

Electronic Supplementary Information

Theoretical Mechanistic Study of Ir^{III}/Cu^I-Metallaphotoredox Catalyzed Asymmetric Radical Decarboxylative Cyanation

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COMPUTATIONAL DETAILS

1. Correction of Translational Entropy in Solution

We evaluated the electronic energy (E_{sol}) with zero-point energy correction in solution. For each species, the E_{sol} is defined through equation (S1):

$$E_{sol} = E_{sol}^{pot} + E_{gas}^{v_0} \quad (S1)$$

where the E_{sol}^{pot} is the potential energy including non-electrostatic energy in solution and $E_{gas}^{v_0}$ delegates the zero-point vibrational energy in the gas phase. In a bimolecular process, such as the benzyl radical capture by Cu(II) complex, the entropy change which can decrease considerably must be taken into consideration. In such case, Gibbs energy (G_{sol}^o) need be computed as follows:

$$\begin{aligned} G_{sol}^o &= H_0 - T(S_r^o + S_v^o + S_t^o) \\ &= E^T + P\Delta V - T(S_r^o + S_v^o + S_t^o) \\ &= E_{sol} + E_{therm} - T(S_r^o + S_v^o + S_t^o) \end{aligned} \quad (S2)$$

where ΔV is 0 in solution, E_{therm} is the thermal correction by translational, vibrational, and rotational movements, and S_r^o , S_v^o , and S_t^o are rotational, vibrational, and translational entropies, respectively.

In general, the Sackur-Tetrode equation is used to evaluate translational entropy S_t^o . In solution, however, the usual Sackur-Tetrode equation cannot be directly applied to the evaluation of S_t^o , because the translation movement is suppressed very much in solution.^{S1} In this context, the translational entropy was corrected with the method developed by Whitesides et al., where the rotational entropy was evaluated in a normal manner. Thermal correction and entropy contributions of vibration movements to the Gibbs energy were evaluated with the frequencies calculated at 298.15 K and 1 atm.

2. Redox Potential

We calculated the standard redox potential ($E_{1/2}^{red}$) according to the equation (S3):^{S2}

$$E_{1/2}^{red} = -\frac{\Delta G_r}{nF} - E_{SHE} \quad (S3)$$

where F is the Faraday constant and n is the number of electrons transferred, $E_{SHE} = 4.51$ V, and ΔG_r is the free energy change of the reaction.

Table S1. The Gibbs free energy (G , a.u.), electronic energy (E_{opt} , a.u.), single point energy (E_{sp} , a.u.), and Gibbs free energy with the single point energy correction ($G_{corr.}$, a.u.) of *Ir(III)_{DFT} and *Ir(III)_{TDDFT}.

	*Ir(III) _{DFT} (a.u.)	*Ir(III) _{TDDFT} (a.u.)	$\Delta(*\text{Ir(III)}_{\text{TDDFT}} - *\text{Ir(III)}_{\text{DFT}})$ (kcal/mol)
G^a	-1539.405209	-1539.409089	-2.4
E_{opt}^a	-1539.81770017	-1539.823742	-3.8
E_{sp}^b	-1539.89767944	-1539.895841	1.1
$G_{corr.}^c$	-1539.485188	-1539.481188	2.5

^a at the (U)M06/[6-31G(d)/LanL2DZ (Ir)] level

^b at the SMD(toluene)/(U)M06/[6-311++G(d,p)/SDD (Ir)] level

^c at the SMD(toluene)/(U)M06/[6-311++G(d,p)/SDD (Ir)]/(U)M06/[6-31G(d)/LanL2DZ (Ir)] level

