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Supporting Information

QM/MM Studies on Photoisomerization Dynamics of Azobenzene Chromophore Tethered to a DNA Duplex: Local Unpaired Nucleobase Plays a Crucial Role

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1. Computational Methods

1.1 System Setup

The initial DNA oligomer with sequence 5'-GCATAAAAAAGGTG-3' was constructed using the NAB module of the AMBER2015 package. [1] Then, a single azobenzene unit was attached to the backbone of this DNA oligomer by replacing the central adenine nucleobase using the XLEAP module. Finally, the azobenzene-modified DNA duplex (**azo-DNA-I**, see Table S1) was constructed with the sequence 5'-GCATAAXAAAG GTG-3' in which X denotes the azobenzene chromophore. [2] In parallel, we built another similar azo-DNA system by removing the unpaired thymine nucleobase that originally matches with the adenine nucleobase in position X (**azo-DNA-II**, see Table S1). These two DNA systems were solvated in two rectangular TIP3P water boxes of 50 x 50 x 80 Å³ and neutralized by adding 28 sodium ions, respectively.

Table S1. Sequences of azobenzene-modified DNA used in this study

azo-DNA-I	DNA1: 5'-GCA TAA AXA AAG GTG-3'
	DNA2: 3'-CGT ATT TTT TTC CAC-5'
azo-DNA-II	DNA1: 5'-GCA TAA AXA AAG GTG-3'
	DNA2: 3'-CGT ATT T T TTC CAC-5'

Equilibrium molecular dynamics (MD) simulations were carried out for these two DNA duplexes. In the first phase, the azobenzene-modified DNA duplexes were restrained with force constants of 10.0 kcal·mol⁻¹·Å⁻² and only sodium ions and water molecules were minimized (1000 steps). In the second phase, the entire systems were minimized (2500 steps), heated (20 ps, NVT, T=300K), and equilibrated (1 ns, NPT, T=300K, P=1 atm). [3] In these simulations, all restraints were removed. The Andersen temperature coupling scheme and periodic boundary conditions were used. [4] A cutoff of 10 Å was

employed for nonbonded interactions. In the MD simulations, the azobenzene chromophores were described using the generalized Amber force field (GAFF) [5]; the nucleic acids and sodium ions were described with the Amber ff99 force field; [6] and water molecules were described using the TIP3P model. [7]

1.2 QM/MM Simulations

1.2.1 CASPT2 and CASSCF Methods

The QM subsystem included the azobenzene chromophore while the MM subsystem consisted of all the remaining atoms. The QM region was treated using the state averaged complete-active-space self-consistent field (CASSCF) and the complete active space second-order perturbation (CASPT2) methods. [8-10] We used the former for structure and path optimizations, and the latter for single-point energy refinements.

In the CASSCF calculations, we employed an active space of 6 electrons in 4 orbitals along with the 3-21G* basis set to balance computational efficiency and accuracy. This choice has been validated and applied in previous ab initio electronic structure calculations and nonadiabatic dynamics simulations of azobenzene in solution and peptides. [11-14] In the CASPT2 calculations, the same active space was used in combination with the larger 6-31G* basis set. In addition, the Cholesky decomposition technique with unbiased auxiliary basis sets was applied for accurate two-electron integral approximation, [15] the imaginary shift technique (0.2 au) was used to avoid intruder-state issues, [16] and the ionization potential electron affinity shift was set to zero. [17, 18]

The MM subsystem was described using the Amber ff99 force field and the TIP3P model. The QM-MM boundary was treated by the hydrogen link-atom scheme. [19] The electrostatic embedding scheme [20] was adopted to account for the polarization of the QM region by the MM environment.

In all QM/MM computations, the QM atoms and all MM atoms within 12 Å from the center of mass of the azobenzene were allowed to move; whereas, the

other atoms were frozen at their positions after the 1 ns MD simulations.

1.2.2 Comparison of CASSCF and CASPT2 Energy Profiles

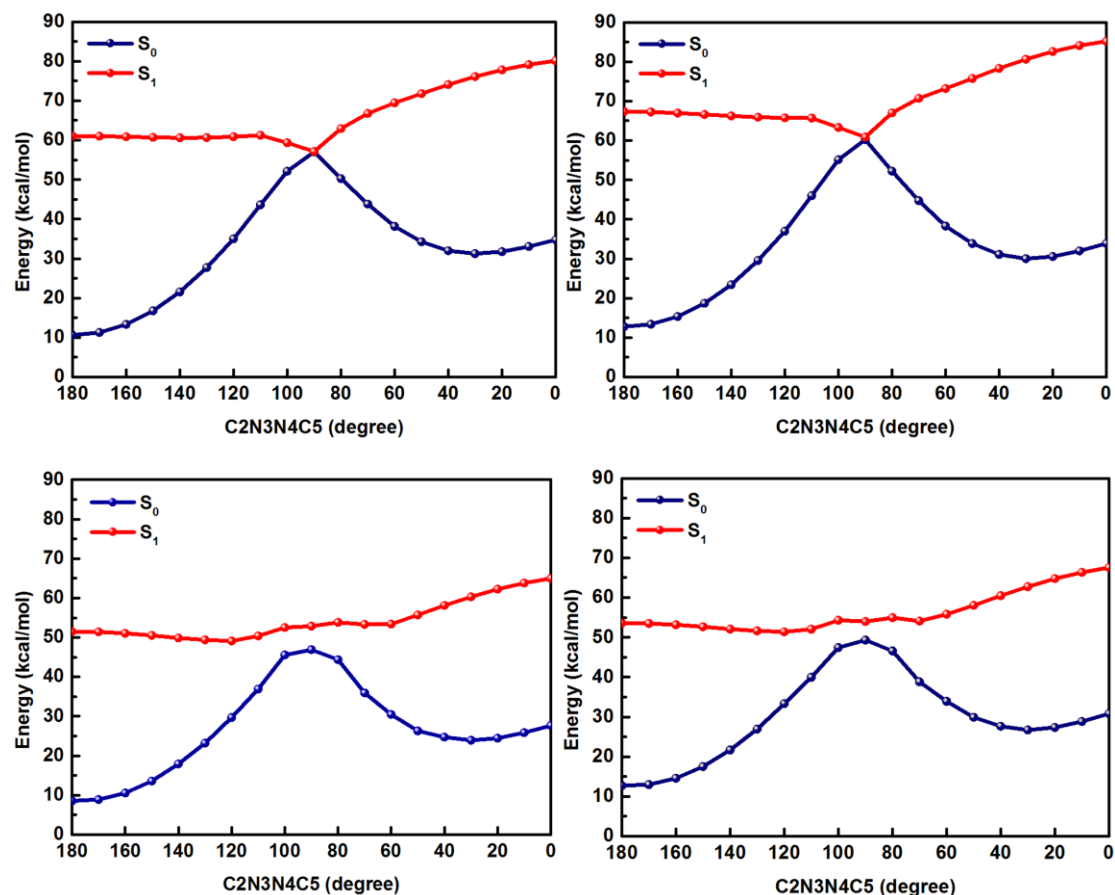


Fig. S1. Computed photoisomerization reaction paths of azobenzene in the gas phase in the S₁ state with respect to the rotation along the central C2-N3-N4-C5 dihedral angle: **(top-left)** CASSCF(6,4)/3-21G*; **(top-right)** CASSCF(6,4)/6-31G*; **(bottom-left)** CASPT2(6,4)/6-31G*; and **(bottom-right)** CASPT2(6,4)/6-31G*. See Ref. S14 for more benchmarks of the same system.

1.2.3 OM2/MRCI Method

Alternatively, the QM region was described by the multi-reference semiempirical OM2/MRCI method implemented in the MNDO99 code. [21-25] During geometry optimizations and dynamics simulations, all required energies, gradients and nonadiabatic coupling elements were computed analytically. Minimum-energy conical intersections were optimized using the

Lagrange-Newton approach. [26, 27]

In the OM2/MRCI calculations, the restricted open-shell Hartree-Fock formalism was applied in the self-consistent field (SCF) treatment. The active space in the MRCI calculations included 10 electrons in 10 orbitals. In terms of the SCF configuration, it comprised the four highest doubly occupied orbitals, the two singly occupied orbitals, and the four lowest unoccupied orbitals. For the MRCI treatment, three configuration state functions were chosen as references, namely the SCF configuration and the two closed-shell configurations derived therefrom (i.e., all singlet configurations that can be generated from the HOMO and LUMO of the closed-shell ground state). The MRCI wavefunction was built by allowing all single and double excitations from these three references.

1.2.4 Nonadiabatic Dynamics Simulations

Trajectory-based surface-hopping nonadiabatic dynamics simulations at the QM(OM2/MRCI)/MM level were employed to investigate the initial photoisomerization dynamics of the azobenzene chromophore tethered to the two modified DNA duplexes (see above). A total of 200 surface-hopping trajectories were run for each of the modified DNA duplexes (**azo-DNA I** and **azo-DNA II**, see Table S1). The corresponding initial conditions (velocities and Cartesian coordinates) were sampled from 10 ps ground-state MD simulations carried out at the QM(OM2)/MM level. All relevant energies, gradients, and nonadiabatic coupling vectors were computed “on-the-fly” when needed. In the excited-state MD simulations, once the system encountered a point with an S_1 - S_0 energy gap of less than 10 kcal/mol, the fewest-switches criterion was applied to decide whether to hop. The time step was chosen to be 0.5 fs for nuclear motion and 0.0005 fs for electronic propagation. The unitary propagator evaluated at mid-point was used to propagate the electronic motion. The translational and rotational motions were removed in each step. The empirical decoherence correction (0.1 au) proposed by Granucci et al. was employed.

[28] The final evaluations were done for the 200 trajectories that finished successfully and satisfied our energy continuity criterion (no changes greater than 30 kcal/mol between any two consecutive MD steps). Further technical details are given in our previous publications. [29-33]

The following computer codes were used: QM/MM calculations in ChemShell3.5; [34] CASSCF calculations in GAUSSIAN09; [35] CASPT2 calculations in MOLCAS8.0; [36, 37] OM2/MRCI calculations in MNDO99; [25] MM calculations in the DL_POLY module implemented in ChemShell3.5. [38]

2. Vertical Excitation Energies

Table S2. Vertical Excitation Energies (E_{\perp} , kcal/mol) for the $S_0 \rightarrow S_1$ (${}^1n\pi^*$) Electronic Transition at Different Computational Levels (**azo-DNA-I** and **azo-DNA-II**).

QM Theory	OM2/MRCI	CASPT2/6-31G* //CASSCF/3-21G*
TRANS-I	58.9	62.4
CIS-I	63.9	60.4
TRANS-II	59.5	63.1
CIS-II	58.0	54.7

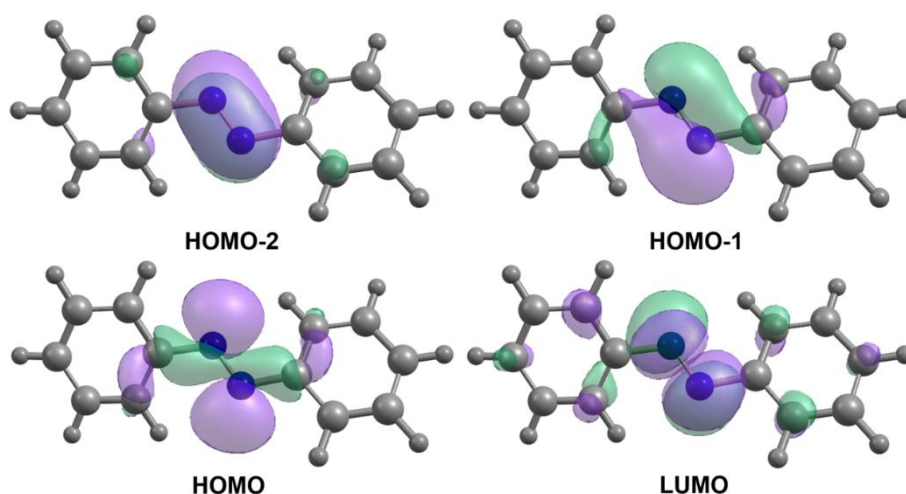


Fig. S2. Active spaces used in the CASSCF and CASPT2 calculations; the

$S_0 \rightarrow S_1$ ($^1n\pi^*$) electronic transition mainly involves a single excitation from HOMO to LUMO.

3. Geometric Parameters and Additional Structures of Key Minima

Table S3. Selected Key Geometric Parameters of Stationary Structures of **azo-DNA-I** (Suffixed with I) and **azo-DNA-II** (Suffixed with II) Optimized at the QM(CASSCF)/MM Level (Minima) and at the QM(OM2/MRCI)/MM Level (Conical Intersections); Distances in Å and Angles in °.

Structures	Distance	Dihedral Angle		
	N3-N4	C1-C2-N3-N4	C2-N3-N4-C5	N3-N4-C5-C6
S0-TRANS-I	1.271	164.0	173.7	173.8
S1S0-CI-I	1.215	-170.1	101.5	166.4
S0-CIS-I	1.234	-91.0	1.651	-168.9
S1-TRANS-I	1.301	174.7	160.1	167.7
S0-TRANS-II	1.269	170.7	-178.9	161.3
S1S0-CI-II	1.204	177.9	-110.4	118.1
S0-CIS-II	1.262	157.0	-7.5	0.9
S1-TRANS-II	1.302	173.4	-176.2	156.2

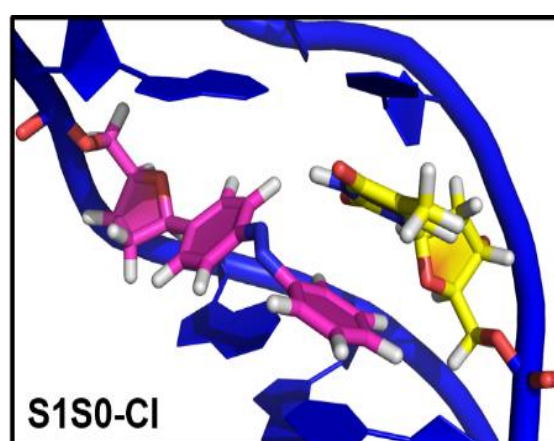


Fig. S3. QM(OM2/MRCI)/MM optimized minimum-energy conical intersection structure of the azobenzene-modified DNA duplex i.e. **azo-DNA-I**.

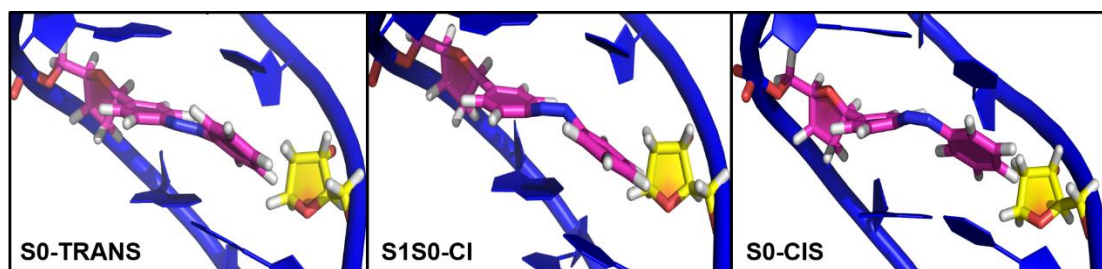


Fig. S4. QM(OM2/MRCI)/MM optimized minimum-energy structures of the azobenzene-modified DNA duplex, i.e. **azo-DNA-II**. See main text and Fig. S3 for the corresponding structures of **azo-DNA-I**.

4. Minimum-Energy Paths

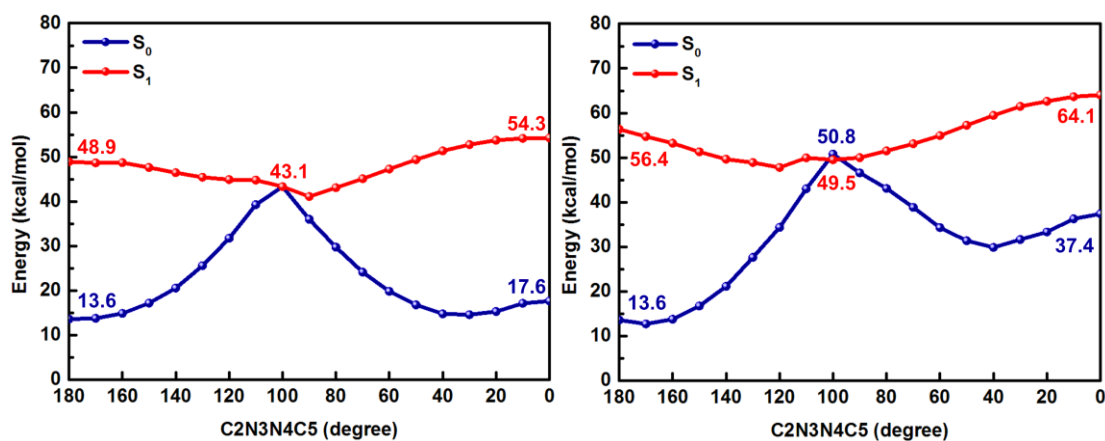


Fig. S5. (Left) QM(OM2/MRCI)/MM and (right) QM(CASPT2//CASSCF)/MM computed minimum-energy reaction paths of **azo-DNA-I** in the S₁ state with respect to the rotation along the central C2-N3-N4-C5 dihedral angle.

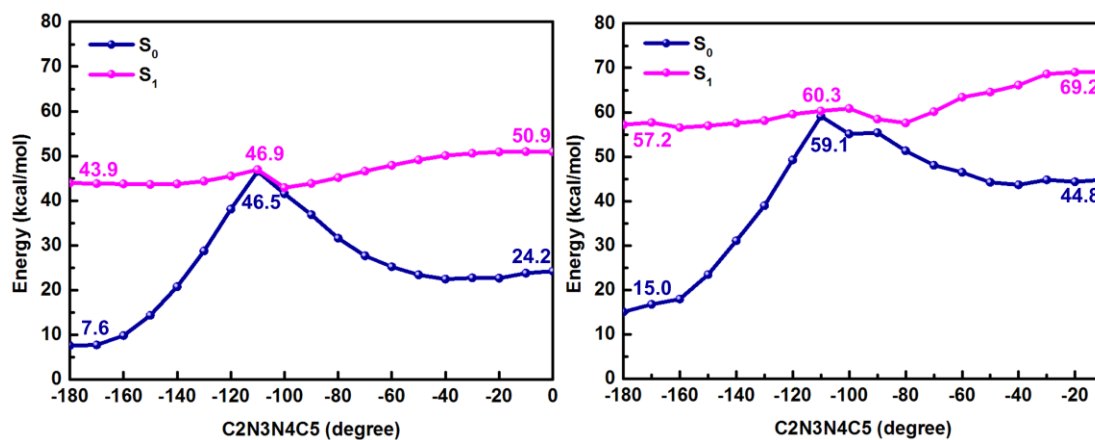


Fig. S6. (Left) QM(OM2/MRCI)/MM and (right) QM(CASPT2//CASSCF)/MM computed minimum-energy reaction paths of **azo-DNA-II** in the S₁ state with respect to the rotation along the central C2-N3-N4-C5 dihedral angle.

respect to the rotation along the central C2-N3-N4-C5 dihedral angle.

