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

PICVib: An Accurate, Fast and Simple Procedure to Investigate Selected Vibrational Modes at High Theoretical Levels. Evaluating Infrared Intensities.

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Supplementary Information

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Table S1. Analytical vibrational frequencies (cm^{-1}) calculated with 6-311+G(2d,p) basis sets for the A_{2u} modes of the YH_4 (D_{4h}) planar system.

Compound	B3LYP	MP2	CCSD	CCSD(T)
CH_4	920i	999i	1016i	1017i
SiH_4	999	995	1062i	1068i
GeH_4	857	850	757	806

Table S2. Analytical infrared intensities (km mol^{-1}) calculated with 6-311+G(2d,p) basis sets for the A_2'' and A_{2u} modes of the XH_3 (D_{3h}) and YH_4 (D_{4h}) planar systems, respectively. For CCSD and CCSD(T) all calculations were performed with the CFOUR program, where the values in brackets are infrared intensities calculated by finite differences. For CCSD calculations with G09 program, the infrared intensities are calculated by finite differences.

Compound	B3LYP	MP2	CCSD (CFOUR)	CCSD (G09)	CCSD(T)
BH_3	84	90	84	84	82
AlH_3	338	390	359	359	353
GaH_3	171	239	218	218	215
NH_3	414	435	438	438	431
PH_3	197	211	216	216	209
AsH_3	124	150	159	159	152
OH_3^+	639	653	816 [648]	648	812 [644]
SH_3^+	276	289	342 [284]	284	340 [283]
SeH_3^+	238	258	283 [261]	261	280 [258]
CH_4	666	719	750	750	731
SiH_4	219	264	324 [242]	242	310 [237]
GeH_4	165	202	205 [180]	180	175

Table S3. Vibrational frequencies (cm^{-1}) calculated with the PICVib procedure for the A_{2u} modes of the YH_4 (D_{4h}) planar systems. All DFT and *ab initio* calculations were performed with 6-311+G(2d,p) basis sets and the following notation is used for the PICVib approach: (method1:method2), where "method1" denotes the higher level quantum chemical method used to obtain the minimized molecular structure and to perform the energy calculations for the displaced geometries, whereas "method2" is the lower level method employed in the analytical vibrational frequency calculation at the structure provided by "method1". The unsigned percentage differences with respect to the analytical vibrational frequencies are in parenthesis. Vibrational frequencies calculated by finite differences from analytical first derivatives are in brackets.

method2	AM1/PM6[a)]				B3LYP			MP2		CCSD
method1	B3LYP	MP2	CCSD	CCSD(T)	MP2	CCSD	CCSD(T)	CCSD	CCSD(T)	CCSD(T)
CH_4	920i	999i	1016i	1017i	999i	1016i	1017i	1016i	1017i	1017i
	(0.0)	(0.0)	(0.0)	(0.0)	(0.0)	(0.0)	(0.0)	(0.0)	(0.0)	(0.0)
SiH_4	999	995	967 [967]	957 [961]	995	967 [967]	957 [961]	967 [967]	957 [961]	957 [961]
	(0.0)	(0.0)	(209.8)	(211.6)	(0.0)	(209.8)	(211.6)	(209.8)	(211.6)	(211.6)
GeH_4	857	850	816 [816]	806	850	816 [816]	806	757	816	806
	(0.0)	(0.0)	(7.2)	(0.0)	(0.0)	(7.2)	(0.0)	(0.0)	(7.2)	(0.0)

[a)] The PM6 method was used when the AM1 parameters were unavailable.

Table S4. Infrared intensities (km mol^{-1}) calculated with the PICVib procedure for the A_2'' and A_{2u} modes of the XH_3 (D_{3h}) and YH_4 (D_{4h}) planar systems, respectively. All DFT and *ab initio* calculations were performed with 6-311+G(2d,p) basis sets and the following notation is used for the PICVib approach: (method1:method2), where "method1" denotes the higher level quantum chemical method used to obtain the minimized molecular structure and to perform the energy and dipole calculations for the displaced geometries, whereas "method2" is the lower level method employed in the analytical vibrational (normal modes) calculation at the structure provided by "method1". The unsigned percentage differences with respect to the analytical infrared intensities (Table S2) are in parenthesis, except for CCSD and CCSD(T) that were considered the finite difference results from Table S2.

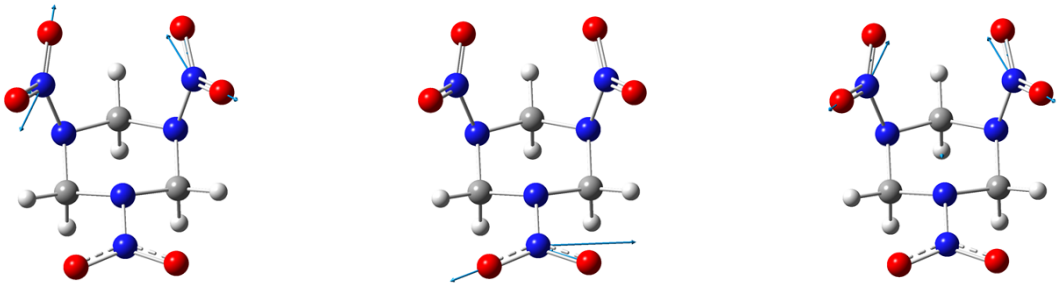
method2	AM1/PM6[a)]				B3LYP			MP2		CCSD
method1	B3LYP	MP2	CCSD	CCSD(T)	MP2	CCSD	CCSD(T)	CCSD	CCSD(T)	CCSD(T)
AlH_3	338 (0.0)	390 (0.0)	359 (0.0)	353 (0.0)	390 (0.0)	359 (0.0)	353 (0.0)	359 (0.0)	353 (0.0)	353 (0.0)
AsH_3	124 (0.0)	150 (0.0)	159 (0.0)	152 (0.0)	150 (0.0)	159 (0.0)	152 (0.0)	159 (0.0)	152 (0.0)	152 (0.0)
BH_3	84 (0.0)	90 (0.0)	84 (0.0)	82 (0.0)	90 (0.0)	84 (0.0)	82 (0.0)	84 (0.0)	82 (0.0)	82 (0.0)
CH_4	666 (0.0)	719 (0.0)	750 (0.0)	730 (0.1)	719 (0.0)	750 (0.0)	730 (0.1)	750 (0.0)	730 (0.1)	730 (0.1)
GaH_3	171 (0.0)	239 (0.0)	218 (0.0)	215 (0.0)	239 (0.0)	218 (0.0)	215 (0.0)	218 (0.0)	215 (0.0)	215 (0.0)
GeH_4	165 (0.0)	202 (0.0)	180 (0.0)	175 (0.0)	202 (0.0)	180 (0.0)	175 (0.0)	180 (0.0)	175 (0.0)	175 (0.0)
NH_3	414 (0.0)	435 (0.0)	438 (0.0)	431 (0.0)	435 (0.0)	438 (0.0)	431 (0.0)	438 (0.0)	431 (0.0)	431 (0.0)
OH_3^+	639 (0.0)	653 (0.0)	648 (0.0)	644 (0.0)	654 (0.1)	648 (0.0)	644 (0.0)	648 (0.0)	644 (0.0)	688 (6.8)
PH_3	197 (0.0)	211 (0.0)	216 (0.0)	209 (0.0)	211 (0.0)	216 (0.0)	209 (0.0)	216 (0.0)	209 (0.0)	209 (0.0)
SeH_3^+	238 (0.0)	258 (0.0)	261 (0.0)	258 (0.0)	258 (0.0)	261 (0.0)	258 (0.0)	261 (0.0)	258 (0.0)	258 (0.0)
SH_3^+	276 (0.0)	289 (0.0)	284 (0.0)	283 (0.0)	289 (0.0)	284 (0.0)	283 (0.0)	284 (0.0)	283 (0.0)	283 (0.0)
SiH_4	219 (0.0)	264 (0.0)	242 (0.0)	237 (0.0)	264 (0.0)	242 (0.0)	237 (0.0)	242 (0.0)	237 (0.0)	237 (0.0)

[a)] The PM6 method was used when the AM1 parameters were unavailable.

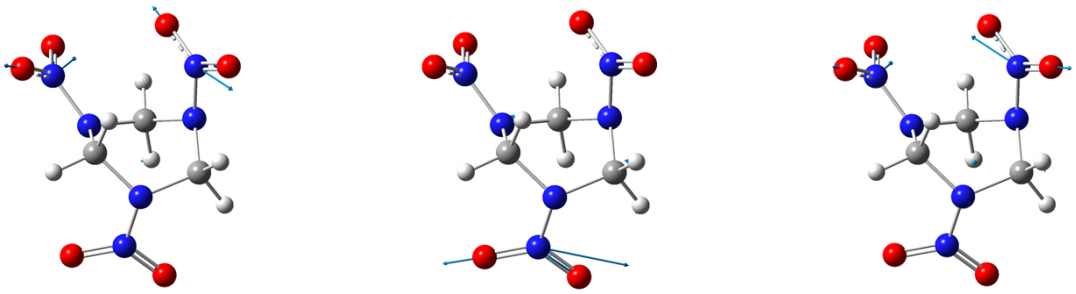
Table S5. Vibrational frequencies (or wavenumbers in cm^{-1}) of three normal modes for each RDX conformer calculated with the PICVib approach (MP2:wB97XD) and compared to the MP2 analytical results. All calculations employed 6-311++G(d,p) basis sets. The value in parenthesis is the difference (in cm^{-1}) between the PICVib and analytical wavenumbers.