Table S2. The experimental and calculated redox potentials of Ir complexes.¹⁷

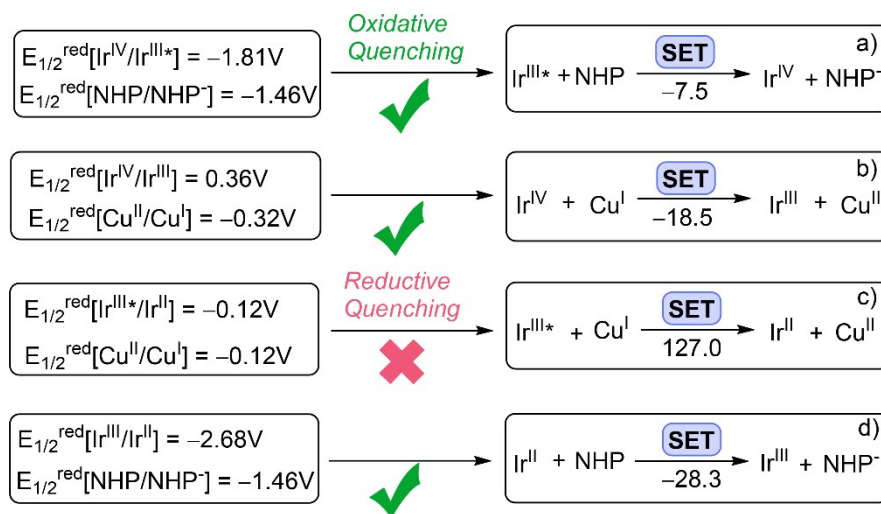
Redox Potential	$E_{1/2}^{red}$ [Ir ^{IV} /*Ir ^{III}]	$E_{1/2}^{red}$ [Ir ^{IV} /Ir ^{III}]
Cal. ^{DMF}	-1.81 V	0.36 V
Cal. ^{MeCN}	-1.81 V	0.36 V
Exp. ^{MeCN}	-1.73 V	0.77 V
Δ	0.08 V	0.41 V

Table S3. The experimental and calculated redox potentials of Cu complexes and NHP ester.¹⁷

Redox Potential	$E_{1/2}^{red}$ [NHP/NHP-]	$E_{1/2}^{red}$ [Cu ^{II} / Cu ^I]
Cal. ^{DMF}	-1.46 V	-0.32 V

Cal. ^{MeCN}	-1.42 V	-0.32 V
Exp. ^{MeCN}	-1.33 V	-
Δ	0.09 V	-

Scheme S1. Possible single electron transfer processes. $\Delta G^{\circ\ddagger}$ values of SET processes are given in kcal/mol.



3. Activation Barrier of Single Electron Transfer Step

According to the Marcus equation, the reorganization energy λ is normally decomposed into internal energy (λ_i) and external energy (λ_o). The internal reorganization energy λ_i can be estimated according to the equation (S4):

$$\lambda_i = [E^{D^+}(Q_R) + E^{A^-}(Q_R)] - [E^{D^+}(Q_P) + E^{A^-}(Q_P)] \quad (\text{S4})$$

where Q_R and Q_P are the equilibrium geometries of the reactants and products, respectively. In addition, the external reorganization energy λ_o may be calculated from equation (S5–S7)

$$\lambda_o = (332 \text{ kcal/mol}) \left(\frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{R} \right) \left(\frac{1}{\epsilon_{op}} - \frac{1}{\epsilon} \right) \quad (\text{S5})$$

$$\lambda = \lambda_o + \lambda_i \quad (\text{S6})$$

$$\Delta G^{\circ\ddagger} = \frac{(\Delta G_r + \lambda)^2}{4\lambda} \quad (\text{S7})$$

where a_1 is the radii of the oxidant, a_2 is the radii of the reductant, $R = a_1 + a_2$, ϵ_{op} is the optical dielectric constant ($\epsilon_{op} = 2.25$), ϵ is the static dielectric constant for the toluene solvent ($\epsilon = 2.37$), and ΔG_r is the free energy change of the reaction.

Table S4. Calculated electron transfer energy barriers related parameters for SET a) and b) in Scheme S1.

SET step	a_1 (Å)	a_2 (Å)	R (Å)	λ (kcal/mol)	ΔG_r (kcal/mol)	ΔG_{SET} (kcal/mol)
(a)	3.73	4.14	7.88	28.3	-7.5	3.6
(b)	4.16	3.87	8.02	38.6	-18.5	2.6

Table S5. The zero-point energy (ZPE , a.u.) correction, Gibbs free energy (G , a.u.), electronic energy (E_{opt} , a.u.), single point energy (E_{sp} , a.u.), and Gibbs free energy with the single point energy correction ($G_{corr.}$, a.u.) of **3** and **TS2**.

