Supplementary Information

Excited State Evolution of DNA Stacked Adenines Resolved at the CASPT2//CASSCF/Amber Level: from the Bright to the Excimer State and Back

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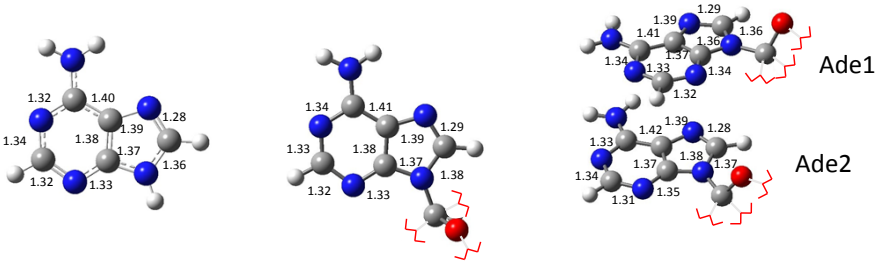
S1. 150 ns MD simulation details

1) Conventional long term MD in explicit TIP3P water using cubic boxes and explicit counterions (Na+) and Particle Mesh Ewald MD; initial dimensions: 63.8916520 64.6173940 68.2374600 (all units of Angstroems); software employed: AMBER 12
1a) 1000 steps of minimization, 500 thereof using conjugate gradient, the remainder using steepest descent, at a cutoff radius of 12 Angstroem; program: sander
1b) 5 ps kickstart heating to a temperature of 300 K (NTV) using a Berndsen theromostat, a timestep of 1 fs and a cutoff of 10 Angstroem with SHAKE constraints; program: pmemd.MPI (4 core)
1c) 500 ps equilibration at 300 K (NTV) at otherwise similar conditions to 1b); program: pmemd.cuda (GeForce GTX 680, method: SPFP)
1d) 200 ps of equilibration at 300 K switching NTV to NTp at 1 bar using isotropic position scaling at otherwise similar conditions to 1b); program: pmemd.cuda (GeForce GTX 680, method: SPFP)
2) Continued MD at 300K, 1 bar, using NTp, 1 fs timesteps, a cutoff of 10 A and SHAKE constraints over a total simulation time of 151.5 ns; program: pmemd.cuda (GeForce GTX 680, method: SPFP)
3) Applied force field in all the above: ff12SB with corresponding frcmod.ionsjc_tip3p;

S2. Ground state optimized geometry for adenine in vacuum (left) and in DNA with one (center) or two QM (right) adenines. Bond lengths in Å and angles in degrees (see ref [1])



Scheme S1

S3. Exciton absorption band details

Table S1. L_a states configurations, configuration coefficients and weights (in parenthesis) in the Franck Condon region. They explicitly show the exciton nature. $L_a(1)$ and $L_a(2)$ are just labels in the FC region because the excitation is shared on both bases, they are exciton,
H_1 and L_1 are the Homo and the Lumo orbitals on Ade1 (H_2 and L_2 on Ade2, respectively).

SA-5-CASSCF(8,8)//CASPT2/6-31g/AMBER*
$L_a(1)$ (os. strength 0.61)

$(H_1+H_2)\rightarrow(L_1+L_2)$	-0.64 0.41
$(H_1-H_2)\rightarrow(L_1-L_2)$	-0.51 0.26
$L_a(2)$ (os. strength 0.06)	
$(H_1-H_2)\rightarrow(L_1+L_2)$	-0.61 (0.37)
$(H_1+H_2)\rightarrow(L_1-L_2)$	-0.52 (0.27)

SA-7-CASSCF(12,10)//CASPT2/6-31g/AMBER*
$L_a(1)$ (os. strength 0.60)

$(H_1+H_2)\rightarrow(L_1+L_2)$	0.58 (0.33)
$(H_1-H_2)\rightarrow(L_1-L_2)$	-0.44 (0.20)
$L_a(2)$ (os. strength 0.05)	
$(H_1-H_2)\rightarrow(L_1+L_2)$	0.51 (0.26)
$(H_1+H_2)\rightarrow(L_1-L_2)$	-0.43 (0.19)

SA-12 CASPT2//CASSCF (8,8)/6-31g/AMBER*
$L_a(1)$ (os. strength 0.58)

$(H1)\rightarrow(L_1)$	0.66 (0.44)
$(H_2)\rightarrow(L_2)$	0.47 (0.22)
$L_a(2)$ (os. strength 0.05)	
$(H_2)\rightarrow(L_2)$	-0.64 (0.07)
$(H_1)\rightarrow(L_1)$	0.45 (0.20)

S4. Correlation between the excited state barriers and the life-time

We affirmed that an allowed process with a lifetime of 100 ps at room temperature corresponds to a barrier of 0.16 eV.
This result originates from the following equation:
$k_v=A\cdot e^{(-\square\square/kT)}$
Where k_v is the *rate costant*,
A is the pre-exponential factor, $6\cdot10^{12}$ (sec^{-1}), coinciding with the velocity of a barrierless process
E_a is the activation energy
kT is 200 (cm^{-1}) at room temperature (k is the Boltzmann constant)

S5. Atom charge re-distribution in CT states

Here we show the atom charges on GS, CT_{12} and CT_{21} at MinGS geometry. Here we report just the charges of QM atoms of the purine rings because we are mainly interested on the ring distortion cause. The QM part is 38 atoms. Bold numbers specify the atoms where a larger part of the negative charge is localized (comparing with GS charges) in the electronic transition from Ade2 to Ade1 for the CT_{21}, and the opposite for the CT_{12} state. Thick border cells shows the net charge of the same atoms. Dotted border cell indicate the atom with an excess of positive charge that stabilize C_2 (with an excess of negative charge) in the C_2 puckering distortion

of CT_{21} state that gets closer the two atoms. This allows a larger stabilization of CT_{21} comparing with CT_{12} in which the puckering does not permit a charge recombination stabilization.

Ground State charges

N_1	C_2	N_3	C_4	C_5	C_6	N_7	C_8	N_9
-0.74	0.27	-0.72	0.67	0.05	0.70	-0.73	0.37	-0.71
N_1'	C_2'	N_3'	C_4'	C_5'	C_6'	N_7'	C_8'	N_9'
-0.75	0.31	-0.69	0.66	0.08	0.74	-0.73	0.33	-0.65

CT_{21} charges

N_1	C_2	N_3	C_4	C_5	C_6	N_7	C_8	N_9
-0.69	0.06	-0.86	0.65	-0.04	0.48	-0.73	0.29	-0.71
N_1'	C_2'	N_3'	C_4'	C_5'	C_6'	N_7'	C_8'	N_9'
-0.72	0.39	-0.62	0.75	0.29	0.81	-0.73	0.41	-0.61

CT_{12} charges

N_1	C_2	N_3	C_4	C_5	C_6	N_7	C_8	N_9
-0.69	0.39	-0.62	0.76	0.32	0.79	-0.73	0.46	-0.67
N_1'	C_2'	N_3'	C_4'	C_5'	C_6'	N_7'	C_8'	N_9'
-0.71	0.07	-0.87	0.63	-0.05	0.48	-0.73	0.23	-0.65

Differences between CT_{21} and GS charges

N_1	C_2	N_3	C_4	C_5	C_6	N_7	C_8	N_9
0.04	**-0.22**	**-0.15**	-0.02	-0.01	**-0.22**	0.00	-0.08	0.00
N_1'	C_2'	N_3'	C_4'	C_5'	C_6'	N_7'	C_8'	N_9'
0.03	0.07	0.07	-0.09	0.22	0.07	0	0.09	0.03

Differences between CT_{12} and GS charges

N_1	C_2	N_3	C_4	C_5	C_6	N_7	C_8	N_9
0.05	0.11	0.09	0.09	0.27	0.09	0	0.09	0.04
N_1'	C_2'	N_3'	C_4'	C_5'	C_6'	N_7'	C_8'	N_9'
0.03	**-0.24**	**-0.18**	-0.03	-0.03	**-0.27**	-0.01	-0.1	-0.01

S6. Intra-monomer stretching and base-base distance coordinates changings

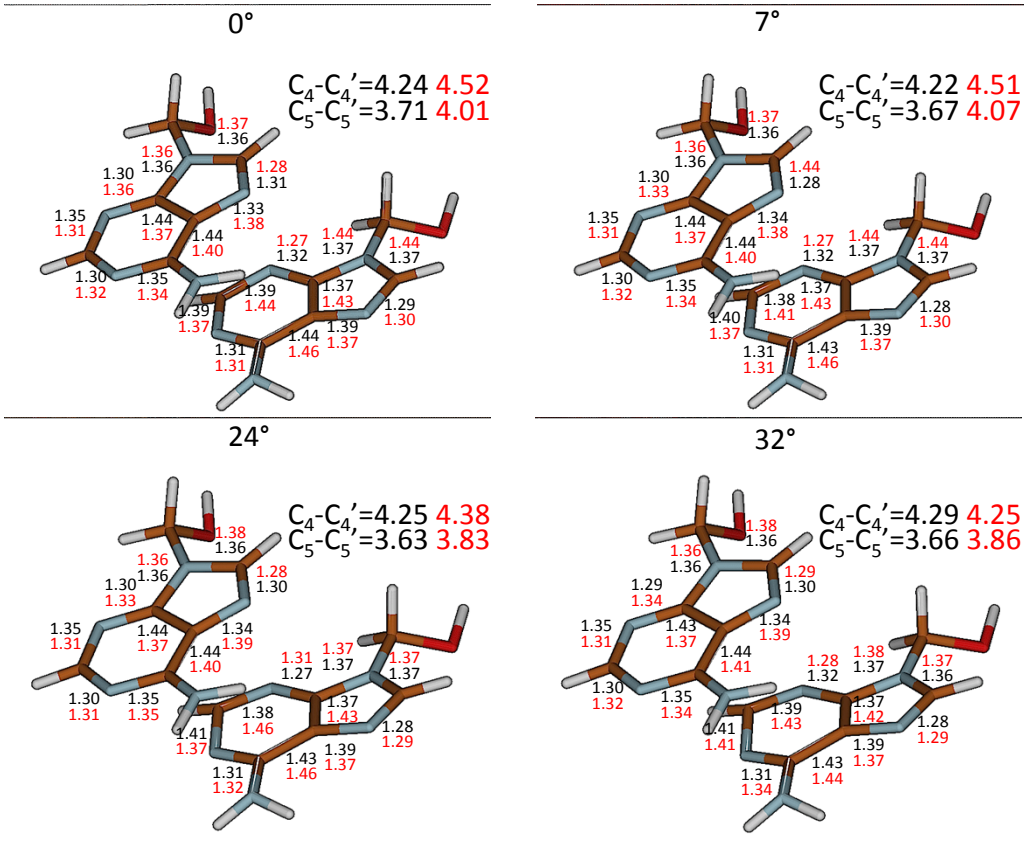


Figure S1. Comparison of bond distances between optimized $L_a(1)$ and CT21 structures at the same $C_6N_1C_2N_3$ dihedral distortion

(0°, 7°, 24° and 32° respectively). $L_a(1)$ and CT_{21} values are the red and the black, respectively. C_4-C_4' and C_5-C_5' inter-base distances are reported.

S7. Energy Tables.

Table S2. SA-7-CASSCF(12,10)//CASPT2/6-31g*/AMBER relative energies (ΔE,eV) of $L_a(1)$, $L_a(2)$, $L_b(1)$, $L_b(2)$, nπ*(1) and nπ*(2) for the relevant points along the $L_a(1)$ (upper table) and $L_a(2)$ (lower table) decay paths ($C_6N_1C_2N_3$ dhiedral angle rotation) of two QM adenines (Ade1 and Ade2, Figure1). See 'Reaction path calculation strategy' section for more information. The active space consists of four π (Homo and Homo-1 orbital for each base) two n orbitals localized on each base and four π* orbitals (Lumo and Lumo+1 for each base).

	MinGS 0°	0_{La1} 0°	Min$L_a(1)$ 7°	24_{La1} 24°	32_{La1} 32°	40_{La1} 40°	48_{La1} 48°	
$L_a(1)$	5.00	4.25	4.21	4.24	4.32	4.35	4.46	
$L_a(2)$	5.04	5.29	5.32	5.59	5.70	6.58	7.18	
$L_b(1)$	5.10	5.15	5.17	5.47	5.52	5.42	5.58	
$L_b(2)$	5.17	5.34	5.36	5.51				
nπ*(1)	6.04	5.60	5.57	5.73	5.70	5.65	6.05	
nπ*(2)	5.98	6.26	6.31	6.73	6.77			
	MinGS 0°	0_{La2} 0°	Min$L_a(2)$ 11°	13_{La2} 13°	24_{La2} 24°	32_{La2} 32°	40_{La2} 40°	48_{La2} 48°
$L_a(1)$	5.00	5.87	5.43	5.68	5.48	5.46	5.88	5.92
$L_a(2)$	5.04	4.12	4.11	4.22	4.17	4.05	4.18	4.14
Lb(1)	5.10	5.36	5.26	5.39	5.65	5.48	5.79	
Lb(2)	5.17	5.35	5.03	5.15	5.25	5.30	5.57	5.32
nπ*(1)	6.04		6.09	6.27	6.34			
nπ*(2)	5.98	5.36	5.51	5.76	5.58	5.43	5.60	5.39

Table S3. SA-5 CASPT2//CASSCF (8,8)/6-31g*/AMBER relative energies (ΔE,eV) for the relevant points along the $L_a(1)$ (upper table) and $L_a(2)$ (lower table) decay paths of two QM adenines in the double strand. The active space consists of four π and four π* orbitals.

