	-4.96	-3.02	-1.16
19_MeOH-Pyridine	-6.65	-7.11	-7.16	-6.96	-6.61	-5.24	-3.23	-1.26
20_AcOH-AcOH	-17.57	-18.74	-18.91	-18.43	-17.58	-14.12	-8.89	-3.50
21_$AcNH_2$-$AcNH_2$	-14.10	-15.10	-15.28	-14.95	-14.30	-11.65	-7.58	-2.92
22_AcOH-Uracil	-17.23	-18.37	-18.58	-18.19	-17.42	-14.23	-9.24	-3.91
23_$AcNH_2$-Uracil	-16.57	-17.67	-17.92	-17.62	-16.97	-14.14	-9.55	-4.40
24_Benzene-Benzene_pi-pi	6.24	3.33	1.70	0.81	0.34	-0.05	0.02	0.04
25_Pyridine-Pyridine_pi-pi	5.37	2.49	0.89	0.02	-0.42	-0.67	-0.36	-0.10
26_Uracil-Uracil_pi-pi	1.53	-1.43	-2.97	-3.68	-3.90	-3.37	-1.99	-0.71
27_Benzene-Pyridine_pi-pi	5.93	2.87	1.22	0.33	-0.11	-0.39	-0.18	-0.03
28_Benzene-Uracil_pi-pi	4.87	1.95	0.34	-0.52	-0.92	-1.00	-0.47	-0.03
29_Pyridine-Uracil_pi-pi	4.92	1.10	-0.81	-1.70	-2.04	-1.84	-1.01	-0.35
30_Benzene-Ethene	3.06	1.66	0.89	0.46	0.24	0.07	0.10	0.07
31_Uracil-Ethene	1.46	0.19	-0.51	-0.87	-1.01	-0.93	-0.51	-0.14
32_Uracil-Ethyne	0.79	-0.50	-1.17	-1.46	-1.54	-1.28	-0.67	-0.18
33_Pyridine-Ethene	2.43	1.21	0.51	0.13	-0.07	-0.18	-0.05	0.03
34_Pentane-Pentane	2.83	1.18	0.25	-0.25	-0.51	-0.60	-0.30	-0.03
35_Neopentane-Pentane	1.94	0.67	0.02	-0.31	-0.45	-0.45	-0.20	-0.02
36_Neopentane-Neopentane	0.95	0.29	-0.07	-0.25	-0.33	-0.31	-0.14	-0.01
37_Cyclopentane-Neopentane	2.10	0.83	0.15	-0.20	-0.37	-0.43	-0.22	-0.03
38_Cyclopentane-Cyclopentane	1.96	0.77	0.02	-0.37	-0.53	-0.52	-0.24	-0.03
39_Benzene-Cyclopentane	3.28	1.39	0.31	-0.27	-0.54	-0.61	-0.30	-0.04
40_Benzene-Neopentane	2.32	0.85	0.05	-0.37	-0.56	-0.57	-0.28	-0.05
41_Uracil-Pentane	3.14	1.24	0.15	-0.44	-0.76	-0.74	-0.30	-0.03
42_Uracil-Cyclopentane	3.26	1.32	0.26	-0.30	-0.57	-0.64	-0.31	-0.04
43_Uracil-Neopentane	2.13	0.58	-0.24	-0.64	-0.81	-0.74	-0.36	-0.06
44_Ethene-Pentane	0.96	0.22	-0.18	-0.37	-0.44	-0.39	-0.18	-0.02
45_Ethyne-Pentane	1.23	0.33	-0.14	-0.38	-0.47	-0.42	-0.19	-0.03
46_Peptide-Pentane	1.56	0.38	-0.32	-0.72	-0.91	-0.93	-0.48	-0.08

47_Benzene-Benzene_TS	2.17	0.66	-0.15	-0.55	-0.72	-0.70	-0.36	-0.09
48_Pyridine-Pyridine_TS	1.19	-0.08	-0.77	-1.11	-1.24	-1.12	-0.65	-0.20
49_Benzene-Pyridine_TS	1.71	0.19	-0.60	-0.98	-1.13	-1.02	-0.58	-0.19
50_Benzene-Ethyne_CH-pi	0.27	-0.79	-1.29	-1.47	-1.49	-1.17	-0.63	-0.19
51_Ethyne-Ethyne_TS	-0.89	-1.17	-1.25	-1.23	-1.15	-0.82	-0.40	-0.11
52_Benzene-AcOH_OH-pi	-1.22	-2.14	-2.56	-2.69	-2.65	-2.13	-1.24	-0.40
53_Benzene-$AcNH_2$_NH-pi	-1.46	-2.17	-2.49	-2.59	-2.54	-2.07	-1.22	-0.36
54_Benzene-Water_OH-pi	-1.60	-2.18	-2.40	-2.42	-2.32	-1.81	-1.04	-0.35
55_Benzene-MeOH_OH-pi	-0.81	-1.71	-2.15	-2.31	-2.31	-1.90	-1.13	-0.38
56_Benzene-$MeNH_2$_NH-pi	0.57	-0.42	-0.95	-1.22	-1.30	-1.09	-0.59	-0.16
57_Benzene-Peptide_NH-pi	1.06	-0.84	-1.79	-2.21	-2.33	-1.99	-1.18	-0.42
58_Pyridine-Pyridine_CH-N	-0.82	-1.99	-2.59	-2.59	-2.38	-1.58	-0.73	-0.17
59_Ethyne-Water_CH-O	-2.59	-2.83	-2.86	-2.76	-2.60	-2.00	-1.19	-0.46
60_Ethyne-AcOH_OH-pi	-3.67	-4.15	-4.25	-4.12	-3.87	-2.91	-1.62	-0.51
61_Pentane-AcOH	0.76	0.10	-0.30	-0.52	-0.63	-0.62	-0.29	-0.03
62_Pentane-$AcNH_2$	0.76	-0.14	-0.65	-0.91	-1.01	-0.91	-0.49	-0.10
63_Benzene-AcOH	1.68	0.15	-0.66	-1.04	-1.19	-1.04	-0.54	-0.13
64_Peptide-Ethene	-0.09	-0.78	-1.14	-1.29	-1.32	-1.08	-0.55	-0.11
65_Pyridine-Ethyne	-3.39	-3.68	-3.71	-3.59	-3.39	-2.61	-1.54	-0.56
66_$MeNH_2$-Pyridine	-0.86	-1.53	-1.88	-2.02	-2.02	-1.70	-1.03	-0.34
MUE (S66x8)				1.50				
B3LYP exchange-correlation functional								
01_Water-Water	-4.45	-4.76	-4.77	-4.59	-4.32	-3.34	-2.03	-0.86
02_Water-MeOH	-4.47	-4.87	-4.94	-4.79	-4.53	-3.52	-2.11	-0.87
03_Water-$MeNH_2$	-6.12	-6.51	-6.54	-6.33	-5.98	-4.65	-2.78	-1.06
04_Water-Peptide	-6.35	-6.84	-6.92	-6.76	-6.45	-5.18	-3.29	-1.28
05_MeOH-MeOH	-4.20	-4.69	-4.83	-4.74	-4.51	-3.55	-2.16	-0.89
06_MeOH-$MeNH_2$	-5.48	-6.12	-6.32	-6.23	-5.96	-4.75	-2.88	-1.11
07_MeOH-Peptide	-5.88	-6.49	-6.67	-6.58	-6.32	-5.12	-3.01	-0.96
08_MeOH-Water	-4.18	-4.56	-4.63	-4.51	-4.27	-3.34	-2.04	-0.87
09_$MeNH_2$-MeOH	-1.20	-1.60	-1.76	-1.76	-1.69	-1.29	-0.74	-0.31
10_$MeNH_2$-$MeNH_2$	-1.35	-2.00	-2.29	-2.35	-2.28	-1.76	-0.85	-0.29
11_$MeNH_2$-Peptide	-1.52	-2.27	-2.63	-2.74	-2.70	-1.87	-0.86	-0.34
12_$MeNH_2$-Water	-5.83	-6.36	-6.47	-6.31	-5.99	-4.69	-2.80	-1.07
13_Peptide-MeOH	-3.22	-3.87	-4.14	-4.18	-4.06	-3.36	-2.22	-1.08
14_Peptide-$MeNH_2$	-4.08	-4.85	-5.19	-5.24	-5.10	-4.23	-2.74	-1.22
15_Peptide-Peptide	-4.52	-5.30	-5.64	-5.70	-5.58	-4.73	-3.22	-1.43
16_Peptide-Water	-3.59	-4.05	-4.20	-4.15	-3.98	-3.24	-2.13	-1.06
17_Uracil-Uracil_BP	-13.24	-14.55	-14.94	-14.75	-14.17	-11.51	-7.24	-2.90
18_Water-Pyridine	-5.83	-6.25	-6.30	-6.11	-5.78	-4.51	-2.72	-1.08
19_MeOH-Pyridine	-5.45	-6.06	-6.24	-6.14	-5.88	-4.68	-2.86	-1.14
20_AcOH-AcOH	-16.36	-17.69	-18.00	-17.64	-16.86	-13.56	-8.43	-3.24
21_$AcNH_2$-$AcNH_2$	-12.93	-14.12	-14.46	-14.23	-13.67	-11.13	-7.16	-2.77
22_AcOH-Uracil	-16.15	-17.48	-17.84	-17.56	-16.88	-13.83	-8.91	-3.74
23_$AcNH_2$-Uracil	-15.50	-16.79	-17.20	-17.02	-16.45	-13.76	-9.24	-4.27
24_Benzene-Benzene_pi-pi	9.28	5.67	3.57	2.35	1.63	0.73	0.30	0.06
25_Pyridine-Pyridine_pi-pi	8.39	4.82	2.75	1.55	0.87	0.15	-0.05	-0.09
26_Uracil-Uracil_pi-pi	4.22	0.74	-1.15	-2.09	-2.48	-2.30	-1.44	-0.67
27_Benzene-Pyridine_pi-pi	9.02	5.23	3.08	1.86	1.18	0.41	0.12	-0.01
28_Benzene-Uracil_pi-pi	7.98	4.40	2.32	1.14	0.51	-0.03	-0.02	0.01