	3 (a.u.)	TS2 (a.u.)	$\Delta(\mathbf{TS2-3})$ (kcal/mol)
ZPE correction ^a	0.375475	0.372299	-2.0
G^a	-1167.482567	-1167.477707	3.0
E_{opt}^a	-1167.800169	-1167.790423	6.1
E_{sp}^b	-1168.21595	-1168.218893	-1.8
$G_{corr.}^c$	-1167.898348	-1167.906177	-4.9

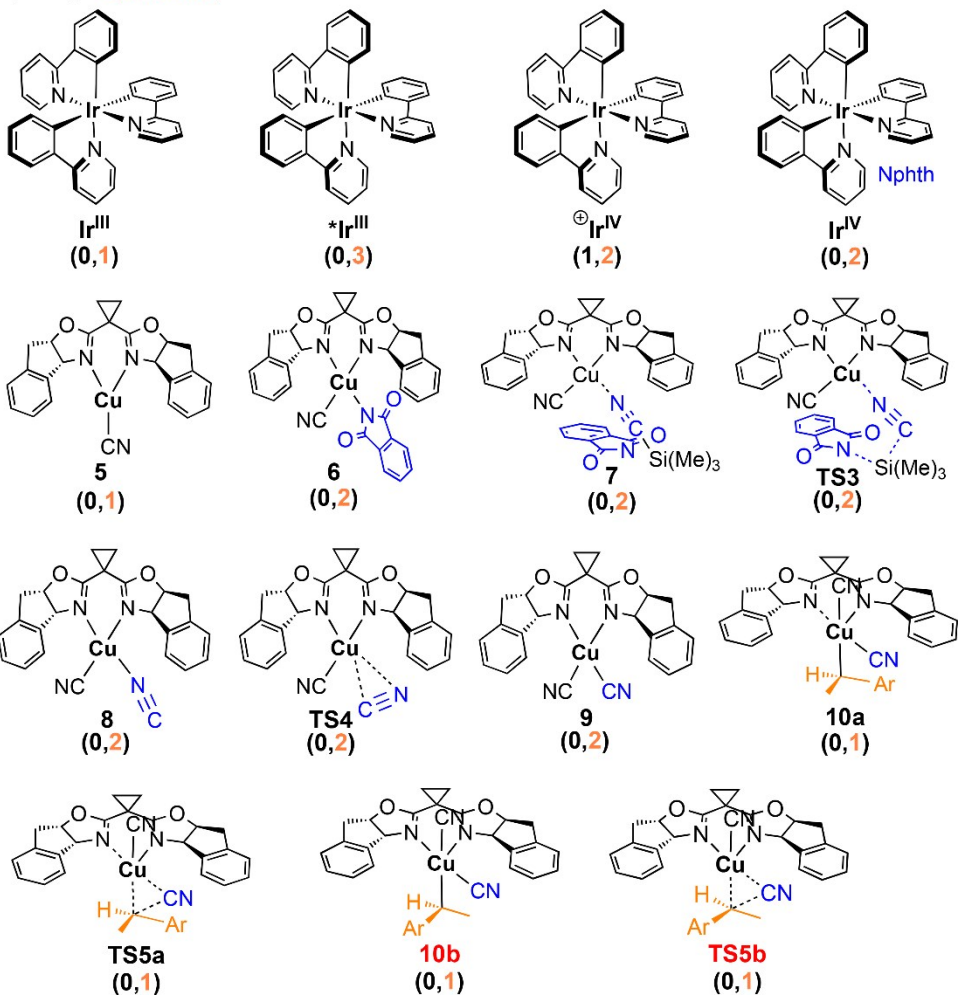
^a at the (U)M06/[6-31G(d)/LanL2DZ (Ir,Cu)] level

^b at the SMD(toluene)/(U)M06/[6-311++G(d,p)/SDD (Ir,Cu)] level

^c at the SMD(toluene)/(U)M06/[6-311++G(d,p)/SDD (Ir,Cu)]/(U)M06/[6-31G(d)/LanL2DZ (Ir,Cu)] level

Scheme S2. Charges and spin states of some structures in Fig. 1 and Fig. 2.

(charge, spin state)



Scheme S3. Evaluation of active species.