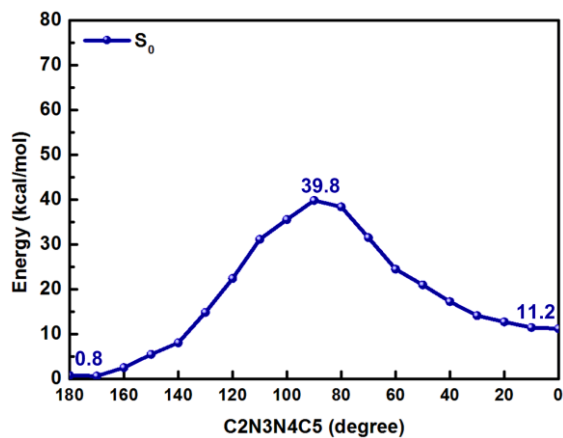


Fig. S7. QM(CASPT2//CASSCF)/MM computed minimum-energy reaction path of **azo-DNA-I** in the S_0 state with respect to the rotation along the central C2-N3-N4-C5 dihedral angle.

5. Additional Figures for QM/MM Dynamics

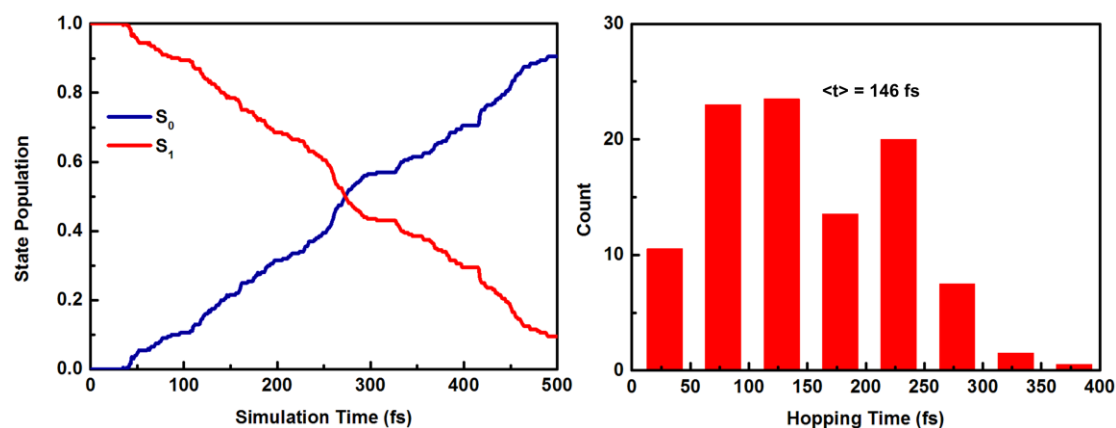


Fig. S8. (Left) Time-dependent state population in the QM(OM2/MRCI)/MM dynamics simulations and (right) distribution of hopping times at all $S_1 \rightarrow S_0$ hopping points.

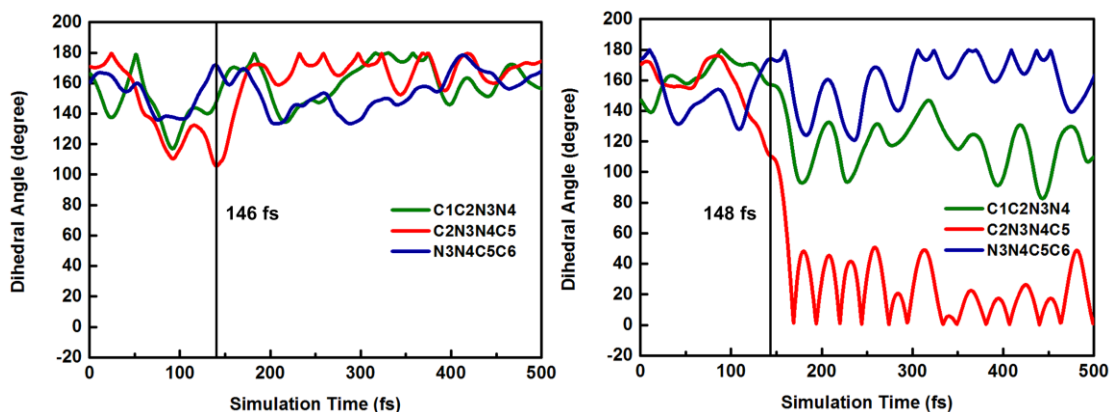


Fig. S9. Evolution of selected geometric parameters in two representative trajectories in which **(left)** trans-to-trans and **(right)** trans-to-cis photoisomerizations take place.

6. Tables

Tables S4-S11 compile various absolute and relative energies of minima and reaction paths calculated by different methods. The total QM/MM energy is decomposed into the QM contribution, i.e. the sum of the QM energy and the electrostatic interaction energy between QM and MM subsystem (denoted as CASSCF A.E., CASPT2 A.E., or OM2/MRCI), and the MM contribution, i.e. the sum of the MM energy and the van-der-Waals interaction energy between QM and MM subsystem (denoted as MM).

Table S4. Absolute Energies (A.E., Hartree), Relative Energies (ΔE , kcal/mol), and MM Energies (A.E., Hartree) of All Optimized Structures of **azo-DNA-I** (Suffixed with I) and **azo-DNA-II** (Suffixed with II) Obtained from QM(CASPT2//CASSCF)/MM Calculations.

Structures	CASSCF A.E.	CASPT2 A.E.	MM	CASPT2 ΔE
S0-TRANS-I				
Root1 (S_0)	-565.96715	-570.93904	-91.05995	0
Root2 (S_1)	-565.85041	-570.83952		62.4

S1S0-CI-I				
Root1 (S ₀)	-565.85589	-570.85811	-91.05681	50.8
Root2 (S ₁)	-565.85580	-570.86015		49.5
S0-CIS-I				
Root1 (S ₀)	-565.93801	-570.91851	-91.05859	12.9
Root2 (S ₁)	-565.82409	-570.82220		73.3
S1-TRANS-I				
Root1 (S ₀)	-565.94447	-570.91498	-91.06055	15.1
Root2 (S ₁)	-565.86624	-570.85447		53.1
S0-TRANS-II				
Root1 (S ₀)	-565.96530	-570.93363	-90.30064	0
Root2 (S ₁)	-565.84503	-570.83299		63.1
S1S0-CI-II				
Root1 (S ₀)	-565.85044	-570.83392	-90.30444	62.6
Root2 (S ₁)	-565.83077	-570.83512		61.8
S0-CIS-II				
Root1 (S ₀)	-565.92615	-570.90446	-90.30048	18.3
Root2 (S ₁)	-565.81623	-570.81726		73.0
S1-TRANS-II				
Root1 (S ₀)	-565.94678	-570.91275	-90.30154	13.1
Root2 (S ₁)	-565.84332	-570.84463		55.8

Table S5. Absolute Energies (A.E., Hartree), Relative Energies (ΔE , kcal/mol), and MM Energies (A.E., Hartree) of All Optimized Structures of **azo-DNA-I** (Suffixed with I) and **azo-DNA-II** (Suffixed with II) Obtained from QM(OM2/MRCI)/MM Calculations.

Structures	OM2/MRCI A.E.	MM	OM2/MRCI ΔE
S0-TRANS-I			
Root1 (S ₀)	0.09777	-91.06077	1.5
Root2 (S ₁)	0.19162		60.4
S1S0-CI-I			
Root1 (S ₀)	0.16103	-91.05681	43.7
Root2 (S ₁)	0.16103		43.7
S0-CIS-I			
Root1 (S ₀)	0.09590	-91.06126	0
Root2 (S ₁)	0.19775		63.9
S1-TRANS-I			
Root1 (S ₀)	0.15091	-91.05821	36.4
Root2 (S ₁)	0.16434		44.9
S0-TRANS-II			
Root1 (S ₀)	0.10154	-90.30175	0
Root2 (S ₁)	0.19632		59.5
S1S0-CI-II			
Root1 (S ₀)	0.17904	-90.30444	46.9
Root2 (S ₁)	0.17904		46.9
S0-CIS-II			
Root1 (S ₀)	0.11101	-90.30174	6.0
Root2 (S ₁)	0.20391		64.3
S1-TRANS-II			
Root1 (S ₀)	0.13311	-90.30923	15.1
Root2 (S ₁)	0.17853		43.6

Table S6. Absolute Energies (A.E., Hartree), Relative Energies (ΔE , kcal/mol), and MM Energies (A.E., Hartree) of All Structures along the C2-N3-N4-C5 Photoisomerization Path of the Azobenzene Chromophore in **azo-DNA-I** (Relaxed in the S_1 State). For Plots of the Corresponding Energy Profile see the Left Panel of Figure 2 in the Main Text and the Right Panel of Figure S4.

(C2N3N4C5)	CASSCF A.E.	CASPT2 A.E.	MM	CASPT2 ΔE
S₁ (180)				
Root1 (S ₀)	-565.94750	-570.91742	-91.06277	13.6
Root2 (S ₁)	-565.86241	-570.84923		56.4
S₁ (170)				
Root1 (S ₀)	-565.94799	-570.91884	-91.06253	12.7
Root2 (S ₁)	-565.86400	-570.85185		54.7
S₁ (160)				
Root1 (S ₀)	-565.94471	-570.91715	-91.06175	13.7
Root2 (S ₁)	-565.86577	-570.85423		53.2
S₁ (150)				
Root1 (S ₀)	-565.94062	-570.91242	-91.06104	16.7
Root2 (S ₁)	-565.86709	-570.85730		51.3
S₁ (140)				
Root1 (S ₀)	-565.93313	-570.90540	-91.06029	21.1
Root2 (S ₁)	-565.86820	-570.85995		49.6
S₁ (130)				
Root1 (S ₀)	-565.92312	-570.89506	-91.05955	27.6
Root2 (S ₁)	-565.86861	-570.86113		48.9
S₁ (120)				
Root1 (S ₀)	-565.91277	-570.88431	-91.05847	34.3
Root2 (S ₁)	-565.86902	-570.86287		47.8

S₁ (110)				
Root1 (S ₀)	-565.89818	-570.87045	-91.05694	43.0
Root2 (S ₁)	-565.87076	-570.85940		49.9
S₁ (100)				
Root1 (S ₀)	-565.88314	-570.85811	-91.05491	50.8
Root2 (S ₁)	-565.87470	-570.86015		49.5
S₁ (90)				
Root1 (S ₀)	-565.88200	-570.86483	-91.05288	46.6
Root2 (S ₁)	-565.87699	-570.85938		50.0
S₁ (80)				
Root1 (S ₀)	-565.88948	-570.87037	-91.05377	43.1
Root2 (S ₁)	-565.86773	-570.85694		51.5
S₁ (70)				
Root1 (S ₀)	-565.89956	-570.87719	-91.06070	38.8
Root2 (S ₁)	-565.86185	-570.85443		53.1
S₁ (60)				
Root1 (S ₀)	-565.90546	-570.88438	-91.06108	34.3
Root2 (S ₁)	-565.85571	-570.85150		54.9
S₁ (50)				
Root1 (S ₀)	-565.90934	-570.88908	-91.06152	31.3
Root2 (S ₁)	-565.85063	-570.84783		57.2
S₁ (40)				
Root1 (S ₀)	-565.91142	-570.89148	-91.06176	29.8
Root2 (S ₁)	-565.84663	-570.84427		59.5
S₁ (30)				
Root1 (S ₀)	-565.91057	-570.88863	-91.06189	31.6
Root2 (S ₁)	-565.84383	-570.84106		61.5
S₁ (20)				

Root1 (S ₀)	-565.90611	-570.88594	-91.06181	33.3
Root2 (S ₁)	-565.84208	-570.83922		62.6
S₁ (10)				
Root1 (S ₀)	-565.90585	-570.88124	-91.06184	36.3
Root2 (S ₁)	-565.84109	-570.83759		63.7
S₁ (0)				
Root1 (S ₀)	-565.90460	-570.87946	-91.06183	37.4
Root2 (S ₁)	-565.84062	-570.83695		64.1

Table S7. Absolute Energies (A.E., Hartree) and Relative Energies (ΔE , kcal/mol) of All Structures along the C2-N3-N4-C5 Photoisomerization Path of the Azobenzene Chromophore in Gas Phase (Relaxed in the S₁ State). For a Plot of the Corresponding Energy Profile see the Right Panel of Figure 2 in the Main Text.

(C2N3N4C5)	CASPT2 A.E.	CASPT2 ΔE
S₀-TRANS		
Root1 (S ₀)	-570.92396	0
S₁ (180)		
Root1 (S ₀)	-570.91037	8.5
Root2 (S ₁)	-570.84194	51.5
S₁ (170)		
Root1 (S ₀)	-570.90982	8.9
Root2 (S ₁)	-570.84204	51.4
S₁ (160)		
Root1 (S ₀)	-570.90716	10.5
Root2 (S ₁)	-570.84260	51.0
S₁ (150)		

Root1 (S_0)	-570.90232	13.6
Root2 (S_1)	-570.84345	50.2
S_1 (140)		
Root1 (S_0)	-570.89542	17.9
Root2 (S_1)	-570.84448	49.9
S_1 (130)		
Root1 (S_0)	-570.88700	23.2
Root2 (S_1)	-570.84524	49.4
S_1 (120)		
Root1 (S_0)	-570.87667	29.7
Root2 (S_1)	-570.84571	49.1
S_1 (110)		
Root1 (S_0)	-570.86517	36.9
Root2 (S_1)	-570.84367	50.4
S_1 (100)		
Root1 (S_0)	-570.85139	45.5
Root2 (S_1)	-570.84027	52.5
S_1 (90)		
Root1 (S_0)	-570.84924	46.9
Root2 (S_1)	-570.83970	52.9
S_1 (80)		
Root1 (S_0)	-570.85328	44.4
Root2 (S_1)	-570.83820	53.8
S_1 (70)		
Root1 (S_0)	-570.86672	35.9
Root2 (S_1)	-570.83902	53.3
S_1 (60)		
Root1 (S_0)	-570.87545	30.4

Root2 (S ₁)	-570.83887	53.4
S₁ (50)		
Root1 (S ₀)	-570.88205	26.3
Root2 (S ₁)	-570.83517	55.7
S₁ (40)		
Root1 (S ₀)	-570.88460	24.7
Root2 (S ₁)	-570.83132	58.1
S₁ (30)		
Root1 (S ₀)	-570.88585	23.9
Root2 (S ₁)	-570.82786	60.3
S₁ (20)		
Root1 (S ₀)	-570.88501	24.4
Root2 (S ₁)	-570.82479	62.2
S₁ (10)		
Root1 (S ₀)	-570.88279	25.8
Root2 (S ₁)	-570.82231	63.8
S₁ (0)		
Root1 (S ₀)	-570.87992	27.6
Root2 (S ₁)	-570.82042	65.0

Table S8. Absolute Energies (A.E., Hartree), Relative Energies (ΔE , kcal/mol), and MM Energies (A.E., Hartree) of All Structures along the C2-N3-N4-C5 Photoisomerization Path of the Azobenzene Chromophore in **azo-DNA-I** (Relaxed in the S₁ State). For a Plot of the Corresponding Energy Profile see Figure S4.

(C2N3N4C5)	OM2/MRCI A.E.	MM	OM2/MRCI ΔE
S₁ (180)			
Root1 (S ₀)	0.11900	-91.06273	13.6

Root2 (S ₁)	0.17531		48..9
S₁ (170)			
Root1 (S ₀)	0.11911	-91.06256	13.7
Root2 (S ₁)	0.17473		48.6
S₁ (160)			
Root1 (S ₀)	0.12013	-91.06182	14.9
Root2 (S ₁)	0.17408		48.7
S₁ (150)			
Root1 (S ₀)	0.12312	-91.06114	17.2
Root2 (S ₁)	0.17166		47.6
S₁ (140)			
Root1 (S ₀)	0.12773	-91.06039	20.5
Root2 (S ₁)	0.16905		46.5
S₁ (130)			
Root1 (S ₀)	0.13504	-91.05966	25.6
Root2 (S ₁)	0.16668		45.4
S₁ (120)			
Root1 (S ₀)	0.14391	-91.05871	31.7
Root2 (S ₁)	0.16492		44.9
S₁ (110)			
Root1 (S ₀)	0.15537	-91.05814	39.3
Root2 (S ₁)	0.16415		44.8
S₁ (100)			
Root1 (S ₀)	0.15950	-91.05583	43.3
Root2 (S ₁)	0.15950		43.3
S₁ (90)			
Root1 (S ₀)	0.15254	-91.05421	36.0
Root2 (S ₁)	0.16146		41.1

S₁ (80)			
Root1 (S ₀)	0.14404	-91.05451	29.7
Root2 (S ₁)	0.16560		43.1
S₁ (70)			
Root1 (S ₀)	0.13450	-91.06142	24.1
Root2 (S ₁)	0.16792		45.1
S₁ (60)			
Root1 (S ₀)	0.12767	-91.06148	19.8
Root2 (S ₁)	0.17144		47.3
S₁ (50)			
Root1 (S ₀)	0.12302	-91.06167	16.8
Root2 (S ₁)	0.17501		49.4
S₁ (40)			
Root1 (S ₀)	0.11991	-91.06176	14.7
Root2 (S ₁)	0.17822		51.3
S₁ (30)			
Root1 (S ₀)	0.11960	-91.06175	14.6
Root2 (S ₁)	0.18047		52.8
S₁ (20)			
Root1 (S ₀)	0.12059	-91.06161	15.3
Root2 (S ₁)	0.18188		53.7
S₁ (10)			
Root1 (S ₀)	0.12351	-91.06160	17.1
Root2 (S ₁)	0.18255		54.2
S₁ (0)			
Root1 (S ₀)	0.12434	-91.06159	17.6
Root2 (S ₁)	0.18272		54.3

Table S9. Absolute Energies (A.E., Hartree), Relative Energies (ΔE , kcal/mol), and MM Energies (A.E., Hartree) of All Structures along the C2-N3-N4-C5 Photoisomerization Path of the Azobenzene Chromophore in **azo-DNA-II** (Relaxed in the S_1 State). For a Plot of the Corresponding Energy Profile see Figure S5.

(C2N3N4C5)	OM2/MRCI A.E.	MM	OM2/MRCI ΔE
S₁ (-180)			
Root1 (S ₀)	0.12097	-90.30913	7.6
Root2 (S ₁)	0.17894		43.9
S₁ (-170)			
Root1 (S ₀)	0.12146	-90.30940	7.7
Root2 (S ₁)	0.17899		43.8
S₁ (-160)			
Root1 (S ₀)	0.12496	-90.30955	9.8
Root2 (S ₁)	0.17903		43.7
S₁ (-150)			
Root1 (S ₀)	0.13188	-90.30928	14.3
Root2 (S ₁)	0.17859		43.6
S₁ (-140)			
Root1 (S ₀)	0.14148	-90.30865	20.7
Root2 (S ₁)	0.17812		43.7
S₁ (-130)			
Root1 (S ₀)	0.15307	-90.30752	28.7
Root2 (S ₁)	0.17797		44.3
S₁ (-120)			
Root1 (S ₀)	0.16694	-90.30645	38.1
Root2 (S ₁)	0.17874		45.5

S₁ (-110)			
Root1 (S ₀)	0.17821	-90.30426	46.5
Root2 (S ₁)	0.17883		46.9
S₁ (-100)			
Root1 (S ₀)	0.17351	-90.30752	41.5
Root2 (S ₁)	0.17565		42.9
S₁ (-90)			
Root1 (S ₀)	0.16629	-90.30778	36.8
Root2 (S ₁)	0.17742		43.8
S₁ (-80)			
Root1 (S ₀)	0.15765	-90.30755	31.6
Root2 (S ₁)	0.17929		45.1
S₁ (-70)			
Root1 (S ₀)	0.15140	-90.30755	27.6
Root2 (S ₁)	0.18160		46.6
S₁ (-60)			
Root1 (S ₀)	0.14768	-90.30773	25.2
Root2 (S ₁)	0.18387		47.9
S₁ (-50)			
Root1 (S ₀)	0.14488	-90.30782	23.4
Root2 (S ₁)	0.18587		49.1
S₁ (-40)			
Root1 (S ₀)	0.14346	-90.30793	22.4
Root2 (S ₁)	0.18753		50.1
S₁ (-30)			
Root1 (S ₀)	0.14403	-90.30807	22.7
Root2 (S ₁)	0.18845		50.6
S₁ (-20)			

Root1 (S ₀)	0.14423	-90.30837	22.6
Root2 (S ₁)	0.18926		50.9
S₁ (-10)			
Root1 (S ₀)	0.14627	-90.30860	23.8
Root2 (S ₁)	0.18960		51.0
S₁ (0)			
Root1 (S ₀)	0.14694	-90.30856	24.2
Root2 (S ₁)	0.18952		50.9

Table S10. Absolute Energies (A.E., Hartree), Relative Energies (ΔE , kcal/mol), and MM Energies (A.E., Hartree) of All Structures along the C2-N3-N4-C5 Photoisomerization Path of the Azobenzene Chromophore in **azo-DNA-II** (Relaxed in the S₁ State). For a Plot of the Corresponding Energy Profile see Figure S5.