29_Pyridine-Uracil_pi-pi	8.08	3.43	0.99	-0.22	-0.78	-1.02	-0.70	-0.35
30_Benzene-Ethene	5.09	3.27	2.20	1.56	1.18	0.66	0.34	0.09
31_Uracil-Ethene	3.16	1.58	0.66	0.16	-0.11	-0.31	-0.23	-0.12
32_Uracil-Ethyne	2.33	0.74	-0.12	-0.56	-0.75	-0.72	-0.41	-0.16
33_Pyridine-Ethene	4.38	2.77	1.81	1.23	0.88	0.44	0.23	0.06
34_Pentane-Pentane	5.25	3.27	2.10	1.42	1.01	0.52	0.27	0.05
35_Neopentane-Pentane	3.82	2.27	1.41	0.94	0.67	0.35	0.18	0.03
36_Neopentane-Neopentane	2.34	1.53	1.04	0.74	0.56	0.31	0.15	0.03
37_Cyclopentane-Neopentane	3.92	2.38	1.51	1.00	0.71	0.36	0.18	0.04
38_Cyclopentane-Cyclopentane	3.85	2.41	1.46	0.93	0.64	0.33	0.18	0.03
39_Benzene-Cyclopentane	5.70	3.37	1.96	1.14	0.69	0.23	0.09	0.00
40_Benzene-Neopentane	4.31	2.49	1.44	0.84	0.50	0.15	0.05	-0.02
41_Uracil-Pentane	5.61	3.33	1.98	1.19	0.68	0.25	0.11	0.01
42_Uracil-Cyclopentane	5.44	3.15	1.85	1.11	0.71	0.29	0.13	0.01
43_Uracil-Neopentane	3.94	2.11	1.10	0.55	0.26	0.02	-0.01	-0.03
44_Ethene-Pentane	2.40	1.47	0.93	0.63	0.46	0.25	0.13	0.02
45_Ethyne-Pentane	2.70	1.57	0.93	0.57	0.36	0.14	0.04	-0.01
46_Peptide-Pentane	3.66	2.24	1.35	0.81	0.50	0.16	0.06	-0.02
47_Benzene-Benzene_TS	3.94	2.08	1.04	0.46	0.16	-0.09	-0.08	-0.06
48_Pyridine-Pyridine_TS	2.76	1.20	0.32	-0.16	-0.39	-0.50	-0.32	-0.17
49_Benzene-Pyridine_TS	3.48	1.61	0.57	0.02	-0.26	-0.42	-0.30	-0.17
50_Benzene-Ethyne_CH-pi	1.63	0.29	-0.40	-0.71	-0.83	-0.72	-0.42	-0.18
51_Ethyne-Ethyne_TS	-0.21	-0.60	-0.76	-0.80	-0.77	-0.56	-0.29	-0.10
52_Benzene-AcOH_OH-pi	0.43	-0.77	-1.40	-1.68	-1.76	-1.50	-0.89	-0.35
53_Benzene-$AcNH_2$_NH-pi	-0.15	-1.05	-1.52	-1.72	-1.76	-1.47	-0.87	-0.30
54_Benzene-Water_OH-pi	-0.35	-1.14	-1.51	-1.64	-1.63	-1.32	-0.80	-0.33
55_Benzene-MeOH_OH-pi	1.04	-0.18	-0.85	-1.19	-1.33	-1.21	-0.77	-0.33
56_Benzene-$MeNH_2$_NH-pi	2.32	1.04	0.29	-0.15	-0.37	-0.45	-0.29	-0.13
57_Benzene-Peptide_NH-pi	3.41	1.05	-0.23	-0.88	-1.18	-1.21	-0.80	-0.38
58_Pyridine-Pyridine_CH-N	0.29	-1.08	-1.85	-1.95	-1.81	-1.16	-0.53	-0.15
59_Ethyne-Water_CH-O	-2.19	-2.47	-2.53	-2.46	-2.31	-1.76	-1.05	-0.44
60_Ethyne-AcOH_OH-pi	-2.51	-3.17	-3.41	-3.39	-3.22	-2.42	-1.31	-0.44
61_Pentane-AcOH	2.31	1.51	1.00	0.67	0.47	0.23	0.12	0.02
62_Pentane-$AcNH_2$	2.56	1.45	0.79	0.40	0.19	0.01	0.00	-0.03
63_Benzene-AcOH	3.60	1.70	0.64	0.07	-0.21	-0.37	-0.24	-0.11
64_Peptide-Ethene	1.12	0.30	-0.16	-0.39	-0.49	-0.45	-0.24	-0.09
65_Pyridine-Ethyne	-2.66	-3.06	-3.18	-3.12	-2.96	-2.28	-1.33	-0.52
66_$MeNH_2$-Pyridine	0.65	-0.25	-0.76	-1.03	-1.13	-1.02	-0.62	-0.26
MUE (S66x8)				2.32				
M11 exchange-correlation functional								
01_Water-Water	-4.78	-5.09	-5.06	-4.84	-4.52	-3.47	-2.19	-0.98
02_Water-MeOH	-5.13	-5.50	-5.49	-5.26	-4.91	-3.73	-2.30	-1.00
03_Water-$MeNH_2$	-6.13	-6.59	-6.66	-6.48	-6.13	-4.75	-2.87	-1.18
04_Water-Peptide	-8.03	-8.44	-8.41	-8.11	-7.64	-5.95	-3.75	-1.49
05_MeOH-MeOH	-4.83	-5.30	-5.37	-5.19	-4.88	-3.74	-2.32	-1.02
06_MeOH-$MeNH_2$	-6.33	-6.87	-6.99	-6.83	-6.49	-5.04	-3.02	-1.24
07_MeOH-Peptide	-7.47	-8.00	-8.06	-7.81	-7.38	-5.76	-3.33	-1.09
08_MeOH-Water	-4.52	-4.91	-4.95	-4.77	-4.48	-3.46	-2.19	-0.99
09_$MeNH_2$-MeOH	-2.23	-2.44	-2.41	-2.28	-2.09	-1.53	-0.92	-0.38
10_$MeNH_2$-$MeNH_2$	-3.42	-3.78	-3.78	-3.58	-3.28	-2.30	-1.08	-0.36

11_$MeNH_2$-Peptide	-4.88	-5.17	-5.09	-4.82	-4.44	-2.69	-1.18	-0.41
12_$MeNH_2$-Water	-6.52	-7.02	-7.10	-6.89	-6.51	-5.01	-2.98	-1.21
13_Peptide-MeOH	-5.22	-5.68	-5.75	-5.56	-5.25	-4.13	-2.67	-1.29
14_Peptide-$MeNH_2$	-5.85	-6.48	-6.67	-6.57	-6.27	-4.96	-3.10	-1.41
15_Peptide-Peptide	-7.41	-7.98	-8.08	-7.88	-7.49	-5.98	-3.89	-1.67
16_Peptide-Water	-4.49	-4.89	-4.94	-4.79	-4.55	-3.64	-2.44	-1.22
17_Uracil-Uracil_BP	-14.47	-15.88	-16.32	-16.09	-15.42	-12.27	-7.58	-3.17
18_Water-Pyridine	-5.89	-6.37	-6.46	-6.29	-5.95	-4.59	-2.79	-1.19
19_MeOH-Pyridine	-5.71	-6.33	-6.52	-6.41	-6.12	-4.81	-2.92	-1.25
20_AcOH-AcOH	-17.99	-19.33	-19.65	-19.27	-18.42	-14.63	-8.85	-3.52
21_$AcNH_2$-$AcNH_2$	-14.17	-15.48	-15.84	-15.56	-14.87	-11.84	-7.51	-3.02
22_AcOH-Uracil	-17.50	-18.92	-19.33	-19.05	-18.30	-14.78	-9.32	-4.06
23_$AcNH_2$-Uracil	-16.80	-18.17	-18.62	-18.41	-17.77	-14.64	-9.67	-4.61
24_Benzene-Benzene_pi-pi	0.18	-1.41	-1.81	-1.67	-1.34	-0.30	0.08	0.06
25_Pyridine-Pyridine_pi-pi	-0.93	-2.54	-2.94	-2.76	-2.39	-1.17	-0.38	-0.12
26_Uracil-Uracil_pi-pi	-7.99	-9.16	-9.02	-8.27	-7.30	-4.56	-2.25	-0.79
27_Benzene-Pyridine_pi-pi	-0.39	-2.10	-2.49	-2.32	-1.91	-0.76	-0.13	-0.03
28_Benzene-Uracil_pi-pi	-3.72	-5.04	-5.12	-4.65	-3.96	-1.97	-0.57	-0.04
29_Pyridine-Uracil_pi-pi	-3.94	-5.98	-6.16	-5.60	-4.79	-2.58	-1.17	-0.39
30_Benzene-Ethene	0.01	-0.66	-0.79	-0.67	-0.48	0.00	0.15	0.09
31_Uracil-Ethene	-2.58	-3.00	-2.94	-2.67	-2.30	-1.32	-0.57	-0.17
32_Uracil-Ethyne	-2.83	-3.40	-3.39	-3.10	-2.73	-1.65	-0.73	-0.21
33_Pyridine-Ethene	-0.59	-1.14	-1.22	-1.08	-0.87	-0.28	0.02	0.04
34_Pentane-Pentane	-3.80	-3.91	-3.55	-3.01	-2.45	-1.09	-0.27	-0.04
35_Neopentane-Pentane	-1.81	-2.10	-1.98	-1.70	-1.38	-0.62	-0.19	-0.03
36_Neopentane-Neopentane	-0.81	-0.98	-0.96	-0.85	-0.71	-0.34	-0.12	-0.01
37_Cyclopentane-Neopentane	-1.57	-1.85	-1.75	-1.52	-1.25	-0.58	-0.18	-0.03
38_Cyclopentane-Cyclopentane	-1.68	-1.98	-1.90	-1.64	-1.32	-0.57	-0.16	-0.03
39_Benzene-Cyclopentane	-2.31	-3.07	-3.10	-2.78	-2.33	-1.13	-0.35	-0.06
40_Benzene-Neopentane	-1.64	-2.22	-2.24	-2.02	-1.72	-0.89	-0.32	-0.08
41_Uracil-Pentane	-4.34	-4.67	-4.37	-3.80	-3.02	-1.24	-0.37	-0.04
42_Uracil-Cyclopentane	-2.90	-3.42	-3.26	-2.84	-2.34	-1.10	-0.35	-0.06
43_Uracil-Neopentane	-2.66	-3.07	-2.93	-2.56	-2.13	-1.07	-0.40	-0.08
44_Ethene-Pentane	-1.85	-1.87	-1.67	-1.40	-1.13	-0.51	-0.17	-0.03
45_Ethyne-Pentane	-1.16	-1.41	-1.35	-1.17	-0.96	-0.46	-0.19	-0.04
46_Peptide-Pentane	-4.46	-4.43	-4.07	-3.57	-3.03	-1.64	-0.52	-0.10
47_Benzene-Benzene_TS	-1.17	-2.01	-2.18	-2.05	-1.80	-1.03	-0.43	-0.12
48_Pyridine-Pyridine_TS	-2.15	-2.78	-2.86	-2.68	-2.40	-1.53	-0.75	-0.28
49_Benzene-Pyridine_TS	-1.76	-2.61	-2.77	-2.61	-2.32	-1.45	-0.69	-0.26
50_Benzene-Ethyne_CH-pi	-2.03	-2.68	-2.77	-2.60	-2.33	-1.52	-0.77	-0.25
51_Ethyne-Ethyne_TS	-0.92	-1.16	-1.21	-1.15	-1.06	-0.76	-0.42	-0.13
52_Benzene-AcOH_OH-pi	-4.14	-4.60	-4.57	-4.28	-3.88	-2.67	-1.42	-0.50
53_Benzene-$AcNH_2$_NH-pi	-3.60	-3.99	-3.98	-3.77	-3.47	-2.48	-1.34	-0.41
54_Benzene-Water_OH-pi	-3.43	-3.65	-3.55	-3.29	-2.98	-2.09	-1.17	-0.43
55_Benzene-MeOH_OH-pi	-3.80	-4.22	-4.19	-3.93	-3.57	-2.46	-1.31	-0.47
56_Benzene-$MeNH_2$_NH-pi	-2.58	-2.98	-2.97	-2.73	-2.39	-1.46	-0.67	-0.20
57_Benzene-Peptide_NH-pi	-3.92	-4.88	-4.95	-4.62	-4.12	-2.68	-1.36	-0.52
58_Pyridine-Pyridine_CH-N	-2.08	-3.07	-3.32	-3.02	-2.61	-1.58	-0.75	-0.21
59_Ethyne-Water_CH-O	-2.64	-2.88	-2.88	-2.76	-2.58	-1.98	-1.24	-0.53
60_Ethyne-AcOH_OH-pi	-4.55	-4.96	-4.93	-4.65	-4.25	-3.00	-1.63	-0.56
61_Pentane-AcOH	-2.63	-2.56	-2.35	-2.06	-1.75	-0.96	-0.29	-0.04

