Supporting Information for

A (Nearly) Universally Applicable Method for Modeling Non-Covalent Interactions Using B3LYP.

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Contents

```
#B3LYP Gen  SCF=Tight Pseudo=Read

Methane-Methane: Demonstration of the use of DCPs without counterpoise.

0 1
C   -0.0000000000000012    0.0000000000000000  -12.9302615371670004
H   -1.0221680029300009    0.0000000000000000  -12.5675320710289995
H   -0.0000000000000012    0.0000000000000000  -14.0149303532539999
H    0.5110840014649981    0.8852234574729996  -12.5675320710289995
H    0.5110840014649981   -0.8852234574729996  -12.5675320710289995
C   -0.0000000000000012    0.0000000000000000   -9.4302615371670004
H   -1.0221680029300009    0.0000000000000000   -9.7929910033049996
H   -0.0000000000000012    0.0000000000000000   -8.3455927210800009
H    0.5110840014649981   -0.8852234574729996   -9.7929910033049996
H    0.5110840014649981    0.8852234574729996   -9.7929910033049996

H C 0
6-31+G(2d,2p)
****

H 0
H 1 0
P an up
 3
  2  0.112790145  0.000226456
  2  0.043193200 -0.000068835
  2  0.005733838 -0.000000390
S-P
 1
  2  0.184641561 -0.000052055
C 0
C 3 0
F an up
 4
  2  0.204353696  0.000103405
  2  0.106552301 -0.000068461
  2  0.103629038  0.001279009
  2  0.010449572 -0.000001033
S-F
 2
  2  0.043390720  0.000020668
  2  0.117045600  0.056519710
P-F
 2
  2  0.064526518 -0.000013344
  2  0.123222363 -0.021488594
D-F
 1
  2  0.066381605 -0.010148271
```

```
#B3LYP Gen  SCF=Tight Pseudo=Read

formamidedimer-formamidedimer: Demonstration of the use of DCPs.

0 1
C    1.1000652940000000    2.0305696410000000    0.0000000000000000
O    1.7041854439999999    3.1009158740000000    0.0000000000000000
N    1.6689117649999998    0.8146382660000002    0.0000000000000000
H    1.0833379169999999    0.0000000000000000    0.0000000000000000
H    2.6865419739999998    0.7138121609999999    0.0000000000000000
H    0.0000000000000000    2.0023083809999997    0.0000000000000000
C    5.4993367580000001    1.7841583940000001    0.0000000000000000
O    4.8952166080000001    0.7138121609999999    0.0000000000000000
N    4.9304902869999996    3.0000897700000002    0.0000000000000000
H    5.5160641349999997    3.8147280349999999    0.0000000000000000
H    3.9128600779999996    3.1009158740000000    0.0000000000000000
H    6.5994020520000003    1.8124196539999999    0.0000000000000000

C O N H 0
6-31+G(2d,2p)
****

C 0
C 3 0
F an up
 4
  2  0.204353696  0.000103405
  2  0.106552301 -0.000068461
  2  0.103629038  0.001279009
  2  0.010449572 -0.000001033
S-F
 2
  2  0.043390720  0.000020668
  2  0.117045600  0.056519710
P-F
 2
  2  0.064526518 -0.000013344
  2  0.123222363 -0.021488594
D-F
 1
  2  0.066381605 -0.010148271
O 0
O 3 0
F an up
 3
  2  0.229218952  0.002292912
  2  0.097343149 -0.000574884
  2  0.008021004 -0.000000082
S-F
 1
  2  0.197820377 -0.000157070
P-F
 1
  2  0.106145399 -0.000206907
D-F
 1
  2  0.057393876 -0.000113868
N 0
N 3 0
F an up
 3
  2  0.124536834  0.000375000
  2  0.030918400 -0.000033729
  2  0.005040192 -0.000000020
S-F
 1
  2  0.066204887 -0.000950120
P-F
 1
  2  0.056034679 -0.000534017
D-F
 1
  2  0.013845593 -0.000127395
H 0
H 1 0
P an up
 3
  2  0.112790145  0.000226456
  2  0.043193200 -0.000068835
  2  0.005733838 -0.000000390
S-P
 1
  2  0.184641561 -0.000052055
```

```
start Methane-Methane
charge 0
geometry units angstroms
C   -0.0000000000000012    0.0000000000000000  -12.9302615371670004
H   -1.0221680029300009    0.0000000000000000  -12.5675320710289995
H   -0.0000000000000012    0.0000000000000000  -14.0149303532539999
H    0.5110840014649981    0.8852234574729996  -12.5675320710289995
H    0.5110840014649981   -0.8852234574729996  -12.5675320710289995
C   -0.0000000000000012    0.0000000000000000   -9.4302615371670004
H   -1.0221680029300009    0.0000000000000000   -9.7929910033049996
H   -0.0000000000000012    0.0000000000000000   -8.3455927210800009
H    0.5110840014649981   -0.8852234574729996   -9.7929910033049996
H    0.5110840014649981    0.8852234574729996   -9.7929910033049996
end
basis
 C library "6-31G"
 C library "Pople-style diffuse"
 C library "Pople (2d,2p) Polarization"
 H library "6-31G"
H library "Pople (2d,2p) Polarization"
end
ecp
   C nelec 0 # ecp replaces 0 electrons on C
   C ul      # F
              2  0.204353696  0.000103405
              2  0.106552301 -0.000068461
              2  0.103629038  0.001279009
              2  0.010449572 -0.000001033
   C s       # s - f
              2  0.043390720  0.000020668
              2  0.117045600  0.056519710
   C p       # p - f
              2  0.064526518 -0.000013344
              2  0.123222363 -0.021488594
   C d       # d - f
              2  0.066381605 -0.010148271
   H nelec 0 # ecp replaces 0 electrons on H
   H ul      # p
            2       0.112790145  0.000226456
            2       0.043193200 -0.000068835
            2       0.005733838 -0.000000390
   H s       # s - p
            2       0.084641561 -0.000052055
end
dft
 xc b3lyp
end
title "6-31+G(2d,2p) single point DFT"
task dft energy
```

```
start formamidedimer-formamidedimer
charge 0
geometry units angstroms
C    1.1000652940000000    2.0305696410000000    0.0000000000000000
O    1.7041854439999999    3.1009158740000000    0.0000000000000000
N    1.6689117649999998    0.8146382660000002    0.0000000000000000
H    1.0833379169999999    0.0000000000000000    0.0000000000000000
H    2.6865419739999998    0.7138121609999999    0.0000000000000000
H    0.0000000000000000    2.0023083809999997    0.0000000000000000
C    5.4993367580000001    1.7841583940000001    0.0000000000000000
O    4.8952166080000001    0.7138121609999999    0.0000000000000000
N    4.9304902869999996    3.0000897700000002    0.0000000000000000
H    5.5160641349999997    3.8147280349999999    0.0000000000000000
H    3.9128600779999996    3.1009158740000000    0.0000000000000000
H    6.5994020520000003    1.8124196539999999    0.0000000000000000
end
basis
 C library "6-31G"
 C library "Pople-style diffuse"
 C library "Pople (2d,2p) Polarization"
 H library "6-31G"
H library "Pople (2d,2p) Polarization"
 N library "6-31G"
 N library "Pople-style diffuse"
 N library "Pople (2d,2p) Polarization"
 O library "6-31G"
 O library "Pople-style diffuse"
 O library "Pople (2d,2p) Polarization"
end
ecp
   C nelec 0 # ecp replaces 0 electrons on C
   C ul      # F
           2  0.204353696  0.000103405
           2  0.106552301 -0.000068461
           2  0.103629038  0.001279009
           2  0.010449572 -0.000001033
   C s       # s - f
           2  0.043390720  0.000020668
           2  0.117045600  0.056519710
   C p       # p - f
           2  0.064526518 -0.000013344
           2  0.123222363 -0.021488594
   C d       # d - f
           2  0.066381605 -0.010148271
   H nelec 0 # ecp replaces 0 electrons on H
   H ul      # p
           2       0.112790145  0.000226456
           2       0.043193200 -0.000068835
           2       0.005733838 -0.000000390
   H s       # s - p
           2       0.084641561 -0.000052055
   N nelec 0 # ecp replaces 0 electrons on N
   N ul      # F
           2       0.209342166  0.000283597
           2       0.164560971  0.002088445
           2       0.014906716 -0.000000109
   N s       # s - f
           2       0.042686780  0.000020569
   N p       # p - f
           2       0.122439426 -0.000111442
   N d       # d - f
           2       0.066959033 -0.005065957
   O nelec 0 # ecp replaces 0 electrons on O
   O ul      # F
           2       0.192168931  0.000242019
           2       0.166560549  0.0030
           2       0.016734867 -0.000000131
   O s       # s - f
           2       0.039337457  0.000016041
   O p       # p - f
           2       0.123780982 -0.000129441
   O d       # d - f
           2       0.061418151 -0.003520223
end
dft
 xc b3lyp
end
title "6-31+G(2d,2p) single point DFT"
task dft energy
```