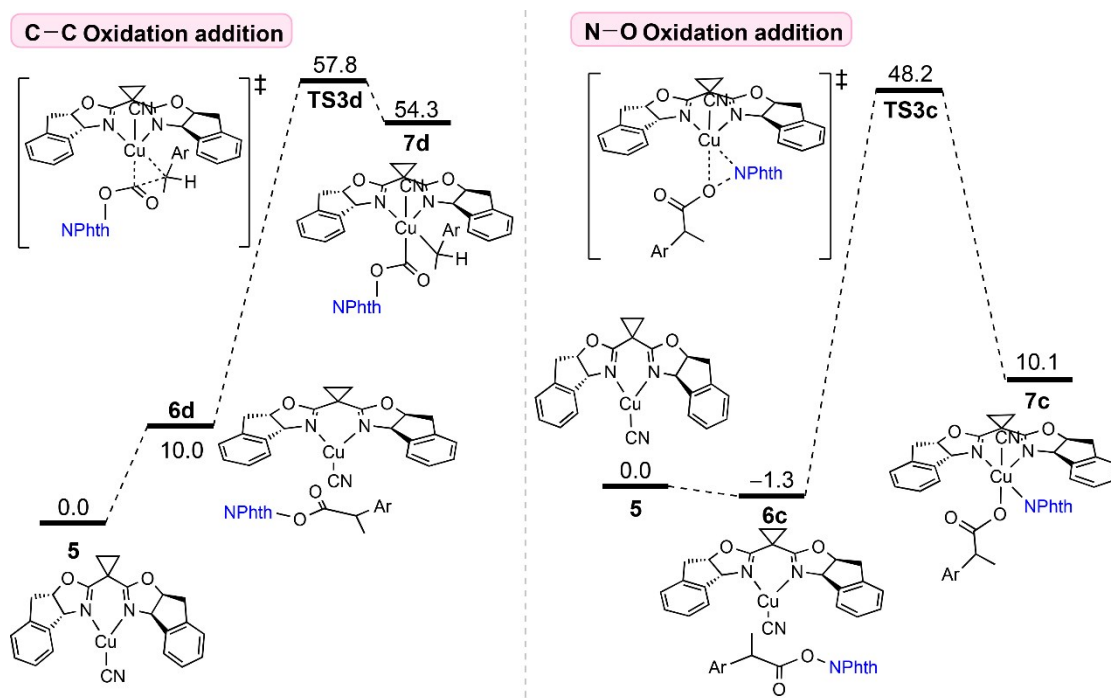
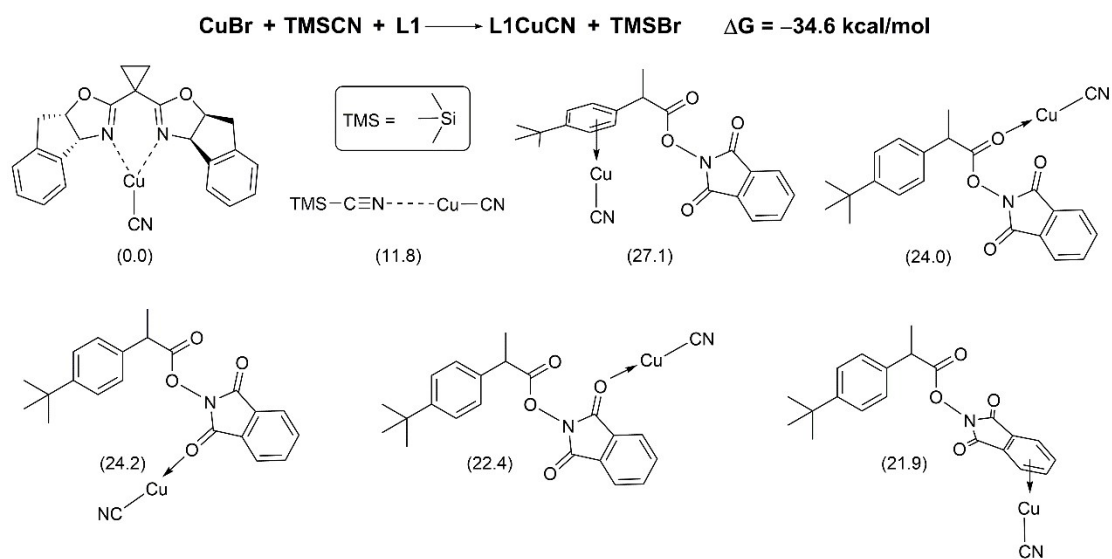


Fig. S1 Gibbs energy profiles ($\Delta G^\circ_{298.15}$) of oxidative additions the C–C and N–O bonds of NHP ester **1** to Cu(I) center of **5**.