62_Pentane-$AcNH_2$	-3.36	-3.34	-3.07	-2.69	-2.28	-1.25	-0.48	-0.11
63_Benzene-AcOH	-3.12	-3.68	-3.60	-3.24	-2.80	-1.60	-0.66	-0.17
64_Peptide-Ethene	-2.41	-2.60	-2.52	-2.31	-2.05	-1.31	-0.60	-0.13
65_Pyridine-Ethyne	-3.05	-3.46	-3.55	-3.44	-3.23	-2.45	-1.48	-0.60
66_$MeNH_2$-Pyridine	-3.10	-3.42	-3.40	-3.18	-2.88	-1.96	-1.03	-0.38
MUE (S66x8)				0.43				
revM11 exchange-correlation functional								
01_Water-Water	-5.21	-5.50	-5.50	-5.30	-4.99	-3.87	-2.31	-0.95
02_Water-MeOH	-5.70	-6.03	-6.02	-5.81	-5.47	-4.22	-2.49	-0.98
03_Water-$MeNH_2$	-6.97	-7.30	-7.28	-7.03	-6.65	-5.22	-3.15	-1.18
04_Water-Peptide	-8.53	-8.91	-8.90	-8.63	-8.20	-6.54	-4.05	-1.45
05_MeOH-MeOH	-5.49	-5.90	-5.95	-5.78	-5.47	-4.27	-2.54	-1.00
06_MeOH-$MeNH_2$	-7.39	-7.80	-7.80	-7.54	-7.13	-5.58	-3.35	-1.24
07_MeOH-Peptide	-8.01	-8.52	-8.59	-8.39	-8.01	-6.44	-3.67	-1.05
08_MeOH-Water	-5.01	-5.38	-5.42	-5.26	-4.98	-3.89	-2.34	-0.96
09_$MeNH_2$-MeOH	-2.89	-3.10	-3.07	-2.89	-2.65	-1.86	-0.97	-0.36
10_$MeNH_2$-$MeNH_2$	-4.00	-4.42	-4.46	-4.28	-3.97	-2.82	-1.16	-0.34
11_$MeNH_2$-Peptide	-5.24	-5.71	-5.77	-5.58	-5.24	-3.16	-1.19	-0.39
12_$MeNH_2$-Water	-7.46	-7.83	-7.80	-7.53	-7.10	-5.54	-3.28	-1.21
13_Peptide-MeOH	-5.74	-6.24	-6.35	-6.22	-5.92	-4.68	-2.84	-1.24
14_Peptide-$MeNH_2$	-6.62	-7.18	-7.32	-7.19	-6.88	-5.53	-3.40	-1.39
15_Peptide-Peptide	-7.78	-8.39	-8.55	-8.42	-8.10	-6.61	-4.19	-1.60
16_Peptide-Water	-4.90	-5.33	-5.43	-5.31	-5.06	-4.02	-2.51	-1.16
17_Uracil-Uracil_BP	-14.34	-15.74	-16.22	-16.09	-15.56	-12.85	-8.13	-3.13
18_Water-Pyridine	-6.70	-7.05	-7.05	-6.82	-6.45	-5.07	-3.06	-1.18
19_MeOH-Pyridine	-6.68	-7.16	-7.24	-7.07	-6.73	-5.36	-3.26	-1.25
20_AcOH-AcOH	-18.18	-19.43	-19.70	-19.33	-18.55	-15.17	-9.61	-3.60
21_$AcNH_2$-$AcNH_2$	-14.17	-15.46	-15.88	-15.71	-15.17	-12.54	-8.05	-2.97
22_AcOH-Uracil	-17.55	-18.90	-19.30	-19.06	-18.41	-15.32	-9.99	-4.08
23_$AcNH_2$-Uracil	-16.69	-18.06	-18.54	-18.42	-17.90	-15.17	-10.23	-4.59
24_Benzene-Benzene_pi-pi	0.53	-1.67	-2.46	-2.49	-2.16	-0.76	0.07	0.06
25_Pyridine-Pyridine_pi-pi	-0.46	-2.71	-3.52	-3.54	-3.19	-1.65	-0.38	-0.11
26_Uracil-Uracil_pi-pi	-7.51	-9.51	-9.91	-9.41	-8.46	-5.18	-2.17	-0.73
27_Benzene-Pyridine_pi-pi	0.09	-2.29	-3.10	-3.11	-2.73	-1.23	-0.15	-0.02
28_Benzene-Uracil_pi-pi	-3.05	-5.15	-5.75	-5.54	-4.91	-2.54	-0.57	-0.02
29_Pyridine-Uracil_pi-pi	-3.00	-6.04	-6.87	-6.58	-5.77	-3.07	-1.11	-0.37
30_Benzene-Ethene	-0.16	-1.17	-1.47	-1.40	-1.16	-0.34	0.13	0.09
31_Uracil-Ethene	-2.73	-3.49	-3.61	-3.38	-2.96	-1.65	-0.56	-0.15
32_Uracil-Ethyne	-2.96	-3.85	-4.02	-3.79	-3.37	-1.97	-0.72	-0.18
33_Pyridine-Ethene	-0.76	-1.64	-1.90	-1.82	-1.57	-0.68	-0.02	0.05
34_Pentane-Pentane	-4.39	-4.99	-4.83	-4.28	-3.59	-1.70	-0.32	-0.01
35_Neopentane-Pentane	-2.43	-3.04	-3.01	-2.67	-2.23	-1.03	-0.21	-0.01
36_Neopentane-Neopentane	-1.69	-1.91	-1.84	-1.63	-1.37	-0.65	-0.13	0.00
37_Cyclopentane-Neopentane	-2.15	-2.74	-2.74	-2.47	-2.10	-1.05	-0.24	-0.01
38_Cyclopentane-Cyclopentane	-2.48	-3.09	-3.14	-2.81	-2.35	-1.07	-0.20	-0.01
39_Benzene-Cyclopentane	-2.21	-3.47	-3.81	-3.60	-3.13	-1.57	-0.35	-0.03
40_Benzene-Neopentane	-1.86	-2.78	-2.98	-2.79	-2.43	-1.24	-0.31	-0.05
41_Uracil-Pentane	-4.64	-5.54	-5.52	-5.01	-4.10	-1.67	-0.31	-0.02
42_Uracil-Cyclopentane	-3.30	-4.32	-4.39	-3.97	-3.35	-1.56	-0.33	-0.04
43_Uracil-Neopentane	-3.11	-3.89	-3.89	-3.49	-2.94	-1.42	-0.36	-0.06

44_Ethene-Pentane	-2.51	-2.69	-2.51	-2.17	-1.77	-0.79	-0.16	-0.01
45_Ethyne-Pentane	-1.74	-2.13	-2.09	-1.85	-1.53	-0.69	-0.16	-0.02
46_Peptide-Pentane	-5.12	-5.45	-5.25	-4.76	-4.12	-2.25	-0.53	-0.07
47_Benzene-Benzene_TS	-1.21	-2.34	-2.71	-2.64	-2.37	-1.32	-0.41	-0.09
48_Pyridine-Pyridine_TS	-2.17	-3.15	-3.45	-3.35	-3.05	-1.88	-0.74	-0.23
49_Benzene-Pyridine_TS	-1.72	-2.89	-3.25	-3.16	-2.86	-1.71	-0.66	-0.22
50_Benzene-Ethyne_CH-pi	-1.99	-2.88	-3.12	-3.00	-2.71	-1.65	-0.70	-0.22
51_Ethyne-Ethyne_TS	-1.13	-1.43	-1.49	-1.42	-1.29	-0.83	-0.38	-0.11
52_Benzene-AcOH_OH-pi	-4.38	-5.00	-5.09	-4.86	-4.47	-3.05	-1.43	-0.44
53_Benzene-$AcNH_2$_NH-pi	-3.82	-4.37	-4.48	-4.33	-4.02	-2.84	-1.38	-0.37
54_Benzene-Water_OH-pi	-3.76	-4.10	-4.06	-3.80	-3.43	-2.28	-1.12	-0.39
55_Benzene-MeOH_OH-pi	-4.10	-4.72	-4.81	-4.59	-4.20	-2.81	-1.29	-0.42
56_Benzene-$MeNH_2$_NH-pi	-2.88	-3.51	-3.63	-3.42	-3.02	-1.74	-0.64	-0.18
57_Benzene-Peptide_NH-pi	-3.81	-5.19	-5.54	-5.32	-4.82	-3.03	-1.31	-0.46
58_Pyridine-Pyridine_CH-N	-2.13	-3.38	-3.90	-3.69	-3.24	-1.87	-0.76	-0.19
59_Ethyne-Water_CH-O	-2.71	-3.04	-3.11	-3.02	-2.84	-2.13	-1.22	-0.48
60_Ethyne-AcOH_OH-pi	-4.79	-5.28	-5.33	-5.13	-4.77	-3.43	-1.72	-0.51
61_Pentane-AcOH	-3.57	-3.62	-3.40	-3.03	-2.60	-1.41	-0.30	-0.02
62_Pentane-$AcNH_2$	-4.16	-4.39	-4.20	-3.77	-3.25	-1.76	-0.52	-0.08
63_Benzene-AcOH	-3.09	-4.05	-4.20	-3.92	-3.44	-1.90	-0.62	-0.15
64_Peptide-Ethene	-3.00	-3.34	-3.31	-3.07	-2.72	-1.64	-0.58	-0.11
65_Pyridine-Ethyne	-3.02	-3.49	-3.65	-3.62	-3.46	-2.68	-1.53	-0.57
66_$MeNH_2$-Pyridine	-3.55	-4.03	-4.12	-3.96	-3.66	-2.51	-1.15	-0.34
MUE (S66x8)				0.30				
CCSD(T) reference values								
01_Water-Water	-4.57	-4.88	-4.89	-4.72	-4.45	-3.46	-2.11	-0.87
02_Water-MeOH	-5.19	-5.55	-5.57	-5.38	-5.08	-3.94	-2.39	-0.95
03_Water-$MeNH_2$	-6.49	-6.87	-6.88	-6.65	-6.28	-4.92	-2.98	-1.14
04_Water-Peptide	-7.63	-8.06	-8.08	-7.84	-7.46	-5.99	-3.83	-1.44
05_MeOH-MeOH	-5.28	-5.69	-5.75	-5.58	-5.28	-4.14	-2.52	-1.01
06_MeOH-$MeNH_2$	-6.97	-7.47	-7.54	-7.34	-6.97	-5.50	-3.35	-1.27
07_MeOH-Peptide	-7.63	-8.14	-8.22	-8.02	-7.66	-6.18	-3.65	-1.10
08_MeOH-Water	-4.59	-4.95	-5.00	-4.85	-4.59	-3.59	-2.20	-0.91
09_$MeNH_2$-MeOH	-2.81	-3.04	-3.04	-2.90	-2.69	-1.98	-1.10	-0.39
10_$MeNH_2$-$MeNH_2$	-3.70	-4.09	-4.15	-4.01	-3.75	-2.79	-1.31	-0.39
11_$MeNH_2$-Peptide	-4.95	-5.36	-5.41	-5.24	-4.94	-3.21	-1.40	-0.46
12_$MeNH_2$-Water	-6.75	-7.20	-7.25	-7.03	-6.66	-5.22	-3.15	-1.20
13_Peptide-MeOH	-5.67	-6.11	-6.18	-6.03	-5.74	-4.60	-2.95	-1.30
14_Peptide-$MeNH_2$	-6.81	-7.34	-7.45	-7.29	-6.97	-5.61	-3.55	-1.49
15_Peptide-Peptide	-8.02	-8.53	-8.62	-8.45	-8.10	-6.66	-4.42	-1.77
16_Peptide-Water	-4.70	-5.06	-5.12	-4.98	-4.74	-3.79	-2.45	-1.13
17_Uracil-Uracil_BP	-15.70	-16.90	-17.18	-16.86	-16.17	-13.15	-8.35	-3.33
18_Water-Pyridine	-6.39	-6.80	-6.83	-6.62	-6.27	-4.93	-3.01	-1.19
19_MeOH-Pyridine	-6.78	-7.31	-7.40	-7.23	-6.88	-5.48	-3.38	-1.33
20_AcOH-AcOH	-17.45	-18.79	-19.09	-18.72	-17.94	-14.56	-9.21	-3.59
21_$AcNH_2$-$AcNH_2$	-14.93	-16.03	-16.26	-15.94	-15.26	-12.42	-8.00	-3.00
22_AcOH-Uracil	-17.90	-19.19	-19.49	-19.15	-18.41	-15.14	-9.86	-4.15
23_$AcNH_2$-Uracil	-17.70	-18.89	-19.19	-18.90	-18.22	-15.21	-10.23	-4.65
24_Benzene-Benzene_pi-pi	-0.23	-2.07	-2.74	-2.80	-2.58	-1.54	-0.49	-0.06
25_Pyridine-Pyridine_pi-pi	-1.32	-3.17	-3.83	-3.86	-3.58	-2.36	-0.96	-0.24