	MinGS 0°	0_{La1} 0°	Min$L_a(1)$ 7°	24_{La1} 24°	32_{La1} 32°	40_{La1} 40°	48_{La1} 48°	55_{La1} 55°	La(1)/GS CI 64°
GS	0.00	0.26	0.30	0.69	0.82	0.95	1.45	3.14	3.58
La(1)	4.97	4.28	4.25	4.28	4.40	4.21	4.25	4.25	3.04
	MinGS 0°	0_{La2} 0°	Min$L_a(2)$ 11°	24_{La2} 24°	32_{La2} 32°	40_{La2} 40°	48_{La2} 48°	55_{La2} 55°	La(2)/GS CI 68°
GS	0.00	0.11	0.13	0.35	0.49	0.80	0.99	1.55	3.90
La(2)	4.93	4.08	4.04	4.13	4.05	4.18	4.09	4.09	3.53

Table S4. SA-12 CASPT2//CASSCF (8,8)/6-31g*/AMBER relative energies (ΔE,eV) of $L_a(1)$, $L_a(2)$, CT_{12} and CT_{21} for the relevant points along the $L_a(1)$ (upper table) and La(2) (lower table) decay paths of two QM adenines in the double strand. CASSCF includes four π and four π* orbitals.

	MinGS 0°	0_{La1} 0°	Min$L_a(1)$ 7°	24_{La1} 24°	32_{La1} 32°	40_{La1} 40°	48_{La1} 48°	55_{La1} 55°	La(1)/GS CI 64°	
GS	0.00	0.22	0.23	0.62	0.73	0.96	1.49	3.06	3.55	
$L_a(1)$	4.81	4.16	4.10	4.19	4.24	4.15	4.23	4.24	2.88	
CT_{12}	6.40	6.69	6.41	6.44	6.78	6.89	7.21	8.38		
CT_{21}	6.99	6.27	5.93	6.27	6.31	6.22	6.38	7.51		
	MinGS 0°	0_{La2} 0°	Min$L_a(2)$ 11°	13_{La2} 13°	24_{La2} 24°	32_{La2} 32°	40_{La2} 40°	48_{La2} 48°	55_{La2} 55°	La(2)/GS CI 68°
GS	0.00	0.08	0.15	0.32	0.37	0.50	0.81	1.00	1.56	3.33
$L_a(2)$	4.80	3.96	3.96	4.15	4.05	4.01	4.13	4.04	4.04	3.64
CT_{12}	6.40	5.98	5.95	6.26	5.64	5.91	6.22	6.30	6.44	
CT_{21}	6.99	6.13	6.34	6.33	6.54	6.72	6.95	6.79	7.66	

Table S5 SA-12 CASPT2//CASSCF (8,8)/6-31g*/AMBER relative energies (ΔE, in eV) of $L_a(1)$ and CT_{21} (upper part), $L_a(2)$ and CT_{12} (middle part) for the relevant points along the CT states optimized scan along the dihedral distortion coordinate characterizing La decay paths. The third part represents energies of geometries obtained optimizing conical intersection between GS and CT states (more information in computational details). In the third and fourth columns the CIs involve proton transfer from Ade1 to Ade2 and conversely from Ade2 to Ade1, respectively. CASSCF includes four π and four π* orbitals.

	0_{CT21} 0°	MinCT_{21} 7°	24_{CT21} 24°	32_{CT21} 32°	40_{CT21} 40°	48_{CT21} 48°
$L_a(1)$	4.95	4.83	4.77	5.36	5.49	5.70
CT_{21}	4.24	4.14	4.20	32	4.48	4.60

	0_{CT12}	11_{CT12}	MinCT_{12}	24_{CT12}	32_{CT12}	40_{CT12}	48_{CT12}	55_{CT12}

	0°	11°	14°	24°	32°	40°	48°	55°
$L_a(2)$	5.18	5.23	4.78	4.75	4.77	4.67	4.61	4.64
CT_{12}	4.72	4.74	4.53	4.58	4.53	4.91	4.96	5.20

	CI CT_{12}/GS	CI CT_{21}/GS	CI CT_{12}/GS PT	CI CT_{21}/GS PT
GS	5.05	5.36	3.72	3.74
CT_{12}	5.25		3.50	
CT_{21}		5.15		3.59

Table S6. SA-8 CASPT2//CASSCF (8,8)/6-31g*/AMBER relative energies (ΔE, in eV) for the linear interpolation between MinCT21 and Min$L_a(1)$ geometries, where each minimum was calculated keeping frozen the dihedral distortion. CASSCF includes four π and four π* orbitals.

	0°							7°						
	0_{CT21}	1	2	3	4	5	0_{La1}	7_{CT21}	1	2	3	4	5	7_{La1}
$L_a(1)$	5.02	4.18	3.74	3.74	3.68	3.62	4.18	4.90	4.08	3.66	3.66	3.61	3.57	4.12
CT_{21}	4.25	3.72	4.09	4.21	4.25	4.38	6.26	4.15	3.63	4.03	4.18	4.27	4.34	5.20
	24°							32°						
	24_{CT21}	1	2	3	4	5	24_{La1}	32_{CT21}	1	2	3	4	5	32_{La1}
$L_a(1)$	4.86	4.15	3.86	3.82	3.72	3.64	4.39	4.84	4.20	3.96	3.89	3.82	3.74	4.26
CT_{21}	4.23	3.79	4.33	4.55	4.64	4.81	5.75	4.33	3.89	4.46	4.72	4.81	4.94	5.71
	40°							48°						
	40_{CT21}	1	2	3	4	5	40_{La1}	48_{CT21}	1	2	3	4	5	48_{La1}
$L_a(1)$	4.88	4.02	4.01	3.81	3.78	3.68	4.16	4.91	4.19	4.11	3.87	3.85	3.76	4.24
CT_{21}	4.50	4.30	4.59	4.75	4.99	4.85	5.98	4.64	4.49	4.83	4.92	5.04	5.67	6.55

Table S7. SA-2 CASPT2//CASSCF (14,12)/6-31+g**/AMBER relative energies (ΔE, in eV) for the calculated MEP values along the forming N_{am}-H distance coordinate between MinCT_{21} and CI CT_{21}/GS PT. The CASSCF(8,8)/6-31g*/AMBER minimum energy path of the proton transfer mechanism was calculate along the N-H bond length coordinate. The state average was on L_a1 and CT_{21} states. Active space includes π(π*), σ(σ*) and lone pair orbitals necessary to describe breaking and creating bonds.

	MinCT_{21}	1_{NH}	2_{NH}	3_{NH}	4_{NH}	5_{NH}	MinCT_{21} PT	CI CT_{21}/GS PT
GS	0.00	0.29	1.03	2.30	2.55	2.70	2.88	4.05
CT_{21}	3.73	4.01	4.63	3.90	3.60	3.49	3.54	3.88

S8. Wave functions and energies of Dyn1, Dyn2 and Dyn3 geometries

Table S8. L_a and CT states configurations, CASPT2 energies (E) at *SA-12 CASPT2//CASSCF (8,8)/6-31g*/AMBER* level, oscillator strength (os) and configuration coefficients (c) in the Franck Condon region.
H_1 and L_1 are the Homo and the Lumo orbitals on Ade1 (H_2 and L_2 on Ade2, respectively). Bold character indicate that the orbital component is larger on that base.

Dyn1				
State	Configuration	C	E (eV)	Os
$L_a(1)$	$(H_1\text{-}\mathbf{H_2})\rightarrow L_2$ $(\mathbf{H_1}+H_2)\rightarrow L_1$ $(H_1\text{-}\mathbf{H_2})\rightarrow L_1$	0.67 0.50 0.30	4.48	0.49
$L_a(2)$	$(H_1\text{-}\mathbf{H_2})\rightarrow L_1$ $(H_1\text{-}\mathbf{H_2})\rightarrow L_2$ $(\mathbf{H_1}+H_2)\rightarrow L_2$	0.44 -0.36 0.34	4.52	0.02
CT_{12}	$(\mathbf{H_1}+H_2)\rightarrow L_2$	-0.78	5.82	0.01
CT_{21}	$(\mathbf{H_1}+H_2)\rightarrow L_1$ $(H_1\text{-}\mathbf{H_2})\rightarrow L_1$	-0.73 0.44	5.39	0.03
Dyn2				
$L_a(1)$	$(H_1\text{-}\mathbf{H_2})\rightarrow L_1$ $\mathbf{H_1}+H_2)\rightarrow L_1$	0.61 -0.29	4.59	0.04
$L_a(2)$	$(H_1\text{-}\mathbf{H_2})\rightarrow L_2$	0.76	4.63	0.40
CT_{12}	$(\mathbf{H_1}+H_2)\rightarrow L_2$	-0.75	5.90	0.03
CT_{21}	$(\mathbf{H_1}+H_2)\rightarrow L_1$ $(H_1\text{-}\mathbf{H_2})\rightarrow L_1$	0.71 0.48	5.43	0.12
Dyn3				
$L_a(1)$	$H_1\rightarrow L_1$ $H_2\rightarrow L_1$	-0.56 -0.55	4.54	0.33
$L_a(2)$	$H_2\rightarrow L_2$	0.55	4.70	0.09

CT_{12}	$H_1 \rightarrow L_2$	-0.77	5.45	0.07
CT_{21}	$H_2 \rightarrow L_1$ $H_1 \rightarrow L_1$	0.58 -0.47	5.38	0.06

S9. Implementation of the gradient projection procedure for optimizing CI in COBRAMM

The gradient projection method is a robust and fast method for locating minimum energy CI. It was originally proposed by Bearpark and co-workers [2] and is implemented in a number of quantum-chemical packages. The geometry optimization procedure follows an effective gradient $\boldsymbol{g}$ composed of two terms:

$$\boldsymbol{g}=2\,(E_I-E_J)\,\boldsymbol{g}_{IJ}/|\boldsymbol{g}_{IJ}| + \boldsymbol{P}_{IS}(\,\nabla_R E_2)$$

In the first term $\boldsymbol{g}_{IJ}$ is the difference vector of the gradients of states I and J. The multiplication of the normalized gradient difference vector with the energy difference E_I - E_J assures that the first term vanishes when both states become degenerate. The second term represents the projection of the excited state gradient $\nabla_R E_2$ onto the orthogonal complement to the plane spanned by the gradient difference $\boldsymbol{g}_{IJ}$ and the scaled derivative coupling vector $\boldsymbol{h}_{IJ}=(E_I - E_J)\langle\Psi_J|\nabla_R|\Psi_I\rangle$. Both vectors define to first order approximation the branching plane in which a geometry deformation lifts the degeneracy between states I and J. Following the projection of the gradient onto th sub-space orthogonal to the branching speace ensures that the optimized structure is the lowest degenerate point. Technically. the projection is performed via the projection matrix $\boldsymbol{P}_{IS} = 1 - \boldsymbol{A}(\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T$, where $\boldsymbol{A}$ is a $3Nx2$ matrix with columns $\boldsymbol{g}_{IJ}$ and $\boldsymbol{h}_{IJ}$.

Implementing the procedure at QM/MM level is straightforward. Thereby, the gradient difference vector $\boldsymbol{g}_{IJ}$ is constructed out of the gradients of the QM and movable MM sub-systems $\boldsymbol{g}_{IJ}^{QM}$ and $\boldsymbol{g}_{IJ}^{MM}$ ($\boldsymbol{g}_{IJ} = [\boldsymbol{g}_{IJ}^{QM}, \boldsymbol{g}_{IJ}^{MM}]$) The construction of the projection matrix $\boldsymbol{P}$ requires also the knowledge of $\boldsymbol{h}_{IJ}$ over the QM and MM sub-systems. As computing $\boldsymbol{h}_{IJ}$ requires a wavefunction description of the system, $\boldsymbol{h}_{IJ}^{MM}$ is set to zero ($\boldsymbol{h}_{IJ} = [\boldsymbol{h}_{IJ}^{QM}, 0^{MM}]$). No weighting factors are used. [3]

The implemented algorithm includes the effect of the MM atoms on the structure and energy of the CI both implicitly via the one-electron Hamiltonian (electrostatic embedding) and explicitly through the force on the movable MM atoms $\boldsymbol{g}_{IJ}^{MM}$. The only approximation is the neglect of structural deformations in the movable MM sub-system, which couple states I and J for the contruction of $\boldsymbol{h}_{IJ}$ and, thus, for the construction of the projection matrix $\boldsymbol{P}_{IS}$.

S10. H-bonds in the adenine-thymine base pair at the CI CT_{21}/GS geometries.

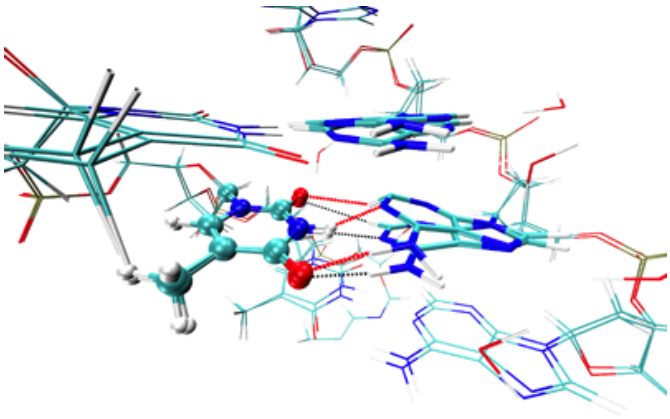


Figure S2. H-bonds in the adenine-thymine base pair at the CI CT_{21}/GS overlaid with the grround state minimum geometry. The deformations towards the CI degrade the H-bonding pattern. A licorice representation is used for the QM adenine dimer, a balls-and-sticks for the paired thymine

S11. Cartesian coordinates (x, y and z in Å) of all the structures (just QM part) discussed in the paper.