Table S1. Signed deviations in binding energies (kcal/mol) calculated for the non-covalently bonded dimers of the S66 benchmark set using B3LYP/6-31+G(d,p) with dispersion-correcting potentials and with (CP) and without (Non-CP) counterpoise corrections. The data are ordered according to interaction type. Overall performance statistics for the entire S66 set are provided at the bottom of the Table.

Dimer	Accepted High-Level Value[a]	CP	Non-CP
Hydrogen Bonded Dimers[b]			
water – water	4.92	0.76	1.16
water – methanol	5.59	0.68	0.90
water – methylamine	6.91	0.90	1.55
water – peptide[c]	8.10	0.52	0.32
methanol – methanol	5.76	0.55	0.81
methanol – methylamine	7.55	0.68	1.45
methanol – peptide[c]	8.23	0.35	0.16
methanol – water	5.01	0.60	1.13
methylamine – methanol	3.06	0.23	0.51
methylamine – methylamine	4.16	0.12	0.71
methylamine – peptide[c]	5.42	0.04	0.23
methylamine – water	7.27	0.79	1.44
peptide[c] – methanol	6.19	0.25	0.54
peptide[c] – methylamine	7.45	0.37	1.16
peptide[c] – peptide[c]	8.63	0.01	-0.03
peptide[c] – water	5.12	0.27	1.00
uracil – uracil (base pair)	17.18	-0.20	-0.18
water – pyridine	6.86	0.31	0.72
methanol – pyridine	7.41	0.14	0.64
formic acid – formic acid	19.09	0.28	-0.53
formamide – formamide	16.27	-0.29	-0.18
formic acid – uracil	19.49	0.01	-0.34
formamide – uracil	19.19	-0.10	-0.02
Dispersion-Dominated Dimers			
benzene – benzene[d] (π-stacked)	2.82	0.09	0.10
pyridine – pyridine (π-stacked)	3.90	0.11	0.06
uracil – uracil (π-stacked)	9.83	-0.55	0.05
benzene – pyridine (π-stacked)	3.44	0.12	0.07
benzene – uracil (π-stacked)	5.71	-0.36	-0.04
pyridine – uracil (π-stacked)	6.82	-0.59	-0.19
benzene – ethene	1.43	0.05	0.00
uracil – ethene	3.38	-0.15	0.05
uracil – ethyne	3.74	-0.22	-0.01
pyridine – ethene	1.87	0.01	-0.02
pentane – pentane	3.78	0.11	-0.16
neopentane – pentane	2.61	-0.10	-0.27

neopentane – neopentane	1.78	-0.20	-0.26
cyclopentane – neopentane	2.40	-0.05	-0.20
cyclopentane – cyclopentane	3.00	0.11	-0.11
benzene – cyclopentane	3.58	0.14	0.04
benzene – neopentane	2.90	-0.04	-0.04
uracil – pentane	4.85	-0.33	-0.10
uracil – cyclopentane	4.85	-0.21	-0.04
uracil – neopentane	4.14	-0.26	-0.02
ethene – pentane	3.71	-0.05	-0.15
ethyne – pentane	2.01	0.07	-0.04
peptide[c] – pentane	1.75	-0.13	-0.16
Mixed Interactions			
benzene – benzene (T-shaped)	2.88	-0.10	0.09
pyridine – pyridine (T-shaped)	3.54	-0.27	-0.04
benzene – pyridine (T-shaped)	3.33	-0.04	0.10
benzene – ethyne (CH-π)	2.87	0.00	0.19
ethyne – ethyne (T-shaped)	1.52	-0.02	0.04
benzene – acetic acid (OH-π)	4.71	-0.47	0.00
benzene – formamide (NH-π)	4.36	-0.26	-0.03
benzene – water (OH-π)	3.28	0.01	0.54
benzene – methanol (OH-π)	4.19	-0.07	0.30
benzene – methylamine (OH-π)	3.23	-0.12	0.07
benzene – peptide (NH-π)	5.28	-0.23	-0.03
pyridine – pyridine (CH-N)[e]	4.15	-0.49	-0.25
ethyne – water (CH-O)[e]	2.85	0.12	0.74
ethyne – acetic acid (OH- π)[e]	4.87	-0.19	0.02
pentane – acetic acid	2.91	-0.01	0.03
pentane – formamide	3.53	-0.15	-0.18
benzene – acetic acid (π-stacked)	3.80	0.05	0.21
peptide – ethene	3.00	-0.06	-0.03
methylamine – pyridine[f]	3.97	-0.28	0.16
pyridine – ethyne	3.99	-0.09	0.18
Performance Statistics for the Entire S66 Set			
Mean Absolute Error		0.20	0.28
Mean Signed Error		-0.01	0.16
Mean Absolute Percent Error		4.21	5.78
Mean Signed Percent Error		-0.56	2.99

[a]Reference values are generally of CCSD(T)/CBS quality and are taken from reference 27. [b]All indicated dimers have a hydrogen-bonded interaction in the form *donor-acceptor*.[c]"Peptide" is the nomenclature used in reference 27 and refers to methylamide. [d]Slipped-parallel configuration. [e]Hydrogen-bonding interaction. [f]NH-N and CH(methylamine)-π interactions.

Table S2. Signed deviations in binding energies (kcal/mol) calculated for the non-covalently bonded dimers of the S66 benchmark set using B3LYP/6-31+G(2d,p) with dispersion-correcting potentials and with (CP) and without (Non-CP) counterpoise corrections. The data are ordered according to interaction type. Overall performance statistics for the entire S66 set are provided at the bottom of the Table.