(C2N3N4C5)	CASSCF A.E.	CASPT2 A.E.	MM	CASPT2 ΔE
S₁ (-180)				
Root1 (S ₀)	-565.94322	-570.90967	-90.30803	15.0
Root2 (S ₁)	-565.85867	-570.84249		57.2
S₁ (-170)				
Root1 (S ₀)	-565.94039	-570.90695	-90.30777	16.7
Root2 (S ₁)	-565.85796	-570.84168		57.7
S₁ (-160)				
Root1 (S ₀)	-565.93927	-570.90505	-90.30947	17.9
Root2 (S ₁)	-565.84345	-570.84352		56.5
S₁ (-150)				
Root1 (S ₀)	-565.92996	-570.89627	-90.30904	23.4
Root2 (S ₁)	-565.84243	-570.84286		57.0

S₁ (-140)				
Root1 (S ₀)	-565.91693	-570.88410	-90.30800	31.1
Root2 (S ₁)	-565.84094	-570.84190		57.6
S₁ (-130)				
Root1 (S ₀)	-565.90237	-570.87154	-90.30694	39.0
Root2 (S ₁)	-565.85166	-570.84104		58.1
S₁ (-120)				
Root1 (S ₀)	-565.88487	-570.85511	-90.30486	49.3
Root2 (S ₁)	-565.84957	-570.83871		59.6
S₁ (-110)				
Root1 (S ₀)	-565.86792	-570.83946	-90.30280	59.1
Root2 (S ₁)	-565.84864	-570.83756		60.3
S₁ (-100)				
Root1 (S ₀)	-565.85826	-570.84580	-90.30538	55.1
Root2 (S ₁)	-565.85031	-570.83665		60.9
S₁ (-90)				
Root1 (S ₀)	-565.86972	-570.84534	-90.30538	55.4
Root2 (S ₁)	-565.84721	-570.84051		58.4
S₁ (-80)				
Root1 (S ₀)	-565.87678	-570.85186	-90.30595	51.3
Root2 (S ₁)	-565.84293	-570.84183		57.6
S₁ (-70)				
Root1 (S ₀)	-565.88154	-570.85701	-90.30776	48.1
Root2 (S ₁)	-565.82129	-570.83783		60.1
S₁ (-60)				
Root1 (S ₀)	-565.88642	-570.85958	-90.30763	46.5
Root2 (S ₁)	-565.83505	-570.83262		63.4
S₁ (-50)				

Root1 (S ₀)	-565.88973	-570.86314	-90.30769	44.2
Root2 (S ₁)	-565.81359	-570.83078		64.5
S₁ (-40)				
Root1 (S ₀)	-565.89095	-570.86404	-90.30777	43.7
Root2 (S ₁)	-565.81224	-570.82827		66.1
S₁ (-30)				
Root1 (S ₀)	-565.89067	-570.86224	-90.30767	44.8
Root2 (S ₁)	-565.80950	-570.82428		68.6
S₁ (-20)				
Root1 (S ₀)	-565.89115	-570.86297	-90.30766	44.3
Root2 (S ₁)	-565.82982	-570.82362		69.0
S₁ (-10)				
Root1 (S ₀)	-565.89066	-570.86222	-90.30770	44.8
Root2 (S ₁)	-565.82944	-570.82340		69.2

Table S11. Absolute Energies (A.E., Hartree), Relative Energies (ΔE , kcal/mol), and MM Energies (A.E., Hartree) of All Structures along the C2-N3-N4-C5 Photoisomerization Path of the Azobenzene Chromophore in **azo-DNA-I** (Relaxed in the S₀ State). For a Plot of the Corresponding Energy Profile see Figure S6.

(C2N3N4C5)	CASSCF A.E.	CASPT2 A.E.	MM	CASPT2 ΔE
S₀ (180)				
Root1 (S ₀)	-565.96678	-570.93783	-91.05997	0.8
S₀ (170)				
Root1 (S ₀)	-565.96803	-570.93803	-91.05986	0.6
S₀ (160)				
Root1 (S ₀)	-565.96442	-570.93505	-91.05950	2.5

S₀ (150)				
Root1 (S ₀)	-565.96045	-570.93033	-91.05838	5.5
S₀ (140)				
Root1 (S ₀)	-565.95557	-570.92619	-91.05615	8.1
S₀ (130)				
Root1 (S ₀)	-565.94580	-570.91542	-91.05428	14.8
S₀ (120)				
Root1 (S ₀)	-565.93434	-570.90337	-91.05237	22.4
S₀ (110)				
Root1 (S ₀)	-565.91976	-570.88945	-91.05149	31.1
S₀ (100)				
Root1 (S ₀)	-565.90567	-570.88239	-91.05385	35.5
S₀ (90)				
Root1 (S ₀)	-565.90066	-570.87565	-91.06002	39.8
S₀ (80)				
Root1 (S ₀)	-565.90597	-570.87792	-91.05562	38.4
S₀ (70)				
Root1 (S ₀)	-565.91650	-570.88885	-91.05611	31.5
S₀ (60)				
Root1 (S ₀)	-565.92621	-570.90007	-91.05547	24.5
S₀ (50)				
Root1 (S ₀)	-565.93054	-570.90568	-91.05798	20.9
S₀ (40)				
Root1 (S ₀)	-565.93631	-570.91160	-91.05809	17.2
S₀ (30)				
Root1 (S ₀)	-565.94077	-570.91659	-91.05774	14.1
S₀ (20)				
Root1 (S ₀)	-565.94224	-570.91881	-91.05567	12.7

S₀ (10)				
Root1 (S ₀)	-565.94164	-570.92080	-91.05508	11.4
S₀ (0)				
Root1 (S ₀)	-565.94257	-570.92119	-91.05461	11.2

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7. Cartesian Coordinates of All Optimized Structures (QM part)

In xyz format (unit: Å)

CASSCF method

S0-TRANS-I

C	20.999074800	23.294267200	37.544472200
C	22.328560300	23.622994900	37.715769100
C	22.678726100	24.902160500	38.101454900
C	21.704073300	25.862764300	38.307632400
C	20.370638300	25.530568400	38.152720300
C	20.011902600	24.241014600	37.776936900
H	20.740566800	22.292374500	37.269049100
H	23.099321000	22.892055700	37.591297500
H	21.980835600	26.840980600	38.638085400
H	19.632740400	26.279340800	38.361187500
C	25.882661500	26.369886700	38.872721000
C	26.468448100	27.619175100	38.830320100
C	26.605950900	25.278710600	39.330931700
C	27.789806500	27.780762500	39.207268900
H	25.883949200	28.454382700	38.504941000
C	27.926529600	25.438661400	39.700241800
H	26.128103100	24.325212000	39.394505400
C	28.523805800	26.688609200	39.632535200
H	28.242181700	28.750850000	39.166525700
H	28.486817900	24.585387100	40.025389600
H	29.550833200	26.811797100	39.907762500
N	24.068255900	25.093573900	38.385871600
N	24.506306000	26.285590800	38.439755100

S0-CIS-I

C	20.898878000	23.601827400	36.748831900
C	22.117950800	24.198442400	36.471948500
C	22.374887100	25.473112000	36.946830200
C	21.446462800	26.114680300	37.747540200
C	20.231892000	25.514328500	38.020372600
C	19.928092700	24.273464700	37.478531300
H	20.703844000	22.622332900	36.362696400
H	22.833404800	23.679897000	35.866736400
H	21.652254700	27.098629400	38.114336200
H	19.529422000	26.046226100	38.632907700
C	25.251588100	25.638117400	37.945224900
C	26.508953700	26.189859700	38.252358300
C	24.803278100	24.530194300	38.612436100
C	27.303544400	25.630768400	39.205720200
H	26.816925100	27.048719200	37.696729900
C	25.629714000	23.933898500	39.576787200
H	23.859506700	24.093239300	38.388489200
C	26.863796400	24.471938800	39.864971900
H	28.263504500	26.052293900	39.431348800
H	25.307955600	23.039088500	40.068131300
H	27.502041800	23.982819300	40.568602600
N	23.471751200	26.274051100	36.443923300
N	24.629634700	26.342000500	36.864866700

S1-TRANS-I

C	20.961237500	23.259965900	37.568427000
C	22.293701600	23.597505300	37.678770600
C	22.650424300	24.879878000	38.059393900
C	21.669266100	25.823115700	38.318966300

C	20.335585200	25.483044600	38.193037100
C	19.970399600	24.199594700	37.813936600
H	20.704713600	22.254348000	37.305536600
H	23.055120800	22.873104500	37.486549600
H	21.946896200	26.806073400	38.630919500
H	19.603308900	26.233583400	38.414078300
C	25.946194900	26.397007800	38.891490100
C	26.550153700	27.645528100	38.865401400
C	26.660859500	25.300932100	39.353807200
C	27.867258000	27.789325500	39.255851600
H	25.987908300	28.492336300	38.531996600
C	27.983528300	25.450395400	39.729878200
H	26.182889300	24.346098000	39.411119200
C	28.597709100	26.690473400	39.674655000
H	28.329028100	28.755460900	39.223449900
H	28.534054700	24.588229200	40.046331500
H	29.627698600	26.802451700	39.946606300
N	24.022802600	25.168951200	38.168336000
N	24.619527600	26.299227200	38.413568900

S1-I C2N3N4C5 (degree)

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C	20.953265200	23.248809800	37.675697500
C	22.272557800	23.592441900	37.884461200
C	22.600842800	24.905097300	38.176752400
C	21.616041000	25.878988800	38.214425200
C	20.295065300	25.527152900	38.012310200
C	19.954539500	24.206655800	37.760985900
H	20.709578700	22.225997600	37.471502500

H	23.040224300	22.850928500	37.854303400
H	21.874242100	26.892198500	38.434233200
H	19.549962500	26.294238600	38.083225400
C	25.917287400	26.389150600	38.977444100
C	26.534375100	27.628814300	38.951864800
C	26.641302500	25.262796700	39.344529200
C	27.875765100	27.737239900	39.264676400
H	25.963279400	28.494493000	38.691543300
C	27.982342900	25.377848800	39.653009500
H	26.150789800	24.314868000	39.392377000
C	28.604820800	26.613346200	39.607128900
H	28.353531800	28.695636400	39.243270000
H	28.537985400	24.501795900	39.921523400
H	29.645245800	26.702174700	39.834512900
N	23.935221500	25.181995300	38.496668600
N	24.547311600	26.321069800	38.647674000

170

C	20.952377300	23.243751000	37.664857500
C	22.275674300	23.582321700	37.852996600
C	22.611470300	24.892671600	38.146061000
C	21.629319500	25.866056700	38.224938100
C	20.304497900	25.518637000	38.040549300
C	19.958764600	24.203851500	37.771439700
H	20.703545400	22.224347800	37.450935200
H	23.042570400	22.843778000	37.788099100
H	21.895858900	26.876711100	38.441603200
H	19.562714100	26.287186500	38.129165600
C	25.905966600	26.392347600	38.960253500

C	26.526649900	27.629944900	38.948410700
C	26.616482300	25.264475400	39.348228800
C	27.861690700	27.733657800	39.286444800
H	25.965401100	28.494904800	38.667029000
C	27.952763300	25.374726900	39.677584800
H	26.122278800	24.318943800	39.382111000
C	28.580618800	26.606658300	39.638027100
H	28.343443100	28.690358700	39.271927600
H	28.500290700	24.495194200	39.952064600
H	29.618476900	26.691347700	39.879912000
N	23.963415200	25.178506100	38.361552700
N	24.558080800	26.319636900	38.554384700

160

C	20.939909700	23.310113300	37.373653300
C	22.269349500	23.648317200	37.508859800
C	22.609999400	24.906636700	37.975058200
C	21.626435300	25.830336700	38.288223600
C	20.295842100	25.482484000	38.147614900
C	19.946041700	24.218841600	37.698427800
H	20.688140300	22.329635000	37.024303500
H	23.038729900	22.949144500	37.272112700
H	21.898242500	26.796836200	38.648470400
H	19.553016000	26.210106500	38.409792600
C	25.901808400	26.320429000	38.880917900
C	26.593481700	27.519468000	38.855915700
C	26.521433900	25.171602500	39.355124700
C	27.913940600	27.560685000	39.255806800
H	26.097608100	28.400509700	38.509320800

C	27.845332100	25.219665500	39.744089400
H	25.970438100	24.259220900	39.402966100
C	28.547310900	26.408842200	39.682347100
H	28.453040100	28.486602400	39.225364200
H	28.325173000	24.320357300	40.075053800
H	29.579486700	26.440872100	39.962302200
N	23.973575500	25.189903100	38.107274600
N	24.580154700	26.303943400	38.388341000

150

C	20.942793200	23.296485500	37.369709800
C	22.274074900	23.639045200	37.461885300
C	22.625662800	24.897635300	37.917392100
C	21.650405200	25.809500500	38.285448300
C	20.317636700	25.460628900	38.184998300
C	19.956436000	24.203923600	37.724389200
H	20.681278200	22.318292000	37.021861400
H	23.037949800	22.943785000	37.190090200
H	21.933597800	26.773969100	38.645701900
H	19.581505100	26.183660600	38.475914800
C	25.880322400	26.322633600	38.842309500
C	26.583170700	27.515770600	38.843310300
C	26.472432200	25.167633200	39.331968300
C	27.895643300	27.540186100	39.270285800
H	26.105596200	28.403831700	38.487528400
C	27.788299300	25.196832000	39.748317600
H	25.908472100	24.260989500	39.361978900
C	28.508747200	26.377099200	39.700089700
H	28.447512000	28.458491700	39.250856800

H	28.251609500	24.290382800	40.082363400
H	29.538377500	26.392442300	39.988613400
N	23.988801600	25.213762400	37.947827400
N	24.586870400	26.314083400	38.280643600

140

C	20.954679700	23.309316700	37.262969400
C	22.285055600	23.664594900	37.295371800
C	22.645579300	24.914322900	37.767092900
C	21.682436200	25.801221800	38.217406300
C	20.349776700	25.441624100	38.171971900
C	19.977777900	24.196614700	37.688208700
H	20.684010500	22.337807500	36.902813300
H	23.040629100	22.985411100	36.962920200
H	21.974351200	26.757782100	38.592826800
H	19.621516000	26.148173200	38.518810400
C	25.865872100	26.302420700	38.752006300
C	26.615796100	27.466466000	38.768797700
C	26.377315500	25.138010800	39.303510700
C	27.901693300	27.448328200	39.268981200
H	26.196602400	28.364075200	38.365656700
C	27.668455700	25.123397300	39.792545800
H	25.774413500	24.255919700	39.323203900
C	28.440108900	26.271044100	39.756217200
H	28.493319100	28.342153000	39.260501100
H	28.074102000	24.207421000	40.173000800
H	29.452906000	26.249985000	40.097858300
N	24.003827300	25.257075200	37.719950300
N	24.611292200	26.332254900	38.104800100

130

C	20.971946700	23.307049500	37.220096000
C	22.298596400	23.676920100	37.198218700
C	22.663127900	24.930569000	37.654297300
C	21.710591400	25.804076100	38.151853900
C	20.380773600	25.432206100	38.157447300
C	20.002901000	24.186662600	37.679288000
H	20.696956500	22.333220200	36.872177100
H	23.046943400	23.007530200	36.829102700
H	22.007366000	26.764583700	38.515154400
H	19.659831800	26.130235000	38.532982900
C	25.845136600	26.292104700	38.673890700
C	26.629707800	27.432702400	38.711843600
C	26.286341000	25.122566500	39.271605900
C	27.888088600	27.382836700	39.275298000
H	26.261025300	28.334656700	38.271537100
C	27.551161400	25.074289300	39.824411500
H	25.654171100	24.260018700	39.274772300
C	28.361700800	26.195715300	39.804885200
H	28.508997200	28.255340100	39.281873400
H	27.907544700	24.154458800	40.240246800
H	29.355645900	26.146792900	40.191423400
N	24.009963600	25.304944100	37.530673500
N	24.633816700	26.354989500	37.945556900

120

C	20.988029400	23.309287800	37.187518900
C	22.308881900	23.696961500	37.104776000

C	22.673837200	24.961191800	37.531313100
C	21.729208000	25.824140800	38.062624900
C	20.405776100	25.434278900	38.125600000
C	20.024257000	24.181276700	37.671594400
H	20.714041500	22.327236200	36.861149500
H	23.050188100	23.033364500	36.712412200
H	22.027151200	26.792362900	38.404134800
H	19.691772800	26.129133800	38.520830400
C	25.804146300	26.288792300	38.583997400
C	26.622821200	27.402345400	38.663487900
C	26.165447700	25.111662900	39.220421700
C	27.843401800	27.316737400	39.301577700
H	26.308981300	28.311320400	38.196123300
C	27.394067800	25.026740200	39.848662100
H	25.504469600	24.270964400	39.197088300
C	28.245606200	26.118089200	39.864296800
H	28.492772400	28.168528500	39.336555500
H	27.694913900	24.100244700	40.295011100
H	29.218991600	26.037624300	40.300429900
N	24.001070100	25.367566200	37.344446800
N	24.648803900	26.395844000	37.771841800

110

C	20.998555800	23.299798100	37.218531500
C	22.318326100	23.692404300	37.117084900
C	22.682291300	24.962877400	37.529574200
C	21.738996500	25.814145100	38.085313400
C	20.418562600	25.419308100	38.163552300
C	20.033181800	24.167448300	37.706462800

H	20.727811500	22.317828200	36.888870800
H	23.048361100	23.028581200	36.708160700
H	22.034820800	26.787983500	38.413672800
H	19.709241300	26.118001000	38.562042800
C	25.798391800	26.290880400	38.538993200
C	26.624101400	27.396828400	38.648847400
C	26.127683000	25.108656700	39.183380500
C	27.822761400	27.303934000	39.328632800
H	26.324269400	28.307413400	38.170882000
C	27.338719100	25.016420000	39.850289800
H	25.464515000	24.267997000	39.143517700
C	28.202727200	26.099509100	39.899549400
H	28.474360300	28.153570400	39.379502900
H	27.620004800	24.083646200	40.297639800
H	29.174606000	26.004265900	40.347517300
N	23.977482400	25.426283800	37.263737300
N	24.675129000	26.443927700	37.671359400

100

C	20.984155500	23.304083000	37.075590800
C	22.298189700	23.703472800	36.951150300
C	22.694373700	24.922637000	37.477307000
C	21.788776800	25.701504400	38.185434500
C	20.468880900	25.302703700	38.281809100
C	20.050127900	24.116144100	37.700769700
H	20.685469500	22.368284500	36.650947900
H	22.997249700	23.093301100	36.420054600
H	22.097406800	26.637134900	38.598351900
H	19.782147100	25.948998900	38.790418300