MinGS

O	0.496396	-7.748811	-7.449307
C	0.911119	-6.545339	-6.871652
H	0.950789	-5.732542	-7.581846
N	-0.014145	-6.155941	-5.854482
C	-0.351878	-6.811857	-4.708896
H	0.088421	-7.753135	-4.449474
N	-1.218276	-6.181719	-3.996315
C	-1.483308	-5.018576	-4.707338
C	-2.274888	-3.881486	-4.446143
N	-3.035064	-3.724674	-3.368966
H	-3.623794	-2.917444	-3.318565
H	-3.187547	-4.457968	-2.699949

N	-2.222612	-2.876873	-5.333703
C	-1.476231	-3.008404	-6.426428
H	-1.484770	-2.168776	-7.095749
N	-0.730475	-4.033554	-6.785306
C	-0.746811	-5.004844	-5.860914
O	3.020615	-2.146126	-7.605099
C	3.270793	-1.345325	-6.476390
H	3.038834	-0.306783	-6.656257
N	2.466235	-1.800232	-5.393501
C	2.571398	-3.003925	-4.754871
H	3.237848	-3.761622	-5.112296
N	1.818383	-3.113885	-3.728248
C	1.134440	-1.910188	-3.661821
C	0.162719	-1.390279	-2.760940
N	-0.293231	-2.061322	-1.715131
H	-1.065704	-1.671259	-1.213876
H	-0.152951	-3.056918	-1.643622
N	-0.266180	-0.156311	-2.991886
C	0.185693	0.527391	-4.047904
H	-0.231275	1.509983	-4.170299
N	1.055663	0.143416	-4.947148
C	1.519583	-1.093950	-4.689625
H	1.354808	-8.064506	-8.042235
H	1.918827	-6.756343	-6.513740
H	3.932354	-2.151998	-8.202424
H	4.334574	-1.457422	-6.266861

0_{La1}

O	0.538975	-7.857376	-6.979051
C	0.878645	-6.561992	-6.549855
H	0.891515	-5.842540	-7.356160
N	-0.080944	-6.107726	-5.608742
C	-0.576135	-6.767341	-4.519434
H	-0.244277	-7.753605	-4.269681
N	-1.451852	-6.084079	-3.852571
C	-1.540529	-4.886036	-4.504404
C	-2.317558	-3.671848	-4.296284
N	-3.180829	-3.591257	-3.323763
H	-3.711702	-2.728890	-3.230076
H	-3.382136	-4.359385	-2.685553
N	-2.144035	-2.640842	-5.086146
C	-1.279090	-2.758034	-6.142105
H	-1.264337	-1.965792	-6.849320
N	-0.512984	-3.932769	-6.490378
C	-0.673672	-4.868599	-5.645626
O	3.119755	-2.279270	-7.322022
C	3.334088	-1.403998	-6.239366
H	3.112370	-0.379923	-6.488945
N	2.499073	-1.809644	-5.169600
C	2.547959	-3.029036	-4.551622
H	3.211702	-3.788429	-4.901216
N	1.747642	-3.128395	-3.563505
C	1.095122	-1.911866	-3.512372
C	0.096001	-1.392773	-2.672173
N	-0.445040	-2.064382	-1.674707
H	-1.172426	-1.643549	-1.128540
H	-0.226049	-3.033738	-1.525331
N	-0.306724	-0.137450	-2.920555
C	0.197838	0.529976	-3.938663
H	-0.196579	1.519841	-4.079730
N	1.113840	0.137694	-4.795780
C	1.537268	-1.094419	-4.519581
H	1.410135	-8.145331	-7.567490
H	1.884605	-6.681144	-6.147429
H	4.039111	-2.307805	-7.906889
H	4.389692	-1.520585	-5.993994

MinLa(1)

O	0.535393	-7.849690	-6.993989

C	0.876556	-6.554109	-6.567384
H	0.891244	-5.836050	-7.374826
N	-0.080843	-6.095156	-5.625947
C	-0.570994	-6.748303	-4.531286
H	-0.243269	-7.736154	-4.282001
N	-1.434010	-6.056889	-3.857202
C	-1.508823	-4.853989	-4.503772
C	-2.320084	-3.658233	-4.327705
N	-3.186878	-3.578623	-3.358925
H	-3.723191	-2.719325	-3.268761
H	-3.360768	-4.333981	-2.697702
N	-2.154460	-2.629444	-5.124942
C	-1.233408	-2.722636	-6.135706
H	-1.235654	-1.943380	-6.860054
N	-0.510306	-3.919720	-6.509494
C	-0.660548	-4.849183	-5.656689
O	3.136796	-2.279141	-7.312051
C	3.353037	-1.400770	-6.232090
H	3.132201	-0.377076	-6.484005
N	2.518213	-1.802939	-5.161036
C	2.566208	-3.021582	-4.541363
H	3.229463	-3.781759	-4.889872
N	1.763760	-3.120197	-3.555066
C	1.110221	-1.904070	-3.506966
C	0.105067	-1.386568	-2.673009
N	-0.439056	-2.057532	-1.676779
H	-1.171280	-1.638131	-1.136008
H	-0.216955	-3.025567	-1.522983
N	-0.301447	-0.133430	-2.926857
C	0.206135	0.533417	-3.943849
H	-0.191029	1.521473	-4.089354
N	1.127785	0.142323	-4.795589
C	1.553712	-1.087725	-4.514703
H	1.407229	-8.140071	-7.580231
H	1.881622	-6.673603	-6.162832
H	4.053848	-2.306978	-7.900558
H	4.409052	-1.518514	-5.989050

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O	0.625258	-7.674387	-7.084245
C	1.011278	-6.396294	-6.646334
H	1.023959	-5.667327	-7.444538
N	0.103328	-5.909947	-5.668556
C	-0.323921	-6.512833	-4.511491
H	0.030915	-7.480777	-4.218146
N	-1.157767	-5.794413	-3.837536
C	-1.264258	-4.619267	-4.523184
C	-2.206839	-3.514263	-4.433694
N	-3.100380	-3.477690	-3.490618
H	-3.716536	-2.672379	-3.447444
H	-3.210252	-4.209483	-2.791200
N	-2.118963	-2.509397	-5.282386
C	-1.099291	-2.563489	-6.191997
H	-1.026952	-1.746050	-6.872546
N	-0.446568	-3.786663	-6.636532
C	-0.492662	-4.672874	-5.724795
O	3.127251	-2.189900	-7.226365
C	3.383829	-1.308367	-6.155087
H	3.117694	-0.290481	-6.391336
N	2.628849	-1.739084	-5.040758
C	2.729737	-2.974252	-4.428636
H	3.422360	-3.706069	-4.781207
N	1.920407	-3.116375	-3.441927
C	1.209547	-1.918838	-3.392954
C	0.171636	-1.455025	-2.572169
N	-0.371366	-2.148328	-1.592630
H	-1.122783	-1.745779	-1.064646
H	-0.118158	-3.107344	-1.425671
N	-0.283770	-0.214620	-2.828566

C	0.209652	0.474984	-3.831313
H	-0.224925	1.447103	-3.977580
N	1.160586	0.130513	-4.671960
C	1.631667	-1.081148	-4.393532
H	1.475850	-7.988442	-7.689192
H	2.023697	-6.551145	-6.273337
H	4.006575	-2.187239	-7.870478
H	4.454408	-1.396806	-5.970319

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O	0.558721	-7.680511	-7.120171
C	0.929197	-6.400192	-6.676097
H	0.946623	-5.672327	-7.474620
N	-0.000586	-5.923418	-5.713021
C	-0.364992	-6.496574	-4.522809
H	-0.000958	-7.461087	-4.230305
N	-1.154608	-5.762689	-3.815555
C	-1.318134	-4.611394	-4.533964
C	-2.204874	-3.490165	-4.386681
N	-3.063866	-3.408443	-3.391689
H	-3.665064	-2.597673	-3.337484
H	-3.168549	-4.129636	-2.685798
N	-2.190205	-2.496237	-5.286402
C	-1.130690	-2.565632	-6.214130
H	-1.078599	-1.754755	-6.904628
N	-0.575459	-3.794434	-6.676216
C	-0.600242	-4.686359	-5.758491
O	3.106030	-2.198142	-7.254881
C	3.354858	-1.325354	-6.175216
H	3.098164	-0.304480	-6.408593
N	2.584716	-1.757066	-5.070684
C	2.692639	-2.980513	-4.441301
H	3.380256	-3.719216	-4.789285
N	1.894952	-3.105599	-3.441291
C	1.189339	-1.906480	-3.400702
C	0.165348	-1.424204	-2.560142
N	-0.339063	-2.102088	-1.548322
H	-1.099698	-1.708121	-1.027207
H	-0.083098	-3.060558	-1.380911
N	-0.296660	-0.198649	-2.832224
C	0.182864	0.482342	-3.859282
H	-0.263545	1.446847	-4.016809
N	1.123758	0.130521	-4.706632
C	1.599187	-1.088867	-4.414813
H	1.418864	-7.990771	-7.713459
H	1.939030	-6.546614	-6.292826
H	3.992755	-2.196611	-7.888771
H	4.423548	-1.417549	-5.981565

40_{La1}

O	0.589219	-7.736863	-7.071186
C	0.955529	-6.439863	-6.670624
H	0.965442	-5.739096	-7.493326
N	0.032057	-5.930942	-5.718678
C	-0.325686	-6.464038	-4.506806
H	0.030170	-7.424886	-4.190800
N	-1.096685	-5.698010	-3.812972
C	-1.240763	-4.561407	-4.558406
C	-2.159182	-3.452540	-4.453436
N	-3.035851	-3.384656	-3.478126
H	-3.663638	-2.593691	-3.441351
H	-3.135217	-4.103886	-2.769394
N	-2.138172	-2.482469	-5.372659
C	-1.019130	-2.559825	-6.216988
H	-0.870498	-1.720769	-6.859240
N	-0.509986	-3.802603	-6.718604
C	-0.534555	-4.679824	-5.785958
O	3.197373	-2.270102	-7.285892
C	3.443288	-1.387629	-6.213323

H	3.200600	-0.366549	-6.460193
N	2.658449	-1.792841	-5.107466
C	2.740931	-2.994150	-4.468910
H	3.425027	-3.742874	-4.804613
N	1.941778	-3.112169	-3.479646
C	1.248840	-1.913638	-3.444956
C	0.211107	-1.415535	-2.612041
N	-0.306101	-2.102922	-1.613234
H	-1.067031	-1.710087	-1.091608
H	-0.051706	-3.060935	-1.443623
N	-0.230075	-0.194290	-2.886453
C	0.260827	0.489978	-3.921160
H	-0.177396	1.457675	-4.077548
N	1.195305	0.122969	-4.762619
C	1.667797	-1.097073	-4.458921
H	1.443001	-8.047006	-7.673653
H	1.968022	-6.571091	-6.288871
H	4.084341	-2.260576	-7.919371
H	4.509578	-1.490637	-6.012040

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O	0.695151	-7.758250	-7.024690
C	1.029741	-6.443629	-6.650590
H	1.014547	-5.758817	-7.486564
N	0.101866	-5.941430	-5.698530
C	-0.221838	-6.456589	-4.465172
H	0.169729	-7.396367	-4.130088
N	-1.006233	-5.698891	-3.781108
C	-1.193248	-4.581601	-4.545459
C	-2.192024	-3.520602	-4.466078
N	-3.079872	-3.505647	-3.502204
H	-3.747046	-2.748846	-3.471385
H	-3.133836	-4.212537	-2.778510
N	-2.193311	-2.568868	-5.390507
C	-1.028173	-2.622497	-6.156282
H	-0.755469	-1.729057	-6.673508
N	-0.527222	-3.844508	-6.728486
C	-0.500087	-4.710311	-5.783724
O	3.017706	-2.208165	-7.146159
C	3.308001	-1.322012	-6.086850
H	3.067982	-0.300199	-6.334093
N	2.555395	-1.710394	-4.955325
C	2.650852	-2.899628	-4.292935
H	3.356082	-3.639231	-4.604933
N	1.837710	-3.019130	-3.316091
C	1.117539	-1.835173	-3.318595
C	0.047386	-1.345218	-2.523072
N	-0.484947	-2.021279	-1.525372
H	-1.267965	-1.633307	-1.034542
H	-0.234810	-2.978835	-1.342791
N	-0.409309	-0.137583	-2.830067
C	0.088944	0.540449	-3.863977
H	-0.364174	1.496968	-4.044429
N	1.046736	0.176038	-4.679904
C	1.537045	-1.027566	-4.339918
H	1.555937	-8.064711	-7.619020
H	2.048107	-6.543848	-6.275110
H	3.881111	-2.207996	-7.811464
H	4.379120	-1.433132	-5.918164

55_{La1}

O	0.632406	-7.699641	-7.173670
C	1.050803	-6.465182	-6.647132
H	1.158542	-5.703900	-7.407166
N	0.100263	-5.976351	-5.715939
C	-0.344627	-6.561255	-4.563056
H	-0.002370	-7.536929	-4.271560
N	-1.166635	-5.844366	-3.881304
C	-1.292329	-4.663846	-4.581006