	PICVib - MP2:wB97XD			Analytical - MP2		
Conformer	$\nu_{(N=O)}$ (1)	$\nu_{(N=O)}$ (2)	$\nu_{(N=O)}$ (3)	$\nu_{(N=O)}$ (1)	$\nu_{(N=O)}$ (2)	$\nu_{(N=O)}$ (3)
AAE	1790 (-22)	1798 (-9)	1813 (-6)	1812	1789	1819
Twist	1786 (-6)	1791 (-8)	1789 (-7)	1792	1799	1796
EEA	1785 (-4)	1813 (-7)	1786 (-7)	1789	1820	1793
EEE	1789 (-2)	1790 (-7)	1791 (-6)	1791	1797	1797

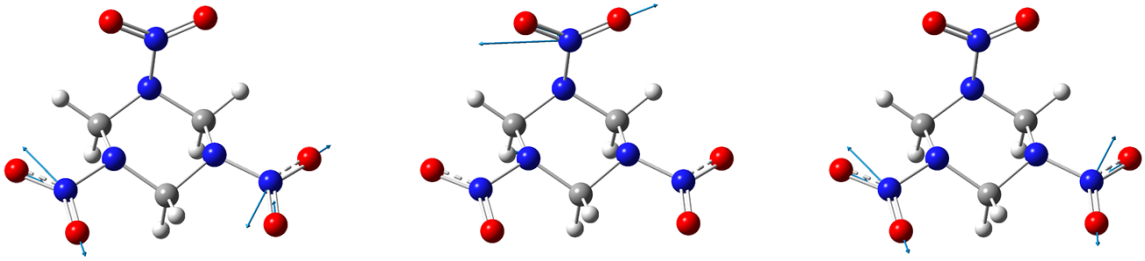
Normal modes of the AAE conformer of RDX



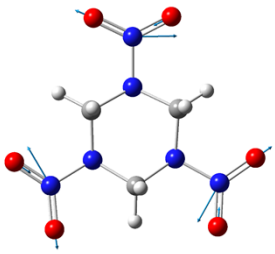
Normal modes of the Twist conformer of RDX



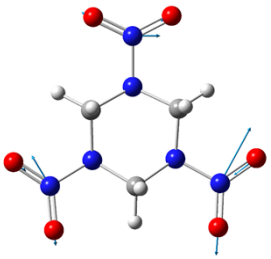
Normal modes of the EEA conformer of RDX



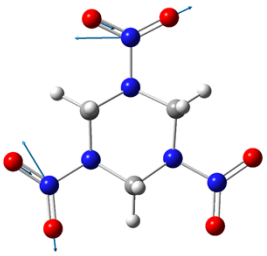
Normal modes of the EEE conformer of RDX



Mode $\nu_{(N-O)}(1)$



Mode $\nu_{(N-O)}(2)$



Mode $\nu_{(N-O)}(3)$

Figure S1. Representation of the vector displacements associated with the N–O normal modes of the main conformers of RDX with all positive frequencies.

Table S6. Vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of selected six normal modes of the intermolecular complex (MeCOOEt···Cl^{-}···BDM) product from the S_N2 reaction between acetate (CH_3COO^-) and chloroethane (CH_3CH_2Cl) mediated by BDM (1,4-$OHCH_2$-C_6H_4-CH_2OH, 1,4-phenylenedimethanol) used to build the PICVib IR spectra at MP2:PBE1PBE level and compared to the MP2 analytical results. All calculations employed 6-31G(d) basis sets. The value in parenthesis is the error (%) between the PICVib and analytical results.

Band	PICVib		Analytical	
	Frequency	Intensity	Frequency	Intensity
ν_{16}	232 (-1.7%)	10 (-16.7%)	236	12
ν_{30}	630 (0.8%)	111 (85.0%)	625	60
ν_{59}	1306 (0.0%)	344 (-3.9%)	1306	358
ν_{81}	1825 (0.1%)	203 (-3.8%)	1824	211
ν_{98}	3301 (-0.1%)	855 (-3.2%)	3305	883
ν_{99}	3658 (-0.1%)	318 (0.6%)	3663	316

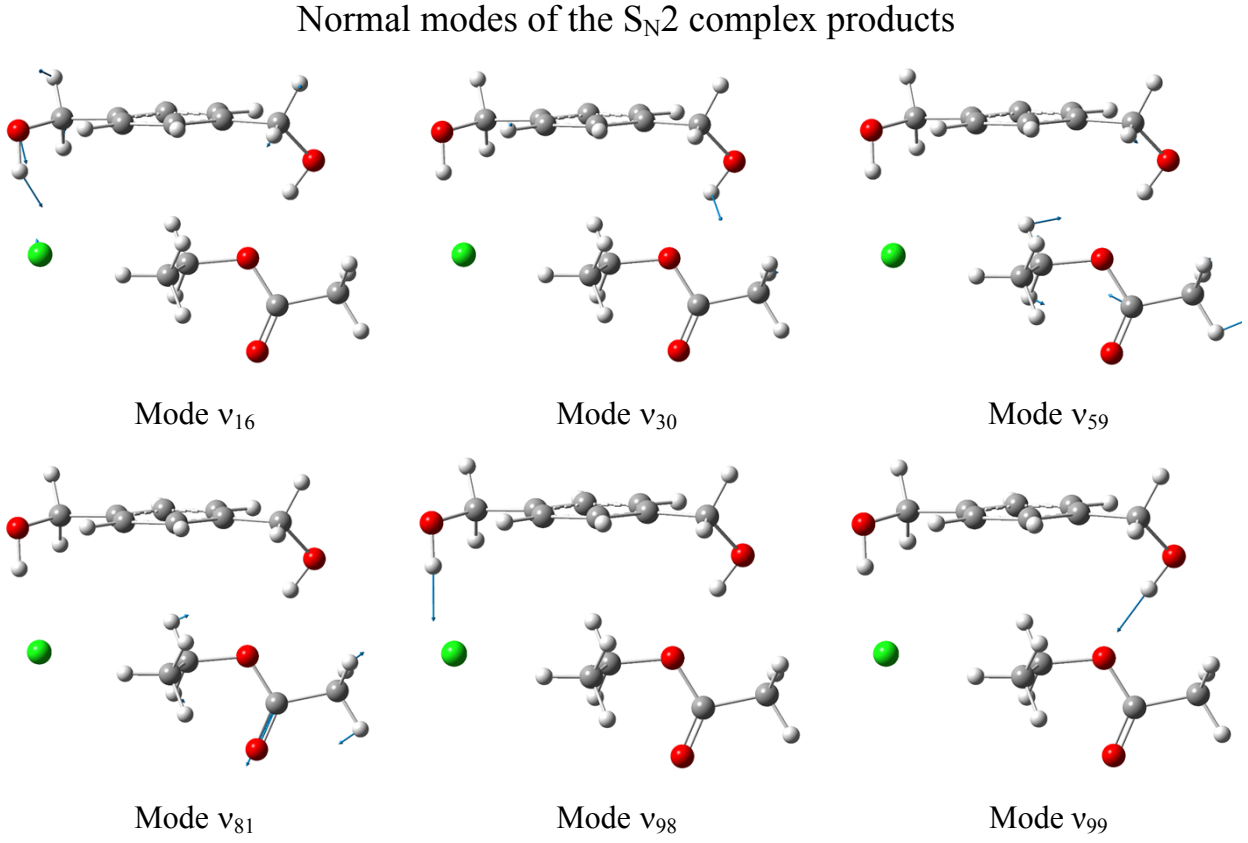
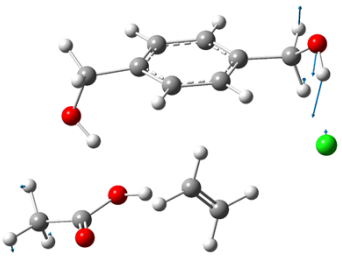


Figure S2. Representation of the vector displacements of the six normal modes of the intermolecular complex (MeCOOEt···Cl^-···BDM) product of the S_N2 reaction between acetate (CH_3COO^-) and chloroethane (CH_3CH_2Cl) mediated by BDM (1,4-$OHCH_2$-C_6H_4-CH_2OH, 1,4-phenylenedimethanol) used to build the PICVib IR spectra at MP2:PBE1PBE level.

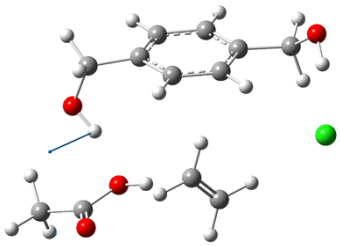
Table S7. Vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of selected ten normal modes of the intermolecular complex (MeCOOH···H_2C=CH_2···Cl^-···BDM) product from the E2 reaction between acetate (CH_3COO^-) and chloroethane (CH_3CH_2Cl) mediated by BDM (1,4-$OHCH_2$-C_6H_4-CH_2OH, 1,4-phenylenedimethanol) used to build the PICVib IR spectra at MP2:PBE1PBE level and compared to the MP2 analytical results. All calculations employed 6-31G(d) basis sets. The value in parenthesis is the error (%) between the PICVib and analytical results.

Band	PICVib		Analytical	
	Frequency	Intensity	Frequency	Intensity
ν_{19}	220 (-0.9)	12 (0.0)	222	12
ν_{29}	589 (1.9)	211 (24.9)	578	169
ν_{44}	970 (-0.4)	56 (19.1)	974	47
ν_{48}	1049 (0.4)	105 (47.9)	1045	71
ν_{67}	1470 (0.0)	117 (-28.7)	1470	164
ν_{81}	1843 (0.0)	235 (-2.1)	1843	240
ν_{87}	3164 (0.0)	109 (10.1)	3164	99
ν_{97}	3391 (-0.1)	756 (-1.8)	3395	770
ν_{98}	3497 (-0.2)	595 (0.7)	3504	591
ν_{99}	3703 (-0.1)	130 (0.0)	3708	130