C	25.771934000	26.269192900	38.482917300
C	26.629747000	27.353362200	38.580248800
C	26.059551300	25.093244000	39.158327800
C	27.808372500	27.248388600	39.291713100
H	26.378416800	28.254859000	38.062011600
C	27.251794400	24.983411700	39.855142100
H	25.384903300	24.262685000	39.108684000
C	28.136538200	26.049799000	39.902417300
H	28.482583700	28.079020500	39.343450500
H	27.502041000	24.056684300	40.330613700
H	29.083342400	25.948093600	40.392758400
N	23.949470200	25.454357300	37.133497600
N	24.675047400	26.453796000	37.573979900

90

C	21.014781100	23.305270000	36.933906600
C	22.304232000	23.739553600	36.702549000
C	22.680271200	25.013303300	37.093337400
C	21.776415400	25.822983300	37.773835200
C	20.488138200	25.380702000	38.004443800
C	20.084935900	24.133256800	37.546888900
H	20.732609900	22.323003400	36.617285800
H	23.014657900	23.113682800	36.209317100
H	22.073482300	26.801527900	38.092587400
H	19.808076200	26.038909300	38.509450600
C	25.660938000	26.137248000	38.153752400
C	26.691073300	27.055946300	38.301543600
C	25.647591800	24.979595000	38.914746400
C	27.745969800	26.795186900	39.152973300

H	26.668831100	27.945122200	37.704453300
C	26.714331700	24.716308900	39.759436700
H	24.848687200	24.275743900	38.817344100
C	27.774931200	25.603264900	39.858864700
H	28.554911900	27.492651000	39.237144100
H	26.740001700	23.798515200	40.309038500
H	28.629622200	25.368161600	40.463061200
N	23.942285900	25.476733800	36.710767800
N	24.720376400	26.453481600	37.120348200

80

C	21.020873600	23.314460000	36.951490500
C	22.305365900	23.764553800	36.713317700
C	22.663151400	25.044627400	37.103647800
C	21.754372200	25.844603400	37.787196900
C	20.471585500	25.390231800	38.017747500
C	20.084045600	24.139437000	37.557519200
H	20.749976200	22.324296200	36.645692900
H	23.022347200	23.147338300	36.212695100
H	22.044665800	26.826805300	38.097973800
H	19.786396900	26.038572600	38.526302600
C	25.674045000	26.128372100	38.140487800
C	26.708433400	27.039092900	38.292226400
C	25.647943900	24.975262700	38.907131000
C	27.748721600	26.780257300	39.157890300
H	26.699090700	27.923182000	37.693147500
C	26.705824000	24.704790800	39.760846200
H	24.843234000	24.278550100	38.809596300
C	27.762846300	25.591813700	39.866461500

H	28.553975000	27.478679100	39.260553800
H	26.721206600	23.787926700	40.316743500
H	28.606541200	25.357964300	40.478503800
N	23.898995900	25.540865600	36.686757400
N	24.759585900	26.441881700	37.089425900
70			
C	20.801279600	23.356913600	36.701416900
C	22.064249000	23.842967400	36.441613200
C	22.401540100	25.118890100	36.861182800
C	21.499990000	25.883140200	37.592746100
C	20.235939300	25.391170400	37.845851900
C	19.867723400	24.143342300	37.363918400
H	20.544278800	22.371358400	36.375170000
H	22.788559300	23.256652700	35.912154100
H	21.783040000	26.860376700	37.928523100
H	19.549804400	26.001619400	38.399248100
C	25.410442600	25.869005600	38.024991600
C	26.593144400	26.560244800	38.237566800
C	25.126609800	24.724537400	38.755149300
C	27.519320900	26.086576300	39.143714100
H	26.783520100	27.441269500	37.662477300
C	26.061623400	24.245370300	39.654120100
H	24.208617100	24.199770100	38.601618800
C	27.261880100	24.913329500	39.829788100
H	28.441533300	26.609742100	39.296253000
H	25.870168500	23.342552500	40.197421500
H	28.002778100	24.501090700	40.475973100
N	23.638779300	25.631683000	36.482526700

N	24.587972500	26.380885100	36.972090800
60			
C	20.803367500	23.369363100	36.709865000
C	22.061717500	23.870442000	36.447737200
C	22.388772600	25.148341400	36.868170900
C	21.477934100	25.900077800	37.600521700
C	20.220374000	25.393723000	37.857105100
C	19.861473400	24.142918900	37.373723800
H	20.557300800	22.381444800	36.380325200
H	22.789069500	23.291937200	35.918496700
H	21.750622600	26.879785000	37.934803100
H	19.531084600	25.997294400	38.413538700
C	25.423343000	25.858760700	37.997790500
C	26.604439400	26.546685000	38.225181300
C	25.124228400	24.722984300	38.733720900
C	27.514219300	26.077669100	39.149727200
H	26.806339900	27.418959700	37.640963900
C	26.046016600	24.248129000	39.649882000
H	24.211744000	24.192861000	38.570094700
C	27.246014100	24.910305700	39.843102600
H	28.436662900	26.599095900	39.306314000
H	25.846406900	23.346584500	40.193438900
H	27.977165700	24.503218500	40.508102900
N	23.613571100	25.685774800	36.472022300
N	24.621089200	26.355424900	36.931116700
50			
C	20.782325700	23.419616600	36.707356900

C	22.033899100	23.934475500	36.441122200
C	22.350533100	25.213635100	36.866002600
C	21.435737600	25.952757100	37.605864800
C	20.183214800	25.434313200	37.863607700
C	19.835377600	24.181650000	37.377519900
H	20.544728900	22.430773900	36.374125100
H	22.763524100	23.365980500	35.904317200
H	21.701964100	26.932110600	37.945869700
H	19.489138700	26.029337700	38.423675800
C	25.425144100	25.840689500	37.959508300
C	26.625602200	26.495932400	38.182263500
C	25.090275400	24.724507500	38.709787100
C	27.516060400	26.013919600	39.118487600
H	26.853991800	27.355386200	37.589313400
C	25.992418500	24.237163500	39.638889700
H	24.162606200	24.220010000	38.550586000
C	27.210017700	24.866650900	39.829665300
H	28.451949200	26.511603400	39.273532300
H	25.761187800	23.352599000	40.197690600
H	27.924631900	24.448852700	40.505748100
N	23.567140300	25.767509500	36.471302300
N	24.637751900	26.349690000	36.890225100

40

C	20.785143200	23.420916200	36.708095400
C	22.035276400	23.942419000	36.443422000
C	22.342558500	25.224811700	36.868064900
C	21.422132900	25.956810900	37.607319300
C	20.173592000	25.431730000	37.865700000

C	19.833688400	24.177937200	37.377271100
H	20.551820300	22.431591000	36.373014300
H	22.767591100	23.376461400	35.906369000
H	21.683767200	26.938098100	37.946032700
H	19.477341300	26.022085100	38.427881500
C	25.432955000	25.833398400	37.952550600
C	26.631676800	26.489978800	38.179487800
C	25.091625100	24.722978200	38.708957200
C	27.517463700	26.010498100	39.121027600
H	26.862810800	27.348284500	37.586484300
C	25.990888000	24.234967800	39.640161700
H	24.161955000	24.222195100	38.550052800
C	27.208380500	24.863801700	39.831530500
H	28.452600000	26.508152000	39.279841600
H	25.758231100	23.349819300	40.197436000
H	27.921437600	24.444311400	40.506615400
N	23.549477500	25.799871500	36.487295800
N	24.662700300	26.324105800	36.863626500

30

C	20.757002200	23.478183900	36.706235000
C	22.007621000	24.011180100	36.469099400
C	22.300854200	25.290771100	36.915153400
C	21.359639900	26.010047500	37.640859200
C	20.110745600	25.474080200	37.871098800
C	19.790177100	24.219424700	37.370104700
H	20.536841500	22.491252600	36.354705500
H	22.752511700	23.456296300	35.938457900
H	21.608871900	26.988824000	37.996183200

H	19.400336300	26.054400100	38.425585500
C	25.460003100	25.815247800	37.952603300
C	26.685715400	26.431382700	38.145097100
C	25.097094700	24.726081200	38.729408800
C	27.573058700	25.934463500	39.075799600
H	26.933499600	27.274763400	37.536886500
C	25.998375900	24.219302700	39.648828000
H	24.147095400	24.257085100	38.597181400
C	27.238158600	24.810206400	39.810253000
H	28.528142900	26.400768600	39.208626900
H	25.747387300	23.348375600	40.220667000
H	27.948788500	24.377544900	40.479432400
N	23.512497000	25.872664700	36.577381400
N	24.680621200	26.324206400	36.878936300

20

C	20.756593700	23.482865400	36.706479300
C	22.008013800	24.018663600	36.479684500
C	22.294182200	25.300047400	36.931504400
C	21.345253300	26.015725600	37.652914400
C	20.097120300	25.475552700	37.873159600
C	19.785737400	24.220629700	37.368590300
H	20.538985600	22.496853000	36.350383200
H	22.756998100	23.467163300	35.949947600
H	21.591254000	26.994062700	38.010828800
H	19.382472100	26.052560900	38.426671600
C	25.474070900	25.809722700	37.942258800
C	26.697894100	26.427987000	38.137898900
C	25.102916300	24.725706800	38.722611600

C	27.577406600	25.934146800	39.077256700
H	26.947615000	27.269597900	37.529281600
C	25.997408600	24.220615100	39.647078200
H	24.151489600	24.259705400	38.587657000
C	27.236466100	24.812559000	39.811245500
H	28.530426000	26.402057900	39.216806000
H	25.742555800	23.351673000	40.219564900
H	27.942377000	24.380465300	40.483863900
N	23.502325500	25.888658900	36.624207300
N	24.702866300	26.305986000	36.852455800

10

C	20.733563300	23.517176900	36.726951300
C	21.989020900	24.052755200	36.528307300
C	22.267153600	25.330640300	36.998089700
C	21.305712500	26.041781400	37.708595800
C	20.052783200	25.502166900	37.897219300
C	19.752161700	24.250249900	37.378785600
H	20.522436800	22.534614200	36.358971700
H	22.746635900	23.505516800	36.005175100
H	21.549402600	27.014938300	38.082673500
H	19.328517200	26.076081300	38.440910600
C	25.503324200	25.805169300	37.964450200
C	26.737247900	26.413624200	38.120082300
C	25.141764200	24.730070900	38.761832800
C	27.636691100	25.918502000	39.039351600
H	26.978355100	27.249743400	37.500138000
C	26.055765100	24.222752000	39.664481100
H	24.181176800	24.275355100	38.655155100

C	27.303354200	24.806215000	39.790542600
H	28.597649600	26.377028300	39.150187500
H	25.807880500	23.359513300	40.247471600
H	28.021639500	24.372620100	40.446796500
N	23.482484500	25.921284700	36.737724500
N	24.704229500	26.303070700	36.891803500
O			
C	20.735084800	23.517110900	36.725915700
C	21.991302200	24.053702200	36.532865900
C	22.264619900	25.332282600	37.005340000
C	21.300189600	26.040512800	37.714534200
C	20.048672800	25.498951000	37.899132700
C	19.751645100	24.247586300	37.377309800
H	20.524352000	22.535831400	36.354048000
H	22.750910600	23.506197800	36.012532300
H	21.543904400	27.012503000	38.091128700
H	19.323130500	26.070457600	38.443361300
C	25.506851100	25.804489700	37.959038700
C	26.738582000	26.415520700	38.117440200
C	25.142924100	24.731229500	38.758191000
C	27.636474800	25.921009900	39.038770200
H	26.979734300	27.252566000	37.498295400
C	26.056334500	24.223128500	39.660669600
H	24.181838100	24.277616200	38.651108100
C	27.303214500	24.807550400	39.788095000
H	28.597004700	26.380055800	39.151169300
H	25.809324800	23.357213000	40.240216300
H	28.020847000	24.374479400	40.445440900

N	23.477045300	25.932898900	36.762640600
N	24.711475900	26.289681100	36.875691600

S0-I C2N3N4C5 (degree)

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C	21.010753600	23.295294400	37.574722400
C	22.335124000	23.624559800	37.789880100
C	22.676986700	24.908180600	38.166639100
C	21.696376400	25.874940800	38.304740500
C	20.367596300	25.544000100	38.109362100
C	20.016030800	24.245494400	37.757795200
H	20.759408100	22.288584200	37.311324200
H	23.104541200	22.885270200	37.712146800
H	21.963806000	26.859765700	38.622151400
H	19.626743800	26.300400600	38.271425200
C	25.891317400	26.384882200	38.912942300
C	26.468888100	27.636096700	38.846618000
C	26.640718000	25.299166800	39.343757800
C	27.802690000	27.809036600	39.172918200
H	25.868546800	28.469171800	38.544898000
C	27.973176900	25.469373500	39.666713000
H	26.173578000	24.342576700	39.424661700
C	28.560476800	26.723158200	39.576212000
H	28.248967200	28.780371100	39.114107900
H	28.552649400	24.623209600	39.975141700
H	29.595373000	26.854135400	39.816817400
N	24.051139100	25.103940000	38.527032300
N	24.498146000	26.293263200	38.533618500

170

C	21.005368100	23.272262200	37.581271100
C	22.338993200	23.598571200	37.728891000
C	22.700248500	24.885683900	38.079110300
C	21.730239700	25.852333400	38.275695600
C	20.393726700	25.524297700	38.139791500
C	20.024507400	24.229719500	37.794539700
H	20.738344800	22.265217900	37.332448800
H	23.103480700	22.861709800	37.606355400
H	22.015506200	26.836319600	38.577390100
H	19.661729100	26.283040300	38.332640400
C	25.889668200	26.386544400	38.845816600
C	26.461536800	27.643567300	38.815524400
C	26.621444600	25.305430000	39.312521400
C	27.774203700	27.821709300	39.214287200
H	25.873727900	28.471780000	38.480704200
C	27.934202800	25.481500800	39.701794700
H	26.155567000	24.346042900	39.365357500
C	28.515793800	26.738760200	39.647976400
H	28.216259400	28.797714500	39.182200000
H	28.502556400	24.634556600	40.030840400
H	29.537374100	26.874996600	39.940895400
N	24.098524500	25.086715500	38.318065700
N	24.524730100	26.284098900	38.381174300

160

C	21.013756800	23.289932500	37.445608400
C	22.350675600	23.624792600	37.519649000
C	22.722525900	24.900351700	37.900038500

C	21.759634200	25.846714200	38.202566000
C	20.419770200	25.511120300	38.132413100
C	20.040577400	24.229226600	37.753031000
H	20.739099400	22.292171100	37.171030600
H	23.111509800	22.903341400	37.311678600
H	22.055018000	26.819792000	38.528120000
H	19.694444700	26.254760100	38.396196100
C	25.871657300	26.390261800	38.765421400
C	26.457572700	27.641659500	38.790713700
C	26.553567800	25.297619400	39.277614000
C	27.737800100	27.801373300	39.288271100
H	25.905842200	28.478650400	38.418891500
C	27.836933400	25.454945100	39.762265300
H	26.074179000	24.343900000	39.292734000
C	28.434700800	26.705283700	39.762558800
H	28.191329700	28.772459300	39.300032200
H	28.368682100	24.597784800	40.123779900
H	29.433550800	26.827677600	40.130387000
N	24.133248800	25.109565700	38.037511700
N	24.546671900	26.304695500	38.199866900

150

C	21.018989000	23.330935900	37.270995300
C	22.352008100	23.685458900	37.266151400
C	22.733479200	24.939870100	37.701822300
C	21.784397100	25.845208200	38.142723900
C	20.447332500	25.491922900	38.144915700
C	20.057756700	24.232941900	37.703517700
H	20.736811600	22.349101300	36.952228700

H	23.105027500	22.993339300	36.951982900
H	22.091105400	26.799117300	38.513004800
H	19.732658100	26.203699800	38.507215900
C	25.838844400	26.379048700	38.672570400
C	26.475009700	27.603937300	38.747121600
C	26.430110600	25.256982500	39.229915400
C	27.723873000	27.705031100	39.330146700
H	25.987503700	28.465645100	38.342837800
C	27.684348300	25.354777300	39.801708100
H	25.906615400	24.326700500	39.213910100
C	28.338763500	26.575621500	39.842797800
H	28.219407000	28.653690700	39.378100500
H	28.147967500	24.474247700	40.198731700
H	29.316358800	26.651969300	40.272672300
N	24.146221800	25.168549500	37.735535400
N	24.557136700	26.346722600	38.018893200

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C	21.012173200	23.382915600	37.025777400
C	22.338234900	23.757368100	36.962701800
C	22.736355100	24.974894800	37.481446600
C	21.813542800	25.819164300	38.073843800
C	20.482757600	25.445832000	38.132473800
C	20.074104300	24.230231500	37.597990600
H	20.718219900	22.430526500	36.637604500
H	23.074988500	23.107909300	36.538325000
H	22.135772500	26.739539000	38.510278400
H	19.787148300	26.109249600	38.606402100
C	25.803985900	26.312809000	38.557212700

C	26.547435200	27.475908800	38.653853600
C	26.249071100	25.152876700	39.168633800
C	27.768742200	27.466992000	39.297726700
H	26.167526800	28.371703600	38.210677300
C	27.476614200	25.141457900	39.806130800
H	25.639977300	24.276146100	39.139314600
C	28.245796700	26.291519800	39.853710700
H	28.353108100	28.363057400	39.355425500
H	27.831090500	24.230094100	40.244750200
H	29.209562000	26.279013600	40.319514000
N	24.142395700	25.230079800	37.418017000
N	24.569602100	26.372096200	37.828270900

130

C	21.031181400	23.360199000	37.034415300
C	22.351128700	23.743472900	36.917571400
C	22.758962300	24.968870600	37.410954400
C	21.855493100	25.802527900	38.048313000
C	20.529270900	25.421800500	38.155254100
C	20.106800100	24.208743200	37.626619100
H	20.729052200	22.404638600	36.661083400
H	23.072818100	23.100844100	36.459571700
H	22.187897900	26.725864400	38.469981700
H	19.847271900	26.081770700	38.653306200
C	25.764823200	26.321802000	38.484940600
C	26.512358800	27.478542700	38.635690500
C	26.163785200	25.153075600	39.111383500
C	27.698196300	27.451017500	39.340276600
H	26.164751300	28.382228400	38.182901800

C	27.360048100	25.122618100	39.806594600
H	25.547411100	24.283541200	39.047190800
C	28.137984400	26.262959700	39.900463600
H	28.287134600	28.340636000	39.437902500
H	27.685583000	24.203037600	40.250963700
H	29.080977700	26.234966800	40.406364700
N	24.147591800	25.258304600	37.244684400
N	24.590258300	26.398055500	37.674074900

120

C	21.047938300	23.358485700	36.961840900
C	22.356808200	23.755905400	36.791761400
C	22.774368800	24.980282000	37.280276200
C	21.891522400	25.797559900	37.968136100
C	20.574881200	25.402506600	38.126974200
C	20.140475600	24.192983700	37.599400100
H	20.738015700	22.405314500	36.589105800
H	23.063374400	23.129374400	36.290021100
H	22.230017000	26.723370400	38.380394700
H	19.907341700	26.051539100	38.658362800
C	25.713660800	26.317518000	38.388756100
C	26.479189600	27.457062800	38.584779300
C	26.039298500	25.142315200	39.045700700
C	27.616442300	27.404013000	39.361098200
H	26.183866100	28.365453600	38.105198500
C	27.190151400	25.086504400	39.813966000
H	25.407363700	24.286517600	38.948208800
C	27.991647200	26.206214300	39.948535300
H	28.221103800	28.278937300	39.490584900

H	27.465654800	24.161802000	40.281690000
H	28.903615400	26.156701700	40.506302900
N	24.144052400	25.293488100	37.031765200
N	24.613652100	26.423663800	37.488529900