Dimer	Accepted High-Level Value[a]	CP	Non-CP
Hydrogen Bonded Dimers[b]			
water – water	4.92	0.30	0.35
water – methanol	5.59	0.21	0.07
water – methylamine	6.91	0.31	0.68
water – peptide[c]	8.10	0.13	-0.17
methanol – methanol	5.76	0.16	0.02
methanol – methylamine	7.55	0.20	0.62
methanol – peptide[c]	8.23	0.15	-0.16
methanol – water	5.01	0.22	0.31
methylamine – methanol	3.06	0.00	0.09
methylamine – methylamine	4.16	-0.24	0.21
methylamine – peptide[c]	5.42	-0.17	-0.07
methylamine – water	7.27	0.13	0.49
peptide[c] – methanol	6.19	-0.19	-0.12
peptide[c] – methylamine	7.45	-0.01	0.50
peptide[c] – peptide[c]	8.63	-0.08	-0.14
peptide[c] – water	5.12	-0.11	0.18
uracil – uracil (base pair)	17.18	-0.21	-0.37
water – pyridine	6.86	-0.07	0.23
methanol – pyridine	7.41	-0.16	0.17
formic acid – formic acid	19.09	0.45	-0.52
formamide – formamide	16.27	-0.21	-0.20
formic acid – uracil	19.49	0.05	-0.47
formamide – uracil	19.19	-0.11	-0.16
Dispersion-Dominated Dimers			
benzene – benzene[d] (π-stacked)	2.82	0.19	0.06
pyridine – pyridine (π-stacked)	3.90	0.17	-0.02
uracil – uracil (π-stacked)	9.83	-0.41	-0.06
benzene – pyridine (π-stacked)	3.44	0.19	0.00
benzene – uracil (π-stacked)	5.71	-0.29	-0.11
pyridine – uracil (π-stacked)	6.82	-0.50	-0.26
benzene – ethene	1.43	0.12	0.03
uracil – ethene	3.38	-0.13	0.05
uracil – ethyne	3.74	-0.17	0.05
pyridine – ethene	1.87	0.04	0.00
pentane – pentane	3.78	0.10	-0.16

neopentane – pentane	2.61	-0.11	-0.30
neopentane – neopentane	1.78	-0.20	-0.30
cyclopentane – neopentane	2.40	-0.06	-0.25
cyclopentane – cyclopentane	3.00	0.11	-0.16
benzene – cyclopentane	3.58	0.18	0.00
benzene – neopentane	2.90	0.00	-0.10
uracil – pentane	4.85	-0.32	-0.15
uracil – cyclopentane	4.85	-0.20	-0.13
uracil – neopentane	4.14	-0.20	-0.01
ethene – pentane	3.71	-0.06	-0.14
ethyne – pentane	2.01	0.10	0.01
peptide[c] – pentane	1.75	-0.11	-0.15
Mixed Interactions			
benzene – benzene (T-shaped)	2.88	-0.08	0.06
pyridine – pyridine (T-shaped)	3.54	-0.26	-0.12
benzene – pyridine (T-shaped)	3.33	-0.03	0.02
benzene – ethyne (CH-π)	2.87	0.02	0.17
ethyne – ethyne (T-shaped)	1.52	0.00	0.10
benzene – acetic acid (OH-π)	4.71	-0.37	-0.03
benzene – formamide (NH-π)	4.36	-0.24	-0.04
benzene – water (OH-π)	3.28	-0.06	0.34
benzene – methanol (OH-π)	4.19	-0.05	0.20
benzene – methylamine (OH-π)	3.23	-0.11	-0.01
benzene – peptide (NH-π)	5.28	-0.13	-0.02
pyridine – pyridine (CH-N)[e]	4.15	-0.60	-0.43
ethyne – water (CH-O)[e]	2.85	-0.14	0.09
ethyne – acetic acid (OH- π)[e]	4.87	-0.07	0.16
pentane – acetic acid	2.91	-0.02	-0.02
pentane – formamide	3.53	-0.15	-0.19
benzene – acetic acid (π-stacked)	3.80	0.09	0.14
peptide – ethene	3.00	-0.07	-0.04
methylamine – pyridine[f]	3.97	-0.39	-0.08
pyridine – ethyne	3.99	-0.22	0.01
Performance Statistics for the Entire S66 Set			
Mean Absolute Error		0.16	0.16
Mean Signed Error		-0.08	-0.02
Mean Absolute Percent Error		3.67	3.40
Mean Signed Percent Error		-1.62	-0.37

[a]Reference values are generally of CCSD(T)/CBS quality and are taken from reference 27. [b]All indicated dimers have a hydrogen-bonded interaction in the form *donor-acceptor*.[c]"Peptide" is the nomenclature used in reference 27 and refers to methylamide. [d]Slipped-parallel configuration. [e]Hydrogen-bonding interaction. [f]NH-N and CH(methylamine)-π interactions.

Table S3. Signed deviations in binding energies (kcal/mol) calculated for the non-covalently bonded dimers of the S66 benchmark set using B3LYP/aug-cc-pVDZ with dispersion-correcting potentials and with (CP) and without (Non-CP) counterpoise corrections. The data are ordered according to interaction type. Overall performance statistics for the entire S66 set are provided at the bottom of the Table.

Dimer	Accepted High-Level Value[a]	CP	Non-CP
Hydrogen Bonded Dimers[b]			
water – water	4.92	0.03	-0.15
water – methanol	5.59	0.01	-0.18
water – methylamine	6.91	0.15	0.48
water – peptide[c]	8.10	-0.03	-0.15
methanol – methanol	5.76	0.05	-0.12
methanol – methylamine	7.55	0.14	0.66
methanol – peptide[c]	8.23	0.11	-0.09
methanol – water	5.01	0.05	-0.10
methylamine – methanol	3.06	-0.13	0.16
methylamine – methylamine	4.16	-0.38	0.44
methylamine – peptide[c]	5.42	-0.28	0.22
methylamine – water	7.27	-0.03	0.45
peptide[c] – methanol	6.19	-0.30	0.12
peptide[c] – methylamine	7.45	-0.13	0.85
peptide[c] – peptide[c]	8.63	-0.14	0.32
peptide[c] – water	5.12	-0.27	0.11
uracil – uracil (base pair)	17.18	-0.18	0.12
water – pyridine	6.86	-0.04	0.27
methanol – pyridine	7.41	-0.07	0.31
formic acid – formic acid	19.09	0.49	-0.42
formamide – formamide	16.27	-0.19	0.18
formic acid – uracil	19.49	0.07	-0.23
formamide – uracil	19.19	-0.15	0.18
Dispersion-Dominated Dimers			
benzene – benzene[d] (π-stacked)	2.82	0.22	0.26
pyridine – pyridine (π-stacked)	3.90	0.18	0.25
uracil – uracil (π-stacked)	9.83	-0.55	-0.12
benzene – pyridine (π-stacked)	3.44	0.21	0.22
benzene – uracil (π-stacked)	5.71	-0.30	0.07
pyridine – uracil (π-stacked)	6.82	-0.52	-0.08
benzene – ethene	1.43	0.20	0.20
uracil – ethene	3.38	-0.09	0.32
uracil – ethyne	3.74	-0.18	0.04
pyridine – ethene	1.87	0.10	0.20
pentane – pentane	3.78	0.20	1.21