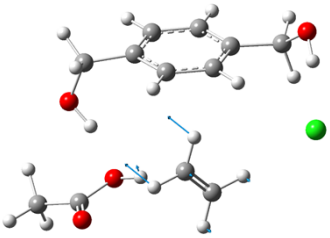
Normal modes of the E2 complex products



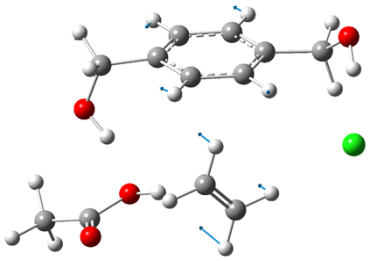
Mode ν_{19}



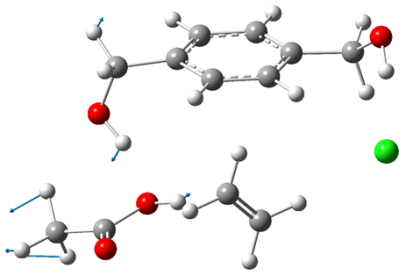
Mode ν_{29}



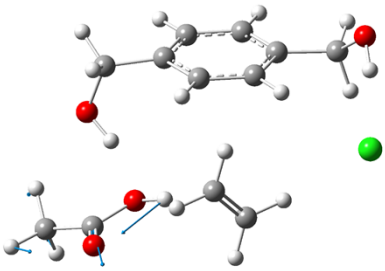
Mode ν_{44}



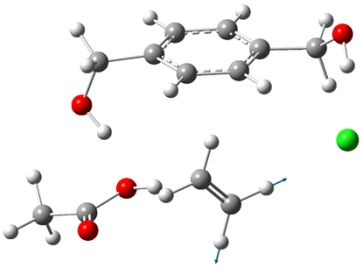
Mode ν_{48}



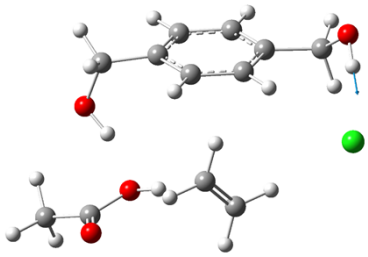
Mode ν_{67}



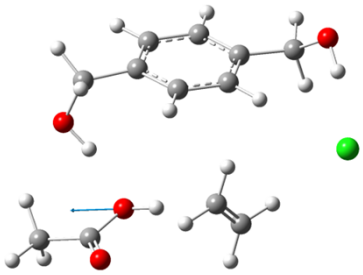
Mode ν_{81}



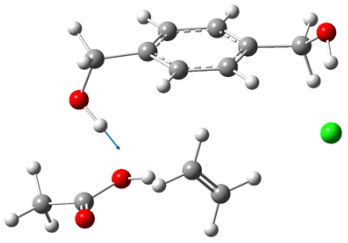
Mode ν_{87}



Mode ν_{97}

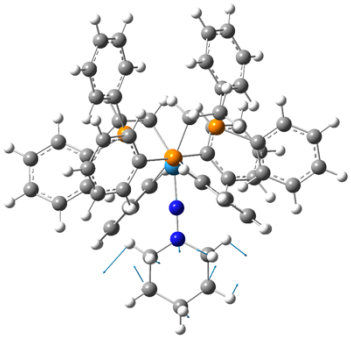


Mode ν_{98}

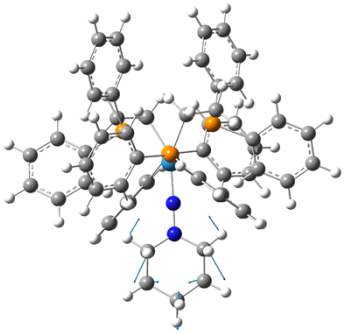


Mode ν_{99}

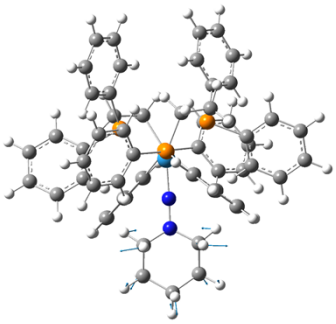
Figure S3. Representation of the ten vector displacements of the product state modes for the E2 reactions between acetate (CH_3COO^-) and chloroethane (CH_3CH_2Cl) mediated by BDM (1,4-$OHCH_2$-C_6H_4-CH_2OH,1,4-phenylenedimethanol).



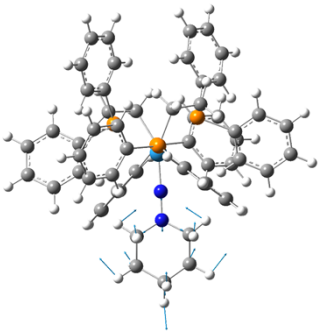
Band I



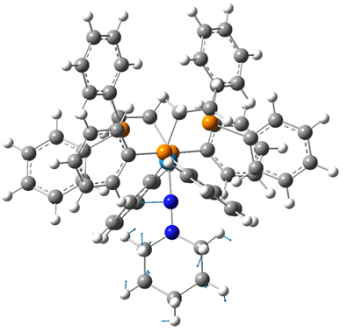
Band III



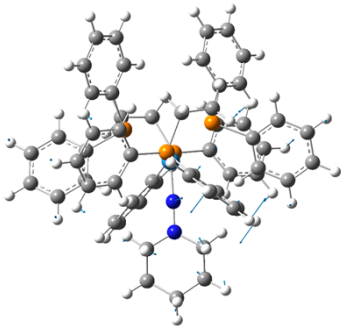
Band V



Band VIb



Band VIIIa



Band VIIIb

Figure S4. Representation of the vector displacements of selected vibrational modes for the $[W(dppe)_2(^{14}N^{14}NC_5H_{10})]$ (^{14}N-**B**^{W}) complex.

Table S8. PICVib calculated infrared intensities (km mol^{-1}) of vibrations involving the N-N moiety in the [W(dppe)$_2$($^{14}N^{14}NC_5H_{10}$)] (^{14}N-**B**^{W}) and [W(dppe)$_2$($^{15}N^{15}NC_5H_{10}$)] (^{15}N-**B**^{W}) complexes. The values in parenthesis are the difference between the PICVib and the analytical calculations and the values in brackets are the percentage relative error (%).

	PICVib[a)]		Analytical[b)]	
Band	^{14}N-**B**^{W}	^{15}N-**B**^{W}	^{14}N-**B**^{W}	^{15}N-**B**^{W}
I	100 (−26) [−20.6]	62 (+5) [+8.5]	126	59
III	202 (+10) [+5.2]	199 (+11) [+5.8]	192	188
V	86 (+16) [+22.2]	69 (−34) [−33.0]	72	103
VIb	57 (−8) [−12.8]	55 (−4) [−7.0]	65	57
VIIIa	40 (+24) [+60.0]	58 (+30) [+52.0]	16	28
VIIIb	129 (−21) [−14.0]	88 (−77) [−45.6]	150	165

[a)]Structure at the B3LYP level and normal modes at the ONIOM(B3LYP:PM6) level, with [Mo(NNC_5H_{10})(PC_2H_4P)$_2$] as the model system for the low-layer. The energies and dipole moment components of the displaced structures at the B3LYP/LANL2DZ level were used in the PICVib approach. All calculations employed LANL2DZ basis sets. [b)]Structure at the B3LYP/ LANL2DZ level.

Table S9. PICVib calculated frequencies (cm^{-1}) of the vibrational modes involving the OH···O and O−H bonds in hydrogen-bonded complexes of water-water, water-methanol (MeOH) and methanol-methanol at the MP2:B3LYP, MP2:PBE1PBE, MP2:M06-2X and MP2:wB97XD levels. Those values were compared with analytical MP2/6-311+G(d,p) frequencies. All calculations employed 6-311+G(d,p) basis sets.

H-bond	Analytical		MP2:B3LYP		MP2:PBE1PBE		MP2:M06-2X		MP2:wB97XD	
complex	OH···O	O-H	OH···O	O-H	OH···O	O-H	OH···O	O-H	OH···O	O-H
H_2O···HOH	172	3808	183	3810	174	3810	174	3809	171	3809
MeHO···HOH	191	3768	194	3769	191	3769	190	3769	190	3769
MeOH···OH_2	172	3823	173	3823	173	3824	173	3823	175	3823
MeOH···OHMe	197	3783	197	3783	197	3783	197	3783	197	3783

Table S10. PICVib calculated frequencies (cm^{-1}) of the vibrational modes involving the OH···O and O−H bonds in hydrogen-bonded complexes of water-water, water-methanol (MeOH) and methanol-methanol at the CCSD(T):B3LYP, CCSD(T):PBE1PBE, CCSD(T):M06-2X and CCSD(T):wB97XD levels. Those values were compared with numerical gradients CCSD(T)/6-311+G(d,p) frequencies. All calculations employed 6-311+G(d,p) basis sets.

H-bond	Frequency		MP2:B3LYP		MP2:PBE1PBE		MP2:M06-2X		MP2:wB97XD	
complex	OH···O	O-H	OH···O	O-H	OH···O	O-H	OH···O	O-H	OH···O	O-H
H_2O···HOH	174	3810	185	3812	176	3812	176	3811	176	3812
MeHO···HOH	195	3776	191	3778	192	3777	181	3777	188	3777
MeOH···OH_2	175	3828	176	3829	173	3829	175	3829	175	3829
MeOH···OHMe	200	3792	192	3793	196	3793	172	3793	189	3793

Table S11. PICVib calculated frequencies (cm^{-1}) of the vibrational modes involving the N-H bending and N-H stretching bonds in the guanine-cytosine (G-C) base pair complex at the MP2:AM1, MP2:PM6, MP2:PDDG, MP2:DFTB and MP2:wB97XD levels. The value in parenthesis is the percentage difference between the PICVib and analytical MP2 frequencies. The 6-31++G(d,p) basis sets were employed in all calculations.

Mode	MP2:AM1	MP2:PM6	MP2:PDDG	MP2:DFTB	MP2:wB97XD	MP2
$\delta_{(N-H)}$	1737 (-2.5%)	1738 (-2.5%)	1764 (-1.0%)	1679 (-6.0%)	1778 (-0.2%)	1781
$\nu_{(N-H)}$	3252 (+0.1%)	3257 (+0.3%)	3248 (0%)	3250 (+0.1%)	3248 (0%)	3248

Cartesian coordinates of equilibrium structures - in Å

B3LYP Equilibrium geometries

AlH_3

Al	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.58010895316	0.00000000000
H	1.36841449418	-0.79005447658	0.00000000000
H	-1.36841449418	-0.79005447658	0.00000000000

AsH3

As	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.46833302778	0.00000000000
H	1.27161370327	-0.73416651389	0.00000000000
H	-1.27161370327	-0.73416651389	0.00000000000

BH3

B	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.18938000000	0.00000000000
H	1.03003329475	-0.59469000000	0.00000000000
H	-1.03003329475	-0.59469000000	0.00000000000

GaH3

Ga	0.00000000000	0.00000000000	0.00000000000
H	0.00000019679	1.56710600000	0.00000000000
H	1.35715350803	-0.78355317042	0.00000000000
H	-1.35715370482	-0.78355282958	0.00000000000

NH3

N	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	0.99942443639	0.00000000000
H	0.86552695107	-0.49971221819	0.00000000000
H	-0.86552695107	-0.49971221819	0.00000000000

OH3+

O	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	0.97546652789	0.00000000000
H	0.84477879369	-0.48773326394	0.00000000000
H	-0.84477879369	-0.48773326394	0.00000000000

PH3

P 0.00000000000 0.00000000000 0.00000000000
H 0.00000000000 1.37915399216 0.00000000000
H 1.19438239295 -0.68957699608 0.00000000000
H -1.19438239295 -0.68957699608 0.00000000000

SH3+

S 0.00000000000 0.00000000000 0.00000000000
H 0.00000000000 1.33997438085 0.00000000000
H 1.16045185424 -0.66998719042 0.00000000000
H -1.16045185424 -0.66998719042 0.00000000000

SeH3+

Se 0.00000000000 0.00000000000 0.00000000000
H 0.00000000000 1.45536497297 0.00000000000
H 1.26038303837 -0.72768248649 0.00000000000
H -1.26038303837 -0.72768248649 0.00000000000

CH4

C 0.00000000000 0.00000000000 0.00000000000
H 0.00000000000 1.08961794290 0.00000000000
H 1.08961794290 0.00000000000 0.00000000000
H -1.08961794290 0.00000000000 0.00000000000
H 0.00000000000 -1.08961794290 0.00000000000

SiH4

Si 0.000000000000 0.000000000000 0.000000000000
H 0.000000000000 1.535606023390 0.000000000000
H 1.535606023390 0.000000000000 0.000000000000
H -1.535606023390 0.000000000000 0.000000000000
H 0.000000000000 -1.535606023390 0.000000000000