26_Uracil-Uracil_pi-pi	-7.86	-9.50	-9.82	-9.43	-8.69	-6.07	-3.10	-0.99
27_Benzene-Pyridine_pi-pi	-0.73	-2.69	-3.37	-3.40	-3.13	-1.97	-0.72	-0.15
28_Benzene-Uracil_pi-pi	-3.53	-5.22	-5.71	-5.55	-5.08	-3.29	-1.36	-0.25
29_Pyridine-Uracil_pi-pi	-3.74	-6.17	-6.81	-6.58	-5.97	-3.87	-1.78	-0.53
30_Benzene-Ethene	-0.26	-1.13	-1.41	-1.40	-1.26	-0.69	-0.17	0.01
31_Uracil-Ethene	-2.57	-3.24	-3.38	-3.24	-2.96	-1.99	-0.93	-0.25
32_Uracil-Ethyne	-2.79	-3.56	-3.74	-3.59	-3.29	-2.23	-1.04	-0.27
33_Pyridine-Ethene	-0.89	-1.62	-1.86	-1.83	-1.67	-1.03	-0.37	-0.05
34_Pentane-Pentane	-2.86	-3.62	-3.77	-3.61	-3.30	-2.24	-1.05	-0.27
35_Neopentane-Pentane	-1.85	-2.49	-2.61	-2.48	-2.25	-1.50	-0.70	-0.18
36_Neopentane-Neopentane	-1.45	-1.74	-1.77	-1.68	-1.54	-1.05	-0.50	-0.14
37_Cyclopentane-Neopentane	-1.61	-2.25	-2.41	-2.33	-2.14	-1.47	-0.71	-0.19
38_Cyclopentane-Cyclopentane	-2.24	-2.84	-3.00	-2.86	-2.60	-1.71	-0.79	-0.20
39_Benzene-Cyclopentane	-2.16	-3.24	-3.57	-3.47	-3.17	-2.07	-0.90	-0.19
40_Benzene-Neopentane	-1.86	-2.68	-2.89	-2.80	-2.57	-1.70	-0.77	-0.19
41_Uracil-Pentane	-3.83	-4.69	-4.84	-4.60	-4.08	-2.44	-0.98	-0.21
42_Uracil-Cyclopentane	-3.05	-3.97	-4.13	-3.92	-3.54	-2.29	-1.02	-0.25
43_Uracil-Neopentane	-2.87	-3.60	-3.70	-3.49	-3.15	-2.05	-0.92	-0.23
44_Ethene-Pentane	-1.66	-1.97	-1.99	-1.86	-1.67	-1.09	-0.49	-0.12
45_Ethyne-Pentane	-1.13	-1.63	-1.75	-1.68	-1.52	-0.98	-0.42	-0.10
46_Peptide-Pentane	-3.75	-4.21	-4.24	-4.05	-3.73	-2.63	-1.19	-0.29
47_Benzene-Benzene_TS	-1.64	-2.58	-2.87	-2.82	-2.60	-1.77	-0.83	-0.22
48_Pyridine-Pyridine_TS	-2.53	-3.31	-3.53	-3.45	-3.22	-2.29	-1.18	-0.37
49_Benzene-Pyridine_TS	-2.09	-3.04	-3.32	-3.26	-3.02	-2.10	-1.05	-0.33
50_Benzene-Ethyne_CH-pi	-1.87	-2.65	-2.86	-2.79	-2.58	-1.79	-0.89	-0.27
51_Ethyne-Ethyne_TS	-1.21	-1.47	-1.52	-1.46	-1.35	-0.93	-0.46	-0.14
52_Benzene-AcOH_OH-pi	-3.97	-4.58	-4.70	-4.55	-4.25	-3.13	-1.70	-0.55
53_Benzene-$AcNH_2$_NH-pi	-3.79	-4.27	-4.36	-4.23	-3.97	-2.97	-1.65	-0.48
54_Benzene-Water_OH-pi	-2.80	-3.21	-3.27	-3.13	-2.90	-2.10	-1.16	-0.42
55_Benzene-MeOH_OH-pi	-3.45	-4.05	-4.19	-4.07	-3.80	-2.80	-1.53	-0.52
56_Benzene-$MeNH_2$_NH-pi	-2.51	-3.09	-3.23	-3.12	-2.86	-1.95	-0.94	-0.26
57_Benzene-Peptide_NH-pi	-3.75	-4.96	-5.28	-5.14	-4.78	-3.41	-1.80	-0.62
58_Pyridine-Pyridine_CH-N	-2.80	-3.82	-4.15	-3.89	-3.45	-2.18	-1.01	-0.28
59_Ethyne-Water_CH-O	-2.52	-2.80	-2.85	-2.76	-2.60	-1.98	-1.17	-0.46
60_Ethyne-AcOH_OH-pi	-4.28	-4.78	-4.86	-4.69	-4.39	-3.26	-1.77	-0.56
61_Pentane-AcOH	-2.70	-2.90	-2.88	-2.73	-2.52	-1.79	-0.78	-0.17
62_Pentane-$AcNH_2$	-3.15	-3.50	-3.51	-3.32	-3.04	-2.12	-1.04	-0.27
63_Benzene-AcOH	-2.73	-3.60	-3.80	-3.65	-3.34	-2.24	-1.02	-0.26
64_Peptide-Ethene	-2.60	-2.95	-2.99	-2.85	-2.63	-1.86	-0.88	-0.19
65_Pyridine-Ethyne	-3.54	-3.91	-3.99	-3.89	-3.68	-2.84	-1.67	-0.62
66_$MeNH_2$-Pyridine	-3.45	-3.88	-3.97	-3.85	-3.62	-2.71	-1.50	-0.49
MUE (S66x8)				0.00				

Table S42. Barrier heights (kcal/mol) of the TMBH22 database

Reaction	PBE	B3LYP	M11	revM11	Ref.
Mo_W					
reaction 1	15.9	24.4	24.9	23.1	25.0
reaction 2	5.9	6.9	8.6	7.8	8.5
reaction 3a	19.6	18.8	18.6	20.9	18.7
reaction 3b	3.7	17.2	25.2	24.3	13.5
reaction 4a_Mo	-0.6	0.8	1.8	0.9	0.1
reaction_4b_Mo	15.7	16.4	15.0	19.1	14.7
reaction 4a_W	-0.9	0.1	0.5	0.0	-0.6
reaction 4b	17.7	19.4	18.7	23.2	14.7
reaction 5a	5.5	1.7	2.8	4.6	4.3
reaction 5b	28.1	23.6	19.1	21.7	19.8
reaction 6_Mo	11.7	22.8	29.0	30.5	17.4
reaction 6_W	9.0	21.0	27.3	28.7	15.8
reaction 7	5.9	9.8	10.8	7.7	8.6
Zr					
reaction 1	5.3	9.9	3.7	4.3	3.4
reaction 2	6.7	11.7	5.1	5.5	4.1
reaction 3	2.1	6.1	-1.5	-0.2	-2.0
reaction 4	9.4	18.1	11.9	10.3	10.2
Re					
reaction 1a	23.3	28.0	27.1	21.7	24.2
reaction 2a	8.7	13.2	12.8	10.1	11.4
reaction 3a	33.8	36.2	38.7	40.7	37.1
reaction 3b	14.7	17.0	15.0	18.5	17.0
reaction 3c	15.2	20.4	21.9	21.7	20.9
MUE (TMBH22)	3.5	3.1	2.7	3.3	0.0

Table S43. Reaction energies[a] (kcal/mol) of the WCCR10/18 database

Reaction	Metal	PBE	B3LYP	M11	revM11	Ref.
Reaction 1	Pt	19.5	20.7	27.5	26.7	25.9
Reaction 2	Cu	43.3	42.5	51.0	54.1	47.6
Reaction 3	Cu	43.7	42.9	51.8	54.8	48.2
Reaction 4	Ru	27.2	22.9	49.4	48.7	30.9
Reaction 5	Pt	34.8	28.4	35.2	39.9	44.5
Reaction 6	Au	63.2	58.5	58.3	65.7	48.2
Reaction 7	Cu	61.2	54.7	49.9	57.9	50.1
Reaction 8	Ag	49.2	44.5	42.2	48.7	44.6
Reaction 9	Pd	35.1	26.3	28.9	34.6	38.7
Reaction 10	Pt	17.6	13.9	19.7	23.5	22.8
MUE		6.8	7.6	6.2	7.0	0.0

[a]The reaction energies presented here differ from those presented in our previous work[1] for the following reasons: (a) A conversion factor of 4.184 is now used consistently in going from kJ/mol to kcal//mol and (b) The WCCR10 database is used instead of its subset WCCR9.

Table S44. Cluster binding energies (kcal/mol) of the ASNC2 database

System	PBE	B3LYP	M11	revM11	Ref.
1A1D	-22.8	-21.1	-26.4	-24.5	-24.5
2A1N	-42.3	-40.1	-49.7	-48.6	-46.0
MUE	2.7	4.7	2.8	1.3	0.0