C	-2.292291	-3.590917	-4.495835
N	-3.231801	-3.604457	-3.584561
H	-3.850290	-2.814968	-3.520085
H	-3.286881	-4.303108	-2.860665
N	-2.131674	-2.591236	-5.323324
C	-0.947651	-2.718005	-5.987962
H	-0.161776	-2.021233	-5.794472
N	-0.573177	-3.878636	-6.743754
C	-0.529767	-4.749493	-5.807381
O	3.085818	-2.173515	-7.101834
C	3.395675	-1.307916	-6.030773
H	3.149073	-0.282970	-6.255829
N	2.652433	-1.723111	-4.900719
C	2.763953	-2.937662	-4.249568
H	3.455777	-3.685528	-4.574135
N	1.943306	-3.049509	-3.241784
C	1.241391	-1.843699	-3.236463
C	0.169567	-1.368547	-2.463484
N	-0.392716	-2.043944	-1.482658
H	-1.199542	-1.668346	-1.020984
H	-0.149619	-3.008888	-1.332304
N	-0.296300	-0.145468	-2.772284
C	0.212534	0.519508	-3.783951
H	-0.230784	1.480175	-3.971547
N	1.181292	0.154640	-4.595923
C	1.668611	-1.038109	-4.259857
H	1.505363	-8.040581	-7.730271
H	2.027108	-6.691844	-6.218703
H	3.953228	-2.198543	-7.761435
H	4.468495	-1.418491	-5.872884

La(1)/GS CI

O	0.675684	-7.751748	-7.299942
O	2.970070	-2.055801	-7.109654
N	0.097466	-6.043197	-5.779367
N	-0.989482	-5.763575	-3.838889
N	-3.141319	-3.601157	-3.568411
N	-2.175781	-2.700590	-5.478801
N	-0.629079	-3.968757	-6.840922
N	2.627706	-1.608904	-4.836431
N	1.879907	-2.911147	-3.180703
N	-0.555976	-1.940358	-1.517501
N	-0.461424	-0.083287	-2.849642
N	1.060925	0.228621	-4.640958
C	1.038662	-6.510384	-6.751645
C	-0.213939	-6.529017	-4.526330
C	-1.220877	-4.673874	-4.630434
C	-2.226759	-3.616547	-4.532126
C	-0.957601	-2.793184	-6.125072
C	-0.548867	-4.833344	-5.880128
C	3.336596	-1.235080	-6.014147
C	2.730008	-2.789935	-4.131238
C	1.126535	-1.748501	-3.246885
C	0.016823	-1.282395	-2.505083
C	0.061879	0.587092	-3.863644
C	1.572076	-0.948658	-4.267333
H	1.093414	-5.745854	-7.513187
H	0.185337	-7.457610	-4.173654
H	-3.791419	-2.840015	-3.537332
H	-3.207978	-4.290145	-2.839881
H	-0.145317	-2.194575	-5.766408
H	3.130894	-0.197801	-6.221987
H	3.473391	-3.514413	-4.387573
H	-1.379758	-1.554254	-1.097896
H	-0.354703	-2.910456	-1.331653
H	-0.397306	1.534280	-4.077872
H	1.436322	-8.020646	-7.795857
H	2.037051	-6.696298	-6.355723

H	3.700682	-2.072409	-7.711932
H	4.407846	-1.392446	-5.888613

0_{La2}

O	0.476003	-7.727571	-7.091953
C	0.850336	-6.462423	-6.611698
H	0.873110	-5.712151	-7.388243
N	-0.081991	-6.019816	-5.630751
C	-0.488978	-6.666639	-4.502623
H	-0.101836	-7.627850	-4.236691
N	-1.353637	-5.998588	-3.824195
C	-1.531808	-4.824538	-4.533985
C	-2.292983	-3.653649	-4.298508
N	-3.077379	-3.482756	-3.251484
H	-3.648109	-2.659505	-3.208733
H	-3.289545	-4.223966	-2.607193
N	-2.170555	-2.664390	-5.180738
C	-1.376037	-2.808155	-6.235337
H	-1.330491	-1.962519	-6.896219
N	-0.646741	-3.850118	-6.566067
C	-0.752395	-4.833622	-5.652136
O	2.968659	-2.203856	-7.330698
C	3.181855	-1.301088	-6.267261
H	2.956982	-0.282296	-6.538777
N	2.347214	-1.681793	-5.192234
C	2.406019	-2.879582	-4.529808
H	3.060884	-3.657145	-4.862242
N	1.626580	-2.951549	-3.513866
C	0.977062	-1.751620	-3.470247
C	-0.023076	-1.205672	-2.613843
N	-0.517292	-1.894475	-1.597544
H	-1.263490	-1.487868	-1.045496
H	-0.275910	-2.871535	-1.449579
N	-0.484958	0.033547	-2.817555
C	0.032986	0.751049	-3.920704
H	-0.153298	1.797562	-3.924708
N	0.996228	0.257098	-4.816885
C	1.402416	-0.918917	-4.542888
H	1.336227	-8.027255	-7.690538
H	1.858028	-6.622674	-6.228325
H	3.881705	-2.222022	-7.925775
H	4.237259	-1.413734	-6.019203

$MinL_a(2)$

O	0.484384	-7.709813	-7.130475
C	0.871234	-6.458767	-6.624369
H	0.914599	-5.695890	-7.387484
N	-0.065682	-6.019981	-5.646899
C	-0.474237	-6.668020	-4.519632
H	-0.084163	-7.627617	-4.250603
N	-1.343736	-6.003720	-3.844567
C	-1.525516	-4.831675	-4.556403
C	-2.292824	-3.664589	-4.324055
N	-3.073382	-3.494109	-3.274119
H	-3.651064	-2.675680	-3.234214
H	-3.280879	-4.235233	-2.627832
N	-2.178192	-2.678049	-5.210246
C	-1.379889	-2.818774	-6.262347
H	-1.339029	-1.974540	-6.925343
N	-0.641384	-3.855765	-6.588275
C	-0.743317	-4.838129	-5.672595
O	2.965748	-2.155347	-7.329711
C	3.180001	-1.249514	-6.268713
H	2.954186	-0.231016	-6.541011
N	2.346886	-1.631220	-5.192094
C	2.389572	-2.841679	-4.552500
H	3.055795	-3.611639	-4.880760
N	1.578965	-2.936148	-3.563199
C	0.914807	-1.743765	-3.524595

C	-0.055307	-1.189496	-2.639379
N	-0.530979	-1.873898	-1.611292
H	-1.264074	-1.463014	-1.045740
H	-0.311904	-2.859235	-1.486774
N	-0.494198	0.063174	-2.817954
C	-0.055399	0.748336	-3.975917
H	-0.248404	1.796384	-3.980008
N	0.965959	0.290901	-4.832221
C	1.369569	-0.889105	-4.566737
H	1.349067	-8.017877	-7.718283
H	1.871518	-6.640903	-6.231485
H	3.878891	-2.180126	-7.924400
H	4.235723	-1.362237	-6.022049

13_{La2}

O	0.459909	-7.767580	-7.127615
C	0.863558	-6.512852	-6.640404
H	0.903636	-5.759922	-7.414021
N	-0.057444	-6.055425	-5.658407
C	-0.455549	-6.688864	-4.526953
H	-0.064179	-7.646979	-4.258562
N	-1.320081	-6.025650	-3.841434
C	-1.513338	-4.855356	-4.560037
C	-2.283445	-3.684266	-4.324374
N	-3.053602	-3.520583	-3.264177
H	-3.630421	-2.702164	-3.212762
H	-3.259126	-4.270411	-2.627465
N	-2.174716	-2.707336	-5.210162
C	-1.378910	-2.844840	-6.273939
H	-1.342900	-1.998919	-6.934213
N	-0.647616	-3.882526	-6.603092
C	-0.741492	-4.864657	-5.686754
O	3.105441	-2.358966	-7.408534
C	3.303407	-1.482163	-6.319968
H	3.093258	-0.457179	-6.580780
N	2.444369	-1.861422	-5.270436
C	2.480217	-3.063039	-4.585075
H	3.146850	-3.838714	-4.894971
N	1.667182	-3.133174	-3.601147
C	0.980328	-1.951977	-3.598900
C	0.072924	-1.348755	-2.642459
N	-0.361963	-2.009995	-1.615132
H	-1.060541	-1.581439	-1.023456
H	-0.161469	-2.997188	-1.493831
N	-0.315076	-0.100445	-2.857124
C	0.057973	0.498935	-4.005770
H	-0.335823	1.472884	-4.184520
N	1.078556	0.080968	-4.975434
C	1.462847	-1.091115	-4.685829
H	1.312656	-8.086712	-7.726844
H	1.867665	-6.699545	-6.259598
H	4.026889	-2.354081	-7.990779
H	4.354915	-1.601611	-6.058888

24_{La2}

O	0.491635	-7.673182	-7.188014
C	0.901427	-6.450891	-6.629910
H	0.984346	-5.664416	-7.365314
N	-0.043212	-6.016734	-5.660480
C	-0.438229	-6.653981	-4.521462
H	-0.033028	-7.603905	-4.238118
N	-1.313855	-5.994535	-3.851179
C	-1.518029	-4.838762	-4.580256
C	-2.299422	-3.681142	-4.352298
N	-3.075250	-3.521501	-3.298480
H	-3.661194	-2.710097	-3.245471
H	-3.242865	-4.258189	-2.636460
N	-2.204400	-2.701553	-5.247432
C	-1.408982	-2.840414	-6.302157

H	-1.381244	-2.000198	-6.970792
N	-0.657669	-3.869866	-6.623888
C	-0.741784	-4.846267	-5.699837
O	2.953542	-2.115222	-7.333161
C	3.173105	-1.223622	-6.260264
H	2.943504	-0.202533	-6.519940
N	2.344096	-1.619794	-5.186631
C	2.399675	-2.830932	-4.546837
H	3.083842	-3.589512	-4.865373
N	1.575233	-2.942155	-3.571651
C	0.879192	-1.766826	-3.549024
C	-0.055850	-1.205969	-2.627261
N	-0.485927	-1.886868	-1.578901
H	-1.198713	-1.480650	-0.986618
H	-0.265897	-2.874127	-1.474863
N	-0.484611	0.052730	-2.791259
C	-0.170249	0.662937	-4.026582
H	-0.460342	1.687203	-4.098842
N	0.915207	0.273260	-4.846231
C	1.335897	-0.900878	-4.582356
H	1.363034	-7.996035	-7.757688
H	1.887907	-6.675103	-6.224095
H	3.867308	-2.150982	-7.926332
H	4.231050	-1.334769	-6.022571

32_{La2}

O	0.491169	-7.660882	-7.217081
C	0.898889	-6.436480	-6.662797
H	0.979387	-5.651346	-7.399895
N	-0.046085	-6.003147	-5.692410
C	-0.438094	-6.641194	-4.552851
H	-0.032164	-7.591783	-4.272360
N	-1.311382	-5.982161	-3.878861
C	-1.517666	-4.825586	-4.606968
C	-2.295625	-3.666839	-4.376781
N	-3.052291	-3.494789	-3.307794
H	-3.654434	-2.693860	-3.271716
H	-3.235185	-4.237177	-2.655707
N	-2.213615	-2.692318	-5.277085
C	-1.420728	-2.830577	-6.333918
H	-1.396138	-1.991025	-7.003310
N	-0.667805	-3.858737	-6.655496
C	-0.745468	-4.833588	-5.729975
O	2.931815	-2.089937	-7.347256
C	3.152051	-1.198619	-6.272632
H	2.922416	-0.177362	-6.531986
N	2.324501	-1.594400	-5.198641
C	2.379617	-2.810565	-4.562571
H	3.075457	-3.561338	-4.873894
N	1.540921	-2.933609	-3.606196
C	0.826295	-1.761410	-3.597436
C	-0.081401	-1.182266	-2.671692
N	-0.479552	-1.875526	-1.597394
H	-1.167350	-1.459417	-0.970163
H	-0.253567	-2.870511	-1.501068
N	-0.497186	0.061937	-2.821743
C	-0.257648	0.628435	-4.085302
H	-0.574668	1.645494	-4.171768
N	0.874729	0.290842	-4.873561
C	1.296051	-0.887685	-4.613472
H	1.363113	-7.985540	-7.784892
H	1.885998	-6.657635	-6.256836
H	3.846021	-2.126950	-7.939672
H	4.209994	-1.310750	-6.035392

40_{La2}

O	0.505519	-7.677268	-7.180465
C	0.908172	-6.449174	-6.631201
H	0.990741	-5.668121	-7.372459

N	-0.040931	-6.011844	-5.666730
C	-0.442465	-6.649226	-4.529839
H	-0.037440	-7.598703	-4.244065
N	-1.322983	-5.991511	-3.865148
C	-1.525681	-4.836973	-4.597109
C	-2.314692	-3.683133	-4.377121
N	-3.091923	-3.522304	-3.324389
H	-3.682720	-2.714149	-3.276499
H	-3.252930	-4.256265	-2.657431
N	-2.227078	-2.708132	-5.278369
C	-1.421386	-2.844788	-6.325784
H	-1.396223	-2.007269	-6.997852
N	-0.658289	-3.868384	-6.637970
C	-0.742366	-4.843841	-5.712149
O	2.956323	-2.092605	-7.321539
C	3.180303	-1.200173	-6.250499
H	2.952840	-0.178500	-6.510485
N	2.351815	-1.594232	-5.174623
C	2.400309	-2.812307	-4.542551
H	3.099611	-3.562547	-4.849494
N	1.548193	-2.941594	-3.595273
C	0.826857	-1.779883	-3.593307
C	-0.055755	-1.199624	-2.617884
N	-0.424132	-1.872224	-1.548180
H	-1.097090	-1.458387	-0.920889
H	-0.218756	-2.862918	-1.454137
N	-0.463925	0.066336	-2.772301
C	-0.282161	0.552677	-4.075729
H	-0.717785	1.511903	-4.252944
N	0.878139	0.275838	-4.859284
C	1.308598	-0.897850	-4.609348
H	1.380249	-8.000573	-7.744752
H	1.893411	-6.667050	-6.218972
H	3.869837	-2.132391	-7.914842
H	4.238108	-1.314144	-6.013519