GeH4

Ge 0.00000000000 0.00000000000 0.00000000000
H 0.00000000000 1.62745100000 0.00000000000
H 1.62745100000 0.00000000000 0.00000000000
H -1.62745100000 0.00000000000 0.00000000000
H 0.00000000000 -1.62745100000 0.00000000000

MP2 Equilibrium geometries in Å

AlH3

Al	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.57308253741	0.00000000000
H	1.36232943964	-0.78654126870	0.00000000000
H	-1.36232943964	-0.78654126870	0.00000000000

AsH3

As	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.46257789736	0.00000000000
H	1.26662961413	-0.73128894868	0.00000000000
H	-1.26662961413	-0.73128894868	0.00000000000

BH3

B	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.18807216851	0.00000000000
H	1.02890067946	-0.59403608426	0.00000000000
H	-1.02890067946	-0.59403608426	0.00000000000

GaH3

Ga	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.57480814602	0.00000000000
H	1.36382386054	-0.78740407301	0.00000000000
H	-1.36382386054	-0.78740407301	0.00000000000

NH3

N	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	0.99881973745	0.00000000000
H	0.86500326643	-0.49940986872	0.00000000000
H	-0.86500326643	-0.49940986872	0.00000000000

OH3+

O	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	0.97417198687	0.00000000000
H	0.84365768828	-0.48708599343	0.00000000000
H	-0.84365768828	-0.48708599343	0.00000000000

PH3

P	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.37112860188	0.00000000000
H	1.18743220109	-0.68556430094	0.00000000000
H	-1.18743220109	-0.68556430094	0.00000000000

SH3+

S	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.32926151783	0.00000000000
H	1.15117424271	-0.66463075892	0.00000000000
H	-1.15117424271	-0.66463075892	0.00000000000

SeH3+

Se	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.44361840630	0.00000000000
H	1.25021021323	-0.72180920315	0.00000000000
H	-1.25021021323	-0.72180920315	0.00000000000

CH4

C	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.08913804641	0.00000000000
H	1.08913804641	0.00000000000	0.00000000000
H	-1.08913804641	0.00000000000	0.00000000000
H	0.00000000000	-1.08913804641	0.00000000000

SiH4

Si	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.52141881356	0.00000000000
H	1.52141881356	0.00000000000	0.00000000000
H	-1.52141881356	0.00000000000	0.00000000000
H	0.00000000000	-1.52141881356	0.00000000000

GeH4

Ge	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.61213676820	0.00000000000
H	1.61213676820	0.00000000000	0.00000000000
H	-1.61213676820	0.00000000000	0.00000000000
H	0.00000000000	-1.61213676820	0.00000000000

CCSD Equilibrium geometries in Å

AlH3

Al	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.57590263828	0.00000000000
H	1.36477171864	-0.78795131914	0.00000000000
H	-1.36477171864	-0.78795131914	0.00000000000

AsH3

As	-0.00008772000	-0.00012372000	0.00000000000
H	0.00007992000	1.45923529000	0.00000000000
H	1.26419110000	-0.72951750000	0.00000000000
H	-1.26418330000	-0.72960407000	0.00000000000

BH3

B	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	1.19115643039	0.00000000000
H	1.03157172860	-0.59557821520	0.00000000000
H	-1.03157172860	-0.59557821520	0.00000000000

GaH3

Ga	-0.00083643000	0.00024221000	0.00000000000
H	0.00144370000	1.55982557000	0.00000000000
H	1.35006952000	-0.77902552000	0.00000000000
H	-1.35067678000	-0.78104226000	0.00000000000

NH3

N	0.00000096000	0.00000228000	0.00000000000
H	-0.00000818000	0.99911798000	0.00000000000
H	0.86527028000	-0.49956693000	0.00000000000
H	-0.86526307000	-0.49955332000	0.00000000000

OH3+

O	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	0.97250191164	0.00000000000
H	0.84221136071	-0.48625095582	0.00000000000
H	-0.84221136071	-0.48625095582	0.00000000000

PH3

P 0.00000000000 0.00000000000 0.00000000000
H 0.00000000000 1.37380324851 0.00000000000
H 1.18974851301 -0.68690162426 0.00000000000
H -1.18974851301 -0.68690162426 0.00000000000

SH3+

S -0.00001568000 -0.00000647000 0.00000000000
H 0.00003809000 1.33108051000 0.00000000000
H 1.15268912000 -0.66550864000 0.00000000000
H -1.15271152000 -0.66556540000 0.00000000000

SeH3+

Se -0.00008501000 0.00006517000 0.00000000000
H 0.00013965000 1.44132942000 0.00000000000
H 1.24809145000 -0.72060089000 0.00000000000
H -1.24814609000 -0.72079370000 0.00000000000

CH4

C 0.00000000000 0.00000000000 0.00000000000
H 0.00000000000 1.09017240550 0.00000000000
H 1.09017240550 0.00000000000 0.00000000000
H -1.09017240550 0.00000000000 0.00000000000
H 0.00000000000 -1.09017240550 0.00000000000

SiH4

Si 0.00000000000 0.00000000000 0.00000000000
H 0.00000000000 1.52642066000 0.00000000000
H 1.52642066000 0.00000000000 0.00000000000
H -1.52642066000 0.00000000000 0.00000000000
H 0.00000000000 -1.52642066000 0.00000000000

GeH4

Ge 0.00000000000 0.00000000000 0.00000000000
H 0.00000000000 1.62101613105 0.00000000000
H 1.62101613105 0.00000000000 0.00000000000
H -1.62101613105 0.00000000000 0.00000000000
H 0.00000000000 -1.62101613105 0.00000000000

CCSD(T) Equilibrium geometries in Å

AlH3

Al	0.00000000000	0.00000000000	0.00000000000
1	0.00000000000	-1.36588597797	-0.78859463700
1	0.00000000000	0.00000000000	1.57718927401
1	0.00000000000	1.36588597797	-0.78859463700

AsH3

As	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	-1.27186881830	-0.73431380443
H	0.00000000000	0.00000000000	1.46862760886
H	0.00000000000	1.27186881830	-0.73431380443

BH3

B	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	-1.03224657532	-0.59596783703
H	0.00000000000	0.00000000000	1.19193567407
H	0.00000000000	1.03224657532	-0.59596783703

GaH3

Ga	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	-1.36949137369	-0.79067621392
H	0.00000000000	0.00000000000	1.58135242784
H	0.00000000000	1.36949137369	-0.79067621392

NH3

N	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	-0.86652659163	-0.50028936243
H	0.00000000000	0.00000000000	1.00057871958
H	0.00000000000	0.86652659163	-0.50028936243

OH3+

O	0.00000000000	0.00000000000	0.00000000000
H	0.00000000000	-0.84337928336	-0.48692525560
H	0.00000000000	0.00000000000	0.97385051120
H	0.00000000000	0.84337928336	-0.48692525560

PH3

P	0.00000000000	0.00000000000	0.00000000000

H 0.00000000000 -1.19073608216 -0.68747179636
H 0.00000000000 0.00000000000 1.37494359272
H 0.00000000000 1.19073608216 -0.68747179636

SH3+

S 0.00000000000 0.00000000000 0.00000000000
H 0.00000000000 -1.15373120398 -0.66610702166
H 0.00000000000 0.00000000000 1.33221404331
H 0.00000000000 1.15373120398 -0.66610702166

SeH3+

Se 0.00000000000 0.00000000000 0.00000000000
H 0.00000000000 -1.25389918132 -0.72393903046
H 0.00000000000 0.00000000000 1.44787806091
H 0.00000000000 1.25389918132 -0.72393903046

CH4

C 0.00000000000 0.00000000000 0.00000000000
H -0.77220519209 -0.77220519209 0.00000000000
H 0.77220519209 -0.77220519209 0.00000000000
H 0.77220519209 0.77220519209 0.00000000000
H -0.77220519209 0.77220519209 0.00000000000

SiH4

Si 0.00000000000 0.00000000000 0.00000000000
H -1.07849360824 -1.07849360824 0.00000000000
H 1.07849360824 -1.07849360824 0.00000000000
H 1.07849360824 1.07849360824 0.00000000000
H -1.07849360824 1.07849360824 0.00000000000

GeH4

Ge 0.00000000000 0.00000000000 0.00000000000
H -1.14854567441 -1.14854567441 0.00000000000
H 1.14854567441 -1.14854567441 0.00000000000
H 1.14854567441 1.14854567441 0.00000000000
H -1.14854567441 1.14854567441 0.00000000000

Equilibrium geometries for the RDX conformers at MP2/6-311++G(d,p) level in Å

Conformer AAE

6	0.75558478476	1.21709185366	0.79092069704
7	1.19555505568	-0.00000781376	0.09364485774
6	0.75555191288	-1.21710843587	0.79089824089
7	-0.69121270270	-1.22211617295	0.85593714004
6	-1.25173804088	0.00001297995	1.43157681632
7	-0.69117976286	1.22213779418	0.85595995287
7	-1.32465541414	1.65136021577	-0.36326731587
8	-2.52565313892	1.44850609987	-0.43377334054
8	-0.61968067509	2.24085851607	-1.16754652587
7	-1.32470005723	-1.65129912940	-0.36329786335
8	-2.52570558566	-1.44847800452	-0.43376493871
8	-0.61975629421	-2.24086696241	-1.16755324679
7	2.56944405245	-0.00002329612	-0.24154157274
8	3.09271128585	-1.09620197101	-0.39495570826
8	3.09274100252	1.09614411587	-0.39493482569
1	1.11771188106	1.22619153626	1.82959535178
1	1.11458306730	2.09304150466	0.26155076395
1	1.11767882457	-1.22623708303	1.82957272251
1	1.11452658019	-2.09305794069	0.26151206254
1	-2.33282473616	0.00002860719	1.32580538378
1	-0.97807851190	-0.00000054580	2.48977148598

Conformer Twist

6	0.29506650916	0.03209078605	1.25707873323
7	0.26910030847	-0.99887817498	0.21195532040
7	0.23644823153	1.36782667777	0.67798048352
1	-0.59443296657	-0.06013991097	1.88602038383
1	1.18606577300	-0.10185077185	1.86624871317
6	-0.37415175348	-0.56135171043	-1.04212187360
6	-1.00810268233	1.58737265704	-0.07150239147
7	1.41685548759	1.71211587580	-0.04346844977
7	1.46986668408	-1.70697250408	0.01890468129
7	-1.46003379869	0.33128729347	-0.68362587308
8	1.34456615154	2.68547492212	-0.78009257458
8	2.40908803214	1.03169823308	0.18789297009
8	1.67679642994	-2.09109979278	-1.12844646763
8	2.14644842765	-1.92866950600	1.01102044258
1	-0.74461777371	-1.42355325274	-1.58858174326
1	0.31390522605	0.00544919542	-1.68081488611
1	-0.81827554813	2.32516906654	-0.84992934303
1	-1.78447605518	1.94614305012	0.60164403968
7	-2.53585869023	-0.33076616208	-0.01392762385
8	-3.26783960623	0.36783204159	0.67398816432