Table S45. Dipole moments (debye) of the DM79 database

System	PBE	B3LYP	M11	revM11	Ref.
acetyl chloride	2.79	2.85	2.91	2.81	2.72
AlF	1.50	1.56	1.43	1.44	1.53
AsH_3	0.27	0.25	0.27	0.33	0.22
aziridine	1.63	1.69	1.74	1.73	1.89
benzonitrile	4.63	4.71	4.77	4.71	4.18
BF_3NH_3	6.03	6.08	6.23	6.24	5.90
BH_2Cl	0.44	0.61	0.74	0.73	0.75
bromoform	0.85	0.88	0.95	0.90	0.99
bromomethane	1.85	1.93	2.01	1.88	1.82
C_2HI	0.22	0.14	0.02	0.03	0.03
CH_3I	1.65	1.70	1.82	1.60	1.64
CrO	3.54	4.15	4.77	4.52	3.88
CuF	4.56	5.12	6.04	5.60	5.77
CuO	4.22	4.59	5.67	5.21	4.45
dimethyl sulfoxide	3.78	3.99	4.21	4.17	3.96
ethanol	1.51	1.58	1.64	1.64	1.44
FeO	4.27	5.17	6.72	5.88	4.70
fluoroacetylene	0.48	0.62	0.75	0.77	0.72
fluorosilane	1.26	1.32	1.30	1.39	1.27
formic acid (*s-cis)*	1.49	1.54	1.59	1.57	1.43
formic acid (*s-trans*)	3.76	3.92	4.11	4.09	3.79
GeO	3.16	3.46	3.54	3.65	3.28
H_2CO	2.21	2.36	2.51	2.51	2.33
H_2O	1.87	1.91	1.98	1.96	1.85
H_2S	1.02	1.02	1.07	1.04	0.98
HCl	1.13	1.14	1.16	1.16	1.11
HCN	2.95	3.03	3.12	3.11	2.99
HF	1.80	1.84	1.89	1.88	1.83
HfO_2	7.44	7.99	8.61	8.49	7.92
HfO	3.24	3.55	3.47	3.74	3.43
imidazole	3.67	3.72	3.83	3.82	3.80
ketene	1.45	1.49	1.53	1.48	1.42
LaO	3.88	4.25	3.64	3.82	3.21
LiOH	4.27	4.34	4.49	4.40	4.50
methylamine	1.27	1.29	1.30	1.30	1.31
methylphosphine	1.18	1.15	1.23	1.16	1.10
methylsilane	0.84	0.78	0.92	0.72	0.73
MgO	7.04	7.45	9.17	3.20	6.20
N_2O	0.14	0.07	0.21	0.26	0.16
NaCl	8.52	8.71	9.07	8.92	9.00
NH_3	1.54	1.53	1.55	1.55	1.47
NiH	2.15	2.46	3.58	3.13	2.40
nitrobenzene	4.51	4.69	4.68	4.64	4.22
nitromethane	3.41	3.59	3.77	3.74	3.46

nitrosyl hydride	1.60	1.71	1.83	1.84	1.62
PbO	4.40	4.78	5.10	5.00	4.64
PbS	3.90	4.12	4.31	4.32	3.59
PH_3	0.60	0.59	0.63	0.65	0.57
phenol	1.25	1.28	1.32	1.32	1.22
propyleneimine (*cis*)	1.75	1.81	1.85	1.83	1.77
propyleneimine (*trans*)	1.57	1.63	1.68	1.67	1.57
propyne	0.88	0.84	0.84	0.76	0.78
ScF	2.19	2.57	1.61	2.79	1.72
ScO	3.47	3.92	3.40	3.79	4.55
SeO_2	2.65	2.88	3.06	3.06	2.62
SO_2	1.57	1.71	1.78	1.78	1.63
TiH	2.57	2.73	2.39	2.44	2.46
TiN	3.83	3.50	2.89	3.13	3.56
TiO	3.26	3.65	3.12	3.50	2.96
VN	3.47	3.23	2.77	2.95	3.07
VO	3.24	3.64	3.39	3.64	3.36
YO	4.38	4.83	4.19	4.64	4.52
ZrO_2	7.39	7.83	8.23	8.12	7.80
ZrO	3.07	3.32	3.90	3.30	2.55
AgBr	4.65	5.18	6.31	5.84	5.62
AgCl	4.91	5.43	6.41	6.02	6.08
AgI	4.13	4.64	6.02	5.39	4.55
HBr	0.89	0.89	0.91	0.90	0.83
HI	0.43	0.43	0.47	0.43	0.45
KF	8.14	8.43	8.70	8.68	8.59
RbCl	10.41	10.78	11.11	10.97	10.51
RbF	8.62	8.94	9.25	9.19	8.55
SrO	7.80	8.67	9.72	9.61	8.90
TlBr	4.45	4.77	4.95	4.64	4.49
TlCl	4.46	4.74	4.86	4.61	4.54
TlF	4.05	4.27	4.39	4.28	4.23
TlI	4.31	4.65	5.03	4.52	4.61
CrN	2.95	3.16	3.01	2.98	2.31
NaLi	0.21	0.03	2.28	0.49	0.46
MUE	0.24	0.22	0.39	0.30	0.00

Table S46. Interaction energies (kcal/mol) of the PEC4 database at various intermonomer distances (Å)

System/distance	PBE	B3LYP	M11	revM11	Ref.
***d* (Ar–Ar)**					
3.0	2.59179	3.13251	2.38954	1.86337	2.25887
3.1	1.66072	2.15023	1.53192	1.00760	1.23823
3.2	1.02262	1.47368	0.97008	0.46076	0.59526
3.3	0.58953	1.01290	0.59901	0.12230	0.19976
3.4	0.30111	0.70109	0.36660	-0.06897	-0.03499
3.5	0.11237	0.48972	0.22433	-0.16525	-0.16651
3.6	-0.00812	0.35030	0.11436	-0.21240	-0.23274
3.7	-0.07995	0.25754	0.05498	-0.21706	-0.25856
3.8	-0.11988	0.19393	0.03161	-0.19772	-0.26014
3.9	-0.13938	0.15305	-0.01022	-0.18312	-0.24789
4.0	-0.14398	0.12629	-0.03990	-0.16283	-0.22840
4.1	-0.13952	0.10569	-0.03224	-0.12953	-0.20578
4.2	-0.13089	0.09091	-0.03892	-0.10697	-0.18250
4.3	-0.11920	0.08138	-0.06390	-0.09694	-0.15998
4.4	-0.10569	0.07336	-0.06848	-0.08044	-0.13899
4.5	-0.09274	0.06463	-0.05067	-0.05766	-0.11989
4.6	-0.08103	0.05744	-0.05284	-0.04764	-0.10277
4.7	-0.06941	0.05219	-0.06347	-0.04489	-0.08758
4.8	-0.05849	0.04721	-0.06378	-0.03868	-0.07422
4.9	-0.04943	0.04098	-0.04668	-0.02562	-0.06251
5.0	-0.04233	0.03510	-0.04202	-0.02010	-0.05227
5.1	-0.03551	0.03064	-0.04384	-0.01905	-0.04335
5.2	-0.02884	0.02736	-0.04479	-0.01886	-0.03556
5.3	-0.02320	0.02375	-0.03505	-0.01358	-0.02878
5.4	-0.01949	0.01962	-0.02754	-0.00921	-0.02286
5.5	-0.01677	0.01595	-0.02649	-0.00836	-0.01769
5.6	-0.01380	0.01339	-0.02432	-0.00777	-0.01317
5.7	-0.01052	0.01187	-0.02154	-0.00750	-0.00921
5.8	-0.00775	0.01036	-0.01635	-0.00511	-0.00574
5.9	-0.00627	0.00844	-0.01417	-0.00372	-0.00269
6.0	-0.00571	0.00645	-0.01336	-0.00356	0.00000
***d* (Ne–Ne)**					
2.5	0.54330	0.67158	0.56224	0.21355	0.50252
2.6	0.23208	0.39840	0.27713	-0.00711	0.22262
2.7	0.05311	0.24222	0.10777	-0.11156	0.06513
2.8	-0.04510	0.15247	0.02360	-0.14492	-0.01942
2.9	-0.09761	0.10259	-0.04824	-0.15577	-0.06118
3.0	-0.11642	0.07568	-0.06083	-0.13408	-0.07841
3.1	-0.12187	0.05894	-0.07667	-0.11489	-0.08204
3.2	-0.11878	0.04890	-0.09669	-0.10084	-0.07855
3.3	-0.10662	0.04303	-0.08003	-0.07200	-0.07170
3.4	-0.09436	0.03803	-0.07679	-0.05643	-0.06362

3.5	-0.08317	0.03349	-0.08859	-0.05241	-0.05546
3.6	-0.06946	0.03001	-0.07306	-0.03633	-0.04780
3.7	-0.05618	0.02723	-0.05754	-0.02400	-0.04090
3.8	-0.04623	0.02379	-0.05740	-0.02249	-0.03485
3.9	-0.03830	0.01991	-0.05637	-0.02170	-0.02960
4.0	-0.03020	0.01668	-0.03955	-0.01265	-0.02511
4.1	-0.02292	0.01490	-0.03287	-0.00930	-0.02128
4.2	-0.01812	0.01247	-0.02915	-0.00827	-0.01802
4.3	-0.01538	0.00930	-0.02548	-0.00856	-0.01526
4.4	-0.01269	0.00687	-0.01865	-0.00580	-0.01291
4.5	-0.00921	0.00639	-0.01489	-0.00388	-0.01092
4.6	-0.00649	0.00606	-0.01218	-0.00284	-0.00922
4.7	-0.00558	0.00461	-0.01012	-0.00314	-0.00777
4.8	-0.00561	0.00270	-0.00807	-0.00302	-0.00654
4.9	-0.00487	0.00194	-0.00638	-0.00225	-0.00547
5.0	-0.00314	0.00240	-0.00493	-0.00123	-0.00456
5.1	-0.00163	0.00281	-0.00377	-0.00073	-0.00377
5.2	-0.00132	0.00227	-0.00296	-0.00090	-0.00309
5.3	-0.00192	0.00111	-0.00246	-0.00115	-0.00250
5.4	-0.00225	0.00035	-0.00217	-0.00109	-0.00199
5.5	-0.00172	0.00046	-0.00185	-0.00069	-0.00154
5.6	-0.00068	0.00102	-0.00129	-0.00021	-0.00115
5.7	0.00009	0.00133	-0.00058	0.00003	-0.00080
5.8	0.00012	0.00107	-0.00025	-0.00007	-0.00050
5.9	-0.00037	0.00047	-0.00044	-0.00032	-0.00023
6.0	-0.00080	0.00000	-0.00073	-0.00045	0.00000
***d* (Kr–Kr)**					
3.0	7.66852	8.89938	7.45673	6.78409	8.02942
3.1	5.31975	6.35525	5.00032	4.41930	5.07071
3.2	3.63595	4.52203	3.29963	2.75393	3.08920
3.3	2.43972	3.21125	2.14538	1.60612	1.77660
3.4	1.59611	2.27780	1.37699	0.83100	0.91974
3.5	1.00233	1.61499	0.86529	0.32292	0.37157
3.6	0.59105	1.14876	0.53235	0.00424	0.03097
3.7	0.31055	0.82139	0.31798	-0.17927	-0.17140
3.8	0.12128	0.59356	0.17321	-0.27617	-0.28282
3.9	-0.00275	0.43606	0.07766	-0.31550	-0.33542
4.0	-0.08072	0.32529	0.03705	-0.31229	-0.35084
4.1	-0.12767	0.24849	0.01349	-0.29084	-0.34356
4.2	-0.15292	0.19647	-0.01475	-0.26444	-0.32317
4.3	-0.16233	0.15900	-0.01775	-0.22596	-0.29591
4.4	-0.16172	0.13101	-0.00816	-0.18357	-0.26578
4.5	-0.15539	0.11193	-0.02849	-0.15649	-0.23525
4.6	-0.14512	0.09821	-0.05595	-0.13674	-0.20580
4.7	-0.13235	0.08567	-0.04946	-0.10733	-0.17826
4.8	-0.11884	0.07476	-0.03696	-0.07998	-0.15302