48_{La2}

O	0.481639	-7.701596	-7.099935
C	0.844789	-6.436004	-6.612840
H	0.868123	-5.683615	-7.387308
N	-0.096386	-6.000507	-5.637822
C	-0.491658	-6.639416	-4.499721
H	-0.084810	-7.588519	-4.219777
N	-1.371453	-5.980176	-3.832975
C	-1.575537	-4.823020	-4.562369
C	-2.365004	-3.667995	-4.346863
N	-3.142216	-3.494139	-3.295192
H	-3.734141	-2.685763	-3.264567
H	-3.328161	-4.226469	-2.632749
N	-2.276289	-2.696220	-5.251255
C	-1.469698	-2.833004	-6.297088
H	-1.443040	-1.996086	-6.969794
N	-0.707449	-3.857790	-6.606210
C	-0.794073	-4.831112	-5.679088
O	2.910745	-2.096476	-7.248344
C	3.153860	-1.186555	-6.194935
H	2.945442	-0.165268	-6.471661
N	2.325670	-1.546506	-5.108222
C	2.330172	-2.773704	-4.492280
H	3.029357	-3.529795	-4.784706
N	1.445453	-2.901753	-3.575948
C	0.741888	-1.728501	-3.582886
C	-0.142105	-1.132729	-2.611096
N	-0.541292	-1.796663	-1.550236
H	-1.217341	-1.364380	-0.935133
H	-0.360703	-2.791478	-1.449063
N	-0.509214	0.145772	-2.772065
C	-0.355800	0.561874	-4.096337
H	-0.836809	1.489021	-4.326561

N	0.845838	0.328398	-4.841905
C	1.265047	-0.846782	-4.582485
H	1.348447	-7.996398	-7.691403
H	1.850868	-6.591350	-6.223262
H	3.813604	-2.137420	-7.857663
H	4.210063	-1.320444	-5.961251

55_{La2}

O	0.429018	-7.766388	-7.059160
C	0.804949	-6.495561	-6.591198
H	0.832561	-5.755433	-7.377629
N	-0.128059	-6.036196	-5.620307
C	-0.519876	-6.657444	-4.472596
H	-0.114889	-7.603803	-4.182426
N	-1.394737	-5.986839	-3.810966
C	-1.598452	-4.839263	-4.555510
C	-2.384338	-3.680734	-4.350674
N	-3.151374	-3.493621	-3.293315
H	-3.745954	-2.687079	-3.269272
H	-3.344903	-4.226231	-2.633249
N	-2.299899	-2.720718	-5.267417
C	-1.493203	-2.869733	-6.311566
H	-1.464179	-2.039513	-6.992449
N	-0.733459	-3.899555	-6.611570
C	-0.821001	-4.863620	-5.674837
O	3.026298	-2.229725	-7.335031
C	3.243799	-1.327018	-6.269893
H	3.041733	-0.304017	-6.546361
N	2.388936	-1.685226	-5.204161
C	2.376696	-2.903469	-4.567992
H	3.070816	-3.669970	-4.848647
N	1.485794	-3.005506	-3.653065
C	0.777521	-1.833652	-3.697161
C	0.001247	-1.168476	-2.649142
N	-0.348158	-1.814707	-1.578494
H	-0.969263	-1.352951	-0.928269
H	-0.200998	-2.815338	-1.477339
N	-0.348382	0.098131	-2.833818
C	-0.274084	0.421567	-4.153204
H	-0.830104	1.283659	-4.456508
N	0.958156	0.226166	-4.924176
C	1.330743	-0.965347	-4.701969
H	1.287967	-8.068451	-7.658378
H	1.810232	-6.656510	-6.201838
H	3.942215	-2.256439	-7.925355
H	4.295597	-1.458489	-6.015853

$L_a(2)$/GS CI

O	0.593286	-7.739514	-6.975004
O	3.055139	-2.169302	-6.801717
N	-0.045625	-5.989670	-5.600161
N	-1.340043	-5.951485	-3.806055
N	-3.152168	-3.476674	-3.319080
N	-2.293093	-2.705575	-5.289113
N	-0.703573	-3.871747	-6.623146
N	2.761885	-1.555882	-4.601859
N	1.962242	-2.891528	-3.001866
N	-0.282530	-1.891704	-1.129193
N	-0.603027	-0.300123	-2.802336
N	0.995465	0.109491	-4.578038
C	0.913840	-6.435889	-6.552111
C	-0.439832	-6.603223	-4.456644
C	-1.565204	-4.810750	-4.562259
C	-2.374233	-3.653037	-4.367371
C	-1.477385	-2.854533	-6.338873
C	-0.774803	-4.827940	-5.676657
C	3.444890	-1.246220	-5.803914
C	2.904325	-2.697158	-3.852631
C	1.090564	-1.852520	-3.170466

C	-0.010955	-1.351953	-2.326206
C	-0.300684	-0.196057	-4.153884
C	1.581556	-0.984059	-4.203228
H	0.906616	-5.723844	-7.364381
H	-0.017749	-7.537067	-4.150493
H	-3.727061	-2.656218	-3.276530
H	-3.314096	-4.194206	-2.634344
H	-1.454638	-2.026388	-7.022392
H	3.209575	-0.230105	-6.080900
H	3.743701	-3.350547	-3.984642
H	-1.145399	-1.589606	-0.716006
H	-0.070589	-2.865799	-1.010157
H	-0.896718	-0.789230	-4.800337
H	1.347972	-7.984089	-7.492150
H	1.927202	-6.540353	-6.164446
H	3.754355	-2.190920	-7.440026
H	4.522917	-1.380473	-5.714842

0_{CT12}

O	0.470918	-7.715435	-6.973295
C	0.904855	-6.473247	-6.483840
H	0.976694	-5.720440	-7.255758
N	-0.018099	-5.990725	-5.508741
C	-0.463511	-6.621279	-4.386589
H	-0.105006	-7.598069	-4.121600
N	-1.340604	-5.948016	-3.703059
C	-1.465870	-4.781441	-4.360385
C	-2.292098	-3.615984	-4.147714
N	-3.116746	-3.489804	-3.170476
H	-3.599520	-2.608349	-3.040340
H	-3.147511	-4.150742	-2.399336
N	-2.177428	-2.627028	-5.069965
C	-1.354555	-2.729856	-6.054014
H	-1.238343	-1.862408	-6.688006
N	-0.591022	-3.830443	-6.416086
C	-0.653602	-4.773953	-5.540159
O	2.915124	-2.297257	-7.246007
C	3.102340	-1.426371	-6.140615
H	2.850231	-0.405616	-6.377849
N	2.262582	-1.864263	-5.099220
C	2.312712	-3.095368	-4.490444
H	2.998975	-3.842643	-4.810990
N	1.475027	-3.190878	-3.526716
C	0.825815	-1.975768	-3.472882
C	-0.145427	-1.415608	-2.568935
N	-0.797547	-2.184354	-1.626866
H	-1.217082	-1.651063	-0.893414
H	-0.303496	-2.994078	-1.307659
N	-0.491494	-0.163190	-2.760968
C	0.034206	0.566197	-3.764047
H	-0.249567	1.589612	-3.809241
N	0.968773	0.120597	-4.690149
C	1.312321	-1.122854	-4.435524
H	1.317412	-8.054598	-7.570385
H	1.900906	-6.689313	-6.097451
H	3.843599	-2.318755	-7.816596
H	4.158923	-1.516122	-5.888274

11_{CT12}

O	0.483115	-7.679610	-7.039552
C	0.937421	-6.450061	-6.537390
H	1.017189	-5.686485	-7.297817
N	0.023967	-5.972340	-5.549358
C	-0.399364	-6.618381	-4.403854
H	-0.000663	-7.581174	-4.140502
N	-1.285849	-5.969060	-3.726891
C	-1.449540	-4.805634	-4.401180
C	-2.316476	-3.666954	-4.200760
N	-3.129544	-3.565744	-3.209837

H	-3.636084	-2.695845	-3.080285
H	-3.124254	-4.214515	-2.427130
N	-2.241777	-2.695123	-5.134306
C	-1.408408	-2.797530	-6.123139
H	-1.335673	-1.936716	-6.770417
N	-0.620908	-3.849727	-6.472704
C	-0.635722	-4.793560	-5.587712
O	2.867578	-2.271980	-7.289403
C	3.042712	-1.392214	-6.189939
H	2.804592	-0.370720	-6.438241
N	2.179248	-1.821907	-5.163950
C	2.171693	-3.076391	-4.602157
H	2.837443	-3.833263	-4.945245
N	1.315166	-3.179976	-3.653039
C	0.718743	-1.938201	-3.556963
C	-0.209499	-1.365664	-2.632680
N	-0.867050	-2.126461	-1.693813
H	-1.280679	-1.590401	-0.959955
H	-0.397429	-2.953778	-1.383983
N	-0.456728	-0.084430	-2.741403
C	0.022470	0.638060	-3.783162
H	-0.199103	1.675496	-3.775124
N	0.963496	0.197662	-4.690868
C	1.249713	-1.070475	-4.487785
H	1.325749	-8.034795	-7.632773
H	1.929421	-6.689513	-6.154379
H	3.800944	-2.293894	-7.851939
H	4.094120	-1.491977	-5.920332

$MinCT_{12}$

O	0.46741600	-7.62631400	-6.90486500
C	0.91987700	-6.37031500	-6.46920200
H	0.95528800	-5.63703300	-7.26242200
N	0.03713400	-5.86022100	-5.46742800
C	-0.30650000	-6.43791300	-4.26499400
H	0.12926900	-7.37086700	-3.95764400
N	-1.16965800	-5.76084000	-3.57888900
C	-1.40444700	-4.65337800	-4.31745200
C	-2.27878600	-3.51085200	-4.14023100
N	-3.05200400	-3.36663400	-3.12228100
H	-3.60211200	-2.51867500	-3.03389600
H	-3.07248200	-4.02392400	-2.34705600
N	-2.25724500	-2.59098000	-5.12284100
C	-1.44591200	-2.72028500	-6.12690200
H	-1.39697500	-1.88398100	-6.80713500
N	-0.65938500	-3.78239700	-6.45609800
C	-0.63962600	-4.68915500	-5.53515300
O	2.94161700	-2.36362800	-7.34982800
C	3.07658000	-1.45111500	-6.26703700
H	2.83122600	-0.44223800	-6.55805400
N	2.20034700	-1.84755500	-5.24766400
C	2.28296000	-3.02320000	-4.53053400
H	2.99699900	-3.76863600	-4.79760800
N	1.45510100	-3.09200100	-3.56827700
C	0.72850300	-1.90658400	-3.61332100
C	-0.11403700	-1.27204800	-2.66798200
N	-0.53968200	-1.92480600	-1.57243800
H	-1.09388800	-1.41800400	-0.91468200
H	-0.16371100	-2.81594000	-1.31756500
N	-0.52226200	-0.05592200	-2.88729700
C	-0.17132700	0.58963000	-4.06051400
H	-0.34142600	1.64026400	-4.08362700
N	0.85488800	0.12276800	-4.95117100
C	1.21363800	-1.07538100	-4.63938100
H	1.28578673	-7.97296913	-7.53589556
H	1.93169811	-6.57733427	-6.12068935
H	3.87806016	-2.35095444	-7.90751392
H	4.12617390	-1.52344553	-5.98204411

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O	0.474724	-7.608863	-6.879247
C	0.918965	-6.350281	-6.448487
H	0.938939	-5.618367	-7.242884
N	0.041696	-5.837474	-5.439095
C	-0.249158	-6.362219	-4.218964
H	0.204044	-7.275207	-3.875396
N	-1.107732	-5.652355	-3.522973
C	-1.354814	-4.576404	-4.283659
C	-2.256850	-3.452390	-4.150076
N	-3.039370	-3.298140	-3.138703
H	-3.609667	-2.461538	-3.069802
H	-3.066706	-3.950664	-2.359548
N	-2.244377	-2.555219	-5.154570
C	-1.462295	-2.717855	-6.174911
H	-1.420357	-1.902773	-6.877634
N	-0.708948	-3.806804	-6.489925
C	-0.651278	-4.664678	-5.525905
O	2.910321	-2.292603	-7.223848
C	3.101412	-1.364929	-6.163806
H	2.838917	-0.359978	-6.455609
N	2.285522	-1.737974	-5.084606
C	2.403821	-2.900038	-4.354383
H	3.164471	-3.614769	-4.571915
N	1.532122	-3.005053	-3.434177
C	0.750840	-1.858162	-3.536695
C	-0.157036	-1.246685	-2.626937
N	-0.575111	-1.910067	-1.525893
H	-1.130895	-1.398563	-0.872142
H	-0.107750	-2.739218	-1.219208
N	-0.596336	-0.056057	-2.877566
C	-0.312986	0.524062	-4.114083
H	-0.521808	1.571976	-4.146520
N	0.797461	0.144662	-4.901833
C	1.229734	-1.022265	-4.539972
H	1.288966	-7.939909	-7.523854
H	1.936878	-6.544617	-6.110573
H	3.817736	-2.282885	-7.827671
H	4.163417	-1.436696	-5.929086