neopentane – pentane	2.61	-0.08	0.75
neopentane – neopentane	1.78	-0.15	0.60
cyclopentane – neopentane	2.40	0.00	0.77
cyclopentane – cyclopentane	3.00	0.17	0.79
benzene – cyclopentane	3.58	0.23	0.61
benzene – neopentane	2.90	0.00	0.40
uracil – pentane	4.85	-0.20	0.67
uracil – cyclopentane	4.85	-0.11	0.56
uracil – neopentane	4.14	-0.14	0.63
ethene – pentane	3.71	0.01	0.39
ethyne – pentane	2.01	0.18	0.30
peptide[c] – pentane	1.75	-0.03	1.01
Mixed Interactions			
benzene – benzene (T-shaped)	2.88	-0.13	0.27
pyridine – pyridine (T-shaped)	3.54	-0.31	0.16
benzene – pyridine (T-shaped)	3.33	-0.09	0.27
benzene – ethyne (CH-π)	2.87	-0.10	0.32
ethyne – ethyne (T-shaped)	1.52	-0.07	0.15
benzene – acetic acid (OH-π)	4.71	-0.52	0.03
benzene – formamide (NH-π)	4.36	-0.34	0.06
benzene – water (OH-π)	3.28	-0.22	0.13
benzene – methanol (OH-π)	4.19	-0.17	0.29
benzene – methylamine (OH-π)	3.23	-0.18	0.25
benzene – peptide (NH-π)	5.28	-0.27	0.48
pyridine – pyridine (CH-N)[e]	4.15	-0.59	0.07
ethyne – water (CH-O)[e]	2.85	-0.24	0.11
ethyne – acetic acid (OH- π)[e]	4.87	-0.23	0.07
pentane – acetic acid	2.91	0.12	0.83
pentane – formamide	3.53	-0.05	0.56
benzene – acetic acid (π-stacked)	3.80	0.06	0.48
peptide – ethene	3.00	-0.11	0.23
methylamine – pyridine[f]	3.97	-0.40	0.20
pyridine – ethyne	3.99	-0.20	0.43
Performance Statistics for the Entire S66 Set			
Mean Absolute Error		0.19	0.34
Mean Signed Error		-0.10	0.30
Mean Absolute Percent Error		4.48	9.38
Mean Signed Percent Error		-1.91	9.04

[a]Reference values are generally of CCSD(T)/CBS quality and are taken from reference 27. [b]All indicated dimers have a hydrogen-bonded interaction in the form *donor-acceptor*.[c]"Peptide" is the nomenclature used in reference 27 and refers to methylamide. [d]Slipped-parallel configuration. [e]Hydrogen-bonding interaction. [f]NH-N and CH(methylamine)-π interactions.

Table S4. Signed deviations in binding energies (kcal/mol) calculated for the non-covalently bonded dimers of the S66 benchmark set using B3LYP/6-311+G(2d,2p) with dispersion-correcting potentials and with (CP) and without (Non-CP) counterpoise corrections. The data are ordered according to interaction type. Overall performance statistics for the entire S66 set are provided at the bottom of the Table.

Dimer	Accepted High-Level Value[a]	CP	Non-CP
Hydrogen Bonded Dimers[b]			
water – water	4.92	0.15	0.14
water – methanol	5.59	0.10	-0.05
water – methylamine	6.91	0.22	0.44
water – peptide[c]	8.10	0.09	-0.29
methanol – methanol	5.76	0.11	-0.01
methanol – methylamine	7.55	0.18	0.45
methanol – peptide[c]	8.23	0.18	-0.15
methanol – water	5.01	0.13	0.16
methylamine – methanol	3.06	-0.05	0.03
methylamine – methylamine	4.16	-0.28	0.04
methylamine – peptide[c]	5.42	-0.20	-0.18
methylamine – water	7.27	0.05	0.25
peptide[c] – methanol	6.19	-0.17	-0.16
peptide[c] – methylamine	7.45	-0.04	0.26
peptide[c] – peptide[c]	8.63	-0.06	-0.18
peptide[c] – water	5.12	-0.15	0.06
uracil – uracil (base pair)	17.18	-0.25	-0.51
water – pyridine	6.86	-0.03	0.18
methanol – pyridine	7.41	-0.08	0.17
formic acid – formic acid	19.09	0.40	-0.61
formamide – formamide	16.27	-0.19	-0.27
formic acid – uracil	19.49	0.00	-0.61
formamide – uracil	19.19	-0.15	-0.33
Dispersion-Dominated Dimers			
benzene – benzene[d] (π-stacked)	2.82	0.28	-0.23
pyridine – pyridine (π-stacked)	3.90	0.24	-0.28
uracil – uracil (π-stacked)	9.83	-0.41	-0.31
benzene – pyridine (π-stacked)	3.44	0.27	-0.28
benzene – uracil (π-stacked)	5.71	-0.25	-0.40
pyridine – uracil (π-stacked)	6.82	-0.49	-0.50
benzene – ethene	1.43	0.21	-0.10
uracil – ethene	3.38	-0.08	-0.06
uracil – ethyne	3.74	-0.17	-0.16
pyridine – ethene	1.87	0.10	-0.13
pentane – pentane	3.78	0.13	-0.28

neopentane – pentane	2.61	-0.08	-0.38
neopentane – neopentane	1.78	-0.16	-0.38
cyclopentane – neopentane	2.40	-0.02	-0.31
cyclopentane – cyclopentane	3.00	0.14	-0.23
benzene – cyclopentane	3.58	0.22	-0.21
benzene – neopentane	2.90	0.01	-0.32
uracil – pentane	4.85	-0.21	-0.15
uracil – cyclopentane	4.85	-0.12	-0.15
uracil – neopentane	4.14	-0.17	-0.05
ethene – pentane	3.71	-0.02	-0.24
ethyne – pentane	2.01	0.16	-0.06
peptide[c] – pentane	1.75	-0.06	-0.21
Mixed Interactions			
benzene – benzene (T-shaped)	2.88	-0.08	-0.30
pyridine – pyridine (T-shaped)	3.54	-0.26	-0.34
benzene – pyridine (T-shaped)	3.33	-0.03	-0.26
benzene – ethyne (CH-π)	2.87	0.00	-0.06
ethyne – ethyne (T-shaped)	1.52	-0.05	-0.11
benzene – acetic acid (OH-π)	4.71	-0.35	-0.08
benzene – formamide (NH-π)	4.36	-0.21	-0.18
benzene – water (OH-π)	3.28	-0.08	0.26
benzene – methanol (OH-π)	4.19	-0.04	0.12
benzene – methylamine (OH-π)	3.23	-0.11	-0.14
benzene – peptide (NH-π)	5.28	-0.14	-0.21
pyridine – pyridine (CH-N)[e]	4.15	-0.61	-0.55
ethyne – water (CH-O)[e]	2.85	-0.16	-0.09
ethyne – acetic acid (OH- π)[e]	4.87	-0.11	-0.01
pentane – acetic acid	2.91	0.09	0.09
pentane – formamide	3.53	-0.06	-0.20
benzene – acetic acid (π-stacked)	3.80	0.10	0.01
peptide – ethene	3.00	-0.09	-0.21
methylamine – pyridine[f]	3.97	-0.37	-0.18
pyridine – ethyne	3.99	-0.22	-0.19
Performance Statistics for the Entire S66 Set			
Mean Absolute Error		0.16	0.22
Mean Signed Error		-0.06	-0.15
Mean Absolute Percent Error		3.84	5.18
Mean Signed Percent Error		-1.08	-3.94

[a]Reference values are generally of CCSD(T)/CBS quality and are taken from reference 27. [b]All indicated dimers have a hydrogen-bonded interaction in the form *donor-acceptor*.[c]"Peptide" is the nomenclature used in reference 27 and refers to methylamide. [d]Slipped-parallel configuration. [e]Hydrogen-bonding interaction. [f]NH-N and CH(methylamine)-π interactions.