110

C	21.060462600	23.352220100	36.977929000
C	22.367742100	23.748189100	36.799846700
C	22.793515300	24.973583600	37.282568500
C	21.915811000	25.787041200	37.985158100
C	20.598696600	25.393240500	38.150307100
C	20.155442700	24.188678000	37.617233900
H	20.746280800	22.402677900	36.598755700
H	23.066418000	23.128381000	36.279334300
H	22.252593100	26.718362100	38.388241900
H	19.932063500	26.045068700	38.680333300
C	25.692431600	26.318210400	38.364582800
C	26.461838900	27.454509700	38.579819200
C	26.002642500	25.140570100	39.025792400
C	27.589377600	27.394066800	39.366930300
H	26.180210900	28.364021300	38.094572400
C	27.146349600	25.077663200	39.805226500
H	25.373093500	24.284280600	38.916267100
C	27.954933800	26.190588800	39.948252800
H	28.198693000	28.264958800	39.502959200
H	27.417327100	24.149060900	40.268408800
H	28.866158900	26.131162500	40.503746000
N	24.133214000	25.313045800	36.937880000
N	24.654833300	26.437104300	37.401284500

100

C	21.050567200	23.302688600	36.771245400
C	22.346212400	23.708572500	36.541831200
C	22.801378400	24.911107300	37.057370700
C	21.964696100	25.687352200	37.848152800
C	20.658620100	25.280061700	38.070677000
C	20.184115400	24.105130700	37.501654100
H	20.715821300	22.372659000	36.364218600
H	23.015327200	23.115997100	35.956579700
H	22.320867500	26.601411900	38.273069100
H	20.024130700	25.896398800	38.677141000
C	25.616048700	26.219162100	38.193596000
C	26.437142700	27.310427400	38.455767400
C	25.798277100	25.034538700	38.889847600
C	27.488943700	27.195020300	39.335839000
H	26.257262400	28.224737200	37.933243300
C	26.866518600	24.916342800	39.764520900
H	25.134792400	24.211875000	38.733654700
C	27.726523700	25.981120300	39.960988700
H	28.138952800	28.028703600	39.510922600
H	27.041633800	23.982228500	40.260580100
H	28.583958000	25.874681300	40.591668500
N	24.114750300	25.264016700	36.643634200
N	24.677134500	26.390113900	37.145586000

90

C	20.778570000	24.147165000	36.679160800
C	22.025381100	24.739684700	36.697011100

C	22.303019000	25.738061700	37.632626300
C	21.315822500	26.139965000	38.531928400
C	20.080479900	25.526370700	38.496185300
C	19.793780800	24.527605900	37.577280500
H	20.608921700	23.368082300	35.966967100
H	22.784873300	24.418943700	36.014561000
H	21.530429600	26.898470400	39.253757800
H	19.359518000	25.833626300	39.228174800
C	25.689184400	26.129657300	38.497402600
C	26.938840300	26.716310000	38.486355300
C	25.458834500	24.939476400	39.162698600
C	27.992617800	26.090906300	39.129925300
H	27.064194400	27.639120100	37.957974200
C	26.514537400	24.307759600	39.791332800
H	24.475988300	24.513331200	39.170597300
C	27.776536600	24.880501400	39.761227100
H	28.967780100	26.531079400	39.119626500
H	26.357872900	23.369954700	40.281486100
H	28.598142900	24.358940000	40.199939900
N	23.536042100	26.308828200	37.675007600
N	24.660738300	26.841279400	37.729560100

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C	20.800424000	24.136403000	36.414368300
C	22.027359300	24.755262700	36.308108600
C	22.442981000	25.653053100	37.278546000
C	21.632974000	25.912171100	38.371595200
C	20.384172300	25.319190600	38.448412800
C	19.953216400	24.430824100	37.474927400

H	20.521967200	23.428766300	35.663942100
H	22.661259200	24.538741000	35.475169900
H	21.956883000	26.590971700	39.132509700
H	19.755985800	25.574301600	39.279443000
C	25.330346400	26.110839400	38.765965300
C	26.524022100	26.747897400	39.052480200
C	25.134298400	24.786210100	39.125086500
C	27.555835900	26.040882500	39.645842000
H	26.640312300	27.775454300	38.777106000
C	26.160287600	24.087022700	39.726042700
H	24.197816000	24.308923600	38.929370900
C	27.379223000	24.705863700	39.962655800
H	28.489723200	26.526102600	39.850622200
H	26.018462400	23.064590200	40.009529600
H	28.184536900	24.135643500	40.376245000
N	23.640206900	26.411354900	37.067934400
N	24.387784100	26.919272200	38.021037800

70

C	20.835439300	24.027668200	36.446056200
C	22.060423900	24.646370600	36.305468900
C	22.464438700	25.603706400	37.220336000
C	21.653614500	25.915139500	38.298505400
C	20.409938400	25.317752600	38.411945700
C	19.982910200	24.380991200	37.483438500
H	20.558982800	23.278097100	35.736477200
H	22.694305900	24.386224700	35.485076800
H	21.973467200	26.640178800	39.017079500
H	19.783593600	25.609912300	39.232036700

C	25.293238900	26.037483000	38.684947000
C	26.498105300	26.642628500	38.996533200
C	25.043103800	24.728594000	39.068310600
C	27.487546500	25.921672900	39.640309900
H	26.652138400	27.658614900	38.697025200
C	26.031815200	24.013578100	39.716398300
H	24.099555200	24.272812200	38.855530800
C	27.260231500	24.600529400	39.980284600
H	28.428541700	26.384056400	39.861293700
H	25.855119900	22.999426600	40.010445200
H	28.034675600	24.016299600	40.431353600
N	23.635487900	26.399995500	36.958977200
N	24.425408300	26.871696300	37.877499100

60

C	20.855189800	23.999134600	36.471516900
C	22.077481000	24.624546000	36.329673500
C	22.470461100	25.594345500	37.236347400
C	21.657086800	25.905064100	38.311895000
C	20.417786800	25.299792600	38.428125900
C	19.995882800	24.358257400	37.501095000
H	20.582889700	23.245683300	35.764314100
H	22.712278700	24.365881500	35.509359900
H	21.968038600	26.641005500	39.024134300
H	19.787301600	25.594162500	39.244474900
C	25.290440400	26.020930300	38.647686300
C	26.496930900	26.619830600	38.970536800
C	25.026678700	24.718159300	39.040885200
C	27.472537500	25.903774700	39.637061800

H	26.661815900	27.630547400	38.658794300
C	26.004471000	24.005333100	39.710450400
H	24.086048500	24.261499800	38.820474800
C	27.231808400	24.587184800	39.987335600
H	28.412736100	26.364683300	39.865550800
H	25.819413500	22.993988400	40.010021600
H	27.995218300	24.004081100	40.457742600
N	23.607213400	26.436271200	36.947509400
N	24.462142300	26.864281300	37.811438000

50

C	20.891423600	23.883660600	36.512580400
C	22.116628200	24.490815900	36.331042900
C	22.510659200	25.520928700	37.162428900
C	21.696576000	25.916009300	38.208959300
C	20.451306600	25.329008700	38.363920000
C	20.026478600	24.325350100	37.504470600
H	20.617554400	23.080783800	35.862674300
H	22.756712200	24.176750200	35.535073900
H	22.009913300	26.699080800	38.868364200
H	19.819386100	25.683573300	39.154398400
C	25.294291800	25.935877200	38.528048900
C	26.504354600	26.514335700	38.871391100
C	24.968725300	24.668281200	38.979187000
C	27.429417000	25.807601800	39.612001500
H	26.711986100	27.498425000	38.508037400
C	25.898754600	23.958216700	39.714571800
H	24.024806100	24.228199800	38.747460900
C	27.132600000	24.516198000	40.011263500

H	28.378848200	26.244765100	39.848391900
H	25.678710400	22.962727600	40.039711200
H	27.856913100	23.930793200	40.534723100
N	23.645155200	26.336065500	36.793291700
N	24.558976200	26.749647000	37.587976600
40			
C	20.911563500	23.850629700	36.548446200
C	22.132595200	24.461194500	36.341787800
C	22.515990000	25.526915100	37.132442200
C	21.699666800	25.950980300	38.165723600
C	20.460272800	25.357738100	38.346702100
C	20.041995100	24.322846000	37.521815700
H	20.642927800	23.021429300	35.929555400
H	22.772777100	24.121418000	35.556991500
H	22.007878900	26.759897400	38.795315800
H	19.828152600	25.732443700	39.128058800
C	25.310243100	25.877309100	38.427177700
C	26.543119100	26.412796600	38.764542600
C	24.925906400	24.641842700	38.920131500
C	27.422727600	25.700827200	39.553226700
H	26.801485500	27.369305200	38.362884900
C	25.812174000	23.924712500	39.702001600
H	23.970978400	24.230136100	38.686809300
C	27.059513500	24.444839800	40.005445900
H	28.388763400	26.102782300	39.785909300
H	25.546931600	22.950093000	40.056285400
H	27.746541600	23.856593400	40.575948500
N	23.635816300	26.350589700	36.729790700

N	24.621169800	26.697108900	37.459443300
30			
C	20.922525400	23.844379200	36.563970300
C	22.141917700	24.461369900	36.361330700
C	22.511877700	25.534868700	37.148054900
C	21.689590000	25.956731100	38.177382300
C	20.455057800	25.353460600	38.357246900
C	20.046384600	24.315387100	37.531602300
H	20.659832200	23.014037500	35.943909000
H	22.787470100	24.125201000	35.578883900
H	21.987766700	26.772599100	38.803201300
H	19.817518600	25.725506800	39.135609200
C	25.323594900	25.852357100	38.387251300
C	26.555387900	26.388653600	38.731502900
C	24.927004800	24.627994200	38.898936900
C	27.420103500	25.691876200	39.548414800
H	26.822434300	27.335127100	38.311636300
C	25.803095100	23.922402300	39.703711600
H	23.974064000	24.213323600	38.662176600
C	27.046772300	24.444223400	40.014166100
H	28.381562200	26.098923500	39.790789100
H	25.531522800	22.953785900	40.069662100
H	27.724558600	23.862540900	40.601350600
N	23.613890600	26.378515700	36.732277900
N	24.658881200	26.662172000	37.394954400
20			
C	20.937286000	23.743667400	36.698783400

C	22.162177700	24.341352600	36.469550600
C	22.490573800	25.509254500	37.128993100
C	21.626351600	26.041747700	38.067769700
C	20.391584700	25.450090300	38.279561300
C	20.019707200	24.319833600	37.565657100
H	20.697619300	22.844131700	36.172882800
H	22.838657700	23.912529800	35.761421700
H	21.892734400	26.934690300	38.594282600
H	19.725650100	25.902732100	38.987534700
C	25.354567100	25.737293600	38.243449700
C	26.612947600	26.235157700	38.545569600
C	24.906131400	24.569208900	38.834711600
C	27.447385100	25.559104400	39.408816100
H	26.920332200	27.139975400	38.065978800
C	25.751417700	23.881325100	39.687066900
H	23.936513200	24.181934400	38.625901400
C	27.016757100	24.368284600	39.966575600
H	28.429425500	25.932143500	39.619884200
H	25.439637000	22.952561100	40.116073200
H	27.667476800	23.803449700	40.596354400
N	23.593750500	26.329313900	36.661351200
N	24.710421300	26.530088900	37.224443300

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C	20.947158100	23.755776800	36.719928100
C	22.169809500	24.365178700	36.500862800
C	22.476129300	25.541932400	37.157997900
C	21.596169700	26.068136100	38.085793100
C	20.368676200	25.460518300	38.292163500

C	20.016239700	24.324756900	37.576902500
H	20.720656600	22.852165500	36.193863000
H	22.858810100	23.941166900	35.801404100
H	21.845676200	26.968677800	38.607633900
H	19.693241800	25.906138800	38.996495100
C	25.371250800	25.699577700	38.195235500
C	26.633141900	26.193790800	38.495355000
C	24.912727400	24.543042600	38.803088300
C	27.452425900	25.535965600	39.387569700
H	26.950844200	27.083229100	37.994185000
C	25.745257300	23.872601200	39.681884800
H	23.946369900	24.150855900	38.586052800
C	27.005664700	24.363757400	39.969136500
H	28.433086400	25.911583000	39.603122400
H	25.425054400	22.952870600	40.126078100
H	27.643657700	23.812336300	40.625470200
N	23.568329400	26.377638600	36.694699600
N	24.733048800	26.494436400	37.176876300
O			
C	20.957480400	23.764835900	36.730901100
C	22.177658400	24.383944900	36.524543700
C	22.465988700	25.565025900	37.182224800
C	21.573580200	26.084253700	38.101215300
C	20.352542100	25.463254700	38.300673900
C	20.015581700	24.325325600	37.581477900
H	20.741645400	22.861783300	36.199784100
H	22.877734000	23.966307100	35.831643100
H	21.808755900	26.988997600	38.622256100

H	19.668771000	25.900226500	39.002070000
C	25.383317500	25.665165900	38.157158300
C	26.641300900	26.166583300	38.460824300
C	24.919185800	24.520246500	38.782106800
C	27.449498200	25.530641400	39.378026600
H	26.963541500	27.046059400	37.944945200
C	25.743036200	23.868621000	39.683177300
H	23.956717000	24.120845900	38.560977100
C	26.999194700	24.367565700	39.975187700
H	28.424245300	25.915933300	39.601780100
H	25.420119900	22.957088500	40.141233400
H	27.631430700	23.827925400	40.645459300
N	23.552973500	26.409476400	36.721967100
N	24.751181000	26.449251400	37.123750100

S0-TRANS-II

C	19.796682500	20.425874800	38.773530500
C	21.072914300	20.931029100	38.611730000
C	21.281585600	22.299203900	38.669225600
C	20.223086600	23.147244500	38.930253500
C	18.944030200	22.645321400	39.073453700
C	18.721641600	21.282392000	38.969241100
H	19.652667400	19.363900400	38.740162400
H	21.899369800	20.278154100	38.435190400
H	20.399426100	24.197523400	39.029556100
H	18.134042300	23.320885600	39.257658700
C	24.854694900	22.593857900	38.228186300
C	25.176682800	23.844214100	37.731230900
C	25.855240200	21.709774300	38.588382900

C	26.503547000	24.213755400	37.627531000
H	24.405698800	24.514882700	37.423598400
C	27.182246300	22.082902900	38.495891400
H	25.570215500	20.744817700	38.950307000
C	27.504876600	23.340259100	38.019379100
H	26.756883600	25.182235300	37.247315100
H	27.953529700	21.405189000	38.803996800
H	28.528994500	23.646069700	37.974872900
N	22.570455500	22.919107400	38.457112800
N	23.528426600	22.087656300	38.409971400

S0-CIS-II

C	20.053321600	21.017156000	38.510831600
C	21.231478900	21.728694200	38.312155200
C	21.302428600	23.064344800	38.664135400
C	20.195284000	23.653899500	39.265083600
C	19.020456800	22.961147800	39.438394600
C	18.929544500	21.639316400	39.022883200
H	20.024812100	19.985406800	38.223133400
H	22.040818100	21.239770800	37.821804300
H	20.267632200	24.683975400	39.540484400
H	18.171316000	23.465950100	39.852817100
C	24.564094300	23.114221400	38.239128500
C	25.796365200	23.679636300	37.940492800
C	24.506101400	21.803741300	38.672469100
C	26.962728800	22.963374200	38.094870800
H	25.809793100	24.693527700	37.603949200
C	25.672792100	21.078182200	38.820783100
H	23.580110900	21.351719500	38.926938200

C	26.899435700	21.658564700	38.550251700
H	27.905105800	23.417608800	37.865840300
H	25.615202400	20.063026900	39.154888000
H	27.803147100	21.107043500	38.703584400
N	22.279245200	24.071949300	38.301526800
N	23.522601000	24.088846300	38.086166200

S1-TRANS-II

C	19.754625600	20.419759600	38.781339200
C	21.028705400	20.927228900	38.627561500
C	21.233075900	22.295978000	38.689858500
C	20.167529000	23.144754600	38.949694300
C	18.894583100	22.633043300	39.078355500
C	18.681108500	21.270079900	38.971210700
H	19.612172100	19.358755100	38.742686900
H	21.853118700	20.271200700	38.450337100
H	20.327670900	24.197043300	39.056054400
H	18.072685500	23.296356800	39.253740000
C	24.914141200	22.584304700	38.214647200
C	25.241323600	23.835648200	37.715900600
C	25.918238600	21.705661200	38.589401200
C	26.564826000	24.213907000	37.628023500
H	24.464050600	24.500308100	37.408710700
C	27.241321500	22.088501200	38.484530500
H	25.661735100	20.743770800	38.977941600
C	27.570708400	23.346778000	38.016135400
H	26.808319400	25.189300900	37.260577000
H	28.015085300	21.413936300	38.791195300
H	28.592521100	23.658433100	37.985364800

N	22.500833500	22.878176800	38.479919200
N	23.586402400	22.170261400	38.353402100

S1-II C2N3N4C5 (degree)

-180

C	19.789736800	20.473396700	38.817151600
C	21.069877700	20.989102300	38.692597800
C	21.260670000	22.359057100	38.726922000
C	20.177872500	23.194414700	38.946915400
C	18.905466000	22.683825600	39.056424800
C	18.701342600	21.317399900	38.964609400
H	19.651661400	19.410177000	38.795318300
H	21.896653700	20.324803800	38.561942300
H	20.349150400	24.244395000	39.035971600
H	18.086527400	23.354292800	39.209994600
C	24.939935800	22.629013900	38.291193400
C	25.309866000	23.924532900	37.948335100
C	25.912352200	21.665177300	38.489625000
C	26.645267800	24.237498900	37.807469200
H	24.560266200	24.669861200	37.808591300
C	27.248170900	21.994820700	38.361721400
H	25.613171700	20.674948900	38.749243100
C	27.620914000	23.279046100	38.017429400
H	26.933232300	25.231195400	37.531174900
H	27.998522300	21.252129200	38.543348800
H	28.652558300	23.532714100	37.911339400
N	22.491472300	23.035230300	38.522772900
N	23.604708600	22.308913500	38.471444500

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C	19.794814400	20.469789000	38.833051700
C	21.071983400	20.985408800	38.695937700
C	21.256899400	22.358316700	38.724662600
C	20.175911400	23.192257600	38.960659700
C	18.906481500	22.681746600	39.080978200
C	18.703770200	21.312863800	38.986221100
H	19.658981000	19.406543700	38.802388100
H	21.897588700	20.319643800	38.550786700
H	20.350167800	24.244888100	39.042346100
H	18.084783900	23.352524500	39.226868600
C	24.936858400	22.628329200	38.281561900
C	25.314617100	23.926412200	37.952569400
C	25.904298300	21.661523400	38.501678300
C	26.651339100	24.240252600	37.830378000
H	24.557592800	24.664864900	37.797366400
C	27.243272100	21.994064900	38.383937200
H	25.612214600	20.664635300	38.760271300
C	27.626564600	23.277758500	38.041040100
H	26.932393000	25.235585900	37.555644200
H	27.992509800	21.249090700	38.562130900
H	28.659519900	23.530042000	37.922557400
N	22.472833700	23.044390900	38.458167200
N	23.586778000	22.313760200	38.354590900

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C	19.792583800	20.467470700	38.830561700
C	21.066219600	20.978661600	38.677723100
C	21.262189900	22.349780800	38.717743000

C	20.197681700	23.190841100	38.993466100
C	18.926790200	22.677270800	39.125113000
C	18.711688900	21.314246100	39.008184900
H	19.654408600	19.404477100	38.791029900
H	21.892762900	20.328119300	38.499516800
H	20.366437900	24.241453200	39.092270200
H	18.109693900	23.345587500	39.306304700
C	24.922537400	22.635372800	38.253830700
C	25.315422800	23.930819400	37.954025300
C	25.872817400	21.660518600	38.503028200
C	26.656143200	24.237171900	37.877007500
H	24.574252300	24.673613800	37.757836500
C	27.215036300	21.980556900	38.442540700
H	25.549545800	20.666389900	38.718580200
C	27.608849300	23.262517300	38.116802500
H	26.964060800	25.229030300	37.612892700
H	27.953559800	21.230398600	38.647559300
H	28.646052500	23.506655900	38.044254000
N	22.499431400	22.942646700	38.399243400
N	23.580070300	22.251316200	38.210283700