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O	0.486230	-7.596222	-6.911488
C	0.928428	-6.340326	-6.471947
H	0.949269	-5.602446	-7.260857
N	0.047698	-5.838686	-5.460892
C	-0.243888	-6.388557	-4.238429
H	0.227430	-7.298690	-3.917323
N	-1.105198	-5.715988	-3.538639
C	-1.383342	-4.625361	-4.296730
C	-2.277305	-3.494788	-4.130504
N	-3.047711	-3.348899	-3.112305
H	-3.615873	-2.511070	-3.032448
H	-3.072845	-4.010483	-2.340339
N	-2.271451	-2.588519	-5.126379
C	-1.491908	-2.737263	-6.151861
H	-1.451809	-1.908051	-6.841042
N	-0.741485	-3.820519	-6.493635
C	-0.657952	-4.682026	-5.536235
O	2.927258	-2.267063	-7.226300
C	3.126524	-1.348892	-6.160148
H	2.863776	-0.341214	-6.441411
N	2.316522	-1.731268	-5.079439
C	2.420561	-2.912519	-4.380205
H	3.191267	-3.617083	-4.596662
N	1.525011	-3.049747	-3.487957
C	0.730972	-1.907824	-3.583528
C	-0.157593	-1.301478	-2.649376
N	-0.545064	-1.966454	-1.537494
H	-1.082302	-1.451963	-0.870577

H	-0.054520	-2.782118	-1.234175
N	-0.587088	-0.103935	-2.882194
C	-0.362467	0.438279	-4.148995
H	-0.629443	1.472319	-4.209816
N	0.784524	0.118631	-4.910343
C	1.231848	-1.044642	-4.557232
H	1.302955	-7.925767	-7.553718
H	1.945431	-6.535473	-6.131768
H	3.832697	-2.260259	-7.833123
H	4.189644	-1.424439	-5.931743

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O	0.418116	-7.573985	-6.955599
C	0.839310	-6.308902	-6.518911
H	0.872404	-5.577773	-7.314105
N	-0.071037	-5.815967	-5.532663
C	-0.498010	-6.446666	-4.384489
H	-0.122634	-7.417235	-4.117425
N	-1.374668	-5.778293	-3.703904
C	-1.513308	-4.619020	-4.377546
C	-2.352142	-3.455716	-4.172987
N	-3.108943	-3.305672	-3.142219
H	-3.645927	-2.450872	-3.037246
H	-3.136334	-3.977936	-2.379996
N	-2.308638	-2.519051	-5.136739
C	-1.488186	-2.636851	-6.136683
H	-1.420739	-1.784658	-6.795574
N	-0.722843	-3.708145	-6.482058
C	-0.714832	-4.625370	-5.572065
O	2.900585	-2.219232	-7.252054
C	3.089575	-1.291868	-6.191740
H	2.831861	-0.285870	-6.483628
N	2.270504	-1.665619	-5.115837
C	2.365818	-2.851310	-4.420810
H	3.126274	-3.564031	-4.648423
N	1.475742	-2.981386	-3.523445
C	0.693287	-1.831013	-3.607575
C	-0.156918	-1.211796	-2.644540
N	-0.477209	-1.845446	-1.500273
H	-1.118797	-1.396823	-0.882127
H	-0.166832	-2.776545	-1.312708
N	-0.558840	-0.000356	-2.867081
C	-0.416197	0.474863	-4.172456
H	-0.727160	1.495443	-4.268530
N	0.737565	0.190806	-4.939826
C	1.190242	-0.974267	-4.592079
H	1.253951	-7.907553	-7.570587
H	1.848724	-6.490446	-6.149826
H	3.814718	-2.227093	-7.845686
H	4.149735	-1.367744	-5.950074

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O	0.471599	-7.591963	-6.923653
C	0.902143	-6.334058	-6.478733
H	0.923793	-5.593938	-7.265543
N	0.009519	-5.842964	-5.472912
C	-0.306009	-6.415944	-4.267386
H	0.155320	-7.335878	-3.959458
N	-1.178987	-5.756527	-3.569994
C	-1.441797	-4.650250	-4.312511
C	-2.339464	-3.521904	-4.144734
N	-3.118136	-3.381742	-3.132374
H	-3.688324	-2.545103	-3.054252
H	-3.149812	-4.047041	-2.363739
N	-2.326863	-2.607225	-5.133308
C	-1.534930	-2.742096	-6.151164
H	-1.493136	-1.907319	-6.833675
N	-0.773222	-3.817073	-6.491232
C	-0.697113	-4.687513	-5.542187

O	2.902719	-2.200055	-7.220951
C	3.109225	-1.282412	-6.155298
H	2.851591	-0.272549	-6.432543
N	2.298618	-1.668223	-5.075043
C	2.360961	-2.884137	-4.434341
H	3.127679	-3.589361	-4.664682
N	1.439386	-3.049339	-3.574085
C	0.663429	-1.890386	-3.634744
C	-0.200084	-1.298993	-2.663342
N	-0.595065	-1.982056	-1.568083
H	-1.108330	-1.463030	-0.885259
H	-0.114087	-2.809367	-1.278085
N	-0.550723	-0.063279	-2.841141
C	-0.426163	0.409235	-4.153174
H	-0.776388	1.416974	-4.250763
N	0.771478	0.190211	-4.875880
C	1.204212	-0.991872	-4.560386
H	1.295424	-7.916070	-7.559552
H	1.917515	-6.523160	-6.130367
H	3.810073	-2.211691	-7.824832
H	4.171501	-1.367851	-5.926454

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O	0.469153	-7.592883	-6.914242
C	0.890877	-6.327373	-6.482676
H	0.901986	-5.593514	-7.275556
N	-0.001752	-5.836739	-5.476039
C	-0.330302	-6.422582	-4.280265
H	0.121126	-7.351158	-3.983303
N	-1.204163	-5.766366	-3.581013
C	-1.454674	-4.648577	-4.312035
C	-2.345451	-3.516717	-4.136357
N	-3.119555	-3.375086	-3.119739
H	-3.691695	-2.539816	-3.041501
H	-3.161099	-4.048155	-2.358126
N	-2.332090	-2.597230	-5.120689
C	-1.540139	-2.727806	-6.139235
H	-1.499842	-1.891107	-6.819686
N	-0.775422	-3.800372	-6.480475
C	-0.703795	-4.678570	-5.538408
O	2.896390	-2.226311	-7.238681
C	3.086725	-1.296403	-6.181130
H	2.823450	-0.291186	-6.471508
N	2.271851	-1.674362	-5.101587
C	2.344285	-2.876291	-4.436362
H	3.105673	-3.588512	-4.664274
N	1.437799	-3.021206	-3.557081
C	0.662787	-1.861971	-3.624869
C	-0.178710	-1.256774	-2.637355
N	-0.535109	-1.905737	-1.523815
H	-1.090396	-1.406195	-0.860654
H	-0.114709	-2.775065	-1.265128
N	-0.516051	-0.014147	-2.845926
C	-0.459893	0.366899	-4.191797
H	-0.867235	1.348784	-4.334627
N	0.747127	0.192234	-4.909649
C	1.188117	-0.984882	-4.581839
H	1.292622	-7.914515	-7.551856
H	1.909185	-6.504218	-6.136449
H	3.806261	-2.227389	-7.838875
H	4.147982	-1.369858	-5.943564

0_{CT21}

O	0.582749	-7.905744	-7.011955
C	0.871255	-6.573424	-6.658289
H	0.769055	-5.891048	-7.489130
N	-0.020778	-6.128193	-5.646600
C	-0.502755	-6.813975	-4.570724
H	-0.215510	-7.822502	-4.378363

N	-1.310530	-6.113167	-3.857102
C	-1.375951	-4.876785	-4.492762
C	-2.041104	-3.639116	-4.192845
N	-2.833587	-3.478455	-3.092271
H	-3.479667	-2.716035	-3.144511
H	-3.232626	-4.301296	-2.682233
N	-1.781235	-2.597406	-4.947029
C	-0.923744	-2.698344	-6.031426
H	-1.016613	-1.934033	-6.762594
N	-0.277707	-3.870108	-6.413580
C	-0.561060	-4.865940	-5.596717
O	3.009222	-2.456267	-7.381479
C	3.173702	-1.548528	-6.325737
H	2.941954	-0.530952	-6.611152
N	2.320850	-1.948984	-5.262318
C	2.317473	-3.173318	-4.671242
H	2.950699	-3.960002	-5.031433
N	1.533662	-3.259001	-3.631989
C	0.899990	-2.085838	-3.583605
C	-0.073660	-1.514407	-2.687100
N	-0.556972	-2.150161	-1.674051
H	-1.299249	-1.726173	-1.126239
H	-0.396209	-3.151898	-1.564308
N	-0.418081	-0.228990	-2.934276
C	0.082541	0.419381	-3.940513
H	-0.270360	1.427904	-4.072285
N	1.007248	0.007734	-4.834662
C	1.371889	-1.217178	-4.624512
H	1.422503	-8.165662	-7.656436
H	1.912895	-6.612726	-6.339636
H	3.915002	-2.402640	-7.985454
H	4.226657	-1.643289	-6.060398

$MinCT_{21}$

O	0.586992	-7.885147	-7.060866
C	0.887776	-6.560751	-6.690852
H	0.807312	-5.868998	-7.516183
N	-0.013673	-6.116174	-5.688014
C	-0.491415	-6.797462	-4.605557
H	-0.213656	-7.810650	-4.419129
N	-1.280026	-6.088958	-3.880201
C	-1.332012	-4.848111	-4.510211
C	-1.978741	-3.605574	-4.206800
N	-2.788250	-3.455318	-3.127200
H	-3.406137	-2.669410	-3.155791
H	-3.197329	-4.272398	-2.716256
N	-1.720511	-2.567504	-4.959769
C	-0.815991	-2.666338	-6.026228
H	-0.898860	-1.891880	-6.747400
N	-0.261138	-3.854689	-6.449987
C	-0.535653	-4.849261	-5.627608
O	3.033745	-2.437769	-7.371941
C	3.198497	-1.527958	-6.317179
H	2.960892	-0.513139	-6.602079
N	2.351064	-1.931453	-5.249823
C	2.363316	-3.155453	-4.657064
H	3.015749	-3.928175	-5.013791
N	1.568579	-3.259423	-3.631744
C	0.909032	-2.096132	-3.589630
C	-0.063378	-1.533097	-2.687633
N	-0.533510	-2.169166	-1.666426
H	-1.266135	-1.740050	-1.108897
H	-0.369973	-3.170025	-1.556553
N	-0.406300	-0.243733	-2.922683
C	0.089534	0.409970	-3.926672
H	-0.264586	1.421812	-4.047355
N	1.014009	0.009866	-4.824490
C	1.376127	-1.218999	-4.628855
H	1.433974	-8.151858	-7.692994

H	1.923178	-6.616419	-6.354783
H	3.938533	-2.384529	-7.977436
H	4.252747	-1.619495	-6.055879

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O	0.569941	-7.892757	-7.084005
C	0.828661	-6.548605	-6.759325
H	0.709525	-5.886860	-7.604441
N	-0.067348	-6.102588	-5.752471
C	-0.484564	-6.758379	-4.630673
H	-0.199818	-7.768861	-4.439174
N	-1.227474	-6.030860	-3.877319
C	-1.301717	-4.799049	-4.522727
C	-1.978065	-3.566824	-4.240121
N	-2.785442	-3.412722	-3.158169
H	-3.420754	-2.641588	-3.203413
H	-3.178736	-4.231198	-2.733618
N	-1.797985	-2.563402	-5.057312
C	-0.806732	-2.645881	-6.054895
H	-0.860622	-1.856697	-6.766904
N	-0.349786	-3.852556	-6.546026
C	-0.576030	-4.829853	-5.688158
O	3.062809	-2.453223	-7.368463
C	3.228184	-1.537737	-6.317981
H	2.996613	-0.522179	-6.610522
N	2.377065	-1.931650	-5.251975
C	2.381783	-3.152190	-4.651562
H	3.026744	-3.933771	-5.003298
N	1.583516	-3.245578	-3.628168
C	0.926602	-2.080611	-3.598373
C	-0.055529	-1.513935	-2.711012
N	-0.533606	-2.148341	-1.693082
H	-1.278150	-1.725869	-1.146587
H	-0.358548	-3.146185	-1.572685
N	-0.405006	-0.229293	-2.961330
C	0.098944	0.418472	-3.965931
H	-0.257790	1.425167	-4.101087
N	1.035730	0.012459	-4.850753
C	1.400394	-1.212201	-4.640095
H	1.418881	-8.145528	-7.719226
H	1.869894	-6.551526	-6.436951
H	3.965057	-2.396358	-7.977408
H	4.282116	-1.632213	-6.056444

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O	0.558152	-7.898896	-7.081599
C	0.782124	-6.541592	-6.787528
H	0.628410	-5.901058	-7.643654
N	-0.109039	-6.100065	-5.774749
C	-0.502310	-6.749058	-4.642468
H	-0.214754	-7.758284	-4.451631
N	-1.229005	-6.017110	-3.877371
C	-1.312300	-4.785739	-4.523694
C	-2.009252	-3.562805	-4.245019
N	-2.822196	-3.409980	-3.163569
H	-3.471240	-2.650290	-3.223264
H	-3.212856	-4.233384	-2.743939
N	-1.867257	-2.574755	-5.092482
C	-0.833497	-2.637464	-6.043501
H	-0.881298	-1.844492	-6.756932
N	-0.406679	-3.853714	-6.575016
C	-0.612658	-4.822412	-5.707307
O	3.077074	-2.459006	-7.367333
C	3.245381	-1.544088	-6.317433
H	3.014538	-0.527841	-6.609258
N	2.395182	-1.937809	-5.250558
C	2.393400	-3.159986	-4.653472
H	3.023770	-3.950028	-5.013042
N	1.601480	-3.244833	-3.622604

C	0.960304	-2.073682	-3.584833
C	-0.033186	-1.510234	-2.706871
N	-0.526905	-2.151914	-1.703013
H	-1.283824	-1.737178	-1.166120
H	-0.343544	-3.149326	-1.582591
N	-0.390435	-0.229912	-2.966102
C	0.117117	0.417630	-3.969126
H	-0.243991	1.421851	-4.111595
N	1.058187	0.009789	-4.849421
C	1.434523	-1.208223	-4.625074
H	1.407003	-8.138901	-7.721872
H	1.827828	-6.502583	-6.482438
H	3.978159	-2.402094	-7.977993
H	4.299407	-1.639916	-6.056769