8 -2.66027051688 -1.52300824974 -0.24811800263

Conformer EEA
6 -1.20830483546 0.66966686143 0.96455866487
7 0.00000165351 1.45602068946 0.82100763241
7 -1.16631096117 -0.41689391767 -0.02334873934
1 -1.21376527544 0.27940317971 1.99163738529
1 -2.08492037057 1.28352662717 0.79073092561
6 1.20830711469 0.66966494514 0.96455789700
6 -0.00000063716 -1.28982089492 0.10211123826
7 -2.37753894315 -1.14033782713 -0.12818631140
7 0.00000123652 2.25552099622 -0.38296142869
7 1.16631056995 -0.41689582453 -0.02334897720
8 -2.30036235757 -2.27579877396 -0.57832789984
8 -3.39431314559 -0.54090369460 0.19688305839
8 1.09479440023 2.58078160272 -0.80990839229
8 -1.09479294858 2.58077779024 -0.80990849944
1 1.21376737206 0.27940150602 1.99163672101
1 2.08492360801 1.28352309621 0.79072965390
1 -0.00000120130 -2.01022827279 -0.70929616950
1 -0.00000103052 -1.81740355506 1.07417053341
7 2.37753724779 -1.14034002872 -0.12819168382
8 2.30035855025 -2.27580019053 -0.57833504913
8 3.39431317891 -0.54090756693 0.19687562053

Conformer EEE
6 -1.33047804189 0.48814517295 0.20610255093
7 -1.02892006394 -0.85885059474 -0.26751662115
7 -0.22931292005 1.32048278085 -0.26749205461
1 -1.40695718957 0.51619175082 1.30890283318
1 -2.25862063030 0.82868656155 -0.23976215050
6 0.24249228076 -1.39632930146 0.20607127457
6 1.08800574212 0.90814291234 0.20610241286
7 -0.46930688037 2.70241719310 -0.05715568394
7 -2.10573569057 -1.75763236308 -0.05715360655
7 1.25824973926 -0.46165876830 -0.26751430688
8 0.51802771183 3.42276764467 -0.00208032564
8 -1.64170599743 3.04769063159 -0.00207472099
8 -1.81860626008 -2.94561015756 -0.00207551113
8 -3.22321803451 -1.26269697702 -0.00204060519
1 0.25643392432 -1.47661612168 1.30886950787
1 0.41164966982 -2.37038090390 -0.23981747191
1 1.84698819289 1.54167314354 -0.23976297160
1 1.15055083995 0.96033442378 1.30890267921
7 2.57503976749 -0.94477922363 -0.05715336704
8 3.46024265742 -0.10207837586 -0.00204006716
8 2.70522712829 -2.16000960664 -0.00207506680

Geometries at MP2/6-31g(d) level of the S_N2 and E2 reactions between acetate (CH_3COO^-) and chloroethane (CH_3CH_2Cl) mediated by 1,4-phenylenedimethanol (BDM, 1,4-$OHCH_2$-C_6H_4-CH_2OH).

S_N2 - BDM complex product

6	1.33039755000	-1.66784505000	-1.37533234000
6	0.12040643000	-2.20904752000	-0.94254432000
6	-0.20372614000	-2.21734897000	0.42268416000
6	0.71123986000	-1.67650866000	1.33307650000
6	1.92443099000	-1.13632212000	0.89784096000
6	2.23959227000	-1.11148463000	-0.46326778000
6	-1.54712178000	-2.73832203000	0.86765096000
6	3.54233491000	-0.49810085000	-0.94630098000
8	-2.61200539000	-2.22269414000	0.06476794000
8	4.27485616000	0.15115990000	0.06667777000
1	1.55911535000	-1.64557783000	-2.44171157000
1	-0.59634552000	-2.60534182000	-1.65994503000
1	0.46439669000	-1.65993717000	2.39508942000
1	2.62156451000	-0.67865073000	1.59302340000
1	-1.60595441000	-3.82923790000	0.77127573000
1	-1.69811108000	-2.49483525000	1.93180522000
1	4.18168143000	-1.29661826000	-1.34954533000
1	3.31306291000	0.19155960000	-1.77169390000
1	-2.39371542000	-1.27881200000	-0.08001485000
1	3.81374481000	1.03051261000	0.18096602000
6	-0.69539514000	1.72451157000	1.43120149000
6	-0.83344445000	1.36141603000	-0.02762673000
1	-0.76899632000	0.82778743000	2.05291115000
1	-1.46603231000	2.44040993000	1.72794694000
1	0.29535689000	2.17124970000	1.55435348000
1	-0.81475641000	2.24255298000	-0.66829558000
1	-0.06244168000	0.66272231000	-0.34466825000
17	2.53128070000	2.67023578000	0.07186529000
6	-4.41524607000	0.50247343000	-0.65157711000
6	-3.21738057000	1.38681880000	-0.39793810000
8	-3.25063633000	2.60615881000	-0.33272181000
8	-2.09687567000	0.63702474000	-0.27707494000
1	-5.31960902000	1.11012712000	-0.62178146000
1	-4.46367593000	-0.29882429000	0.08887682000
1	-4.31883015000	0.03158802000	-1.63397947000

E2 - BDM complex product

6	-0.60066035000	-3.03439154000	-0.08785845000
6	-1.89146990000	-2.64818059000	-0.45478125000
6	-2.36002035000	-1.35474028000	-0.18785820000
6	-1.52205296000	-0.45660260000	0.48828909000
6	-0.23664041000	-0.84961314000	0.86271217000
6	0.23760360000	-2.14172190000	0.59245392000
6	-3.73544159000	-0.90176075000	-0.63742742000
6	1.66678947000	-2.50362548000	0.88480590000
8	-4.42247269000	-0.15068889000	0.34272293000
8	2.49813799000	-2.36384348000	-0.27958438000
1	-0.24297623000	-4.03925977000	-0.31324614000
1	-2.54130216000	-3.35787399000	-0.96794801000
1	-1.87663377000	0.55730404000	0.66474557000
1	0.40778652000	-0.14299692000	1.38526305000
1	-3.62836425000	-0.32044641000	-1.56509548000
1	-4.34341260000	-1.78759486000	-0.86916921000
1	2.04798603000	-1.88212586000	1.70972770000
1	1.75766071000	-3.55284656000	1.18401579000
1	-4.12616253000	0.78932451000	0.21478854000
1	2.29736325000	-1.47187649000	-0.62517056000
6	4.78684882000	-0.02228017000	-0.83272458000
6	3.78881513000	0.98044402000	-0.32081766000
8	2.51977978000	0.58878578000	-0.61037759000
8	4.06018466000	2.01381377000	0.27099315000
1	5.78626653000	0.27182610000	-0.51415013000
1	4.53059161000	-1.01737226000	-0.46111669000
1	4.73960488000	-0.05517141000	-1.92492902000
6	0.86003415000	2.82516257000	1.13528390000
6	0.36436416000	3.04731496000	-0.09412006000
17	-3.20831992000	2.62430354000	-0.33081850000
1	1.88500517000	1.25883971000	-0.24942159000
1	1.90553613000	2.99443137000	1.37730730000
1	0.20843583000	2.48179671000	1.93406167000
1	1.00986596000	3.42077638000	-0.88797762000
1	-0.69125672000	2.89600774000	-0.31855574000

Nanotube equilibrium geometry at B3LYP/6-31G(d) level

Nanotube (8,0)×3 Pure

C	0.00000000	3.19156554	5.69616320
C	1.21351885	2.92969365	5.01470269
C	2.25677764	2.25677764	5.69616320
C	2.92969365	1.21351885	5.01470269
C	3.19156554	0.00000000	5.69616320
C	2.92969365	-1.21351885	5.01470269
C	2.25677764	-2.25677764	5.69616320
C	1.21351885	-2.92969365	5.01470269
C	0.00000000	-3.19156554	5.69616320
C	-1.21351885	-2.92969365	5.01470269
C	-2.25677764	-2.25677764	5.69616320
C	-2.92969365	-1.21351885	5.01470269
C	-3.19156554	0.00000000	5.69616320
C	-2.92969365	1.21351885	5.01470269
C	-2.25677764	2.25677764	5.69616320
C	-1.21351885	2.92969365	5.01470269
C	1.21424118	2.93143752	3.56953275
C	2.24089893	2.24089893	2.85979045
C	2.93143752	1.21424118	3.56953275
C	3.16910965	0.00000000	2.85979045
C	2.93143752	-1.21424118	3.56953275
C	2.24089893	-2.24089893	2.85979045
C	1.21424118	-2.93143752	3.56953275
C	0.00000000	-3.16910965	2.85979045
C	-1.21424118	-2.93143752	3.56953275
C	-2.24089893	-2.24089893	2.85979045
C	-2.93143752	-1.21424118	3.56953275
C	-3.16910965	0.00000000	2.85979045
C	-2.93143752	1.21424118	3.56953275
C	-2.24089893	2.24089893	2.85979045
C	-1.21424118	2.93143752	3.56953275
C	0.00000000	3.16910965	2.85979045
C	2.24390660	2.24390660	1.42731758
C	2.93205342	1.21449629	0.71499988
C	3.17336315	0.00000000	1.42731758
C	2.93205342	-1.21449629	0.71499988
C	2.24390660	-2.24390660	1.42731758
C	1.21449629	-2.93205342	0.71499988
C	0.00000000	-3.17336315	1.42731758
C	-1.21449629	-2.93205342	0.71499988
C	-2.24390660	-2.24390660	1.42731758
C	-2.93205342	-1.21449629	0.71499988