Table S5. Signed deviations in binding energies (kcal/mol) calculated for the non-covalently bonded dimers of the S66 benchmark set using B3LYP/aug-cc-pVTZ with dispersion-correcting potentials and with (CP) and without (Non-CP) counterpoise corrections. The data are ordered according to interaction type. Overall performance statistics for the entire S66 set are provided at the bottom of the Table.

Dimer	Accepted High-Level Value[a]	CP	Non-CP
Hydrogen Bonded Dimers[b]			
water – water	4.92	0.09	-0.28
water – methanol	5.59	0.05	-0.41
water – methylamine	6.91	0.20	0.14
water – peptide[c]	8.10	0.05	-0.55
methanol – methanol	5.76	0.10	-0.33
methanol – methylamine	7.55	0.19	0.19
methanol – peptide[c]	8.23	0.19	-0.37
methanol – water	5.01	0.12	-0.20
methylamine – methanol	3.06	-0.09	-0.17
methylamine – methylamine	4.16	-0.31	-0.10
methylamine – peptide[c]	5.42	-0.22	-0.32
methylamine – water	7.27	0.01	-0.03
peptide[c] – methanol	6.19	-0.23	-0.36
peptide[c] – methylamine	7.45	-0.08	0.11
peptide[c] – peptide[c]	8.63	-0.07	-0.27
peptide[c] – water	5.12	-0.20	-0.22
uracil – uracil (base pair)	17.18	0.01	-0.50
water – pyridine	6.86	0.00	-0.02
methanol – pyridine	7.41	-0.05	-0.01
formic acid – formic acid	19.09	0.70	-0.60
formamide – formamide	16.27	-0.12	-0.30
formic acid – uracil	19.49	0.25	-0.61
formamide – uracil	19.19	-0.01	-0.34
Dispersion-Dominated Dimers			
benzene – benzene[d] (π-stacked)	2.82	0.37	-0.24
pyridine – pyridine (π-stacked)	3.90	0.31	-0.32
uracil – uracil (π-stacked)	9.83	-0.30	-0.72
benzene – pyridine (π-stacked)	3.44	0.35	-0.31
benzene – uracil (π-stacked)	5.71	-0.11	-0.56
pyridine – uracil (π-stacked)	6.82	-0.35	-0.69
benzene – ethene	1.43	0.28	-0.06
uracil – ethene	3.38	-0.01	-0.06
uracil – ethyne	3.74	-0.10	-0.18
pyridine – ethene	1.87	0.19	-0.08
pentane – pentane	3.78	0.21	-0.21

neopentane – pentane	2.61	-0.03	-0.33
neopentane – neopentane	1.78	-0.16	-0.36
cyclopentane – neopentane	2.40	0.01	-0.29
cyclopentane – cyclopentane	3.00	0.15	-0.23
benzene – cyclopentane	3.58	0.27	-0.20
benzene – neopentane	2.90	0.05	-0.28
uracil – pentane	4.85	-0.11	-0.27
uracil – cyclopentane	4.85	-0.03	-0.26
uracil – neopentane	4.14	-0.11	-0.13
ethene – pentane	3.71	0.01	-0.19
ethyne – pentane	2.01	0.20	-0.03
peptide[c] – pentane	1.75	0.01	-0.22
Mixed Interactions			
benzene – benzene (T-shaped)	2.88	-0.07	-0.31
pyridine – pyridine (T-shaped)	3.54	-0.26	-0.39
benzene – pyridine (T-shaped)	3.33	-0.02	-0.29
benzene – ethyne (CH-π)	2.87	0.00	-0.09
ethyne – ethyne (T-shaped)	1.52	-0.03	-0.07
benzene – acetic acid (OH-π)	4.71	-0.36	-0.25
benzene – formamide (NH-π)	4.36	-0.27	-0.27
benzene – water (OH-π)	3.28	-0.14	-0.06
benzene – methanol (OH-π)	4.19	-0.03	-0.06
benzene – methylamine (OH-π)	3.23	-0.08	-0.18
benzene – peptide (NH-π)	5.28	-0.12	-0.24
pyridine – pyridine (CH-N)[e]	4.15	-0.59	-0.57
ethyne – water (CH-O)[e]	2.85	-0.20	-0.25
ethyne – acetic acid (OH- π)[e]	4.87	-0.11	-0.06
pentane – acetic acid	2.91	0.12	-0.01
pentane – formamide	3.53	-0.01	-0.21
benzene – acetic acid (π-stacked)	3.80	0.10	-0.10
peptide – ethene	3.00	-0.08	-0.22
methylamine – pyridine[f]	3.97	-0.37	-0.28
pyridine – ethyne	3.99	-0.19	-0.11
Performance Statistics for the Entire S66 Set			
Mean Absolute Error		0.16	0.25
Mean Signed Error		-0.02	-0.24
Mean Absolute Percent Error		3.94	5.57
Mean Signed Percent Error		-0.26	-5.44

[a]Reference values are generally of CCSD(T)/CBS quality and are taken from reference 27. [b]All indicated dimers have a hydrogen-bonded interaction in the form *donor-acceptor*.[c]"Peptide" is the nomenclature used in reference 27 and refers to methylamide. [d]Slipped-parallel configuration. [e]Hydrogen-bonding interaction. [f]NH-N and CH(methylamine)-π interactions.

Table S6. Signed deviations in binding energies (kcal/mol) calculated for the non-covalently bonded dimers of the S22 benchmark set using B3LYP/6-31+G(d,p) with dispersion-correcting potentials and with (CP) and without (Non-CP) counterpoise corrections. The data are ordered according to interaction type. Overall performance statistics for the entire S22 set are provided at the bottom of the Table.

Dimer	Accepted High-Level Value[a]	CP	Non-CP
2-pyridoxine - 2-aminopyridine	**16.934**	-0.20	0.23
Adenine-Thymine (H-bonded)	**16.66**	-0.58	-0.23
Adenine-Thymine (Stacked)	**11.73**	-0.87	-0.28
Benzene-H_2O	**3.275**	0.04	0.54
Benzene-HCN	**4.541**	-0.01	0.11
Benzene-Indole (Stacked)	**4.524**	0.24	0.33
Benzene-Indole (T-shaped)	**5.627**	-0.52	-0.07
Benzene-Methane	**1.448**	0.08	0.09
Benzene-NH_3	**2.312**	-0.03	0.25
Ethylene Dimer	**1.472**	-0.12	-0.08
Ethylene-Ethyne	**1.496**	0.03	0.10
Formamide Dimer	**16.062**	-0.52	-0.36
Formic Acid Dimer	**18.753**	-0.03	-0.76
H_2O Dimer	**4.989**	0.68	1.19
Methane Dimer	**0.527**	-0.14	-0.18
NH_3 Dimer	**3.133**	0.23	0.67
Phenol Dimer	**7.097**	-0.26	0.17
Pyrazine Dimer	**4.255**	-0.47	-0.22
Slipped parallel Benzene Dimer	**2.654**	0.23	0.23
T-shaped Benzene Dimer	**2.717**	-0.08	0.10
Uracil Dimer (H-bonded)	**20.641**	-0.53	-0.49
Uracil Dimer (Stacked)	**9.805**	-0.47	0.10
Performance Statistics for the Entire S22 Set			
Mean absolute error		0.29	0.31
Mean signed error		-0.15	0.07
Mean absolute percent error		5.91	7.78
Mean signed percent error		-1.93	2.42

[a]High-level binding energies are of CCSD(T)/CBS quality and are taken from reference 29

Table S7. Signed deviations in binding energies (kcal/mol) calculated for the non-covalently bonded dimers of the S22 benchmark set using B3LYP/6-31+G(2d,p) with dispersion-correcting potentials and with (CP) and without (Non-CP) counterpoise corrections. The data are ordered according to interaction type. Overall performance statistics for the entire S22 set are provided at the bottom of the Table.