40_{CT21}

O	0.488196	-7.875207	-7.067372
C	0.639730	-6.497039	-6.835868
H	0.403197	-5.906037	-7.709229
N	-0.229343	-6.062734	-5.799266
C	-0.611601	-6.708173	-4.661681
H	-0.334520	-7.721025	-4.477581
N	-1.312180	-5.966201	-3.881333
C	-1.377224	-4.726844	-4.516577
C	-2.092103	-3.510889	-4.249879
N	-2.920824	-3.366269	-3.180682
H	-3.576116	-2.612723	-3.247284
H	-3.299078	-4.193646	-2.758098
N	-1.965205	-2.538157	-5.114570
C	-0.875714	-2.593351	-6.009908
H	-0.880389	-1.779180	-6.701820
N	-0.497779	-3.807625	-6.587086
C	-0.704523	-4.774988	-5.718048
O	3.070970	-2.485348	-7.306788
C	3.250473	-1.580798	-6.251297
H	3.009550	-0.566402	-6.526233
N	2.404854	-1.974617	-5.175543
C	2.393820	-3.190717	-4.564087
H	3.014802	-3.994876	-4.913120
N	1.589823	-3.259655	-3.537594
C	0.958960	-2.083468	-3.517139
C	-0.057213	-1.515357	-2.667077
N	-0.580686	-2.151377	-1.676084
H	-1.353979	-1.737883	-1.164237
H	-0.403869	-3.148119	-1.546382
N	-0.410942	-0.237829	-2.945727
C	0.114014	0.394570	-3.947397
H	-0.249805	1.402283	-4.110160
N	1.066800	-0.020457	-4.810402
C	1.443523	-1.233763	-4.564213
H	1.337790	-8.091545	-7.715049
H	1.690846	-6.363566	-6.580056
H	3.970668	-2.430582	-7.919686
H	4.306775	-1.672564	-5.998502

48_{CT21}

O	0.484494	-7.868735	-7.088490
C	0.634476	-6.489537	-6.859634
H	0.401012	-5.899737	-7.734260
N	-0.238788	-6.054039	-5.827117
C	-0.589791	-6.685829	-4.671094
H	-0.306283	-7.696474	-4.483164
N	-1.268401	-5.935312	-3.880643
C	-1.350196	-4.701986	-4.526037
C	-2.086224	-3.495243	-4.265967
N	-2.921122	-3.355517	-3.201433
H	-3.594567	-2.619908	-3.284972
H	-3.287733	-4.188259	-2.777144
N	-1.995748	-2.547850	-5.164095

C	-0.861183	-2.593900	-6.011758
H	-0.835061	-1.762008	-6.683492
N	-0.522694	-3.800881	-6.628222
C	-0.709371	-4.764782	-5.747930
O	3.075012	-2.484439	-7.302702
C	3.260284	-1.579738	-6.247988
H	3.020523	-0.565082	-6.523044
N	2.418718	-1.969721	-5.168269
C	2.417704	-3.178691	-4.542261
H	3.040265	-3.984171	-4.885525
N	1.619367	-3.239998	-3.512396
C	0.979117	-2.067890	-3.505389
C	-0.047798	-1.501622	-2.668696
N	-0.573339	-2.136480	-1.678789
H	-1.359228	-1.734429	-1.178097
H	-0.393563	-3.130399	-1.541414
N	-0.411958	-0.229218	-2.958134
C	0.108837	0.400032	-3.965696
H	-0.257581	1.397205	-4.141670
N	1.067868	-0.021022	-4.821933
C	1.453376	-1.228120	-4.561983
H	1.336746	-8.086852	-7.732067
H	1.684580	-6.355621	-6.599929
H	3.971587	-2.428679	-7.920070
H	4.317614	-1.672815	-6.000019

CI CT_{12}/GS

O	0.615247	-7.579428	-7.551794
O	3.034698	-2.178096	-7.517974
N	0.182284	-6.080381	-5.777027
N	-1.103897	-5.974950	-3.907720
N	-2.800518	-3.527034	-3.277193
N	-2.308041	-2.805448	-5.377465
N	-0.608363	-3.992074	-6.666629
N	2.210365	-1.875836	-5.366980
N	1.315212	-3.218659	-3.861086
N	-0.667529	-2.072283	-1.805127
N	-0.378785	-0.071611	-2.884166
N	1.081019	0.165333	-4.983330
C	1.128826	-6.521712	-6.815979
C	-0.179060	-6.665767	-4.649670
C	-1.249752	-4.872938	-4.524196
C	-2.170111	-3.731589	-4.315312
C	-1.464510	-2.841219	-6.270802
C	-0.479432	-4.843994	-5.781389
C	3.142253	-1.401022	-6.289043
C	2.255923	-3.096282	-4.682822
C	0.430202	-2.039656	-4.035383
C	-0.152614	-1.307661	-2.870340
C	-0.115525	0.626822	-4.211397
C	1.185583	-1.121514	-4.799045
H	1.312351	-5.641698	-7.411427
H	0.194439	-7.611139	-4.315793
H	-3.366757	-2.684530	-3.175742
H	-2.748855	-4.147673	-2.463349
H	-1.324204	-2.007120	-6.926370
H	2.917507	-0.371206	-6.499291
H	2.987141	-3.830279	-4.958483
H	-0.903206	-1.501733	-1.014088
H	-0.149859	-2.887333	-1.540408
H	0.019133	1.675047	-3.957566
H	1.354093	-7.991825	-7.977050
H	2.064884	-6.870591	-6.379885
H	3.866806	-2.241584	-7.965606
H	4.187542	-1.516682	-6.002525

CI CT_{21}/GS

O	0.561798	-7.849744	-7.366970
O	3.189481	-2.343868	-7.628659

N	-0.008080	-6.137292	-5.812630
N	-1.203486	-6.122583	-3.934142
N	-2.540969	-3.518240	-3.003531
N	-1.384092	-2.431753	-4.630815
N	-0.021796	-3.895592	-6.504555
N	2.459720	-1.986202	-5.462986
N	1.594574	-3.343199	-3.871452
N	-0.623493	-2.323758	-1.956178
N	-0.528087	-0.365143	-3.184789
N	1.103571	-0.081891	-4.960371
C	0.853530	-6.563324	-6.861832
C	-0.514666	-6.845965	-4.696267
C	-1.177849	-4.814054	-4.500376
C	-1.711799	-3.630198	-4.077336
C	-0.474413	-2.531124	-5.937370
C	-0.386474	-4.823009	-5.690872
C	3.344775	-1.542113	-6.511668
C	2.441222	-3.194718	-4.892412
C	0.906048	-2.263320	-3.862624
C	-0.205879	-1.767095	-3.020867
C	0.023305	0.317123	-4.036593
C	1.445578	-1.261423	-4.846241
H	0.803892	-5.819290	-7.639050
H	-0.293872	-7.882500	-4.561101
H	-3.138049	-2.709762	-3.047417
H	-3.033836	-4.328302	-2.667694
H	-0.905231	-1.896043	-6.703413
H	3.113950	-0.510033	-6.718242
H	3.099279	-3.967592	-5.214324
H	-1.352809	-1.895231	-1.404986
H	-0.398200	-3.293781	-1.742973
H	-0.262647	1.343373	-4.162940
H	1.320131	-8.092964	-7.879399
H	1.881571	-6.650576	-6.510238
H	3.986191	-2.315722	-8.139804
H	4.388684	-1.661798	-6.221792

CI CT_{12}/GS PT

O	0.450881	-7.783846	-7.501727
O	2.838015	-2.370743	-7.423856
N	0.027281	-6.188328	-5.771346
N	-1.086099	-5.961942	-3.815848
N	-2.854527	-3.517890	-3.362581
N	-2.112720	-2.806558	-5.472403
N	-0.626825	-4.112191	-6.772924
N	2.194424	-2.139711	-5.185680
N	1.517272	-3.473406	-3.550554
N	-0.640890	-2.371063	-1.368515
N	-0.473987	-0.380327	-2.720638
N	0.853695	-0.125481	-4.686304
C	0.936760	-6.683360	-6.786477
C	-0.305899	-6.699342	-4.520131
C	-1.344976	-4.876258	-4.616603
C	-2.141554	-3.746058	-4.475673
C	-1.361904	-2.995380	-6.489234
C	-0.625777	-4.996323	-5.847474
C	3.031476	-1.643818	-6.220916
C	2.268957	-3.360504	-4.586990
C	0.880552	-2.239101	-3.429963
C	0.119586	-1.605601	-2.385677
C	-0.034896	0.240384	-3.778706
C	1.262496	-1.419561	-4.449141
H	1.116366	-5.844047	-7.440845
H	0.099293	-7.630721	-4.185175
H	-3.464282	-2.718662	-3.483797
H	-1.491071	-2.822948	-1.666777
H	-1.296816	-2.210306	-7.215164
H	2.794615	-0.604186	-6.369294
H	2.920290	-4.121823	-4.960904

H	-0.902710	-1.748762	-0.613174
H	-0.081262	-3.142384	-1.009444
H	-0.469502	1.216605	-3.937116
H	1.198936	-8.171788	-7.933841
H	1.885086	-7.011428	-6.360861
H	3.643425	-2.422227	-7.919308
H	4.089126	-1.756665	-5.982709

CI CT_{21}/GS PT

O	0.772808	-7.907282	-7.419178
O	3.092803	-2.148553	-7.609099
N	0.048960	-6.312140	-5.844655
N	-1.176097	-6.414156	-3.999328
N	-2.617658	-3.744506	-2.994915
N	-2.076324	-2.944039	-5.182918
N	-0.577133	-4.062057	-6.654282
N	2.437039	-1.770278	-5.387206
N	1.642423	-3.029315	-3.701606
N	-0.314615	-1.852565	-1.715585
N	-0.205172	0.109082	-2.979818
N	1.155966	0.203464	-4.942660
C	0.979657	-6.625039	-6.884668
C	-0.292623	-7.016004	-4.735939
C	-1.442580	-5.220541	-4.668947
C	-2.331158	-4.098776	-4.405389
C	-1.299004	-3.054440	-6.213792
C	-0.679396	-5.134084	-5.778937
C	3.300228	-1.367403	-6.466971
C	2.408869	-2.977325	-4.745221
C	1.082326	-1.818027	-3.618929
C	0.145437	-1.227016	-2.692036
C	0.244264	0.704628	-3.986308
C	1.536845	-0.989129	-4.702732
H	0.877259	-5.867462	-7.645963
H	0.150045	-7.962490	-4.510799
H	-3.227469	-2.936219	-2.990184
H	-3.096212	-4.479564	-2.482308
H	-1.233718	-2.161656	-6.820890
H	3.117311	-0.326756	-6.671915
H	3.001548	-3.790569	-5.095692
H	-0.960740	-1.311803	-1.155084
H	-1.791370	-3.540537	-2.448772
H	-0.077515	1.712256	-4.160981
H	1.551541	-8.121632	-7.913584
H	2.007605	-6.650362	-6.523033
H	3.888609	-2.157018	-8.122354
H	4.343957	-1.533883	-6.200486

MinCT_{21} PT

O	0.669436	-7.910830	-7.069963
C	0.895601	-6.578771	-6.687548
H	0.739788	-5.878557	-7.494374
N	-0.012130	-6.221755	-5.650157
C	-0.355854	-6.935011	-4.552225
H	0.073271	-7.886768	-4.343869
N	-1.226514	-6.333244	-3.815232
C	-1.463131	-5.128048	-4.459288
C	-2.315038	-4.018813	-4.178936
N	-2.635898	-3.682444	-2.793225
H	-3.177613	-2.826741	-2.783541
H	-3.201439	-4.395475	-2.342975
N	-2.130249	-2.894639	-4.963959
C	-1.377235	-2.991005	-6.046906
H	-1.352470	-2.122664	-6.669255
N	-0.641128	-4.036870	-6.465911
C	-0.722210	-5.049875	-5.600269
O	2.950423	-2.320735	-7.316236
C	3.163876	-1.399630	-6.271205
H	2.948482	-0.387721	-6.573058

N	2.324056	-1.757131	-5.190108
C	2.358894	-2.948864	-4.525141
H	2.996350	-3.745589	-4.860563
N	1.574201	-3.002479	-3.498626
C	0.940999	-1.808686	-3.474864
C	-0.048224	-1.222396	-2.607784
N	-0.535386	-1.881789	-1.633502
H	-1.213636	-1.341103	-1.097314
H	-1.788739	-3.567830	-2.235191
N	-0.412060	0.075932	-2.931429
C	0.066485	0.669468	-3.963914
H	-0.290463	1.666974	-4.160327
N	0.981136	0.198150	-4.857000
C	1.387073	-0.998596	-4.559759
H	1.528477	-8.137780	-7.701344
H	1.939598	-6.563516	-6.374600
H	3.842682	-2.282274	-7.941132
H	4.219189	-1.518800	-6.025823