C	-3.17336315	0.00000000	1.42731758
C	-2.93205342	1.21449629	0.71499988
C	-2.24390660	2.24390660	1.42731758
C	-1.21449629	2.93205342	0.71499988
C	0.00000000	3.17336315	1.42731758
C	1.21449629	2.93205342	0.71499988
C	2.93205342	1.21449629	-0.71499988
C	3.17336315	0.00000000	-1.42731758
C	2.93205342	-1.21449629	-0.71499988
C	2.24390660	-2.24390660	-1.42731758
C	1.21449629	-2.93205342	-0.71499988
C	0.00000000	-3.17336315	-1.42731758
C	-1.21449629	-2.93205342	-0.71499988
C	-2.24390660	-2.24390660	-1.42731758
C	-2.93205342	-1.21449629	-0.71499988
C	-3.17336315	0.00000000	-1.42731758
C	-2.93205342	1.21449629	-0.71499988
C	-2.24390660	2.24390660	-1.42731758
C	-1.21449629	2.93205342	-0.71499988
C	0.00000000	3.17336315	-1.42731758
C	1.21449629	2.93205342	-0.71499988
C	2.24390660	2.24390660	-1.42731758
C	3.16910965	0.00000000	-2.85979045
C	2.93143752	-1.21424118	-3.56953275
C	2.24089893	-2.24089893	-2.85979045
C	1.21424118	-2.93143752	-3.56953275
C	0.00000000	-3.16910965	-2.85979045
C	-1.21424118	-2.93143752	-3.56953275
C	-2.24089893	-2.24089893	-2.85979045
C	-2.93143752	-1.21424118	-3.56953275
C	-3.16910965	0.00000000	-2.85979045
C	-2.93143752	1.21424118	-3.56953275
C	-2.24089893	2.24089893	-2.85979045
C	-1.21424118	2.93143752	-3.56953275
C	0.00000000	3.16910965	-2.85979045
C	1.21424118	2.93143752	-3.56953275
C	2.24089893	2.24089893	-2.85979045
C	2.93143752	1.21424118	-3.56953275
C	2.92969365	-1.21351885	-5.01470269
C	2.25677764	-2.25677764	-5.69616320
C	1.21351885	-2.92969365	-5.01470269
C	0.00000000	-3.19156554	-5.69616320
C	-1.21351885	-2.92969365	-5.01470269
C	-2.25677764	-2.25677764	-5.69616320
C	-2.92969365	-1.21351885	-5.01470269
C	-3.19156554	0.00000000	-5.69616320
C	-2.92969365	1.21351885	-5.01470269

C	-2.25677764	2.25677764	-5.69616320
C	-1.21351885	2.92969365	-5.01470269
C	0.00000000	3.19156554	-5.69616320
C	1.21351885	2.92969365	-5.01470269
C	2.25677764	2.25677764	-5.69616320
C	2.92969365	1.21351885	-5.01470269
C	3.19156554	0.00000000	-5.69616320
H	-2.23732693	2.23732693	-6.78318034
H	0.00000000	3.16405809	-6.78318034
H	2.23732693	2.23732693	-6.78318034
H	-3.16405809	0.00000000	-6.78318034
H	0.00000000	-3.16405809	-6.78318034
H	2.23732693	-2.23732693	-6.78318034
H	-2.23732693	-2.23732693	-6.78318034
H	3.16405809	0.00000000	-6.78318034
H	0.00000000	3.16405809	6.78318034
H	2.23732693	2.23732693	6.78318034
H	-2.23732693	2.23732693	6.78318034
H	3.16405809	0.00000000	6.78318034
H	-3.16405809	0.00000000	6.78318034
H	-2.23732693	-2.23732693	6.78318034
H	0.00000000	-3.16405809	6.78318034
H	2.23732693	-2.23732693	6.78318034

Nanotube (11,0)×3 Pure

6	4.35725958756	-0.00003006991	5.69294062633
6	4.16309057558	-1.22248429290	5.01238389939
6	4.33199499759	-0.00003468159	2.85865818977
6	3.66554376448	-2.35573768170	5.69294062633
6	2.84128974676	-3.27915592216	5.01238389939
6	4.16027404351	-1.22165474227	3.56711626265
6	3.64428734565	-2.34208249273	2.85865818977
6	1.81004369567	-3.96351522441	5.69294062633
6	0.61739949894	-4.29471871554	5.01238389939
6	2.83936881814	-3.27693532756	3.56711626265
6	1.79954421076	-3.94053566078	2.85865818977
6	-0.62013245736	-4.31290468822	5.69294062633
6	-1.80251072746	-3.94673866177	5.01238389939
6	0.61698405503	-4.29181210006	3.56711626265
6	-0.61654149607	-4.28789659903	2.85865818977
6	-2.85342093682	-3.29297738705	5.69294062633
6	-3.65013653382	-2.34569696921	5.01238389939
6	-1.80128878615	-3.94406885529	3.56711626265
6	-2.83687963417	-3.27388066392	2.85865818977
6	-4.18076843015	-1.22755303256	5.69294062633

6	-4.33886978133	0.00008693717	5.01238389939
6	-3.64766516503	-2.34411161642	3.56711626265
6	-4.15652853286	-1.22043075015	2.85865818977
6	-4.18075148681	1.22761073629	5.69294062633
6	-3.65004253025	2.34584324162	5.01238389939
6	-4.33593362717	0.00008449796	3.56711626265
6	-4.15650899099	1.22049730364	2.85865818977
6	-2.85337548618	3.29301677026	5.69294062633
6	-1.80235256579	3.94681089178	5.01238389939
6	-3.64757379894	2.34425378483	3.56711626265
6	-2.83682721297	3.27392608715	2.85865818977
6	-0.62007292968	4.31291324701	5.69294062633
6	0.61757160350	4.29469397064	5.01238389939
6	-1.80113506206	3.94413905873	3.56711626265
6	-0.61647283890	4.28790647045	2.85865818977
6	1.81009840077	3.96349024142	5.69294062633
6	2.84142115223	3.27904205868	5.01238389939
6	0.61715133080	4.29178804944	3.56711626265
6	1.79960730574	3.94050684627	2.85865818977
6	3.66557627852	2.35568708887	5.69294062633
6	4.16313956165	1.22231746169	5.01238389939
6	2.83949653672	3.27682465877	3.56711626265
6	3.64432484622	2.34202414070	2.85865818977
6	4.16032165516	1.22149259188	3.56711626265
6	4.33507699094	-0.00003477630	1.42629007539
6	4.15991595618	-1.22155038583	0.71532515507
6	4.33507699094	-0.00003477630	-1.42629007539
6	3.64688003223	-2.34374882380	1.42629007539
6	2.83912399526	-3.27665394071	0.71532515507
6	4.15991595618	-1.22155038583	-0.71532515507
6	3.64688003223	-2.34374882380	-1.42629007539
6	1.80082443092	-3.94333917988	1.42629007539
6	0.61693022614	-4.29144302114	0.71532515507
6	2.83912399526	-3.27665394071	-0.71532515507
6	1.80082443092	-3.94333917988	-1.42629007539
6	-0.61698020319	-4.29094720865	1.42629007539
6	-1.80113453077	-3.94372926425	0.71532515507
6	0.61693022614	-4.29144302114	-0.71532515507
6	-0.61698020319	-4.29094720865	-1.42629007539
6	-2.83889798217	-3.27620981706	1.42629007539
6	-3.64735180036	-2.34390933102	0.71532515507
6	-1.80113453077	-3.94372926425	-0.71532515507
6	-2.83889798217	-3.27620981706	-1.42629007539
6	-4.15948571050	-1.22129895715	1.42629007539
6	-4.33556064429	0.00008525354	0.71532515507
6	-3.64735180036	-2.34390933102	-0.71532515507
6	-4.15948571050	-1.22129895715	-1.42629007539

6 -4.15946611526 1.22136569238 1.42629007539
6 -3.64725961727 2.34405277070 0.71532515507
6 -4.33556064429 0.00008525354 -0.71532515507
6 -4.15946611526 1.22136569238 -1.42629007539
6 -2.83884541782 3.27625536433 1.42629007539
6 -1.80097943207 3.94380009545 0.71532515507
6 -3.64725961727 2.34405277070 -0.71532515507
6 -2.83884541782 3.27625536433 -1.42629007539
6 -0.61691135854 4.29095710702 1.42629007539
6 0.61709899770 4.29141875545 0.71532515507
6 -1.80097943207 3.94380009545 -0.71532515507
6 -0.61691135854 4.29095710702 -1.42629007539
6 1.80088769819 3.94331028668 1.42629007539
6 2.83925285591 3.27654228232 0.71532515507
6 0.61709899770 4.29141875545 -0.71532515507
6 1.80088769819 3.94331028668 -1.42629007539
6 3.64691763521 2.34369031243 1.42629007539
6 4.15996399358 1.22138678549 0.71532515507
6 2.83925285591 3.27654228232 -0.71532515507
6 3.64691763521 2.34369031243 -1.42629007539
6 4.15996399358 1.22138678549 -0.71532515507
6 4.33199499759 -0.00003468159 -2.85865818977
6 4.16027404351 -1.22165474227 -3.56711626265
6 4.35725958756 -0.00003006991 -5.69294062633
6 3.64428734565 -2.34208249273 -2.85865818977
6 2.83936881814 -3.27693532756 -3.56711626265
6 4.16309057558 -1.22248429290 -5.01238389939
6 3.66554376448 -2.35573768170 -5.69294062633
6 1.79954421076 -3.94053566078 -2.85865818977
6 0.61698405503 -4.29181210006 -3.56711626265
6 2.84128974676 -3.27915592216 -5.01238389939
6 1.81004369567 -3.96351522441 -5.69294062633
6 -0.61654149607 -4.28789659903 -2.85865818977
6 -1.80128878615 -3.94406885529 -3.56711626265
6 0.61739949894 -4.29471871554 -5.01238389939
6 -0.62013245736 -4.31290468822 -5.69294062633
6 -2.83687963417 -3.27388066392 -2.85865818977
6 -3.64766516503 -2.34411161642 -3.56711626265
6 -1.80251072746 -3.94673866177 -5.01238389939
6 -2.85342093682 -3.29297738705 -5.69294062633
6 -4.15652853286 -1.22043075015 -2.85865818977
6 -4.33593362717 0.00008449796 -3.56711626265
6 -3.65013653382 -2.34569696921 -5.01238389939
6 -4.18076843015 -1.22755303256 -5.69294062633
6 -4.15650899099 1.22049730364 -2.85865818977
6 -3.64757379894 2.34425378483 -3.56711626265
6 -4.33886978133 0.00008693717 -5.01238389939

6	-4.18075148681	1.22761073629	-5.69294062633
6	-2.83682721297	3.27392608715	-2.85865818977
6	-1.80113506206	3.94413905873	-3.56711626265
6	-3.65004253025	2.34584324162	-5.01238389939
6	-2.85337548618	3.29301677026	-5.69294062633
6	-0.61647283890	4.28790647045	-2.85865818977
6	0.61715133080	4.29178804944	-3.56711626265
6	-1.80235256579	3.94681089178	-5.01238389939
6	-0.62007292968	4.31291324701	-5.69294062633
6	1.79960730574	3.94050684627	-2.85865818977
6	2.83949653672	3.27682465877	-3.56711626265
6	0.61757160350	4.29469397064	-5.01238389939
6	1.81009840077	3.96349024142	-5.69294062633
6	3.64432484622	2.34202414070	-2.85865818977
6	4.16032165516	1.22149259188	-3.56711626265
6	2.84142115223	3.27904205868	-5.01238389939
6	3.66557627852	2.35568708887	-5.69294062633
6	4.16313956165	1.22231746169	-5.01238389939
1	4.34157497632	-0.00006693693	-6.78023684706
1	4.34157497632	-0.00006693693	6.78023684706
1	3.65232909805	-2.34728895517	-6.78023684706
1	3.65232909805	-2.34728895517	6.78023684706
1	1.80349453727	-3.94926331530	-6.78023684706
1	1.80349453727	-3.94926331530	6.78023684706
1	-0.61793679621	-4.29737447698	-6.78023684706
1	-0.61793679621	-4.29737447698	6.78023684706
1	-2.84317756303	-3.28109960602	-6.78023684706
1	-2.84317756303	-3.28109960602	6.78023684706
1	-4.16572954251	-1.22309879329	-6.78023684706
1	-4.16572954251	-1.22309879329	6.78023684706
1	-4.16569182589	1.22322724431	-6.78023684706
1	-4.16569182589	1.22322724431	6.78023684706
1	-2.84307638792	3.28118727475	-6.78023684706
1	-2.84307638792	3.28118727475	6.78023684706
1	-0.61780428500	4.29739352921	-6.78023684706
1	-0.61780428500	4.29739352921	6.78023684706
1	1.80361631321	3.94920770209	-6.78023684706
1	1.80361631321	3.94920770209	6.78023684706
1	3.65240147572	2.34717633332	-6.78023684706
1	3.65240147572	2.34717633332	6.78023684706