Dimer	Accepted High-Level Value[a]	CP	Non-CP
2-pyridoxine - 2-aminopyridine	**16.934**	-0.49	-0.20
Adenine-Thymine (H-bonded)	**16.66**	-0.84	-0.65
Adenine-Thymine (Stacked)	**11.73**	-0.79	-0.55
Benzene-H_2O	**3.275**	-0.04	0.34
Benzene-HCN	**4.541**	0.08	0.14
Benzene-Indole (Stacked)	**4.524**	0.35	0.28
Benzene-Indole (T-shaped)	**5.627**	-0.43	-0.11
Benzene-Methane	**1.448**	0.10	0.07
Benzene-NH_3	**2.312**	-0.07	0.10
Ethylene Dimer	**1.472**	-0.10	-0.07
Ethylene-Ethyne	**1.496**	0.04	0.14
Formamide Dimer	**16.062**	-0.39	-0.32
Formic Acid Dimer	**18.753**	0.31	-0.59
H_2O Dimer	**4.989**	0.27	0.46
Methane Dimer	**0.527**	-0.13	-0.17
NH_3 Dimer	**3.133**	-0.21	0.18
Phenol Dimer	**7.097**	-0.56	-0.42
Pyrazine Dimer	**4.255**	-0.40	-0.35
Slipped parallel Benzene Dimer	**2.654**	0.33	0.18
T-shaped Benzene Dimer	**2.717**	-0.07	0.06
Uracil Dimer (H-bonded)	**20.641**	-0.60	-0.73
Uracil Dimer (Stacked)	**9.805**	-0.35	0.00
Performance Statistics for the Entire S22 Set			
Mean absolute error		0.32	0.28
Mean signed error		-0.18	-0.10
Mean absolute percent error		6.04	6.02
Mean signed percent error		-2.54	-0.39

[a]High-level binding energies are of CCSD(T)/CBS quality and are taken from reference 29.

Table S8. Signed deviations in binding energies (kcal/mol) calculated for the non-covalently bonded dimers of the S22 benchmark set using B3LYP/aug-cc-pVDZ with dispersion-correcting potentials and with (CP) and without (Non-CP) counterpoise corrections. The data are ordered according to interaction type. Overall performance statistics for the entire S22 set are provided at the bottom of the Table.

Dimer	Accepted High-Level Value[a]	CP	Non-CP
2-pyridoxine - 2-aminopyridine	**16.934**	-0.33	0.54
Adenine-Thymine (H-bonded)	**16.66**	-0.68	0.12
Adenine-Thymine (Stacked)	**11.73**	-0.80	-0.14
Benzene-H_2O	**3.275**	-0.20	0.12
Benzene-HCN	**4.541**	-0.10	0.17
Benzene-Indole (Stacked)	**4.524**	0.45	0.58
Benzene-Indole (T-shaped)	**5.627**	-0.60	0.23
Benzene-Methane	**1.448**	0.08	0.26
Benzene-NH_3	**2.312**	-0.17	0.13
Ethylene Dimer	**1.472**	-0.07	0.21
Ethylene-Ethyne	**1.496**	-0.05	0.23
Formamide Dimer	**16.062**	-0.40	0.01
Formic Acid Dimer	**18.753**	0.34	-0.51
H_2O Dimer	**4.989**	-0.03	-0.08
Methane Dimer	**0.527**	-0.10	0.19
NH_3 Dimer	**3.133**	-0.53	-0.03
Phenol Dimer	**7.097**	-0.58	-0.46
Pyrazine Dimer	**4.255**	-0.41	0.00
Slipped parallel Benzene Dimer	**2.654**	0.40	0.45
T-shaped Benzene Dimer	**2.717**	-0.16	0.28
Uracil Dimer (H-bonded)	**20.641**	-0.63	-0.33
Uracil Dimer (Stacked)	**9.805**	-0.48	-0.06
Performance Statistics for the Entire S22 Set			
Mean absolute error		0.34	0.23
Mean signed error		-0.23	0.09
Mean absolute percent error		6.78	7.27
Mean signed percent error		-3.86	5.88

[a]High-level binding energies are of CCSD(T)/CBS quality and are taken from reference 29.

Table S9. Signed deviations in binding energies (kcal/mol) calculated for the non-covalently bonded dimers of the S22 benchmark set using B3LYP/6-31+G(2d,2p) with dispersion-correcting potentials and with (CP) and without (Non-CP) counterpoise corrections. The data are ordered according to interaction type. Overall performance statistics for the entire S22 set are provided at the bottom of the Table.

Dimer	Accepted High-Level Value[a]	CP	Non-CP
2-pyridoxine - 2-aminopyridine	**16.934**	-0.32	-0.02
Adenine-Thymine (H-bonded)	**16.66**	-0.69	-0.47
Adenine-Thymine (Stacked)	**11.73**	-0.79	-0.59
Benzene-H_2O	**3.275**	-0.10	0.28
Benzene-HCN	**4.541**	0.02	0.09
Benzene-Indole (Stacked)	**4.524**	0.38	0.37
Benzene-Indole (T-shaped)	**5.627**	-0.45	-0.12
Benzene-Methane	**1.448**	0.10	0.09
Benzene-NH_3	**2.312**	-0.10	0.06
Ethylene Dimer	**1.472**	-0.11	-0.09
Ethylene-Ethyne	**1.496**	0.00	0.12
Formamide Dimer	**16.062**	-0.29	-0.20
Formic Acid Dimer	**18.753**	0.57	-0.20
H_2O Dimer	**4.989**	0.21	0.37
Methane Dimer	**0.527**	-0.12	-0.14
NH_3 Dimer	**3.133**	-0.30	0.06
Phenol Dimer	**7.097**	-0.52	-0.39
Pyrazine Dimer	**4.255**	-0.40	-0.34
Slipped parallel Benzene Dimer	**2.654**	0.35	0.26
T-shaped Benzene Dimer	**2.717**	-0.09	0.07
Uracil Dimer (H-bonded)	**20.641**	-0.49	-0.60
Uracil Dimer (Stacked)	**9.805**	-0.37	-0.03
Performance Statistics for the Entire S22 Set			
Mean absolute error		0.31	0.23
Mean signed error		-0.16	-0.06
Mean absolute percent error		6.05	5.44
Mean signed percent error		-2.73	-0.20

[a]High-level binding energies are of CCSD(T)/CBS quality and are taken from reference 29.

Table S10. Signed deviations in binding energies (kcal/mol) calculated for the non-covalently bonded dimers of the S22 benchmark set using B3LYP/6-311+G(2d,2p) with dispersion-correcting potentials and with (CP) and without (Non-CP) counterpoise corrections. The data are ordered according to interaction type. Overall performance statistics for the entire S22 set are provided at the bottom of the Table.