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C	19.800932400	20.460367100	38.848433700
C	21.071427100	20.973166200	38.675857200
C	21.266285100	22.343539900	38.707114400
C	20.207790700	23.183290900	39.010989400
C	18.938989600	22.670004000	39.159215900
C	18.721004300	21.307595600	39.035201100
H	19.662138200	19.397790900	38.809889200

H	21.895067900	20.323201100	38.477202200
H	20.377727700	24.234386000	39.108557800
H	18.123906800	23.337578200	39.351479500
C	24.909552300	22.640841500	38.219722300
C	25.321898800	23.936413500	37.946955800
C	25.841516100	21.658992000	38.498714800
C	26.665107600	24.235527000	37.915020600
H	24.591233100	24.683640400	37.726188000
C	27.188751600	21.969646100	38.481093800
H	25.506595900	20.664278000	38.696535400
C	27.602727300	23.249162800	38.170586600
H	26.988099900	25.227077700	37.670352900
H	27.916131600	21.214164000	38.705042800
H	28.642600700	23.483570000	38.118933200
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N	23.563987800	22.275412200	38.074963700

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C	19.813589800	20.451444900	38.867394600
C	21.079060600	20.972298300	38.663224300
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C	20.210459400	23.175766700	39.024870400
C	18.947282600	22.656380800	39.207276700
C	18.733284400	21.293045900	39.081622200
H	19.680904500	19.389130100	38.817874600
H	21.898463300	20.324435800	38.437283200
H	20.374703000	24.228377200	39.110101500
H	18.134659600	23.324316600	39.409172600
C	24.895171100	22.665408500	38.163253500

C	25.339385300	23.959303700	37.927072100
C	25.802961500	21.669476500	38.472894400
C	26.686727900	24.245913800	37.958429700
H	24.623881300	24.715880400	37.684087100
C	27.157021900	21.967098500	38.512767100
H	25.457507900	20.672683600	38.655107400
C	27.605017700	23.245718800	38.235639000
H	27.023732100	25.236273500	37.730974100
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H	28.652996400	23.464663200	38.209257200
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C	19.835382700	20.453465700	38.872771100
C	21.096761200	20.982069100	38.656837500
C	21.277789700	22.353853400	38.686899900
C	20.225077600	23.178157200	39.055581300
C	18.966537200	22.650655800	39.247738700
C	18.754109400	21.288926800	39.100515800
H	19.704221100	19.390823200	38.817383900
H	21.915430900	20.342096300	38.408639300
H	20.387389200	24.230438800	39.152287100
H	18.152863400	23.309772600	39.472494700
C	24.869401100	22.694560600	38.141168400
C	25.341256900	23.984233900	37.930511400
C	25.749031900	21.678003700	38.457653100
C	26.690645700	24.246395700	37.992323400
H	24.646052000	24.753884000	37.672916200

C	27.107074600	21.951875100	38.536626400
H	25.381329400	20.684990100	38.602060600
C	27.580211900	23.223918400	38.279740300
H	27.056724100	25.231266500	37.785606900
H	27.799469600	21.173030900	38.787001400
H	28.630531500	23.425872300	38.286676400
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C	20.218685400	23.173250600	39.065999200
C	18.971679400	22.637891200	39.291145500
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H	19.729539600	19.387211000	38.815199400
H	21.920361000	20.353971700	38.361873500
H	20.376897100	24.226930300	39.144826800
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C	27.574206700	23.206171800	38.327239900
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C	18.957586200	22.646360800	39.327467900
C	18.790953700	21.278519100	39.154280900
H	19.795234800	19.419697300	38.787376700
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H	18.126943200	23.271452400	39.599701800
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C	18.678397300	21.597974300	38.968418800
H	19.842855300	19.903095100	38.383672300
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H	19.950131700	24.670237000	39.471644200
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H	23.809312500	21.244950300	39.037678600
C	27.011195000	21.945396300	38.270032300
H	27.671016000	23.751415000	37.337460800
H	26.013317400	20.263974800	39.130928300
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C	18.677060500	21.592166800	38.959574500
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C	27.010881900	21.933808300	38.261981500
H	27.687334200	23.739451200	37.345143900
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C	19.890833400	23.633133800	39.230296900
C	18.706833700	22.936092500	39.291695100
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H	19.855965100	19.888355100	38.404210800
H	21.923020300	21.147842400	38.223207300
H	19.922807600	24.670219200	39.482228400
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C	25.906066900	21.245677900	38.731183500
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C	19.895265800	23.623147900	39.083946000
C	18.696769500	22.950493500	39.168640300
C	18.644860000	21.574818400	38.981815700
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H	21.917970100	21.001913400	38.421771000
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C	19.871808000	23.637852400	39.045055900
C	18.680509200	22.960899200	39.150992200
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C	27.012051300	21.875944700	38.307350300
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C	19.867030400	23.637719200	39.049266300
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C	18.638413500	21.580416000	38.996474800
H	19.824091500	19.826829300	38.676958000
H	21.909044600	21.028747400	38.456106300
H	19.906528000	24.700464400	39.157866900
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C	25.858792300	21.174836600	38.596466400
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H	27.969828800	21.396997600	38.361004600
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C	18.674090800	22.954029200	39.161080600
C	18.628800300	21.574312400	39.011440700
H	19.807509400	19.811042200	38.683361400
H	21.881782400	21.008538700	38.418369400
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C	24.567624900	23.174966300	38.241580600
C	25.730825400	23.849002800	37.910662500
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C	26.951965800	23.210260300	37.940573700
H	25.656506700	24.878874900	37.642746600
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C	27.022645700	21.873155400	38.293781300
H	27.838088300	23.760631500	37.698059400
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H	27.976193000	21.387226100	38.357432200
N	22.198712300	23.660757900	38.553838100
N	23.397039000	23.980880700	38.232647600
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C	19.869492700	23.629781000	39.050535000
C	18.674151900	22.954000900	39.161085200
C	18.628749400	21.574304700	39.011393000
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H	17.777840900	23.506816100	39.353532300
C	24.567063000	23.174173300	38.238627100
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C	24.632661700	21.828080200	38.561262500
C	26.951968200	23.210262400	37.940569400
H	25.656527500	24.878920800	37.642748300
C	25.856930200	21.187148200	38.587652700
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C	27.022650500	21.873183100	38.293821100
H	27.838101500	23.760611900	37.698057700
H	25.887669900	20.151962100	38.854584100
H	27.976169400	21.387222200	38.357405200
N	22.193757600	23.662810900	38.536140400
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C	20.996530100	21.553355100	38.644835500
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C	19.869781900	23.629211100	39.055409700
C	18.675298400	22.952526100	39.161997300

C	18.627760100	21.573847500	39.008445000
H	19.805170600	19.810284700	38.683071500
H	21.881431200	21.006968500	38.416503500
H	19.900121300	24.691293800	39.171673600
H	17.779084100	23.506679800	39.353637100
C	24.566566800	23.174648500	38.238088000
C	25.731564500	23.850179000	37.908926600
C	24.632823100	21.828383300	38.559415700
C	26.952218700	23.210836500	37.940195300
H	25.658024300	24.881726600	37.643094900
C	25.857913000	21.187934900	38.587620000
H	23.757577100	21.276944800	38.811438400
C	27.022795500	21.874534500	38.296130400
H	27.839041000	23.759354100	37.697973700
H	25.887052000	20.152053300	38.855024900
H	27.974857400	21.386955300	38.355752100
N	22.191177200	23.655885400	38.516536600
N	23.401128000	23.983275200	38.263180100

OM2/MRCI method

S0-TRANS-I

C	20.998592200	23.283924500	37.535563900
C	22.340483100	23.598019500	37.719645500
C	22.679607900	24.895240000	38.138094300
C	21.696100200	25.877379600	38.328685100
C	20.356854500	25.536848400	38.150039000
C	20.003240800	24.239668000	37.769261700
H	20.731921100	22.270686900	37.225523100
H	23.117693900	22.852755000	37.557402300

H	21.969377300	26.877060000	38.670208800
H	19.598860300	26.299951200	38.347590100
C	25.864687500	26.366900200	38.885916000
C	26.457880000	27.637679100	38.827476300
C	26.594758000	25.254418700	39.336550600
C	27.789332900	27.780834000	39.207562900
H	25.876387300	28.499502900	38.492821600
C	27.927703000	25.416809200	39.700951200
H	26.109394400	24.281324700	39.411504700
C	28.529161200	26.674168100	39.627285800
H	28.261724500	28.767723500	39.179739700
H	28.500686300	24.551531500	40.038446500
H	29.580743300	26.795872000	39.897312700
N	24.058770600	25.117409300	38.460651400
N	24.481323000	26.256616700	38.475780800

S0-CIS-I

C	20.908851900	23.578992700	36.762838700
C	22.154571100	24.150613500	36.511467100
C	22.403375800	25.447407500	36.979648700
C	21.473750700	26.117568300	37.783518500
C	20.235169200	25.524761500	38.021072000
C	19.923487900	24.282713700	37.461256100
H	20.700173900	22.578950000	36.380047600
H	22.900860500	23.614104800	35.923019900
H	21.704759000	27.099627100	38.195010200
H	19.511404500	26.067480800	38.637643500
C	25.255220300	25.659764200	37.919163600
C	26.503415600	26.228451900	38.235019600

C	24.772898000	24.528097000	38.591293100
C	27.298988600	25.637008100	39.209501200
H	26.839926100	27.119548600	37.699855400
C	25.599396600	23.941533100	39.550907500
H	23.802111500	24.096423000	38.363917300
C	26.852513900	24.477228900	39.842709600
H	28.277792000	26.058356900	39.451313500
H	25.272076100	23.033771200	40.061619600
H	27.504049700	23.966061600	40.554854200
N	23.490290200	26.219451500	36.421501200
N	24.614690200	26.303154000	36.801458000

S1-TRANS-I

C	21.003558800	23.293622000	37.205710800
C	22.336114300	23.674569600	37.097262300
C	22.683542700	24.961521300	37.535159400
C	21.744340300	25.854938000	38.073978600
C	20.413878100	25.446913200	38.147014400
C	20.035945300	24.181273000	37.689775300
H	20.720394500	22.286599800	36.889335200
H	23.089694500	22.998992300	36.697685800
H	22.041429800	26.842123000	38.429275200
H	19.682775400	26.144640800	38.565190000
C	25.777739900	26.299668100	38.569799100
C	26.611462000	27.429857700	38.641766000
C	26.120708300	25.087770000	39.195634000
C	27.824624900	27.318161900	39.312063000
H	26.304923600	28.365585100	38.173809300
C	27.347632800	25.000696400	39.846338400

H	25.437186200	24.239410600	39.166151600
C	28.208090700	26.100211100	39.877467100
H	28.493416500	28.180761400	39.380422100
H	27.641041900	24.061832500	40.314426800
H	29.194705700	26.009523200	40.337643700
N	24.021054400	25.410681700	37.304751300
N	24.641902300	26.366407700	37.702222900

S1S0-CI-I

C	21.026143500	23.274056200	37.201353300
C	22.354690600	23.652173000	37.055705800
C	22.724165100	24.932162300	37.508905000
C	21.810234400	25.799263500	38.138637400
C	20.479996900	25.400278700	38.232293400
C	20.077077500	24.158762200	37.728500400
H	20.725127000	22.276974400	36.871366000
H	23.092387000	22.986959700	36.611608500
H	22.128897900	26.769811900	38.521189900
H	19.762949100	26.085320300	38.693730600
C	25.711018100	26.296934200	38.494702000
C	26.557691800	27.417920200	38.605795200
C	26.003870200	25.087697500	39.153902800
C	27.744188900	27.288184300	39.317109800
H	26.280199800	28.358073200	38.128869100
C	27.210789700	24.977032200	39.836099000
H	25.306306900	24.251824300	39.104292100
C	28.091107800	26.061491700	39.888049600
H	28.424278800	28.139679300	39.409231200
H	27.480039500	24.033019000	40.309061100

H	29.063805200	25.953652000	40.374484200
N	24.011353300	25.416648400	37.172287300
N	24.652864300	26.381767700	37.536093900

S1-I C2N3N4C5 (degree)

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C	20.956456900	23.234663700	37.677989100
C	22.291137900	23.560856000	37.885475400
C	22.600742000	24.900339400	38.185643100
C	21.619274300	25.910639700	38.208561500
C	20.292857200	25.540135400	38.010369400
C	19.954101200	24.207521900	37.762478100
H	20.701846200	22.193955900	37.456836100
H	23.073962100	22.807566200	37.851479600
H	21.882579000	26.942256300	38.437784900
H	19.528188200	26.318926400	38.087727200
C	25.912338300	26.391226900	38.978330300
C	26.520653700	27.660915100	38.945881100
C	26.635080500	25.232106800	39.336386600
C	27.871355600	27.750727700	39.264256000
H	25.938310300	28.543233500	38.678299100
C	27.981714200	25.362660000	39.652165500
H	26.129222000	24.269234400	39.394085800
C	28.603956400	26.612400100	39.605849900
H	28.369614700	28.726128200	39.242941100
H	28.552455600	24.475420500	39.935310000
H	29.666374800	26.702693000	39.837220100
N	23.929965300	25.230605900	38.500321300
N	24.544181400	26.270762100	38.655881300

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C	20.957371900	23.230646500	37.660025800
C	22.296733200	23.551835500	37.844234800
C	22.609595100	24.884504000	38.168738800
C	21.634049400	25.898570000	38.210937500
C	20.303213500	25.534382200	38.031370400
C	19.958534500	24.205256900	37.770417800
H	20.695683100	22.191934200	37.440047500
H	23.077631200	22.798555800	37.783858200
H	21.905209400	26.926922200	38.446395700
H	19.541710200	26.312004700	38.137169200
C	25.898037100	26.396231400	38.971150600
C	26.513761100	27.661661800	38.933101300
C	26.611249600	25.233423000	39.332612800
C	27.858418300	27.746248200	39.277668100
H	25.939439700	28.545368200	38.653826600
C	27.953031300	25.357879100	39.670463400
H	26.098690100	24.273690200	39.384506700
C	28.580437900	26.605614500	39.634905700
H	28.357589800	28.720660300	39.275856900
H	28.512632200	24.469376000	39.968256200
H	29.639154800	26.691771600	39.883820300
N	23.955764200	25.223973400	38.389837300
N	24.553492700	26.271500600	38.567388600

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C	20.946051000	23.299479300	37.362434200
C	22.291492200	23.622621900	37.492408900

C	22.608550100	24.895945800	37.995258800
C	21.629913700	25.863178900	38.283662100
C	20.292960000	25.501625500	38.139494700
C	19.946755400	24.222170900	37.693152900
H	20.682984000	22.298561800	37.011192800
H	23.075870600	22.906569700	37.260456600
H	21.906223800	26.845984200	38.664793800
H	19.531686000	26.233709700	38.422482700
C	25.894355400	26.324976200	38.892425600
C	26.582764000	27.550066000	38.837307300
C	26.513554600	25.142425200	39.344575400
C	27.912521100	27.572556800	39.244177000
H	26.073439300	28.451110600	38.495455600
C	27.845226400	25.200820000	39.737370000
H	25.944425900	24.215974200	39.409303300
C	28.547944600	26.406687100	39.676577400
H	28.467327600	28.515646000	39.228823200
H	28.335757600	24.294602900	40.092739400
H	29.599053400	26.440147900	39.966169800
N	23.971201700	25.228004000	38.144054300
N	24.573176800	26.256840600	38.394492700

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C	20.948187300	23.286528900	37.358940500
C	22.296306600	23.613421300	37.444760900
C	22.626656200	24.886802100	37.936793800
C	21.655135400	25.841049800	38.282784500
C	20.314728400	25.479140000	38.177715500
C	19.957434900	24.207513700	37.718628400

H	20.676115200	22.287267200	37.010262300
H	23.074100500	22.902205600	37.179444900
H	21.942440700	26.820655800	38.664220900
H	19.560545100	26.207301800	38.488188900
C	25.870164400	26.329123400	38.856611300
C	26.572062300	27.546247300	38.825374000
C	26.462689600	25.139964800	39.323251000
C	27.894236300	27.551094200	39.257541500
H	26.081756300	28.454750300	38.475761200
C	27.788143800	25.178943100	39.740385100
H	25.881602100	24.219474000	39.366752900
C	28.508592500	26.374637000	39.692044700
H	28.461430200	28.486407400	39.253312200
H	28.261674000	24.264331300	40.096779300
H	29.558299000	26.390891700	39.990109300
N	23.993563000	25.244934600	37.987021100
N	24.574652500	26.270499200	38.284443700

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C	20.959353300	23.299538700	37.252731800
C	22.306479100	23.639838000	37.277823300
C	22.648568100	24.905072500	37.782495800
C	21.686960000	25.831597700	38.218839000
C	20.345977500	25.459867800	38.166793200
C	19.978724800	24.200848900	37.682295600
H	20.677475000	22.307539500	36.892197100
H	23.075754900	22.945104600	36.948679900
H	21.981892800	26.803939700	38.613931700
H	19.600061600	26.171388100	38.531257100

C	25.855635400	26.308875600	38.763296800
C	26.606684100	27.496007800	38.750225400
C	26.366498600	25.111592400	39.297842000
C	27.901852100	27.459128300	39.256780000
H	26.176588100	28.415589600	38.353000600
C	27.668417200	25.105707200	39.786428600
H	25.746986800	24.215814600	39.330189300
C	28.440642900	26.268544300	39.749046600
H	28.508933100	28.369002400	39.262985800
H	28.083114400	24.181503500	40.187665800
H	29.473420000	26.247689600	40.101541000
N	24.015039500	25.284245400	37.751371100
N	24.593215400	26.290034600	38.106369400

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C	20.975856600	23.297389500	37.212550400
C	22.318702000	23.653957600	37.180280000
C	22.668338200	24.923388300	37.668408600
C	21.715584300	25.833788600	38.153869200
C	20.377112300	25.448785300	38.154472500
C	20.002414000	24.190188400	37.674945100
H	20.691048600	22.302302100	36.863321400
H	23.080888800	22.970452500	36.812551900
H	22.014218500	26.810272600	38.535788100
H	19.638079800	26.152720100	38.545993900
C	25.833427100	26.298473900	38.684140500
C	26.622421900	27.460778500	38.692925900
C	26.274731900	25.097050000	39.267557400
C	27.888599700	27.393017900	39.265010700

H	26.244183300	28.385489400	38.256812200
C	27.550910500	25.057916200	39.820190100
H	25.626377100	24.221485100	39.281935500
C	28.362924700	26.193429900	39.799599800
H	28.525835800	28.281587800	39.284405500
H	27.916164200	24.128473600	40.255473700
H	29.378512500	26.144060000	40.197373700
N	24.027637800	25.328420400	37.553562600
N	24.610838500	26.313210700	37.947608900

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C	20.993385900	23.299575100	37.179750000
C	22.328322200	23.674765500	37.088482100
C	22.678549600	24.955032800	37.544334800
C	21.734475200	25.854077600	38.065445000
C	20.401888600	25.452567000	38.123251000
C	20.025789700	24.186257600	37.665726700
H	20.708544400	22.296395800	36.854071000
H	23.085458600	22.999326700	36.695734300
H	22.034126800	26.838382900	38.425285800
H	19.668879300	26.152677200	38.533515100
C	25.791186100	26.294736400	38.596923200
C	26.616373200	27.430534000	38.646585500
C	26.152998500	25.086616200	39.218866500
C	27.844337700	27.327077000	39.291130400
H	26.293287300	28.362262800	38.182445000
C	27.393211700	25.009784900	39.845071900
H	25.473082500	24.235033900	39.205176500
C	28.246201300	26.115350900	39.857367700