W Complex equilibrium geometry at B3LYP/LANDLDZ2 level

^{14}N- BW Complex

W	0.00341482338	0.13178765598	0.25434493661
P	1.72081190686	-1.65696440806	0.79145294643
P	-1.26076942769	-1.95357316444	-0.36174226052
C	1.36844363781	-3.17372467173	-0.32012817667
H	1.64899999581	-2.89826920877	-1.34305828699
H	1.98512053464	-4.01996507086	0.00920376295
C	-0.12202147641	-3.52717582314	-0.22755380421
H	-0.34447907409	-3.98216135696	0.74391366935
H	-0.40808562199	-4.23970506970	-1.00848060995
C	3.60493813944	-1.46857909017	0.66809551594
C	4.22884702160	-0.48457355986	1.46640598365
H	3.62267755524	0.14328956891	2.11587500252
C	5.62329187841	-0.31261692930	1.43800326330
H	6.08658526245	0.45006872693	2.05980411964
C	6.41898966401	-1.12237648994	0.60252567320
H	7.49807044480	-0.98865605732	0.57631966313
C	5.80599158619	-2.10291256746	-0.19840226126
H	6.40973889600	-2.73439340920	-0.84669500344
C	4.40771914690	-2.27584768709	-0.16393919313
H	3.96018433553	-3.03595235452	-0.79628208016
C	1.62714283268	-2.48228227567	2.51061591491
C	0.50139939500	-2.26343537227	3.32734264225
H	-0.27546735372	-1.58689371879	2.98544996058
C	0.38130703701	-2.91484871109	4.57047115530
H	-0.49960436124	-2.74268057408	5.18507909816
C	1.39103722270	-3.79025739995	5.01149629447
H	1.29991930895	-4.29450547288	5.97114936997
C	2.52296412391	-4.00974824258	4.20119856095
H	3.31113024285	-4.68133995799	4.53497943018
C	2.63979256231	-3.35996601164	2.95844126595
H	3.52518155861	-3.52933121511	2.35092902672
C	-2.18494853497	-2.35447008321	-1.99261921682
C	-1.45852688889	-2.82455574620	-3.10955083416
H	-0.38589371639	-2.98198113617	-3.03072003654
C	-2.10259144059	-3.08888137326	-4.33212848643
H	-1.52691828002	-3.46596183582	-5.17512113626
C	-3.48888446225	-2.86904139246	-4.46362903394
H	-3.99032843711	-3.07386483448	-5.40699020635
C	-4.21788500374	-2.38652565428	-3.36051151912
H	-5.28840578152	-2.21268660129	-3.44719671175
C	-3.57164863790	-2.13359856683	-2.13435179232
H	-4.15439225968	-1.77736814962	-1.29053045562

C	-2.62243554998	-2.51242386863	0.86991455914
C	-3.22934879444	-3.78385265701	0.76679376659
H	-2.96758814347	-4.44707704813	-0.05506403282
C	-4.18263605962	-4.20172475656	1.71326495372
H	-4.63895990702	-5.18540182909	1.62413211194
C	-4.54812322442	-3.34637961152	2.77274501316
H	-5.28735685635	-3.66712884932	3.50383646594
C	-3.95270051819	-2.07502790081	2.87549934542
H	-4.23472378801	-1.40590295882	3.68641483259
C	-2.99332369130	-1.66546730371	1.92894166208
H	-2.51882238918	-0.68808475184	1.99963963426
P	1.23633154259	0.76873371714	-1.82999900110
P	-1.72583975646	1.57412942631	-0.90596660808
C	0.10617410582	1.80916568288	-3.02750188500
H	0.34478609188	2.86028249259	-2.83067635084
H	0.38762702577	1.58609392140	-4.06198125477
C	-1.38755410000	1.55272881721	-2.78966707824
H	-1.68999157769	0.56955306560	-3.16822093488
H	-1.99361885812	2.32797825562	-3.27593263898
C	2.10068392355	-0.36969957987	-3.11154567793
C	3.48054381880	-0.65711827188	-3.03472952234
H	4.09190791436	-0.18468239836	-2.27219511333
C	4.08431564064	-1.53943371202	-3.95242558720
H	5.15037084912	-1.74385471607	-3.87677504025
C	3.31938719343	-2.14433848611	-4.96744094171
H	3.78775124201	-2.81763364019	-5.68201295577
C	1.94070533883	-1.86312534011	-5.05239165960
H	1.33808207179	-2.31775401924	-5.83626057926
C	1.33871681347	-0.99081734167	-4.12685313162
H	0.27109232905	-0.79924659366	-4.20004131773
C	2.64446278963	2.05669565694	-1.62297801562
C	3.06268871938	2.42756310356	-0.33346442746
H	2.59685007502	1.93915596214	0.52023104222
C	4.05936396056	3.40682420119	-0.15407858665
H	4.37917713156	3.67817413147	0.85041013596
C	4.64504216900	4.03106063299	-1.27139863814
H	5.41306934369	4.78988461657	-1.13657079342
C	4.23250214099	3.66374976979	-2.56862033937
H	4.68110608706	4.13877417007	-3.43861847394
C	3.24189080241	2.67980382521	-2.74120455180
H	2.94439354530	2.39362547852	-3.74792349555
C	-3.60717554045	1.35920398836	-0.80648666916
C	-4.42299489486	1.15754132463	-1.93864113695
H	-3.98694549224	1.09042324164	-2.93048291124
C	-5.81965428913	1.02852778968	-1.80159844514
H	-6.43430533913	0.87296274685	-2.68562996251
C	-6.41707211559	1.10383506436	-0.53015006417

H	-7.49507853033	1.00521865753	-0.42413173475
C	-5.60782928657	1.30787903123	0.60591895501
H	-6.05924579150	1.36601021509	1.59371698345
C	-4.21493744140	1.43196783783	0.46647439792
H	-3.59750662046	1.59463556624	1.34719746583
C	-1.63161278333	3.45156193524	-0.57607347609
C	-2.64758596616	4.32369678411	-1.02735145004
H	-3.53159836593	3.92605147180	-1.51961403139
C	-2.53561895665	5.71243167197	-0.83044402177
H	-3.32522054453	6.37284098646	-1.18263693538
C	-1.40651467429	6.24571762392	-0.17733476927
H	-1.31940374889	7.31950554339	-0.02564176830
C	-0.39488605345	5.38004263286	0.27818203076
H	0.48194094794	5.78230801194	0.78095273545
C	-0.50868949945	3.99010715276	0.08068190069
H	0.26679382051	3.31750551503	0.43308695086
N	-0.00719435762	1.76015970889	2.96775582525
C	1.20627340663	2.54406320731	3.28917076368
H	1.60490148344	2.93746384311	2.34979190719
H	1.97740019578	1.88124718977	3.73233401925
C	0.87658387513	3.68607065774	4.26964892873
H	1.80574611795	4.20328498140	4.54867132865
H	0.22962249537	4.41409872986	3.76043042911
C	0.15622886105	3.14846759287	5.52655014725
H	-0.12081511617	3.97763840921	6.19151281505
H	0.84223118030	2.49803026484	6.09268628991
C	-0.73483202130	1.21419894881	4.13675417549
H	-0.11550141445	0.45528694824	4.65251245597
H	-1.63207707613	0.71333328703	3.75963555494
N	0.01231835283	1.02209984246	1.83024096645
C	-1.09884289020	2.34252960806	5.12170245951
H	-1.58047472370	1.90686235082	6.00871747310
H	-1.82554586032	3.01425913104	4.64332250069

^{15}N- BW Complex

W	0.00338990046	0.13155807825	0.25441097801
P	1.72074772360	-1.65766757201	0.79007841070
P	-1.26079245893	-1.95326694796	-0.36352008711
C	1.36841277184	-3.17349519930	-0.32279121466
H	1.64905137687	-2.89719938763	-1.34547192103
H	1.98504244084	-4.02003103183	0.00587135314
C	-0.12206402812	-3.52699605777	-0.23060758114
H	-0.34458398052	-3.98281758171	0.74045366293
H	-0.40808331622	-4.23885202017	-1.01216543887
C	3.60487433830	-1.46916919070	0.66694193413

C	4.22879969461	-0.48615013440	1.46645316847
H	3.62264284751	0.14092842830	2.11669293177
C	5.62324870673	-0.31418772528	1.43826327495
H	6.08655591626	0.44772606607	2.06099926117
C	6.41893053394	-1.12293652157	0.60179216096
H	7.49801413600	-0.98920685277	0.57575059460
C	5.80591228770	-2.10247264728	-0.20034321875
H	6.40964662861	-2.73316636491	-0.84941408947
C	4.40763711407	-2.27542507766	-0.16609030335
H	3.96008560754	-3.03473453525	-0.79937737463
C	1.62702730574	-2.48440861165	2.50854704783
C	0.50136784337	-2.26605682107	3.32552177364
H	-0.27541056595	-1.58910669506	2.98423362722
C	0.38125099511	-2.91848162776	4.56811757810
H	-0.49959512902	-2.74668700006	5.18292348619
C	1.39087189175	-3.79441316278	5.00835428162
H	1.29973170712	-4.29944208348	5.96759466420
C	2.52271983343	-4.01340676845	4.19781013604
H	3.31080476813	-4.68539113514	4.53099113598
C	2.63957524131	-3.36261187407	2.95558590544
H	3.52491071327	-3.53159335565	2.34788838586
C	-2.18490132049	-2.35283145556	-1.99476377117
C	-1.45836853268	-2.82172663362	-3.11212306728
H	-0.38569947266	-2.97897118466	-3.03342720668
C	-2.10236370035	-3.08507510898	-4.33494755263
H	-1.52660025730	-3.46124878562	-5.17828382535
C	-3.48870584453	-2.86542770874	-4.46625403013
H	-3.99009842117	-3.06949341885	-5.40980667404
C	-4.21782076453	-2.38409104120	-3.36269763205
H	-5.28837857165	-2.21040627142	-3.44923201157
C	-3.57164915218	-2.13214174267	-2.13630240699
H	-4.15447490637	-1.77680594816	-1.29216116707
C	-2.62251555296	-2.51311886567	0.86761732121
C	-3.22924370173	-3.78456391843	0.76360445543
H	-2.96729766858	-4.44722309462	-0.05864985425
C	-4.18258298741	-4.20317489149	1.70969611536
H	-4.63876180510	-5.18685699427	1.61987727813
C	-4.54831406137	-3.34856113607	2.76968237261
H	-5.28758764929	-3.66988473470	3.50048114236
C	-3.95308298032	-2.07719147910	2.87332256073
H	-4.23529607965	-1.40862580789	3.68463300957
C	-2.99364944118	-1.66689119171	1.92714293846
H	-2.51929304977	-0.68948637945	1.99852486591
P	1.23646460189	0.77034663449	-1.82926789113
P	-1.72577435440	1.57488558327	-0.90479059409
C	0.10634859711	1.81167556215	-3.02603630841
H	0.34492404691	2.86264590598	-2.82838742156