4.9	-0.10536	0.06707	-0.04971	-0.06915	-0.13021
5.0	-0.09226	0.06100	-0.06885	-0.06488	-0.10979
5.1	-0.08020	0.05418	-0.06532	-0.05196	-0.09164
5.2	-0.06956	0.04701	-0.04977	-0.03591	-0.07558
5.3	-0.05978	0.04155	-0.04934	-0.02966	-0.06141
5.4	-0.05040	0.03763	-0.05509	-0.02886	-0.04893
5.5	-0.04234	0.03381	-0.05730	-0.02750	-0.03796
5.6	-0.03601	0.02910	-0.04608	-0.01994	-0.02832
5.7	-0.03102	0.02456	-0.03860	-0.01433	-0.01983
5.8	-0.02624	0.02126	-0.03805	-0.01273	-0.01237
5.9	-0.02136	0.01907	-0.03728	-0.01219	-0.00580
6.0	-0.01721	0.01711	-0.03449	-0.01167	0.00000
***d* (Kr–He)**					
3.0	0.29664	0.56804	0.48402	0.12273	0.32571
3.1	0.13673	0.39844	0.33164	0.01862	0.16589
3.2	0.03185	0.28335	0.21823	-0.03765	0.06652
3.3	-0.03089	0.20632	0.14795	-0.06069	0.00660
3.4	-0.06602	0.15577	0.08893	-0.06713	-0.02784
3.5	-0.08538	0.12080	0.03716	-0.06818	-0.04605
3.6	-0.09136	0.09632	0.01897	-0.05853	-0.05411
3.7	-0.08926	0.08035	-0.00026	-0.05096	-0.05599
3.8	-0.08499	0.06795	-0.02466	-0.04811	-0.05426
3.9	-0.07809	0.05727	-0.02300	-0.03834	-0.05056
4.0	-0.06818	0.05019	-0.01897	-0.03025	-0.04594
4.1	-0.05829	0.04521	-0.02859	-0.02896	-0.04101
4.2	-0.05101	0.03888	-0.03098	-0.02552	-0.03614
4.3	-0.04472	0.03228	-0.02197	-0.01935	-0.03156
4.4	-0.03696	0.02853	-0.02116	-0.01630	-0.02735
4.5	-0.02871	0.02661	-0.02540	-0.01507	-0.02355
4.6	-0.02310	0.02342	-0.02412	-0.01226	-0.02017
4.7	-0.02061	0.01846	-0.01881	-0.00988	-0.01719
4.8	-0.01840	0.01433	-0.01717	-0.00825	-0.01457
4.9	-0.01435	0.01265	-0.01962	-0.00722	-0.01227
5.0	-0.00952	0.01239	-0.01925	-0.00557	-0.01027
5.1	-0.00633	0.01136	-0.01326	-0.00357	-0.00852
5.2	-0.00591	0.00870	-0.00862	-0.00262	-0.00700
5.3	-0.00680	0.00550	-0.00949	-0.00262	-0.00567
5.4	-0.00673	0.00349	-0.01252	-0.00288	-0.00451
5.5	-0.00477	0.00340	-0.01131	-0.00245	-0.00349
5.6	-0.00190	0.00434	-0.00517	-0.00097	-0.00260
5.7	0.00002	0.00482	-0.00064	0.00029	-0.00182
5.8	-0.00010	0.00390	-0.00145	0.00050	-0.00114
5.9	-0.00175	0.00185	-0.00520	-0.00042	-0.00053
6.0	-0.00334	-0.00006	-0.00686	-0.00158	0.00000

Table S47. Internuclear distances (Å) of the TSG48 database

System	PBE	B3LYP	M11	revM11	Ref.
R1					
	NA[a]	2.535	2.552	2.548	2.530
	NA	1.325	1.372	1.376	1.341
	NA	1.213	1.189	1.182	1.192
R2					
	1.469	1.202	1.200	1.218	1.215
	0.804	0.907	0.919	0.892	0.894
	2.272	2.109	2.119	2.110	2.109
R3					
	1.380	1.380	1.418	1.402	1.426
	2.889	2.792	2.620	2.663	2.578
	1.511	1.415	1.204	1.265	1.160
R4					
	1.484	1.471	1.428	1.432	1.431
	2.302	2.282	2.215	2.195	2.187
	1.227	1.223	1.217	1.217	1.226
R5					
	1.493	1.489	1.490	1.482	1.480
	2.986	2.979	2.980	2.964	2.960
	1.493	1.489	1.490	1.482	1.480
R6					
	NA	1.717	1.754	1.763	1.767
	NA	4.103	3.852	3.830	3.814
	NA	2.387	2.098	2.067	2.047
R7					
	2.336	2.355	2.312	2.292	2.305
	4.672	4.710	4.624	4.584	4.610
	2.336	2.355	2.312	2.292	2.305
R8					
	2.552	2.157	2.005	1.995	2.020
	4.354	4.234	4.155	4.123	4.134
	1.878	2.077	2.150	2.128	2.114
R9					
	1.756	1.771	1.763	1.743	1.758
	3.842	3.821	3.766	3.729	3.745
	2.087	2.051	2.004	1.987	1.988
R10					
	1.119	1.110	1.106	1.108	1.127

	2.353	2.285	2.207	2.228	2.201
	1.583	1.526	1.461	1.478	1.439
R11					
	1.339	1.333	1.332	1.333	1.351
	2.242	2.210	2.041	1.996	1.925
	2.941	2.875	2.724	2.686	2.662
R12					
	1.193	1.180	1.170	1.174	1.187
	1.201	1.190	1.177	1.173	1.183
	1.376	1.388	1.444	1.438	1.387
R13					
	1.404	1.345	1.296	1.278	1.289
	2.549	2.528	2.509	2.506	2.501
	1.168	1.201	1.253	1.266	1.240
R14					
	1.276	1.302	1.293	1.274	1.301
	2.745	2.722	2.711	2.703	2.697
	1.468	1.421	1.421	1.435	1.398
R15					
	0.974	1.288	1.254	1.256	1.246
	2.872	2.349	2.345	2.336	2.337
	2.031	1.093	1.108	1.098	1.103
R16					
	1.209	1.205	1.247	1.265	1.248
	2.516	2.506	2.495	2.492	2.490
	1.309	1.302	1.259	1.239	1.248
MUE	[0.141][b]	0.065	0.020	0.019	0.000

[a]NA = not available. The saddle points could not be located in these cases.

[b]The MUE for the PBE functional cannot be calculated for all 16 reactions because we could not locate a transition structure for two of the reactions. The value listed is obtained by averaging over 14 transition structures (42 internuclear distances excluding those for R1 and R6). For the other three functionals we include all 16 reactions (48 internuclear distances).

Table S48. Bond lengths (Å) of the MGBL193 database

System	PBE	B3LYP	M11	revM11	Ref.
aziridine					
r (1,2)	1.4852	1.4800	1.4805	1.4788	1.4777
r (1,3)	1.4776	1.4700	1.4578	1.4527	1.4714
r (1,4)	1.0918	1.0830	1.0847	1.0840	1.0805
r (1,5)	1.0908	1.0819	1.0838	1.0829	1.0791
r (3,8)	1.0230	1.0134	1.0104	1.0134	1.0126
benzene					
r (1,2)	1.3974	1.0819	1.0844	1.3861	1.3919
r (1,7)	1.0909	1.0819	1.0844	1.0836	1.0795
butadiene					
r (1,2)	1.3443	1.3344	1.3263	1.3253	1.3386
r (1,5)	1.0895	1.0808	1.0838	1.0829	1.0793
r (1,6)	1.0920	1.0831	1.0862	1.0852	1.0815
r (2,3)	1.4514	1.4527	1.4614	1.4645	1.4543
r (2,7)	1.0952	1.0858	1.0881	1.0868	1.0839
CCl_2F_2					
r (1,2)	1.7824	1.7794	1.7637	1.7595	1.7519
r (1,3)	1.3447	1.3342	1.3365	1.3304	1.3286
CH_2CHF					
r (1,2)	1.3265	1.3172	1.3121	1.3126	1.3234
r (1,3)	1.0875	1.0790	1.0812	1.0806	1.0768
r (1,4)	1.0886	1.0801	1.0826	1.0820	1.0782
r (2,5)	1.0910	1.0811	1.0848	1.0834	1.0784
r (2,6)	1.3561	1.3494	1.3508	1.3437	1.3412
CH_2Cl_2					
r (2,3)	1.7855	1.7862	1.7733	1.7655	1.7642
r (2,4)	1.0916	1.0817	1.0848	1.0836	1.0810
CH_2ClF					
r (1,2)	1.0957	1.0855	1.0888	1.0870	1.0842
r (1,4)	1.3738	1.3654	1.3685	1.3605	1.3591
r (1,5)	1.7910	1.7908	1.7763	1.7695	1.7645
CH_2F_2					
r (1,2)	1.3723	1.3633	1.3645	1.3576	1.3533
r (2,4)	1.1004	1.0899	1.0931	1.0907	1.0867
$CHClF_2$					
r (1,2)	1.7884	1.7847	1.7684	1.7639	1.7558
r (2,4)	1.3534	1.3435	1.3457	1.3395	1.3363
r (2,5)	1.0969	1.0864	1.0905	1.0879	1.0849
cis-CHFCHCl					
r (1,2)	1.3325	1.3215	1.3154	1.3162	1.3266
r (1,3)	1.0869	1.0774	1.0799	1.0794	1.0795
r (1,4)	1.7264	1.7295	1.7214	1.7182	1.7124
r (2,5)	1.0901	1.0805	1.0838	1.0827	1.0776
r (2,6)	1.3447	1.3379	1.3391	1.3325	1.3306

cis-acrolein					
r (1,2)	1.4837	1.4817	1.4879	1.4901	1.4809
r (1,3)	1.1184	1.1070	1.1079	1.1050	1.1021
r (1,4)	1.2205	1.2095	1.2037	1.2037	1.2102
r (2,5)	1.0930	1.0837	1.0853	1.0845	1.0807
r (2,6)	1.3404	1.3310	1.3234	1.3228	1.3368
r (6,7)	1.0917	1.0823	1.0863	1.0845	1.0800
r (6,8)	1.0897	1.0811	1.0841	1.0829	1.0786
cis-formic acid					
r (1,2)	1.3619	1.3520	1.3471	1.3442	1.3485
r (1,4)	0.9751	0.9652	0.9610	0.9641	0.9619
r (2,3)	1.2013	1.1910	1.1875	1.1885	1.1910
r (2,5)	1.1132	1.1024	1.1051	1.1021	1.0985
cis-hexatriene					
r (1,2)	1.3613	1.3489	1.3360	1.3344	1.3509
r (2,3)	1.4451	1.4476	1.4581	1.4620	1.4510
r (2,8)	1.0943	1.0850	1.0875	1.0866	1.0813
r (3,5)	1.3475	1.3370	1.3281	1.3268	1.3418
r (3,9)	1.0932	1.0836	1.0857	1.0844	1.0866
r (5,11)	1.0921	1.0831	1.0863	1.0852	1.0815
r (5,12)	1.0894	1.0807	1.0838	1.0829	1.0800
cis-methyl formate					
r (1,2)	1.4485	1.4417	1.4356	1.4279	1.4358
r (1,3)	1.3499	1.3382	1.3326	1.3310	1.3343
r (2,6)	1.0935	1.0849	1.0876	1.0865	1.0845
r (2,7)	1.0971	1.0881	1.0913	1.0900	1.0875
r (3,4)	1.2102	1.2002	1.1972	1.1977	1.2001
r (3,8)	1.1068	1.0967	1.0995	1.0965	1.0925
cyclobutene					
r (1,2)	1.5708	1.5700	1.5648	1.5603	1.5646
r (1,4)	1.5162	1.5154	1.5139	1.5130	1.5149
r (1,5)	1.1004	1.0914	1.0919	1.0912	1.0892
r (3,4)	1.3455	1.3349	1.3284	1.3279	1.3409
r (3,9)	1.0911	1.0819	1.0843	1.0832	1.0801
cyclopropane					
r (1,2)	1.5088	1.0807	1.5012	1.4975	1.5031
r (1,4)	1.0892	1.0807	1.0820	1.0818	1.0787
dimethyl ether					
r (1,2)	1.4174	1.4116	1.4082	1.4017	1.4074
r (1,4)	1.0968	1.0881	1.0905	1.0889	1.0855
r (1,5)	1.1067	1.0971	1.0994	1.0982	1.0949
dioxirane					
r (1,2)	1.5094	1.4985	1.4576	1.4523	1.5140
r (1,3)	1.3977	1.3879	1.3834	1.3787	1.3850
r (3,4)	1.0982	1.0879	1.0900	1.0877	1.0850
ethene					