1_{NH}

O	0.669286	-7.898965	-7.078386
O	3.009337	-2.390791	-7.304593
N	0.030186	-6.126140	-5.730323
N	-1.260750	-6.106553	-3.934585
N	-2.845889	-3.530995	-3.237329
N	-1.735762	-2.592938	-5.006648
N	-0.220315	-3.855013	-6.472473
N	2.392385	-1.904982	-5.158685
N	1.593729	-3.261732	-3.563097
N	-0.629810	-2.194460	-1.688404
N	-0.418892	-0.234484	-2.885377
N	1.055038	0.028771	-4.754402
C	0.945959	-6.566096	-6.718230
C	-0.460525	-6.805310	-4.655512
C	-1.298544	-4.856590	-4.548895
C	-1.994410	-3.650923	-4.277079
C	-0.804402	-2.648378	-6.024640
C	-0.486622	-4.845594	-5.669236
C	3.218925	-1.502568	-6.241285
C	2.377635	-3.150642	-4.575654
C	0.942323	-2.068664	-3.502056
C	-0.089019	-1.528104	-2.648387
C	0.101833	0.421124	-3.874509
C	1.421278	-1.194114	-4.544910
H	0.859453	-5.883233	-7.551207
H	-0.181514	-7.818032	-4.466964
H	-3.468086	-2.746399	-3.265451
H	-3.235002	-4.354575	-2.819324
H	-0.913636	-1.903116	-6.775865
H	2.987977	-0.481220	-6.497815
H	3.012081	-3.927669	-4.955912
H	-1.392760	-1.793352	-1.157881
H	-0.506068	-3.303827	-1.634492
H	-0.252249	1.430603	-4.005349
H	1.413512	-8.127606	-7.617513
H	1.980189	-6.602845	-6.376008
H	3.784335	-2.356352	-7.847733
H	4.276891	-1.613621	-6.003643

2_{NH}

O	0.701785	-7.907569	-7.090381
O	2.972983	-2.386765	-7.337499
N	0.084795	-6.155341	-5.704906
N	-1.186130	-6.163520	-3.900492
N	-2.760812	-3.573118	-3.124056
N	-1.716594	-2.648615	-4.965634
N	-0.209636	-3.893109	-6.451915
N	2.347865	-1.921258	-5.190421
N	1.574747	-3.279270	-3.567828

N	-0.554594	-2.194100	-1.617601
N	-0.418278	-0.261197	-2.867537
N	0.999583	-0.000748	-4.777960
C	0.991100	-6.582776	-6.711320
C	-0.382688	-6.851833	-4.630960
C	-1.254329	-4.916548	-4.516415
C	-1.945779	-3.697943	-4.213812
C	-0.809746	-2.713333	-6.019720
C	-0.460862	-4.893900	-5.637021
C	3.173757	-1.503205	-6.268270
C	2.376078	-3.177473	-4.597434
C	0.929349	-2.103051	-3.511309
C	-0.073239	-1.548034	-2.617047
C	0.077142	0.389474	-3.878153
C	1.393043	-1.221046	-4.567959
H	0.903526	-5.883764	-7.530056
H	-0.087403	-7.860014	-4.449746
H	-3.411454	-2.812143	-3.171224
H	-3.176205	-4.407875	-2.758358
H	-0.919718	-1.946364	-6.747790
H	2.935002	-0.482437	-6.521009
H	3.016815	-3.948393	-4.974059
H	-1.311357	-1.803043	-1.071259
H	-0.444219	-3.462951	-1.591724
H	-0.289381	1.394985	-4.006379
H	1.443049	-8.138316	-7.632683
H	2.026588	-6.634227	-6.374845
H	3.750792	-2.348854	-7.876372
H	4.231936	-1.607292	-6.028433

3_{NH}

O	0.673682	-7.936293	-7.123416
O	2.843398	-2.290853	-7.331899
N	0.021613	-6.235571	-5.693211
N	-1.215678	-6.299697	-3.868421
N	-2.685512	-3.610094	-2.934449
N	-2.048905	-2.858103	-5.075796
N	-0.552696	-4.014177	-6.537998
N	2.204959	-1.795709	-5.198725
N	1.316919	-3.119943	-3.633631
N	-0.993312	-2.044154	-1.912036
N	-0.510297	0.013852	-2.907505
N	0.949959	0.192198	-4.778528
C	0.937382	-6.618387	-6.711408
C	-0.349623	-6.923290	-4.594471
C	-1.418953	-5.088588	-4.522470
C	-2.255639	-3.962479	-4.268226
C	-1.286958	-2.968471	-6.130202
C	-0.662796	-5.042591	-5.654381
C	3.062350	-1.408284	-6.262077
C	2.151882	-3.031683	-4.625231
C	0.731186	-1.911134	-3.557162
C	-0.301113	-1.340370	-2.721386
C	0.044766	0.654883	-3.871944
C	1.274627	-1.041285	-4.556685
H	0.832804	-5.900900	-7.511450
H	0.054675	-7.884574	-4.373652
H	-3.433282	-2.930072	-3.004040
H	-3.058256	-4.401344	-2.422691
H	-1.253993	-2.111701	-6.770557
H	2.860522	-0.382145	-6.522555
H	2.770414	-3.831512	-4.987364
H	-1.632364	-1.472183	-1.360896
H	-1.854057	-3.137714	-2.387196
H	-0.228115	1.690998	-3.984306
H	1.538126	-8.180858	-7.740687
H	1.973296	-6.654797	-6.374279
H	3.743902	-2.270231	-7.945712
H	4.114632	-1.544667	-6.012675

4_{NH}

O	0.643271	-7.935090	-7.108416
O	2.845684	-2.281772	-7.338956
N	-0.045019	-6.223580	-5.704257
N	-1.266365	-6.278381	-3.868148
N	-2.721638	-3.586105	-2.928810
N	-2.092980	-2.843101	-5.075947
N	-0.625967	-4.010845	-6.549863
N	2.216482	-1.769612	-5.201777
N	1.363977	-3.061425	-3.592017
N	-0.893751	-1.969186	-1.845064
N	-0.500400	0.070426	-2.927134
N	0.937175	0.216395	-4.818092
C	0.870361	-6.601871	-6.726118
C	-0.405682	-6.905569	-4.600131
C	-1.472138	-5.070232	-4.522279
C	-2.311609	-3.943803	-4.276884
C	-1.343440	-2.958918	-6.139154
C	-0.726609	-5.027987	-5.663140
C	3.070650	-1.395475	-6.271501
C	2.186341	-2.990397	-4.591533
C	0.769081	-1.852640	-3.538008
C	-0.251798	-1.272479	-2.696980
C	0.034830	0.691922	-3.914733
C	1.286674	-1.006475	-4.566114
H	0.730988	-5.906958	-7.540856
H	-0.001782	-7.867034	-4.379243
H	-3.434717	-2.867245	-2.991363
H	-3.135169	-4.365967	-2.428113
H	-1.304223	-2.099832	-6.775184
H	2.872961	-0.369931	-6.537466
H	2.809278	-3.792907	-4.940295
H	-1.544865	-1.402862	-1.301665
H	-1.913754	-3.208714	-2.384667
H	-0.256963	1.719345	-4.056830
H	1.505203	-8.161969	-7.735869
H	1.911216	-6.595825	-6.402569
H	3.743344	-2.260906	-7.956913
H	4.123385	-1.535693	-6.026172

5_{NH}

O	0.689911	-7.924769	-7.066713
O	2.894476	-2.284632	-7.296924
N	0.032037	-6.223548	-5.643387
N	-1.186745	-6.293209	-3.805226
N	-2.659314	-3.628949	-2.848490
N	-2.051614	-2.859482	-5.000013
N	-0.580134	-4.008692	-6.492442
N	2.279365	-1.769949	-5.153573
N	1.459366	-3.051019	-3.519919
N	-0.720506	-1.942494	-1.700406
N	-0.464484	0.057761	-2.899878
N	0.971468	0.200932	-4.792176
C	0.940714	-6.601052	-6.670154
C	-0.323788	-6.911033	-4.541162
C	-1.402280	-5.083970	-4.458643
C	-2.251614	-3.965899	-4.205639
C	-1.305139	-2.967882	-6.070676
C	-0.662170	-5.035686	-5.599167
C	3.123242	-1.396916	-6.230941
C	2.265094	-2.985325	-4.532687
C	0.854262	-1.844718	-3.469365
C	-0.158506	-1.265542	-2.620512
C	0.049678	0.668984	-3.903686
C	1.343744	-1.011631	-4.520158
H	0.815000	-5.892729	-7.475540
H	0.086648	-7.871129	-4.324139
H	-3.270416	-2.822389	-2.893934

H	-3.183683	-4.375579	-2.403139
H	-1.282974	-2.108971	-6.707155
H	2.921680	-0.372000	-6.496776
H	2.888919	-3.786755	-4.882058
H	-1.387273	-1.384640	-1.167571
H	-1.842225	-3.411547	-2.268649
H	-0.276436	1.681425	-4.075255
H	1.549654	-8.161489	-7.693534
H	1.980554	-6.617774	-6.343731
H	3.790666	-2.265586	-7.917070
H	4.177506	-1.533887	-5.990386

Dyn1

O	9.302997	-3.532999	1.399000
C	8.042998	-4.032999	1.179000
H	7.752998	-4.722999	1.978999
N	7.262998	-2.782999	1.019000
C	7.352998	-1.862999	-0.051000
H	8.012998	-1.942999	-0.911000
N	6.762998	-0.693000	0.219000
C	6.182998	-0.903000	1.459000
C	5.302999	-0.163000	2.288999
N	4.902999	1.077000	2.028999
H	4.332999	1.527000	2.718999
H	5.152999	1.587000	1.189000
N	4.882999	-0.623000	3.528999
C	5.272999	-1.852999	3.798999
H	4.892999	-2.142999	4.768999
N	5.972998	-2.692999	3.088999
C	6.432998	-2.162999	1.918999
O	4.672999	-5.852998	2.098999
C	3.712999	-5.572998	1.019000
H	2.722999	-5.712998	1.439000
N	3.962999	-4.132999	0.479000
C	4.672999	-3.692999	-0.651000
H	5.192999	-4.472999	-1.181000
N	4.542999	-2.452999	-1.011000
C	3.652999	-2.052999	-0.011000
C	2.922999	-0.863000	0.259000
N	3.062999	0.317000	-0.291000
H	2.402999	1.057000	-0.111000
H	3.822999	0.477000	-0.931000
N	2.192999	-0.763000	1.339000
C	2.072999	-1.832999	2.128999
H	1.303000	-1.733000	2.878999
N	2.532999	-3.072999	2.018999
C	3.442999	-3.012999	0.969000
H	10.034531	-4.287393	1.109434
H	8.130823	-4.662410	0.293433
H	4.732364	-6.936411	2.202888
H	3.969420	-6.363631	0.313841

Dyn2

O	3.419999	6.808998	-5.098999
C	3.378999	6.021998	-3.949999
H	2.785999	6.508998	-3.175999
N	2.741999	4.738999	-4.246999
C	3.295999	3.666999	-4.918999
H	4.263999	3.608999	-5.393998
N	2.423999	2.702999	-5.120999
C	1.216000	3.256999	-4.598999
C	-0.127000	2.764999	-4.500999
N	-0.552000	1.541000	-4.803999
H	-1.515000	1.298000	-4.617999
H	-0.023000	0.869000	-5.340999
N	-1.099000	3.542999	-3.984999
C	-0.744000	4.734999	-3.466999
H	-1.480000	5.394998	-3.030999
N	0.447000	5.316999	-3.466999

C	1.401000	4.497999	-4.042999
O	2.415999	6.454998	-0.578000
C	2.574999	5.284999	0.180000
H	1.710000	5.169999	0.833000
N	2.589999	4.125999	-0.790000
C	3.682999	3.455999	-1.301000
H	4.687999	3.802999	-1.112000
N	3.392999	2.297999	-1.887999
C	2.001999	2.265999	-1.668000
C	1.083000	1.266000	-1.832999
N	1.321000	0.105000	-2.360999
H	0.633000	-0.582000	-2.088999
H	2.262999	-0.122000	-2.647999
N	-0.188000	1.469000	-1.499000
C	-0.501000	2.572999	-0.939000
H	-1.479000	2.621999	-0.483000
N	0.270000	3.596999	-0.641000
C	1.542000	3.386999	-1.040000
H	4.437012	7.072098	-5.389794
H	4.385833	5.986496	-3.533917
H	2.714148	7.274344	0.076125
H	3.495359	5.412573	0.749880

Dyn3

O	3.071999	6.642998	-5.813998
C	2.785999	5.325999	-5.394998
H	3.768999	4.922999	-5.149999
N	1.891999	5.244999	-4.239999
C	0.488000	5.229999	-4.234999
H	-0.141000	5.407998	-5.094999
N	-0.063000	5.031999	-3.079999
C	1.006000	4.769999	-2.236999
C	1.247000	4.568999	-0.869000
N	0.320000	4.623999	0.052000
H	0.691000	4.564999	0.990000
H	-0.569000	5.069999	-0.122000
N	2.484999	4.242999	-0.358000
C	3.484999	4.218999	-1.243000
H	4.463999	4.000999	-0.844000
N	3.414999	4.462999	-2.546999
C	2.183999	4.710999	-2.987999
O	4.165999	2.221999	-5.202999
C	3.449999	1.161000	-4.773999
H	4.011999	0.612000	-4.017999
N	2.100999	1.620000	-4.261999
C	0.943000	1.666000	-5.017999
H	0.878000	1.615000	-6.094998
N	-0.146000	1.717000	-4.285999
C	0.335000	1.659000	-2.982999
C	-0.215000	1.505000	-1.619000
N	-1.505000	1.474000	-1.236000
H	-1.763000	1.281000	-0.279000
H	-2.210999	1.698000	-1.922999
N	0.669000	1.369000	-0.613000
C	1.934999	1.322000	-0.783000
H	2.580999	1.325000	0.082000
N	2.558999	1.428000	-1.941999
C	1.706000	1.612000	-2.967999
H	2.890629	6.698504	-6.887368
H	2.524040	4.753095	-6.284525
H	5.078528	1.851574	-5.670090
H	3.426934	0.600961	-5.708838

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