Dimer	Accepted High-Level Value[a]	CP	Non-CP
2-pyridoxine - 2-aminopyridine	**16.934**	-0.35	-0.20
Adenine-Thymine (H-bonded)	**16.66**	-0.70	-0.58
Adenine-Thymine (Stacked)	**11.73**	-0.74	-0.82
Benzene-H_2O	**3.275**	-0.07	0.25
Benzene-HCN	**4.541**	0.08	0.00
Benzene-Indole (Stacked)	**4.524**	0.47	-0.16
Benzene-Indole (T-shaped)	**5.627**	-0.41	-0.42
Benzene-Methane	**1.448**	0.11	-0.01
Benzene-NH_3	**2.312**	-0.08	0.00
Ethylene Dimer	**1.472**	-0.08	-0.18
Ethylene-Ethyne	**1.496**	-0.01	-0.08
Formamide Dimer	**16.062**	-0.37	-0.38
Formic Acid Dimer	**18.753**	0.25	-0.67
H_2O Dimer	**4.989**	0.10	0.23
Methane Dimer	**0.527**	-0.10	-0.14
NH_3 Dimer	**3.133**	-0.34	-0.01
Phenol Dimer	**7.097**	-0.53	-0.67
Pyrazine Dimer	**4.255**	-0.36	-0.46
Slipped parallel Benzene Dimer	**2.654**	0.44	-0.11
T-shaped Benzene Dimer	**2.717**	-0.08	-0.29
Uracil Dimer (H-bonded)	**20.641**	-0.65	-0.93
Uracil Dimer (Stacked)	**9.805**	-0.34	-0.25
Performance Statistics for the Entire S22 Set			
Mean absolute error		0.30	0.31
Mean signed error		-0.17	-0.27
Mean absolute percent error		5.84	5.85
Mean signed percent error		-2.22	-4.74

[a]High-level binding energies are of CCSD(T)/CBS quality and are taken from reference 29.

Table S11. Signed deviations in binding energies (kcal/mol) calculated for the non-covalently bonded dimers of the S22 benchmark set using B3LYP/aug-cc-pVTZ with dispersion-correcting potentials and with (CP) and without (Non-CP) counterpoise corrections. The data are ordered according to interaction type. Overall performance statistics for the entire S22 set are provided at the bottom of the Table.

Dimer	Accepted High-Level Value[a]	CP	Non-CP
2-pyridoxine - 2-aminopyridine	**16.934**		-0.22
Adenine-Thymine (H-bonded)	**16.66**		-0.57
Adenine-Thymine (Stacked)	**11.73**		-1.14
Benzene-H_2O	**3.275**		-0.09
Benzene-HCN	**4.541**		0.17
Benzene-Indole (Stacked)	**4.524**		-0.25
Benzene-Indole (T-shaped)	**5.627**		-0.64
Benzene-Methane	**1.448**		0.01
Benzene-NH_3	**2.312**		-0.13
Ethylene Dimer	**1.472**		-0.22
Ethylene-Ethyne	**1.496**		0.07
Formamide Dimer	**16.062**		-0.36
Formic Acid Dimer	**18.753**		-0.47
H_2O Dimer	**4.989**		-0.20
Methane Dimer	**0.527**		-0.11
NH_3 Dimer	**3.133**		-0.21
Phenol Dimer	**7.097**		-1.02
Pyrazine Dimer	**4.255**		-0.49
Slipped parallel Benzene Dimer	**2.654**		-0.11
T-shaped Benzene Dimer	**2.717**		-0.33
Uracil Dimer (H-bonded)	**20.641**		-0.63
Uracil Dimer (Stacked)	**9.805**		-0.66
Performance Statistics for the Entire S22 Set			
Mean absolute error			0.37
Mean signed error			-0.35
Mean absolute percent error			6.89
Mean signed percent error			-6.08

[a]High-level binding energies are of CCSD(T)/CBS quality and are taken from reference 29.

Table S12. Structure file and associated binding energies (kcal/mol) taken from reference 27 for use in the fitting set described in Table 1. The Distance Scaling represents that scaling factor used on the equilibrium distance between monomers. See www.begdb.com for additional information.

Distance Scaling	Binding Energy
Uracil Dimer (H-bonded)	
0.9	-18.730
1.0	-20.460
1.2	-17.160
1.5	-10.460
2.0	-4.580
Uracil Dimer (Stacked)	
0.9	-6.760
1.0	-9.870
1.2	-6.260
1.5	-2.420
2.0	-0.690
Benzene Dimer (T-Shaped)	
0.9	-2.200
1.0	-2.800
1.2	-2.250
1.5	-1.120
2.0	-0.350
Benzene Dimer (Stacked)	
0.9	-0.150
1.0	-2.810
1.2	-1.920
1.5	-0.530
2.0	-0.070
Formamide dimer (H-bonded)	
0.9	-14.140
1.0	-15.950
1.2	-13.400
1.5	-8.100
2.0	-3.510
Formic acid dimer (H-bonded)	
0.9	-16.340
1.0	-18.590
1.2	-15.620
1.5	-9.240
2.0	-3.630

Table S13. Separation coordinate (Å)and binding energies (kcal/mol) for dimers used in the fitting set described in Table 1.[a] Representative coordinates for this structures are listed in the Table S14.

Distance	Binding Energy
CH_4-NH_3	
3.6	-0.568
3.92	-0.766
4.5	-0.497
7	-0.038
10	-0.005
$(CH_3CN)_2$	
3.0	-4.607
3.3	-6.347
3.5	-6.081
4.0	-4.372
10.0	-0.219
H_2NH-NH_3	
2.8	-1.446
3.2	-3.093
3.6	-2.433
5.0	-0.583
10.0	0.010
H_3N-NH_3	
4.0	1.991
5.0	0.965
6.0	0.540
10.0	0.100
$(CO_2)_2$	
3.36	-1.403
3.56	-1.521
4.5	-0.651
10.0	-0.008
$(H_2CO)_2$	
3.30	-1.201
3.62	-3.343
5.0	-1.042
10.0	-0.043
HOH-OH_2	
1.70	-3.745
1.95	-4.998
2.75	-2.746
5.0	-0.437
10.0	-0.055
H_2O-OH_2	
3.0	2.737
4.0	1.167
6.0	0.403
10.0	0.094
$(C_2H_6)_2$	
3.500	0.73

3.9	-0.988
4.1	-1.031
4.3	-0.922
5.0	-0.433
10.0	-0.005
C3v $(CH_4)_2$	
3.25	0.054
3.5	-0.431
3.65	-0.492
4.25	-0.321
5.0	-0.126
10.0	-0.002
D3h $(CH_4)_2$	
3.75	-0.227
3.85	-0.344
4.1	-0.424
4.5	-0.325
5.0	-0.183
10.0	-0.002

[a]Calculations were performed using the Ave-CCSD/T + Ave-(T)/D + Ave-ΔMP2((Q-T)-T) approach described in reference 21.

Table S14. Cartesian coordinates (Å) for representative structures for those given in Table S13.