r (1,4)	1.3329	1.3248	1.3203	1.3199	1.3317
r (4,5)	1.0913	1.0825	1.0851	1.0839	1.0805
ethenol					
r (1,2)	1.3346	1.3250	1.3200	1.3196	1.3316
r (1,4)	1.0868	1.0784	1.0807	1.0804	1.0770
r (1,5)	1.0892	1.0807	1.0829	1.0825	1.0812
r (2,3)	1.3738	1.3681	1.3633	1.3612	1.3598
r (2,6)	1.0939	1.0843	1.0877	1.0863	1.0798
r (3,7)	0.9691	0.9601	0.9568	0.9596	0.9605
furan					
r (1,2)	1.3644	1.3547	1.3504	1.3479	1.3542
r (1,5)	1.4334	1.4322	1.4312	1.4336	1.4344
r (1,6)	1.0848	1.0760	1.0784	1.0780	1.0743
r (2,3)	1.3693	1.3618	1.3532	1.3509	1.3598
r (2,7)	1.0835	1.0746	1.0782	1.0775	1.0739
glycolaldehyde					
r (1,2)	1.5039	1.5031	1.5058	1.5075	1.5014
r (1,4)	1.2183	1.2065	1.2022	1.2025	1.2083
r (1,5)	1.1156	1.1055	1.1064	1.1035	1.1011
r (2,3)	1.4030	1.3997	1.3953	1.3905	1.3970
r (2,6)	1.1097	1.0992	1.0998	1.0984	1.0964
r (3,8)	0.9813	0.9690	0.9662	0.9685	0.9618
glyoxylic acid					
r (1,2)	1.5384	1.5341	1.5369	1.5391	1.5211
r (1,5)	1.2070	1.1963	1.1907	1.1916	1.2087
r (1,6)	1.1147	1.1032	1.1052	1.1020	1.0963
r (2,3)	1.3470	1.3360	1.3293	1.3273	1.3317
r (2,4)	1.2151	1.2035	1.1979	1.1987	1.1977
r (3,7)	0.9793	0.9694	0.9659	0.9691	0.9697
H_2CCCH_2					
r (1,2)	1.3078	1.0831	1.2971	1.2984	1.3075
r (2,4)	1.0920	1.0831	1.0845	1.0838	1.0800
H_2CO					
r (1,2)	1.2096	1.2002	1.1969	1.1982	1.2051
r (1,3)	1.1173	1.1058	1.1076	1.1036	1.1002
H_2O					
r (1,2)	0.9703	0.9618	0.9581	0.9610	0.9572
HCCCCH					
r (1,2)	1.0699	1.0614	1.0658	1.0660	1.0610
r (2,3)	1.2174	1.2042	1.1967	1.1960	1.2070
r (3,4)	1.3608	1.3638	1.3776	1.3858	1.3726
HCCH					
r (1,2)	1.0703	1.0616	1.0656	1.0658	1.0611
r (2,3)	1.2072	1.1963	1.1920	1.1920	1.2036
HCN					
r (1,2)	1.1583	1.1460	1.1396	1.1414	1.1536

r (1,3)	1.0749	1.0656	1.0690	1.0685	1.0645
HCO^+					
r (1,2)	1.1038	1.0953	1.1009	1.1003	1.0916
r (2,3)	1.1138	1.1020	1.0967	1.0991	1.1057
$HNCCN^+$					
r (1,2)	1.0213	1.0148	1.0193	1.0216	1.0138
r (2,3)	1.1511	1.1382	1.1312	1.1321	1.1392
r (3,4)	1.3631	1.3648	1.3761	1.3827	1.3735
r (4,5)	1.1711	1.1555	1.1453	1.1465	1.1607
HNC					
r (1,2)	1.0056	0.9969	0.9979	1.0007	0.9946
r (2,3)	1.1759	1.1644	1.1596	1.1610	1.1688
imidazole					
r (1,2)	1.3768	1.3670	1.3635	1.3601	1.3627
r (1,4)	1.3791	1.3750	1.3693	1.3718	1.3794
r (1,6)	1.0854	1.0763	1.0794	1.0786	1.0752
r (2,3)	1.3800	1.3763	1.3701	1.3716	1.3743
r (2,7)	1.0837	1.0747	1.0774	1.0771	1.0764
r (3,5)	1.3688	1.3627	1.3574	1.3568	1.3616
r (3,8)	1.0132	1.0046	1.0042	1.0070	1.0011
r (4,5)	1.3206	1.3100	1.3043	1.3023	1.3103
r (5,9)	1.0859	1.0772	1.0807	1.0799	1.0770
maleic anhydride					
r (1,2)	1.2019	1.1901	1.1836	1.1848	1.1896
r (1,3)	1.4038	1.3912	1.3824	1.3771	1.3843
r (1,4)	1.4878	1.4871	1.4952	1.4960	1.4857
r (4,6)	1.3386	1.3285	1.3196	1.3191	1.3320
r (4,8)	1.0867	1.0776	1.0806	1.0795	1.0761
NH_3					
r (1,2)	1.0220	1.0132	1.0102	1.0133	1.0111
oxirane					
r (1,3)	1.4376	1.4296	1.4193	1.4109	1.4281
r (2,3)	1.4693	1.4632	1.4629	1.4632	1.4615
r (2,4)	1.0939	1.0844	1.0865	1.0853	1.0814
propanal					
r (1,2)	1.2145	1.2046	1.2003	1.2011	1.2075
r (1,3)	1.5075	1.5052	1.5054	1.5052	1.5037
r (1,5)	1.1240	1.1119	1.1134	1.1099	1.1040
r (3,4)	1.5348	1.5336	1.5308	1.5286	1.5165
r (3,6)	1.1051	1.0959	1.0962	1.0951	1.0946
r (4,8)	1.0974	1.0892	1.0905	1.0899	1.0879
r (4,9)	1.0984	1.0902	1.0917	1.0911	1.0888
propene					
r (1,2)	1.4967	1.4966	1.4981	1.4984	1.4956
r (1,5)	1.1016	1.0931	1.0936	1.0928	1.0895
r (1,6)	1.0984	1.0900	1.0915	1.0908	1.0880

r (2,3)	1.3359	1.3271	1.3221	1.3215	1.3326
r (2,7)	1.0954	1.0863	1.0883	1.0872	1.0841
r (3,8)	1.0903	1.0816	1.0843	1.0835	1.0804
r (3,9)	1.0927	1.0837	1.0866	1.0856	1.0818
pyrazole					
r (1,2)	1.4129	1.4098	1.4085	1.4095	1.4090
r (1,4)	1.3394	1.3275	1.3201	1.3183	1.3289
r (1,6)	1.0860	1.0772	1.0801	1.0793	1.0757
r (2,3)	1.3851	1.3764	1.3719	1.3697	1.3765
r (2,7)	1.0839	1.0751	1.0774	1.0771	1.0739
r (3,5)	1.3600	1.3537	1.3485	1.3482	1.3519
r (3,8)	1.0848	1.0759	1.0787	1.0783	1.0745
r (4,5)	1.3501	1.3451	1.3316	1.3330	1.3441
r (5,9)	1.0125	1.0042	1.0047	1.0074	1.0014
pyridazine					
r (1,2)	1.3859	1.3777	1.3710	1.3704	1.3778
r (1,3)	1.3977	1.3924	1.3895	1.3902	1.3926
r (1,7)	1.0904	1.0812	1.0837	1.0826	1.0791
r (3,5)	1.3411	1.3304	1.3218	1.3217	1.3324
r (3,9)	1.0922	1.0826	1.0856	1.0839	1.0804
pyridine					
r (1,2)	1.3949	1.3883	1.3834	1.3834	1.3888
r (1,7)	1.0908	1.0818	1.0846	1.0835	1.0802
r (2,4)	1.3970	1.3905	1.3861	1.3858	1.3907
r (2,8)	1.0904	1.0812	1.0835	1.0826	1.0796
r (4,6)	1.3419	1.3337	1.3275	1.3276	1.3358
r (4,10)	1.0937	1.0841	1.0873	1.0856	1.0818
pyrrole					
r (1,2)	1.4240	1.4214	1.4193	1.4214	1.4228
r (1,6)	1.0851	1.0764	1.0789	1.0787	1.0745
r (2,4)	1.3827	1.3735	1.3692	1.3660	1.3732
r (3,5)	1.3758	1.3713	1.3653	1.3657	1.3694
r (4,9)	1.0842	1.0755	1.0785	1.0783	1.0744
r (5,10)	1.0112	1.0032	1.0033	1.0062	1.0007
SH_3^+					
r (1,2)	1.3713	1.3598	1.3586	1.3559	1.3502
thiophene					
r (1,2)	1.4240	1.4230	1.4223	1.4253	1.4233
r (1,6)	1.0885	1.0797	1.0819	1.0814	1.0792
r (2,4)	1.3736	1.3634	1.3583	1.3552	1.3625
r (4,5)	1.7271	1.7257	1.7150	1.7131	1.7127
r (4,9)	1.0853	1.0765	1.0793	1.0792	1.0772
trans-acrolein					
r (1,2)	1.4718	1.4705	1.4781	1.4799	1.4703
r (1,3)	1.2201	1.2092	1.2023	1.2028	1.2109
r (1,4)	1.1214	1.1092	1.1112	1.1077	1.1044

r (2,5)	1.0923	1.0831	1.0852	1.0840	1.0817
r (2,6)	1.3409	1.3314	1.3238	1.3233	1.3355
r (6,7)	1.0931	1.0838	1.0874	1.0859	1.0826
r (6,8)	1.0898	1.0811	1.0841	1.0829	1.0792
trans-formic acid					
r (1,2)	1.3551	1.3450	1.3404	1.3375	1.3417
r (1,4)	0.9804	0.9703	0.9664	0.9695	0.9656
r (2,3)	1.2082	1.1977	1.1943	1.1953	1.1973
r (2,5)	1.1062	1.0960	1.0992	1.0960	1.0918
trans-glyoxal					
r (1,2)	1.5290	1.5243	1.5296	1.5295	1.5149
r (1,3)	1.1169	1.1052	1.1069	1.1036	1.1006
r (2,5)	1.2127	1.2019	1.1961	1.1972	1.2051
MUE	0.0103	0.0037	0.0060	0.0057	0.0000

Table S49. Bond lengths (Å) of the TMDBL10 database

System	PBE	B3LYP	M11	revM11	Ref.
Ag_2	2.560	2.585	2.556	2.555	2.530
Au_2	2.520	2.545	2.489	2.504	2.472
Cu_2	2.252	2.280	2.308	2.273	2.219
Fe_2	2.156	2.421	2.505	2.320	2.020
FeC	1.555	1.609	1.725	1.680	1.596
Ir_2	2.213	2.304	2.267	2.273	2.270
Ni_2	2.120	2.295	2.330	2.295	2.155
Os_2	2.236	2.238	2.247	2.236	2.280
Pd_2	2.472	2.496	2.484	2.472	2.480
Pt_2	2.331	2.335	2.416	2.424	2.333
MUE	0.043	0.084	0.104	0.078	0.000

Table S50. Dipole charges[a] on Na atom (kcal/mol) of the NaCl database

System	PBE	B3LYP	M11	revM11	Ref.
Na atom	0.462	0.445	0.908	0.000	0.000

[a]The values tabulated are the charges on Na atom in NaCl with an internuclear distance of 10 Å.