H	0.38786377377	1.58940916751	-4.06067217653
C	-1.38739067416	1.55503106587	-2.78848935119
H	-1.68979850156	0.57216323346	-3.16786447309
H	-1.99344052911	2.33067039583	-3.27415231523
C	2.10109620866	-0.36694057716	-3.11164599253
C	3.48089904945	-0.65458700372	-3.03466871487
H	4.09206680140	-0.18296685233	-2.27147228432
C	4.08487028512	-1.53607704607	-3.95302718276
H	5.15087829604	-1.74069038679	-3.87723055603
C	3.32020325027	-2.13991162080	-4.96887524473
H	3.78872230932	-2.81256538104	-5.68394925468
C	1.94157852503	-1.85846834328	-5.05399060132
H	1.33915672695	-2.31227223045	-5.83849233539
C	1.33938709827	-0.98699718336	-4.12779506277
H	0.27180781533	-0.79524354937	-4.20114472315
C	2.64444593608	2.05827935727	-1.62102041020
C	3.06240102915	2.42822843790	-0.33115414962
H	2.59643993789	1.93915593008	0.52209190505
C	4.05895365398	3.40744634133	-0.15085550615
H	4.37855385349	3.67808192484	0.85389368836
C	4.64478493030	4.03256356913	-1.26760219642
H	5.41271915133	4.79135580359	-1.13206778381
C	4.23252159818	3.66617705601	-2.56517296402
H	4.68124768596	4.14188534260	-3.43473431054
C	3.24202965791	2.68227189918	-2.73867235994
H	2.94475015273	2.39681473845	-3.74566095247
C	-3.60711515570	1.35991069875	-0.80557400172
C	-4.42293024855	1.15953897049	-1.93795976627
H	-3.98687360818	1.09351027103	-2.92987132535
C	-5.81959729360	1.03044129492	-1.80107304422
H	-6.43424729123	0.87589037960	-2.68528329492
C	-6.41702432473	1.10436029353	-0.52954748482
H	-7.49503644807	1.00567586818	-0.42365026946
C	-5.60778390705	1.30710056355	0.60675684747
H	-6.05920690708	1.36415063307	1.59461497941
C	-4.21488576962	1.43128597286	0.46746190770
H	-3.59745411111	1.59294798761	1.34836999068
C	-1.63153080813	3.45203488856	-0.57332749384
C	-2.64753803498	4.32454665343	-1.02379812089
H	-3.53158438697	3.92731297505	-1.51633186512
C	-2.53556213589	5.71311442671	-0.82572120135
H	-3.32518792703	6.37382089863	-1.17730168284
C	-1.40641537626	6.24584888195	-0.17223446184
H	-1.31929956589	7.31950755486	-0.01963232869
C	-0.39474996866	5.37979246119	0.28247469170
H	0.48210770986	5.78163465301	0.78553061963
C	-0.50855932902	3.99002486420	0.08379865605

H	0.26695561490	3.31712282963	0.43556135138
N	-0.00742840932	1.75742141482	2.96933875165
C	1.20601046470	2.54099285388	3.29167612863
H	1.60475699701	2.93532522458	2.35273799987
H	1.97707877272	1.87772934117	3.73427183136
C	0.87621588751	3.68202857283	4.27324680923
H	1.80535100516	4.19895775572	4.55288716252
H	0.22932059081	4.41056605577	3.76467356378
C	0.15570897939	3.14319180412	5.52953243510
H	-0.12141229256	3.97170829829	6.19527779506
H	0.84164173495	2.49219558322	6.09511095477
C	-0.73519779961	1.21030114195	4.13771324073
H	-0.11592417574	0.45087627121	4.65278678241
H	-1.63240297379	0.70981408831	3.75999790255
N	0.01218974602	1.02050921113	1.83107883306
C	-1.09931569233	2.33765650297	5.12373759530
H	-1.58105516651	1.90111100612	6.01026237150
H	-1.82595977141	3.00986220805	4.64593794469

C-G base pair equilibrium geometry at MP2/6-31++g(d,p) level in Å

CG pair

N	1.979240	-2.342729	0.259816
C	2.768360	-1.271404	0.089221
N	2.172546	-0.082015	-0.061521
C	2.914930	1.058622	-0.186176
N	4.310476	0.923102	-0.175239
C	4.935578	-0.279403	-0.031002
C	4.200692	-1.415794	0.099830
O	2.424066	2.194783	-0.312976
H	4.834597	1.782955	-0.263704
H	6.016654	-0.267001	-0.033709
H	4.676635	-2.377412	0.219372
H	2.385928	-3.263583	0.255775
H	0.960840	-2.249110	0.134123
O	-0.796508	-2.029764	-0.104342
C	-1.421287	-0.953390	-0.012830
N	-0.728230	0.256191	0.151496
C	-1.288554	1.512859	0.183615
N	-2.591087	1.735857	0.130650
C	-3.296685	0.580790	0.021556
C	-2.837380	-0.738644	-0.015310
N	-3.879310	-1.634962	-0.156784
C	-4.957901	-0.865465	-0.176451
N	-4.662224	0.476263	-0.069670
N	-0.421754	2.551733	0.368625
H	-5.972271	-1.219748	-0.263093
H	-5.309781	1.250525	-0.065441
H	-0.830852	3.456336	0.190229
H	0.552577	2.437073	0.088646
H	0.301069	0.176701	0.110008

Water/Methanol cluster equilibrium geometry at MP2/6-311+G(d,p) level in Å

HOH---OHH

O	1.37530994997	-0.00102318392	0.09398510000
H	1.83050693142	-0.75336319514	-0.29261290000
H	1.82657696876	0.76078880495	-0.27842590000
O	-1.52911704997	0.00128288771	-0.11899890000
H	-0.56981205002	-0.00100813595	-0.01063590000
H	-1.85681505021	-0.00849510421	0.78178510000

MeHO---HOH

O	0.64620204528	0.66310417016	-0.08180910714
H	0.99548209087	1.33076114631	0.51371589286
O	-2.06687301448	-0.21209664458	0.09875789286
H	-1.17901998875	0.16474029480	0.02381889286
C	1.49640196699	-0.48337488790	-0.00462510714
H	1.06250191572	-1.23427685827	-0.66353810714
H	2.50876298292	-0.25011795703	-0.34762710714
H	1.53528393945	-0.88665989055	1.01167689286
H	-2.53605498855	0.16774238746	-0.64588610714

MeOH---OHH

O	-1.98967210396	-0.19343321132	0.00011503571
H	-2.53323510775	0.03663577974	0.75799103571
H	-2.53673610766	0.03115277968	-0.75687896429
O	0.76775388089	0.72718583406	-0.00040396429
H	-0.14765311412	0.42391981900	-0.00161296429
C	1.58635989991	-0.42873115246	0.00024803571
H	2.62394389436	-0.09130313539	0.00139003571
H	1.42449391012	-1.04918015513	0.89053803571
H	1.42637291012	-1.04885915510	-0.89060396429

MeOH---OHMe

O	-1.25076681147	0.63427720823	-0.15371694444
H	-1.68619674324	1.19328126138	-0.80205594444
O	1.32078404414	-0.54864010566	-0.45389094444
H	0.47231410036	-0.08807800210	-0.41562094444
C	2.23389613650	0.20798578288	0.32024305556
H	3.18513907122	-0.32678933323	0.31716905556

H	2.40070825866	1.20880676252	-0.09790794444
H	1.90226714973	0.31640182336	1.36058205556
C	-2.17454893531	-0.38034167902	0.24718205556
H	-1.64417901331	-1.01929174375	0.95221105556
H	-3.04739088248	0.05246542753	0.74504305556
H	-2.49888300946	-0.98775763943	-0.60310794444

Water/Methanol cluster equilibrium geometry at CCSD(T)/6-311+G(d,p) level in Å

HOH---OHH

O	1.37551042217	-0.00100796406	0.09429196644
H	1.82999497579	-0.75357541848	-0.29404370997
H	1.82623430343	0.76089248628	-0.27998858761
O	-1.52931170511	0.00125034667	-0.11898449927
H	-0.57018735411	-0.00102161789	-0.01164391591
H	-1.85563166159	-0.00823451079	0.78321647606

MeHO---HOH

O	0.644767	0.664126	-0.081904
H	0.994170	1.331819	0.513944
O	-2.067713	-0.212829	0.098910
H	-1.180529	0.164169	0.023976
6	1.498179	-0.483452	-0.004743
H	1.065435	-1.239090	-0.665449
H	2.513753	-0.247104	-0.348369
H	1.538012	-0.887047	1.015487
H	-2.536348	0.167589	-0.647184

MeOH---OHH

O	-0.767236	0.728969	-0.000400
H	0.147448	0.425299	-0.000022
O	1.990415	-0.194085	0.000321
H	2.535882	0.031908	-0.758172
C	-1.587627	-0.429465	0.000144
H	-2.629350	-0.091975	0.000022
H	-1.425153	-1.052060	-0.893349
H	-1.425097	-1.051273	0.894169
H	2.536600	0.035817	0.757122

MeOH---OHMe

O	-1.250071	0.635115	-0.154445
H	-1.685471	1.193895	-0.803363
O	1.320408	-0.549674	-0.455048
H	0.472869	-0.088910	-0.416610
C	2.235823	0.208005	0.321008
H	3.190695	-0.328404	0.318604
H	2.402809	1.212436	-0.098739
H	1.901957	0.316696	1.364726
C	-2.176577	-0.380286	0.248001
H	-1.646135	-1.022417	0.956114
H	-3.052082	0.056003	0.746639
H	-2.502806	-0.989136	-0.605481