H	28.509211700	28.193939900	39.339915100
H	27.701623900	24.074454300	40.311282400
H	29.239266400	26.034748400	40.305153300
N	24.025793500	25.385169200	37.356359000
N	24.621143600	26.348666400	37.776034200

110

C	21.007845300	23.292962000	37.207787400
C	22.340820600	23.673154500	37.101369300
C	22.686246000	24.960518600	37.536929600
C	21.751139900	25.852058700	38.085494500
C	20.419601900	25.444969300	38.152275400
C	20.039952900	24.181562100	37.690679000
H	20.725673000	22.285933400	36.891198700
H	23.096125300	23.000237300	36.701619000
H	22.050472400	26.836991000	38.444925700
H	19.689291800	26.143435700	38.571417700
C	25.767181100	26.297889500	38.567181800
C	26.604441100	27.427823400	38.643067400
C	26.110648700	25.086452700	39.196585300
C	27.817840700	27.315093300	39.311067500
H	26.296455600	28.364438900	38.176821300
C	27.338347400	24.996509200	39.843927700
H	25.426437300	24.238183600	39.168003400
C	28.200912700	26.095434500	39.873341100
H	28.486582100	28.177941500	39.379251400
H	27.633523200	24.057388800	40.310853600
H	29.187346900	26.002399300	40.332740400
N	24.019144400	25.416266300	37.293445200

N	24.663319600	26.368388100	37.662283100
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C	21.030746300	23.307373400	37.012298000
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C	22.348739900	23.706607300	36.831977300
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C	22.729777100	24.960883400	37.344281800
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C	21.833081100	25.786307200	38.051376200
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C	20.512702200	25.366608100	38.183271800
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C	20.099153800	24.147205800	37.634660000
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H	20.723464100	22.327158300	36.641682200
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H	23.073739100	23.072083500	36.324529200
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H	22.157253000	26.739667000	38.470152800
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H	19.810799200	26.019422200	38.710396500
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C	25.704285600	26.256565500	38.390969200
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C	26.614968900	27.325766700	38.502496000
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C	25.896509500	25.050470200	39.090880500
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C	27.763996600	27.145502300	39.262982800
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H	26.419081900	28.264431700	37.984925800
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C	27.066109700	24.888784000	39.825852200
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H	25.156107000	24.252888600	39.033325400
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C	28.009646600	25.918413800	39.882187200
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H	28.492418800	27.955691500	39.354354000
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H	27.257529100	23.945386500	40.335249100
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H	28.956258600	25.763172100	40.405861300
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N	24.014885600	25.451332700	37.018652200
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N	24.662449600	26.398735600	37.419049400
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C	21.019184300	23.291100100	36.930607500
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C	22.316591200	23.716273200	36.675448100
C	22.679510300	25.009306600	37.102330600
C	21.774808400	25.856328600	37.776955700
C	20.481585100	25.400952500	38.004033600
C	20.086078600	24.141095600	37.537868000
H	20.725741500	22.285250200	36.624422500
H	23.039925000	23.074347200	36.173983900
H	22.082911100	26.844574000	38.120766800
H	19.783034100	26.058814400	38.528213000
C	25.673861600	26.126810900	38.144294500
C	26.702459100	27.077143600	38.273694900
C	25.642512300	24.957070000	38.922195000
C	27.752366900	26.806135600	39.143582200
H	26.679287000	27.991905800	37.683679900
C	26.718244400	24.698952100	39.766836300
H	24.813498400	24.255407000	38.841947500
C	27.780713800	25.601790800	39.848943900
H	28.572547000	27.521048500	39.251733200
H	26.743722600	23.771681400	40.338994300
H	28.652983100	25.363410300	40.461712200
N	23.942321600	25.507850100	36.729816100
N	24.672803400	26.380719700	37.141673500

80

C	21.028256000	23.302890400	36.950518200
C	22.320568300	23.743915400	36.691297000
C	22.667758300	25.041066300	37.112803100
C	21.755948300	25.877471400	37.787075300
C	20.468249200	25.406827800	38.020310400

C	20.084909900	24.144341800	37.552778200
H	20.747025100	22.293207500	36.646274000
H	23.049655900	23.112372900	36.184974700
H	22.051254800	26.872920500	38.119628900
H	19.764993700	26.057362200	38.547494800
C	25.686877300	26.119394300	38.131450900
C	26.718647900	27.064852900	38.267042600
C	25.637325100	24.950946900	38.908746900
C	27.753345700	26.794401500	39.154737000
H	26.707708700	27.973608000	37.668245300
C	26.701971900	24.691614400	39.767733100
H	24.806205600	24.253550500	38.817346400
C	27.764503000	25.592783900	39.864735200
H	28.576338700	27.505324700	39.269136800
H	26.719538300	23.761654600	40.336171200
H	28.629652500	25.350833600	40.485181600
N	23.910675600	25.571831900	36.696466800
N	24.704702400	26.375827100	37.112758500

70

C	20.808956600	23.347726100	36.701231100
C	22.083332600	23.826558000	36.423801700
C	22.411713600	25.117547100	36.874743300
C	21.503481300	25.913538900	37.597331300
C	20.233707200	25.404931300	37.850686100
C	19.867107300	24.145854400	37.361121400
H	20.541236000	22.343722300	36.370274400
H	22.815077500	23.224445500	35.887059700
H	21.788145700	26.904525000	37.949619700

H	19.529655400	26.020068500	38.418360600
C	25.421280700	25.859489500	38.015295700
C	26.606498300	26.586124600	38.217772100
C	25.104954300	24.707083500	38.754169400
C	27.525458900	26.099118000	39.141844900
H	26.802112000	27.488023900	37.638684600
C	26.051627700	24.237235800	39.659610200
H	24.166173700	24.178163900	38.601952800
C	27.262055200	24.913068200	39.828624000
H	28.468936400	26.628162000	39.302975200
H	25.862129700	23.316345300	40.214133300
H	28.021913200	24.489398700	40.487408500
N	23.659993500	25.659180900	36.480347800
N	24.526633900	26.321674800	36.987598100

60

C	20.814416600	23.359125800	36.711120400
C	22.083716100	23.851686500	36.432047300
C	22.396842400	25.147150000	36.881217500
C	21.482070100	25.932853900	37.606099700
C	20.219406500	25.409068300	37.863265700
C	19.864372300	24.147997900	37.370272800
H	20.556474600	22.353395000	36.377738100
H	22.819501300	23.257135400	35.892046000
H	21.755910200	26.927072800	37.957200200
H	19.509847300	26.014656800	38.434076100
C	25.433412700	25.846800800	37.991063200
C	26.618568000	26.572064000	38.202793600
C	25.102979600	24.700605600	38.733714900

C	27.521424400	26.091643000	39.145787000
H	26.827151400	27.465761500	37.615915400
C	26.036050800	24.237257400	39.656509400
H	24.167331300	24.169709300	38.571581100
C	27.244636400	24.912728000	39.839200300
H	28.464518000	26.618994800	39.314871700
H	25.838347300	23.319089900	40.212723400
H	27.991901300	24.494410100	40.515530000
N	23.630436000	25.710393700	36.470111700
N	24.558402100	26.305066300	36.947931700

50

C	20.793680100	23.410025900	36.707666300
C	22.056810900	23.915671400	36.424415000
C	22.358606400	25.211424100	36.880989000
C	21.439694500	25.985465500	37.612613600
C	20.181948600	25.450264100	37.869453700
C	19.838558200	24.187334100	37.373504000
H	20.543430400	22.403349700	36.371436200
H	22.794803600	23.331172900	35.877118000
H	21.708884400	26.978411900	37.968988600
H	19.468593400	26.047487500	38.443724900
C	25.435819800	25.827208900	37.952051900
C	26.640914600	26.521431000	38.158700800
C	25.067127500	24.701296800	38.708433200
C	27.523814200	26.027691700	39.113595600
H	26.875429200	27.402750300	37.563267300
C	25.980508300	24.226747900	39.645147000
H	24.116001600	24.197211100	38.550900400

C	27.207872400	24.869214400	39.824598200
H	28.479830000	26.531875600	39.282367900
H	25.749233700	23.327727000	40.220046300
H	27.939028200	24.439428700	40.511682100
N	23.583764400	25.788321900	36.471172700
N	24.575399700	26.304753000	36.908351500

40

C	20.796321000	23.410404800	36.706043400
C	22.058276100	23.921637700	36.425060500
C	22.350490100	25.219629100	36.882431000
C	21.426739000	25.989421400	37.613248200
C	20.173292700	25.446438700	37.871024900
C	19.837245100	24.182089300	37.373481900
H	20.549173800	22.403027800	36.369418300
H	22.799129500	23.340075300	35.878707900
H	21.690729300	26.984930200	37.967347600
H	19.459835100	26.040355600	38.448553000
C	25.442261100	25.822328500	37.947394400
C	26.646109000	26.518094900	38.157814900
C	25.066274200	24.701488700	38.708472100
C	27.524344800	26.024810600	39.117074500
H	26.883396700	27.397389500	37.560861500
C	25.977938200	24.224938400	39.645689500
H	24.113919800	24.199917900	38.550792000
C	27.205829900	24.866359300	39.827149600
H	28.481023800	26.527653100	39.286825800
H	25.747542700	23.322531200	40.215978800
H	27.936160000	24.434074500	40.513383100

N	23.567191600	25.816532600	36.488294100
N	24.600013500	26.282608700	36.883309000
30			
C	20.768244400	23.468218900	36.702293600
C	22.031121900	23.991523700	36.450190600
C	22.309636200	25.285105800	36.932323600
C	21.364892700	26.043945000	37.648703300
C	20.110976200	25.488885800	37.875553300
C	19.794058600	24.224054100	37.366081700
H	20.534164500	22.463389100	36.348854400
H	22.785662900	23.420360900	35.910936400
H	21.613916100	27.036697600	38.018233200
H	19.382380600	26.071842800	38.444560900
C	25.466783900	25.806878100	37.949584200
C	26.700976800	26.460072100	38.122070000
C	25.070760000	24.705703100	38.729986500
C	27.580858400	25.947410300	39.069604400
H	26.957203700	27.323122800	37.509812300
C	25.985019600	24.208268600	39.653092200
H	24.098129200	24.236183900	38.599509000
C	27.235613700	24.812903100	39.805114700
H	28.557726000	26.418379300	39.214460100
H	25.736156000	23.321708700	40.240046100
H	27.962018400	24.367891400	40.486705400
N	23.530242500	25.885724700	36.576527900
N	24.615222800	26.284095800	36.901641900

20

C	20.766919700	23.472566900	36.701620000
C	22.029818000	23.999296700	36.459099500
C	22.304547700	25.292634600	36.949521600
C	21.351158200	26.049970200	37.659713800
C	20.098859100	25.490166800	37.878199900
C	19.789278400	24.224555800	37.365378300
H	20.535879700	22.468696200	36.343198500
H	22.789617200	23.432398500	35.922349200
H	21.594494400	27.042706100	38.032255700
H	19.365633700	26.069382400	38.444977800
C	25.477409000	25.804595100	37.939966200
C	26.711377000	26.456828500	38.115973700
C	25.076450400	24.707163700	38.722432300
C	27.584305100	25.946453800	39.071302900
H	26.969883500	27.317902100	37.502097200
C	25.984444000	24.209386700	39.651167200
H	24.103553300	24.238868900	38.588898900
C	27.234799000	24.813691400	39.807458900
H	28.559075200	26.420033400	39.222590400
H	25.730717800	23.324246600	40.237946300
H	27.956725400	24.369382000	40.494184500
N	23.521308700	25.897698400	36.623249200
N	24.637871000	26.268245300	36.872850500

10

C	20.743546700	23.508016800	36.720558600
C	22.010551500	24.035375700	36.505880700
C	22.280771400	25.322679200	37.018702000
C	21.312264900	26.076110700	37.715784200

C	20.054549400	25.517143500	37.900783100
C	19.754594900	24.253640400	37.375940600
H	20.519451800	22.506379100	36.351561100
H	22.778659500	23.470862800	35.978271500
H	21.552994000	27.063332300	38.105019100
H	19.311712900	26.093408400	38.458709800
C	25.502100700	25.804626000	37.963145200
C	26.748581700	26.442810700	38.099213100
C	25.114507900	24.714544900	38.762164200
C	27.642802900	25.929151300	39.032702500
H	26.999390900	27.296121400	37.471510600
C	26.042878600	24.212043500	39.667699300
H	24.134505900	24.253300800	38.658006900
C	27.301882100	24.806827900	39.788408600
H	28.625971300	26.394059300	39.153790400
H	25.796895400	23.332725300	40.266291600
H	28.037697800	24.360613000	40.458911300
N	23.501745100	25.926652400	36.737702500
N	24.643726200	26.267475800	36.909101500
O			
C	20.745057600	23.507539800	36.718759900
C	22.013192400	24.035413600	36.510936900
C	22.280060600	25.322850800	37.026661000
C	21.307443400	26.073938300	37.722346800
C	20.050821400	25.513253600	37.903302600
C	19.754117900	24.251029700	37.373866200
H	20.519802800	22.507438800	36.345914700
H	22.783196000	23.470591800	35.985779000

H	21.547350500	27.060374700	38.112988300
H	19.306437600	26.087476300	38.460733300
C	25.502638600	25.807259500	37.960507200
C	26.749031200	26.445051400	38.096963600
C	25.115663800	24.716307100	38.758510600
C	27.642366000	25.930912400	39.031206500
H	27.000257400	27.299153600	37.470452500
C	26.043875700	24.211222800	39.662629800
H	24.134767900	24.256554500	38.654072900
C	27.301864000	24.807571500	39.785240100
H	28.624909700	26.396565900	39.154678100
H	25.798899000	23.329462300	40.257734500
H	28.036004500	24.363321500	40.458534200
N	23.495932700	25.938810300	36.760575400
N	24.651257000	26.254624100	36.892453500

S0-TRANS-II

C	19.788574400	20.421860100	38.757741000
C	21.081749900	20.915551700	38.608520000
C	21.300392800	22.299895000	38.693013300
C	20.244086200	23.173836800	38.988327500
C	18.955710800	22.663902500	39.110424300
C	18.718902100	21.295619300	38.968085800
H	19.628722400	19.341250400	38.711587800
H	21.915721000	20.240228500	38.417991000
H	20.426363300	24.236966200	39.149747900
H	18.128453200	23.346780800	39.329995300
C	24.850929100	22.571947300	38.217719400
C	25.170411300	23.835310300	37.699818400

C	25.857805900	21.669796100	38.600565300
C	26.511236700	24.201862600	37.609594600
H	24.387721800	24.515257200	37.364074300
C	27.189673100	22.062752900	38.519174300
H	25.578921300	20.689171000	38.991746500
C	27.514416000	23.330575800	38.035603400
H	26.779923400	25.186835600	37.213364200
H	27.980423700	21.387561200	38.857359800
H	28.558933900	23.648152700	38.012987000
N	22.606281200	22.888651700	38.465424500
N	23.509654500	22.082938300	38.391641700

S0-CIS-II

C	20.059723200	21.007437500	38.509073200
C	21.250482300	21.710683600	38.313122000
C	21.316559700	23.065131300	38.666025300
C	20.196507000	23.682881800	39.262283200
C	19.015299400	22.975672700	39.436471200
C	18.926263800	21.642034600	39.023307700
H	20.027122600	19.954417900	38.219772500
H	22.082994200	21.212072900	37.811990000
H	20.265916900	24.726968000	39.577824200
H	18.146505700	23.480745100	39.869614900
C	24.549087700	23.123479900	38.248298800
C	25.795171000	23.709247300	37.941502100
C	24.478306100	21.791815500	38.668524100
C	26.966753900	22.977109700	38.094370000
H	25.825973300	24.741335100	37.582052000
C	25.662128900	21.069557500	38.815436800

H	23.530078200	21.324120200	38.927172000
C	26.897226100	21.660489800	38.550552500
H	27.929308500	23.428038700	37.853931400
H	25.610685400	20.035391900	39.165936000
H	27.823126600	21.098585400	38.710310100
N	22.306670500	24.030929500	38.284968900
N	23.483043900	24.071284400	38.093277000

S1S0-CI-II

C	19.889966900	20.486557700	38.853697600
C	21.139132700	21.049760200	38.617104700
C	21.277369200	22.452233400	38.700888600
C	20.192094100	23.262313400	39.100465000
C	18.957191900	22.672368800	39.319975400
C	18.784547500	21.296768500	39.137406900
H	19.783881000	19.400054000	38.794812800
H	21.991691000	20.427757100	38.342944200
H	20.333928800	24.333682000	39.247505500
H	18.109000700	23.301098800	39.611596900
C	24.779976400	22.825695900	38.061951500
C	25.359216900	24.089306100	37.832613700
C	25.543666600	21.712871600	38.441114900
C	26.731582300	24.226833900	37.993137200
H	24.735003900	24.932687400	37.533064700
C	26.914534900	21.891758200	38.613261800
H	25.068819700	20.741766000	38.588398100
C	27.509969600	23.127734500	38.360865700
H	27.207875000	25.190060400	37.804924800
H	27.537952000	21.062533400	38.950666200

H	28.594969500	23.237239100	38.421312200
N	22.362262700	23.111786400	38.082072700
N	23.417843300	22.700984400	37.674256600

S1-TRANS-II

C	19.804752900	20.447985300	38.836841300
C	21.088532800	20.951412100	38.662418400
C	21.279500400	22.347991200	38.725844300
C	20.210216200	23.220085400	38.999232500
C	18.937145800	22.686102000	39.149554800
C	18.720701000	21.310915400	39.030787000
H	19.660728000	19.363852000	38.813813600
H	21.932650700	20.288662700	38.474402100
H	20.382217100	24.288245400	39.125867200
H	18.100168900	23.358998900	39.364051000
C	24.899328900	22.642659300	38.238987500
C	25.298407900	23.959740000	37.928937000
C	25.836426000	21.624401600	38.491766200
C	26.658033500	24.245165600	37.905208700
H	24.554616400	24.728361000	37.719287300
C	27.188094500	21.952103200	38.478303900
H	25.490384400	20.612228500	38.705582400
C	27.601276400	23.249449200	38.170854300
H	26.995552300	25.256801200	37.665575500
H	27.935822200	21.193019800	38.717842000
H	28.664948700	23.486256600	38.113669000
N	22.509819000	22.902241500	38.301835400
N	23.545228900	22.296511000	38.108489300

S1-II C2N3N4C5 (degree)

-180

C	19.791594600	20.461905800	38.810479600
C	21.082208200	20.964640400	38.690233800
C	21.262089600	22.362879700	38.730024000
C	20.181109000	23.239517200	38.932317500
C	18.905490200	22.702932500	39.044076200
C	18.700258200	21.324162700	38.960267100
H	19.649297000	19.377325000	38.796600800
H	21.935540200	20.300194000	38.563143500
H	20.345168900	24.308819600	39.050855600
H	18.061105700	23.376845100	39.226084200
C	24.936095200	22.644005600	38.302708200
C	25.290695700	23.962463000	37.947594600
C	25.903206500	21.634023500	38.485564800
C	26.640669300	24.255363600	37.796825800
H	24.527243200	24.724973400	37.800987000
C	27.243271100	21.977020700	38.357236200
H	25.585726400	20.625930600	38.753099200
C	27.615158000	23.278724600	38.017848600
H	26.947006400	25.267541300	37.518054900
H	28.016136800	21.230596800	38.558074700
H	28.670238100	23.535113500	37.915155400
N	22.548044900	22.914697500	38.535644400
N	23.595371800	22.297206900	38.482357400