CH_4-NH_3				
C	0.0000000000000000	0.0000000000000000	-12.3348508455473009	1
H	1.0254197585872136	0.0000000000000000	-12.7021283193990797	1
H	-0.5127126841450675	0.8880453362351374	-12.7021306544230157	1
H	-0.5127139388729051	-0.8880390935671613	-12.7021341575584028	1
H	-0.0000020504473206	-0.0000048200948200	-11.2460839235329679	1
N	0.0000000000000000	0.0000000000000000	-8.4148508455473010	2
H	0.4687923364987370	-0.8119668577364032	-8.0324407533978786	2
H	0.4687939599524392	0.8119722556778979	-8.0324362207988997	2
H	-0.9375808575225234	-0.0000056460971746	-8.0324351146006645	2
$(CH_3CN)_2$				
C	0.0000000000000000	-0.0000000000000012	-12.4191728274274027	1
N	1.1428110343906399	-0.0000000000000012	-12.2541099649325442	1
C	-1.4510577323613796	-0.0000000000000012	-12.6079437917048871	1
H	-1.7485669542476516	-0.8872899999999989	-13.1633476936470899	1
H	-1.9321778933488869	-0.0000000000000012	-11.6315430168222793	1
H	-1.7485669542476516	0.8872900000000001	-13.1633476936470899	1
C	0.0000000000000000	-0.0000000000000012	-9.1191728274274020	2
N	-1.1428209316862681	-0.0000000000000012	-9.2842371194463897	2
C	1.4510464055416177	-0.0000000000000012	-8.9303933953784167	2
H	1.7485669542476516	0.8872900000000001	-8.3749979612077112	2
H	1.7485669542476516	-0.8872899999999989	-8.3749979612077112	2
H	1.9321665665291277	-0.0000000000000012	-9.9067941702610227	2
H_2NH-NH_3				
N	0.0000000000000000	0.0000000000000000	-12.1860393281001116	1
H	0.8257344458621967	0.0000000000000000	-12.7720771925053516	1
H	0.1582133107728458	0.6661546038097967	-11.4400560122563135	1
H	-0.7375564287362828	0.3712808892121492	-12.7720789126297003	1
N	0.0000000000000000	0.0000000000000000	-8.9860393281001123	2
H	0.7375522363723639	-0.3712877834383226	-8.4000056506620435	2
H	-0.1582133107728433	-0.6661546038097979	-9.7320226439439104	2
H	-0.8257344458621955	0.0000000000000000	-8.4000014636948741	2
H_3N-NH_3				
N	0.0000000000000000	0.0000000000000000	-11.8816876810593897	1
H	0.9378681864665914	0.0000000000000000	-12.2633695098302535	1
H	-0.4689370158404720	0.8122226934405790	-12.2633741917389880	1
H	-0.4689378638265722	-0.8122194769351301	-12.2633762754095414	1
N	0.0000000000000000	0.0000000000000000	-7.8816876810593888	2
H	0.4689286014797857	0.8122194769351313	-7.4999953172355385	2
H	0.4689256927558694	-0.8122143200970717	-7.5000024645488725	2
H	-0.9378681864665914	0.0000000000000000	-7.5000058522885258	2
$(CO_2)_2$				
C	0.0000000000000000	0.0000000000000000	-12.3972502138259308	1
O	0.9879661127696175	0.0000000000000000	-11.7871023363438496	1
O	-0.9811041305954901	0.0000000000000000	-13.0125041764661269	1

C	0.0000000000000000	0.0000000000000000	-9.0372502138259314	2
O	-0.9879661127696175	0.0000000000000000	-9.6473980913080108	2
O	0.9811041305954913	0.0000000000000000	-8.4219962511857300	2
$(H_2CO)_2$				
C	0.0000000000000000	0.0000000000000000	-12.9098056241358083	1
O	0.0000000000000000	1.0127955699354381	-12.2429361744084311	1
H	0.0000000000000000	-0.9979617142634707	-12.4465319632626592	1
H	0.0000000000000000	0.0312673746114162	-14.0096112473888130	1
C	0.0000000000000000	0.0000000000000000	-9.6098056241358076	2
O	0.0000000000000000	-1.0127955699354381	-10.2766750738631902	2
H	0.0000000000000000	0.9979617142634756	-10.0730792850089639	2
H	0.0000000000000000	-0.0312673746114125	-8.5100000008828101	2
$HOH\text{-}OH_2$				
O	-0.1395785790362273	-0.0000000000000012	-12.7749627410050515	1
H	0.7446136119241541	-0.0000000000000012	-13.1509159370396045	1
H	0.0000000000000000	-0.0000000000000012	-11.8243553262936576	1
O	0.0000000000000000	-0.0000000000000012	-9.8743553262936583	2
H	-0.4734672687524294	-0.7606267999999994	-9.5273506292175831	2
H	-0.4734672687524294	0.7606267999999982	-9.5273506292175831	2
$H_2O\text{-}OH_2$				
O	0.0000000000000000	0.0000000000000000	-12.0870143696566945	1
H	0.7606262623466677	0.0000000000000000	-12.6740274266056332	1
H	-0.7606320284416230	0.0000000000000000	-12.6740246188080903	1
O	0.0000000000000000	0.0000000000000000	-9.0870143696566945	2
H	0.7606320284416230	0.0000000000000000	-8.5000041205053023	2
H	-0.7606262623466689	0.0000000000000000	-8.5000013127077594	2
$(C_2H_6)_2$				
C	0.0000000000000000	-13.0744959999999999	1.5460059999999987	1
C	0.0000000000000000	-13.0744959999999999	0.0000000000000000	1
H	0.0000000000000000	-12.0499999999999989	1.9439980000000010	1
H	-0.8872400000000003	-13.5867439999999995	1.9439980000000010	1
H	0.8872399999999990	-13.5867439999999995	1.9439980000000010	1
H	0.0000000000000000	-14.0989920000000009	-0.3979920000000011	1
H	-0.8872400000000003	-12.5622480000000003	-0.3979920000000011	1
H	0.8872399999999990	-12.5622480000000003	-0.3979920000000011	1
C	0.0000000000000000	-9.1744959999999995	1.5460059999999987	2
C	0.0000000000000000	-9.1744959999999995	0.0000000000000000	2
H	0.0000000000000000	-8.1500000000000004	1.9439980000000010	2
H	-0.8872400000000003	-9.6867440000000009	1.9439980000000010	2
H	0.8872399999999990	-9.6867440000000009	1.9439980000000010	2
H	0.0000000000000000	-10.1989920000000023	-0.3979920000000011	2
H	-0.8872400000000003	-8.6622480000000017	-0.3979920000000011	2
H	0.8872399999999990	-8.6622480000000017	-0.3979920000000011	2
$(CH_4)_2$ C_{3v}				
C	0.0000000000000000	0.0000000000000000	-12.7533125118164996	1
H	1.0224540862679996	0.0000000000000000	-13.1153753200394991	1
H	0.0000000000000000	0.0000000000000000	-11.6687308011525008	1

H	-0.5112270431339998	0.8854712129109996	-13.1153753200394991	1
H	-0.5112270431339998	-0.8854712129109996	-13.1153753200394991	1
C	0.0000000000000000	0.0000000000000000	-8.9033125118165000	2
H	1.0227386764609996	0.0000000000000000	-9.2648380781394994	2
H	0.0000000000000000	0.0000000000000000	-7.8186909185444993	2
H	-0.5113693382310007	0.8857176752479990	-9.2648380781394994	2
H	-0.5113693382310007	-0.8857176752479990	-9.2648380781394994	2
$(CH_4)_2$ D_{3h}				
C	-0.0000000000000012	0.0000000000000000	-12.9302615371670004	1
H	-1.0221680029300009	0.0000000000000000	-12.5675320710289995	1
H	-0.0000000000000012	0.0000000000000000	-14.0149303532539999	1
H	0.5110840014649981	0.8852234574729996	-12.5675320710289995	1
H	0.5110840014649981	-0.8852234574729996	-12.5675320710289995	1
C	-0.0000000000000012	0.0000000000000000	-9.4302615371670004	2
H	-1.0221680029300009	0.0000000000000000	-9.7929910033049996	2
H	-0.0000000000000012	0.0000000000000000	-8.3455927210800009	2
H	0.5110840014649981	-0.8852234574729996	-9.7929910033049996	2
H	0.5110840014649981	0.8852234574729996	-9.7929910033049996	2