Table S51. Excitation energies of atoms (eV) in the EEA11 database

System	states	orbitals	type	PBE	B3LYP	M11	revM11	Ref.
H	^{2}S–^{2}S	1s−2s	Rydberg	8.1	8.5	8.4	9.0	10.2
He	^{1}S–^{1}S	$1s^2$−1s2s	Rydberg	17.6	18.6	18.0	18.3	20.6
Li	^{2}S–^{2}P	2s−2p	valence	2.0	2.0	1.9	1.8	1.9
Be	^{1}S–^{1}P	$2s^2$−2s2p	valence	5.0	4.9	5.0	5.0	5.3
B	^{2}P–^{2}S	2p−3s	Rydberg	4.1	4.5	4.3	5.0	5.0
Ne	^{1}S–^{1}P	$2p^6$–$2p^5$3s	Rydberg	15.9	16.6	16.9	16.4	16.7
Na	^{2}S–^{2}P	3s−3p	valence	2.1	2.2	1.9	2.1	2.1
Mg	^{1}S–^{1}P	$3s^2$−3s3p	valence	4.2	4.3	4.2	4.1	4.4
Al	^{2}P–^{2}S	3p−4s	Rydberg	2.7	2.8	2.9	3.3	3.1
Ar	^{1}S–^{1}P	$3p^6$–$3p^5$4s	Rydberg	11.0	11.4	11.5	12.6	11.7
K	^{2}S–^{2}P	4s−4p	valence	1.6	1.7	1.3	1.6	1.6
	MUE			0.8	0.5	0.6	0.5	0.0

Table S52. Adiabatic excitation energies (eV) of the AEE15 database

System	PBE	B3LYP	M11	revM11	Ref.
acetaldehyde	3.6	3.8	3.6	3.6	3.7
anisole	4.4	4.7	5.0	5.0	4.5
benzene	4.9	5.1	5.4	5.3	4.7
benzophenone ketyl radical	1.9	2.3	2.8	2.7	2.3
BF	6.1	6.1	6.1	6.0	6.3
C_2H_2	4.9	4.7	4.5	4.5	5.2
cinnoline	1.8	2.4	2.7	2.7	2.8
CO	7.8	8.0	7.8	7.8	8.1
glyoxal	2.0	2.4	2.4	2.5	2.7
p-diethynylbenzene	3.9	4.2	4.6	4.5	4.3
propynal	2.9	3.2	3.3	3.3	3.2
pyridone lactim	4.2	4.6	4.8	4.8	4.5
quinoline	2.9	3.5	3.8	3.9	4.0
ScO	2.1	2.2	1.9	2.0	2.0
VO	1.5	1.4	0.8	1.1	1.6
MUE	0.4	0.2	0.3	0.3	0.4

Table S53. Charge transfer excitation energies (eV) of the EEAroT5 database

System[a]	PBE	B3LYP	M11	revM11	Ref.
Benzene–TCNE	1.5	2.1	3.6	4.0	3.6
Toluene–TCNE	1.4	1.8	3.3	3.7	3.4
Xylene–TCNE	1.1	1.5	3.1	3.5	3.2
Naphtalene–TCNE	0.4	0.9	2.6	3.0	2.6
Anthracene–TCNE	1.1[b]	1.2[b]	1.8[b]	2.1[b]	1.7[c]
MUE	1.8	1.4	0.1	0.4	0.0

[a]TCNE = tetracyanoethylene

[b]These values are obtained by subtracting 0.32 eV from the gas phase values to obtain solution phase values that can be compared to the reference value.

[c]Solution phase value

Table S54. Excitation energies (eV) of the EE69 database

System	State	Type	PBE	B3LYP	M11	revM11	Ref.
acetaldehyde							
	A"	valence	4.14	4.26	3.92	3.91	4.28
	2 A'	Rydberg	5.39	6.17	6.28	7.03	6.82
	3 A'	Rydberg	5.86	6.66	6.94	7.75	7.46
	4 A'	Rydberg	6.18	6.88	7.08	7.96	7.75
	6 A'	Rydberg	6.58	7.31	7.91	8.74	8.43
	7 A'	Rydberg	6.64	7.42	7.94	8.89	8.69
acetone							
	1 A_2	valence	4.22	4.38	4.09	4.05	4.43
	1 B_2	Rydberg	4.90	5.73	6.05	6.79	6.36
	2 A_2	Rydberg	5.76	6.59	6.67	7.66	7.36
	2 A_1	Rydberg	5.63	6.50	6.92	7.85	7.41
	2 B_2	Rydberg	5.85	6.67	6.87	7.79	7.49
	3 A_1	Rydberg	6.16	7.07	7.85	8.49	7.80
	3 B_2	Rydberg	6.02	6.91	7.37	8.23	8.09
	1 B_1	Rydberg	6.21	7.12	7.66	8.62	8.17
ethylene							
	1 B_{3u}	Rydberg	6.30	6.49	6.48	7.20	7.11
	1 B_{1u}	valence	7.22	7.31	7.37	7.50	7.65
	1 B_{1g}	Rydberg	6.77	6.99	6.91	7.77	7.80
	1 B_{2g}	Rydberg	6.73	6.98	7.01	7.95	7.90
	2 A_g	Rydberg	7.06	7.32	7.58	8.26	8.28
	2 B_{3u}	Rydberg	7.32	7.64	7.88	8.79	8.62
	3 B_{3u}	Rydberg	7.51	7.81	8.56	9.21	8.90
	4 B_{3u}	Rydberg	8.13	8.35	8.76	9.29	9.08
	3 B_{1g}	Rydberg	7.73	8.08	8.89	9.42	9.20
	2 B_{1u}	Rydberg	7.93	8.08	8.59	9.32	9.33
	5 B_{3u}	Rydberg	9.45	9.63	10.01	10.61	9.51
formaldehyde							
	1 A_2	valence	3.80	3.92	3.56	3.62	4.00
	1 B_2	Rydberg	5.74	6.44	6.42	7.17	7.08
	2 B_2	Rydberg	6.51	7.22	7.16	7.93	7.97
	2A_1	Rydberg	6.38	7.17	7.23	8.07	8.14
	2 A_2	Rydberg	6.64	7.42	7.26	8.23	8.37
	3 B_2	Rydberg	6.78	7.68	8.35	9.23	8.88
	1 B_1	valence	8.82	8.96	8.70	8.78	9.00
	3 A_2	Rydberg	8.00	8.68	8.76	9.65	9.22
	4 B_2	Rydberg	7.73	8.46	8.78	9.48	9.26
	4 A_1	Rydberg	7.87	8.57	9.23	9.69	9.58
	5 B_2	Rydberg	7.86	8.57	8.86	9.58	9.63
isobutene							
	B_1	Rydberg	5.27	5.60	5.76	6.53	6.17
	A_1	Rydberg	5.87	6.17	6.27	6.82	6.70

pyrazine							
	B_{3u}	valence	3.57	3.97	4.02	4.07	3.83
	B_{2u}	valence	5.23	5.33	5.46	5.36	4.81
	B_{2g}	valence	5.14	5.60	5.71	5.74	5.46
	B_{1g}	valence	5.59	6.42	7.11	7.19	6.10
	B_{1u}	valence	6.40	6.46	6.67	6.62	6.51
pyridazine							
	1 B_1	valence	3.13	3.59	3.69	3.70	3.60
	2 A_1	valence	5.46	5.60	5.77	5.69	5.00
	1 A_2	valence	3.50	4.16	4.53	4.55	5.30
	2 B_1	valence	5.45	6.12	6.47	6.54	6.00
	2 B_2	valence	6.32	6.28	6.63	6.84	6.50
pyridine							
	1 B_1	valence	4.37	4.82	4.92	4.97	4.59
	1 B_2	valence	5.33	5.47	5.62	5.56	4.99
	1 A_2	valence	4.46	5.12	5.50	5.53	5.43
	2 A_1	valence	6.18	6.26	6.42	6.46	6.38
pyrimidine							
	1 B_1	valence	3.79	4.29	4.47	4.52	3.85
	1 A_2	valence	4.01	4.61	4.91	4.95	4.62
	1 B_2	valence	5.58	5.73	5.89	5.82	5.12
	2 A_2	valence	5.12	5.69	5.92	5.96	5.52
	2 B_1	valence	5.33	5.97	6.27	6.32	5.90
	2 A_1	valence	6.43	6.53	6.78	6.76	6.70
***s*-tetrazine**							
	1 B_{3u}	valence	1.84	2.26	2.33	2.34	2.25
	1 A_u	valence	2.81	3.48	3.86	3.90	3.40
	2 A_u	valence	4.63	5.10	5.32	5.38	5.00
	2 B_{3u}	valence	5.63	6.31	6.60	6.71	6.34
***t*-butadiene**							
	1 B_u	valence	5.40	5.54	5.79	5.88	5.91
	1 B_g	Rydberg	5.39	5.57	5.53	6.30	6.22
	2 A_u	Rydberg	5.67	5.88	5.98	6.82	6.66
	2 B_u	Rydberg	6.23	6.41	6.51	7.17	7.07
	2 B_g	Rydberg	6.18	6.43	6.55	7.48	7.36
	3 A_g	Rydberg	6.54	6.75	7.16	7.80	7.62
	3 B_u	Rydberg	7.02	7.20	7.76	8.44	8.00
MUE			0.97	0.58	0.49	0.30	0.00

Table S55. Charge transfer excitation energies (eV) of the EER5 database

System	PBE	B3LYP	M11	revM11	Ref.
11-*Z-cis*-retinal					
S_1	2.1	2.3	2.4	2.4	2.1
S_2	2.6	3.0	3.8	3.9	3.3
11-*Z-cis*-7,8-dihydroretinal					
S_1	1.0	1.5	3.9	4.2	2.6
S_2	3.2	3.1	3.0	3.1	3.0
S_3	2.2	3.2	5.3	5.5	4.4
MUE	0.9	0.5	0.6	0.7	0.0

Table S56. Charge transfer excitation energies (eV) of the LRCTEE2 database

System	PBE	B3LYP	M11	revM11	Ref.
$C_2F_4\cdots C_2H_4$ (8 Å)	5.2	6.8	11.4	10.8	10.9
$NH_3\cdots F_2$ (6 Å)	0.1	2.2	6.4	6.9	7.7
MUE	6.7	4.8	0.9	0.4	0.0

Table S57. Geometries (Å), total electronic energies (*E* in hartrees), charges, and spin multiplicities of selected systems in the SR-MGN-BE107 database[a]

System			
H_2O (*E* = -76.427690)			
Charge, spin multiplicity = 0, 1			
O	0.000000	0.000000	0.117145
H	0.000000	0.756709	-0.468582
H	0.000000	-0.756709	-0.468582
C_2H_2 (*E* = -77.292447)			
Charge, spin multiplicity = 0, 1			
C	0.000000	0.000000	0.601571
C	0.000000	0.000000	-0.601571
H	0.000000	0.000000	-1.664176
H	0.000000	0.000000	1.664176
CH ($^2\prod$) (*E* = -38.458990)			
Charge, spin multiplicity = 0, 2			
C	0.000000	0.000000	0.159876
H	0.000000	0.000000	-0.959254
CH_2 ($^3B_1$) (*E* = -39.131921)			
Charge, spin multiplicity = 0, 3			
C	0.000000	0.000000	0.105529
H	0.000000	0.990531	-0.316586
H	0.000000	-0.990531	-0.316586

[a]The basis set is MG3S, which for these four systems (or for any system with no atom heavier than Ne) is the same as 6-311+G(2df,2p).

Reference

1. Wang, Y.; Verma, P.; Jin, X. S.; Truhlar, D. G.; He, X. Revised M06 Density Functional for Main-Group and Transition-Metal Chemistry. *Proc. Natl. Acad. Sci. USA* **2018**, *115*, 10257–10262.