-170

C	19.793907700	20.460175900	38.818224000
C	21.084555700	20.961034400	38.694146000

C	21.269775700	22.359168900	38.745199200
C	20.188606400	23.236317200	38.945849500
C	18.912211000	22.701921600	39.058796600
C	18.703542200	21.323527300	38.970935400
H	19.650161700	19.375951800	38.802950600
H	21.936236500	20.296126500	38.557487200
H	20.353364200	24.306152000	39.060451100
H	18.068732700	23.376645500	39.240320600
C	24.929454500	22.644727300	38.310144500
C	25.287717500	23.962154700	37.952958900
C	25.895068900	21.634384300	38.493715700
C	26.638700600	24.255830900	37.813452800
H	24.524820100	24.723739400	37.798942100
C	27.236531500	21.976700100	38.375004700
H	25.576378500	20.624073400	38.751988500
C	27.611629100	23.277454400	38.034456400
H	26.946616900	25.267390700	37.535794000
H	28.007835800	21.229353600	38.575975300
H	28.666779300	23.529919900	37.923253300
N	22.541295100	22.908527200	38.478634500
N	23.583862400	22.281647300	38.388185700

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C	19.797254500	20.454544700	38.818029600
C	21.084398400	20.956253500	38.665786700
C	21.273553700	22.353249200	38.732520700
C	20.200074500	23.227702500	38.979553500
C	18.925266800	22.693794100	39.113457800
C	18.711541900	21.317627100	39.003149100

H	19.651863700	19.370830900	38.793136700
H	21.931806200	20.293052400	38.496411500
H	20.370364600	24.295588300	39.105942400
H	18.086759600	23.367060000	39.320296200
C	24.913839900	22.637444000	38.273026300
C	25.291477300	23.955002300	37.938296400
C	25.866561500	21.624271700	38.494176200
C	26.647952000	24.246861000	37.864619600
H	24.537544300	24.718784600	37.751310100
C	27.213722200	21.961783900	38.436313000
H	25.533688200	20.611890100	38.726425300
C	27.607339400	23.262535100	38.117073900
H	26.970671000	25.258236500	37.604955000
H	27.972479300	21.209118100	38.660502100
H	28.667020600	23.510673700	38.042896800
N	22.527481800	22.904379100	38.393286800
N	23.563165500	22.277378000	38.250008200

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C	19.804976100	20.448407800	38.835657500
C	21.088513300	20.951679200	38.659826400
C	21.278486400	22.348155400	38.722968000
C	20.209442600	23.220131700	38.997287900
C	18.936664700	22.686054700	39.148891700
C	18.720699500	21.311025200	39.030000400
H	19.660411200	19.364604400	38.814145500
H	21.932990700	20.288971900	38.474790900
H	20.381846600	24.287530700	39.125612900
H	18.100359400	23.359175600	39.364646300

C	24.900071900	22.642117800	38.236062200
C	25.297751000	23.959497600	37.927133800
C	25.837382000	21.623827700	38.489487600
C	26.657223400	24.245050400	37.903825700
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C	27.188437700	21.952254500	38.476874200
H	25.490931700	20.612575800	38.705668000
C	27.601026300	23.249886000	38.170457300
H	26.995123300	25.256736900	37.665541000
H	27.934932400	21.193029600	38.718559300
H	28.664521600	23.486644300	38.113625100
N	22.511193000	22.902966800	38.308430600
N	23.546116400	22.294268200	38.117720100

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C	19.819049700	20.445465700	38.848013200
C	21.098056800	20.954670700	38.652785700
C	21.285975900	22.351133200	38.716514600
C	20.218580900	23.216190100	39.019980000
C	18.950045400	22.677788700	39.191097100
C	18.734917400	21.303631500	39.060137400
H	19.676763300	19.361520200	38.818923900
H	21.940555200	20.295050700	38.446795100
H	20.388618400	24.284655900	39.147872700
H	18.114464200	23.347960900	39.418826400
C	24.883607500	22.663389000	38.196166200
C	25.307888000	23.978580500	37.914750700
C	25.800875700	21.633143800	38.468444600
C	26.669770400	24.251726000	37.937951400

H	24.580343500	24.757792500	37.686963000
C	27.155729400	21.947838600	38.504398800
H	25.439532800	20.620653700	38.655149400
C	27.592928700	23.242576300	38.221479700
H	27.025326700	25.260827400	37.716080600
H	27.887779900	21.178126400	38.757355900
H	28.660430600	23.468315900	38.195411100
N	22.489405700	22.919138800	38.227671100
N	23.527996200	22.341316900	37.991916100

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C	19.838860100	20.443134400	38.857317600
C	21.110517000	20.962838200	38.639757700
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C	20.225642900	23.213454200	39.045233400
C	18.964263300	22.666600400	39.238361000
C	18.753308100	21.293074300	39.092836000
H	19.702138600	19.358592700	38.821633600
H	21.951262900	20.309203500	38.407793900
H	20.390943700	24.282713900	39.175085800
H	18.128635000	23.329734600	39.485153300
C	24.860201600	22.696189300	38.158299500
C	25.319428800	24.006282100	37.909833800
C	25.747625600	21.646207700	38.448676400
C	26.683880400	24.255775900	37.980275000
H	24.613391500	24.800998800	37.666341800
C	27.106444800	21.936729000	38.534159400
H	25.365610600	20.636449000	38.607299000
C	27.577690900	23.224914300	38.278092200

H	27.064742700	25.260193500	37.781159100
H	27.817638900	21.152396500	38.800104600
H	28.650140100	23.429452900	38.281486900
N	22.459134500	22.949936100	38.151932300
N	23.505644000	22.413101700	37.875816800

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C	19.855313400	20.445917800	38.863030200
C	21.121502600	20.972616300	38.629068300
C	21.298164900	22.369906400	38.697055600
C	20.232015300	23.214997200	39.064269200
C	18.976198800	22.662910600	39.274572300
C	18.768232000	21.290305200	39.113714700
H	19.721838300	19.361075000	38.821874400
H	21.960516200	20.323537300	38.377845600
H	20.395880900	24.284326100	39.197650600
H	18.141416800	23.320659700	39.539422400
C	24.836859700	22.733014900	38.132353400
C	25.326439100	24.036831700	37.909669200
C	25.694550000	21.664201700	38.438489000
C	26.693349400	24.260949300	38.007708100
H	24.638823200	24.846660800	37.660743100
C	27.057251600	21.928804200	38.552588100
H	25.291604700	20.660721000	38.584625900
C	27.559589800	23.207259800	38.306334400
H	27.097534100	25.259225700	37.824555300
H	27.749194400	21.130935700	38.829492500
H	28.636657200	23.386003700	38.315834000
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N	23.485782300	22.495368400	37.781079600
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C	21.278248500	22.448807100	38.696957100
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C	20.195687700	23.258730000	39.101928200
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C	18.960004000	22.670362300	39.324392600
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C	18.785218100	21.295281300	39.140197400
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H	19.782776400	19.397034800	38.796436100
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H	21.990567200	20.424411300	38.341061400
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H	20.335434900	24.331249000	39.243052700
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H	18.112418500	23.301408800	39.612232600
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C	24.776302800	22.828153500	38.068412400
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C	25.540208100	21.712978800	38.439999700
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H	24.737541100	24.932362200	37.532767700
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H	27.211269700	25.190847900	37.805027900
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H	27.534429600	21.063757400	38.951686300
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H	28.595205600	23.234330500	38.419768000
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N	22.359847000	23.118277200	38.071760500
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N	23.415746300	22.700164900	37.669300200
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C	19.807961600	20.860112100	38.724057700
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C	21.043107400	21.503540900	38.663382700
C	21.081805400	22.895114700	38.839726900
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C	18.700640700	22.967139800	39.160240000
C	18.636712000	21.585083100	38.957870300
H	19.776521600	19.775113700	38.594704600
H	21.955565100	20.935207300	38.465143700
H	19.989409000	24.707598600	39.290766900
H	17.788012200	23.537752400	39.358563300
C	24.513135800	23.138846600	38.142395600
C	25.629325500	23.877749900	37.704902900
C	24.638745100	21.812084100	38.592394800
C	26.887294200	23.291362800	37.780247900
H	25.494309100	24.894189900	37.331775700
C	25.908502900	21.256197300	38.666492500
H	23.757534300	21.248115600	38.904860500
C	27.028957000	21.992169700	38.274231900
H	27.768663100	23.847656200	37.458402900
H	26.017315900	20.239760300	39.049918000
H	28.025396300	21.545370600	38.343965100
N	22.303807000	23.629037000	38.869892900
N	23.237847200	23.757091100	38.118545400

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C	19.826871300	20.879402300	38.735134000
C	21.050447400	21.540656300	38.653639000
C	21.072886800	22.937119800	38.806673100
C	19.899222000	23.657173600	39.098756800
C	18.693842400	22.974493400	39.164393600

C	18.647042500	21.590146600	38.970574500
H	19.810340900	19.793037800	38.611955000
H	21.967587800	20.983190700	38.446200600
H	19.954663900	24.735782500	39.256639400
H	17.774132900	23.531748400	39.368379000
C	24.526169400	23.108211100	38.181803700
C	25.671785800	23.839165900	37.815094200
C	24.604328200	21.758626800	38.563836700
C	26.912514500	23.218267500	37.899151500
H	25.573159000	24.875741600	37.490087000
C	25.858629200	21.167783600	38.648285300
H	23.702088100	21.199784100	38.822035400
C	27.008257900	21.893003900	38.328954600
H	27.814953500	23.770458000	37.635049200
H	25.928227800	20.131477000	38.984712400
H	27.992498700	21.421800400	38.405733200
N	22.273083700	23.693847800	38.793252700
N	23.267284100	23.758241700	38.123582100

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C	19.832661100	20.877450000	38.743780700
C	21.053156500	21.543570600	38.649157300
C	21.067123400	22.942141100	38.785392600
C	19.890224500	23.657574400	39.083433500
C	18.690387500	22.968024900	39.166249100
C	18.649284000	21.582772600	38.977959800
H	19.820626600	19.790399000	38.627724200
H	21.971260600	20.988422400	38.440640300
H	19.940951700	24.737711000	39.233357800

H	17.770249400	23.522255900	39.377326800
C	24.535884000	23.110715700	38.198689200
C	25.686894400	23.834826900	37.830516600
C	24.602686800	21.757122300	38.568751700
C	26.922460800	23.203488100	37.903907300
H	25.594980100	24.873910200	37.512081000
C	25.853798400	21.158169500	38.646229600
H	23.698138400	21.201590500	38.825240800
C	27.008515100	21.875856700	38.328468000
H	27.828390600	23.746361700	37.632183300
H	25.916843600	20.119302900	38.976170500
H	27.988792200	21.396536600	38.401706300
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N	23.288966300	23.779155800	38.143423800

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C	19.831533000	20.875422600	38.749807200
C	21.050192300	21.543571900	38.648100500
C	21.057484700	22.943942900	38.772894000
C	19.881101400	23.659065300	39.077366300
C	18.685271900	22.965001800	39.171827900
C	18.647684300	21.579842300	38.983432300
H	19.821822900	19.788269600	38.634483300
H	21.968180200	20.987471200	38.441878700
H	19.930371800	24.738424600	39.226794700
H	17.765068600	23.514937400	39.391604200
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C	25.694520700	23.839373200	37.839687700
C	24.605177200	21.759069700	38.569508500

C	26.927574000	23.202558400	37.903774800
H	25.603353600	24.878028400	37.521067800
C	25.855503000	21.157995100	38.642762400
H	23.699604200	21.203627700	38.821949300
C	27.011691600	21.874223900	38.326556400
H	27.832541900	23.742843500	37.624389600
H	25.915678600	20.118091700	38.969459600
H	27.990754900	21.392219600	38.397948500
N	22.230505100	23.726860500	38.692581700
N	23.302467400	23.792251200	38.166218400

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C	19.832795300	20.883629800	38.771422400
C	21.048053900	21.555178700	38.654327700
C	21.048975500	22.958773600	38.751026000
C	19.868943000	23.674564300	39.042709200
C	18.677619700	22.975586700	39.154462100
C	18.645751100	21.586113500	38.995136700
H	19.827128100	19.794622700	38.671808400
H	21.966738900	20.999958400	38.450743200
H	19.911622500	24.758371400	39.163236300
H	17.755186100	23.527375800	39.361628300
C	24.549505100	23.141329200	38.225348700
C	25.708180500	23.871142100	37.889133900
C	24.601297400	21.772335900	38.540881000
C	26.935859500	23.223543800	37.937937900
H	25.627677100	24.922279200	37.610985700
C	25.846761800	21.160343500	38.597509800
H	23.691827700	21.216361900	38.776896700

C	27.008940500	21.879124000	38.309501400
H	27.846005900	23.769216400	37.686644300
H	25.897097700	20.109092900	38.888596700
H	27.984903100	21.389074900	38.363400800
N	22.214898200	23.743741400	38.651778900
N	23.315476200	23.823275300	38.195193800

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C	19.831548900	20.883639600	38.775087500
C	21.046470600	21.555183700	38.660216600
C	21.042797000	22.959754400	38.750081600
C	19.863323000	23.676878500	39.043443500
C	18.674253800	22.974845900	39.160395800
C	18.643726500	21.585983600	38.996249900
H	19.826340300	19.795299400	38.672044200
H	21.967098900	21.001838800	38.460702300
H	19.905230600	24.760692700	39.162104200
H	17.751689600	23.523741300	39.373873400
C	24.553286600	23.143848300	38.226830500
C	25.712812800	23.874445500	37.893257500
C	24.601952600	21.772395800	38.535475700
C	26.938841300	23.223542900	37.936372800
H	25.631497400	24.926857000	37.619711700
C	25.847207500	21.160627700	38.594074200
H	23.691852900	21.215743200	38.767742600
C	27.010305600	21.878812100	38.307812900
H	27.849756500	23.767453200	37.683880900
H	25.898237500	20.111143500	38.891489100
H	27.985813500	21.387876600	38.362716800

N	22.204604000	23.740185800	38.620105900
N	23.323899500	23.830287500	38.218041800
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C	19.826003800	20.881014500	38.780242300
C	21.040285300	21.551906400	38.662126400
C	21.036643100	22.958044400	38.745647900
C	19.858648600	23.678803900	39.036978500
C	18.670850100	22.975806800	39.161541100
C	18.639758700	21.586650900	38.999558600
H	19.820850400	19.792164500	38.679696600
H	21.962285700	20.999900400	38.466914400
H	19.900318000	24.762028000	39.155824700
H	17.748335700	23.523226100	39.380299500
C	24.558582600	23.149559700	38.228533600
C	25.719787500	23.880030100	37.899924200
C	24.604290200	21.776206500	38.532910200
C	26.943838500	23.225258700	37.937849400
H	25.640146700	24.932336400	37.627476100
C	25.848342700	21.162365500	38.590232900
H	23.693306500	21.219420400	38.760759800
C	27.012858300	21.879659500	38.306954300
H	27.855445900	23.765860600	37.680315000
H	25.897197100	20.111478800	38.883429800
H	27.987373400	21.386981300	38.362575400
N	22.198355300	23.727724800	38.591316400
N	23.332278200	23.840964700	38.241684200

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C	19.802176000	20.858434400	38.834713800
C	21.022107900	21.517738800	38.714171700
C	21.023939300	22.927597500	38.752618200
C	19.842267400	23.662949100	38.994688400
C	18.649639200	22.969465100	39.120162400
C	18.615031200	21.575371500	39.008365800
H	19.790208500	19.766254500	38.775825000
H	21.944801000	20.954836100	38.555205000
H	19.885972100	24.750214800	39.069445700
H	17.725371000	23.528820400	39.296277200
C	24.556630300	23.189949200	38.246490800
C	25.720048700	23.945731800	37.988971100
C	24.606048600	21.800224500	38.464726800
C	26.945966500	23.293631300	38.000313200
H	25.641475500	25.015473400	37.792611600
C	25.851435000	21.187710900	38.492847000
H	23.693407600	21.227147500	38.643319000
C	27.016332900	21.925236600	38.271660200
H	27.859548800	23.854890700	37.799233200
H	25.899401100	20.118101000	38.708227400
H	27.992373000	21.433032200	38.299241200
N	22.186973600	23.681249000	38.591075000
N	23.326006400	23.874001300	38.297554600

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C	19.791643400	20.847111700	38.834805000
C	21.015624400	21.497326300	38.712715200
C	21.028332700	22.908229900	38.753610400
C	19.852878400	23.654762600	38.995822400

C	18.656119600	22.968542700	39.124486900
C	18.611383800	21.575105100	39.009012800
H	19.771831400	19.754643000	38.775482300
H	21.935231900	20.930147200	38.552338800
H	19.904691300	24.741338800	39.073369300
H	17.736503900	23.534034300	39.304276200
C	24.558473600	23.210703700	38.238701700
C	25.726763100	23.958909300	37.984215400
C	24.599563000	21.820616300	38.457230800
C	26.948580100	23.298719800	37.993539700
H	25.655060400	25.028871000	37.787491000
C	25.840226800	21.198587100	38.485470500
H	23.683043200	21.254002600	38.635837600
C	27.009572900	21.929772300	38.265704800
H	27.866201700	23.853404300	37.790449100
H	25.881455300	20.127659600	38.700095600
H	27.982250100	21.431504400	38.294624600
N	22.194948600	23.640916300	38.566023100
N	23.330315800	23.905822100	38.314936000

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C	19.773257800	20.811157900	38.843360800
C	21.008525200	21.437048200	38.719417600
C	21.045873000	22.849088800	38.754872500
C	19.883867800	23.620816400	38.983397100
C	18.674943000	22.955178300	39.112070700
C	18.605842800	21.562053000	39.007631000
H	19.735593600	19.718677900	38.796899200
H	21.919958300	20.854058300	38.571582300

H	19.956844800	24.706102700	39.058157700
H	17.764378700	23.537650400	39.286575600
C	24.566096000	23.246748700	38.229806600
C	25.734934700	23.992445700	37.980901700
C	24.603278000	21.856266900	38.445142600
C	26.954241000	23.326628200	37.983633300
H	25.668222900	25.064097600	37.791817500
C	25.840360100	21.227407900	38.466665000
H	23.683580300	21.294385500	38.622363700
C	27.010941100	21.955871400	38.245866600
H	27.873297400	23.878133300	37.781131600
H	25.878626700	20.155032500	38.673987100
H	27.982294900	21.454246500	38.268094500
N	22.225633200	23.538731800	38.540298400
N	23.330658900	23.943151500	38.328150500
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C	19.767910800	20.798224700	38.848607800
C	21.004935300	21.420372000	38.724736800
C	21.045023400	22.832412400	38.759574200
C	19.883038500	23.608115900	38.974907200
C	18.672424500	22.945770400	39.103929600
C	18.601749100	21.552261400	39.007057100
H	19.726641800	19.705451900	38.811300100
H	21.917428100	20.838144200	38.581019200
H	19.956531600	24.693338600	39.043322600
H	17.763070700	23.531068900	39.276991900
C	24.568179000	23.247736200	38.230889900
C	25.731544700	24.000177100	37.976791400

C	24.615085200	21.856998700	38.442260100
C	26.955172000	23.341596200	37.974828600
H	25.657253600	25.072026100	37.789821200
C	25.856037700	21.235532200	38.458727300
H	23.698654500	21.289838000	38.619608700
C	27.021817100	21.971127000	38.236774200
H	27.869924600	23.899255500	37.769577800
H	25.900018800	20.162877400	38.662741400
H	27.996022300	21.474673500	38.256715600
N	22.226783300	23.513886200	38.531998300
N	23.328676200	23.937372200	38.339441700