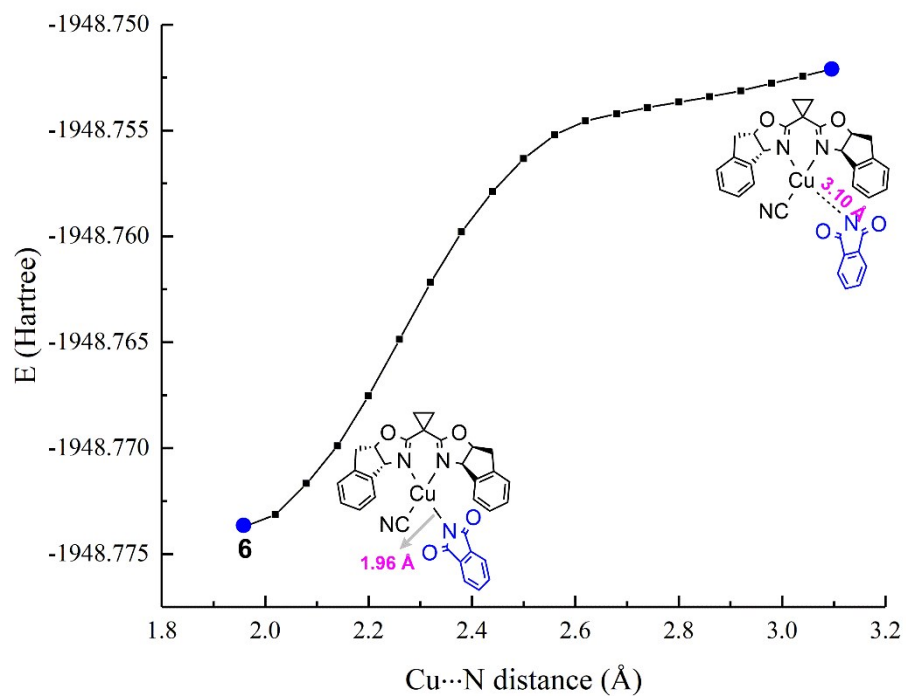


Fig. S2 Relaxed scanning the potential energy surface of Nphth⁻ anion dissociation by modulating Cu...N distance of **6** calculated at the (U)M06/[6-31G(d)/LanL2DZ (Ir, Cu)] level.

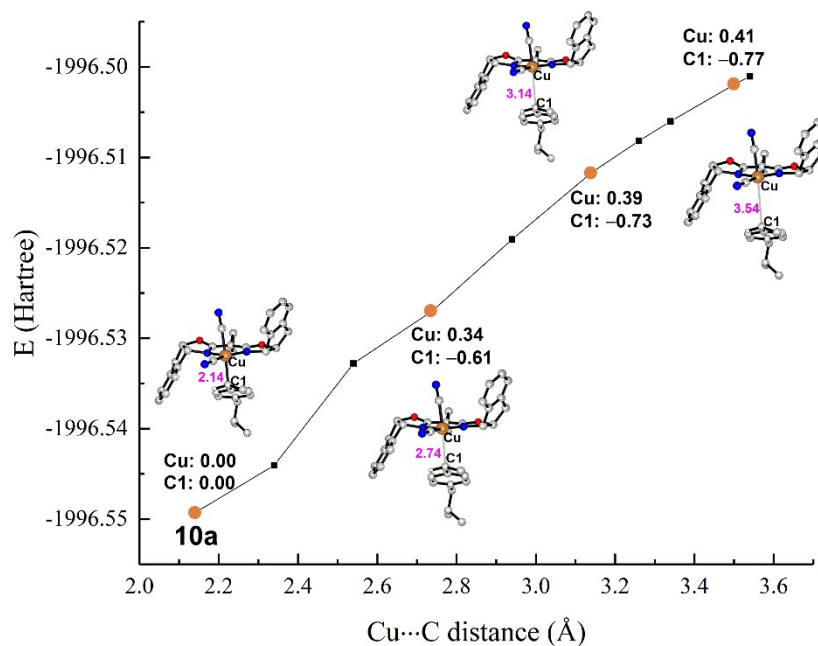


Fig. S3 Relaxed scanning the potential energy surface of benzyl radical dissociation by modulating Cu...C distance of **10a** calculated at the (U)M06/[6-31G(d)/LanL2DZ (Ir, Cu)] level. As the distance of Cu...C increases, the spin polarization becomes more and more obvious.

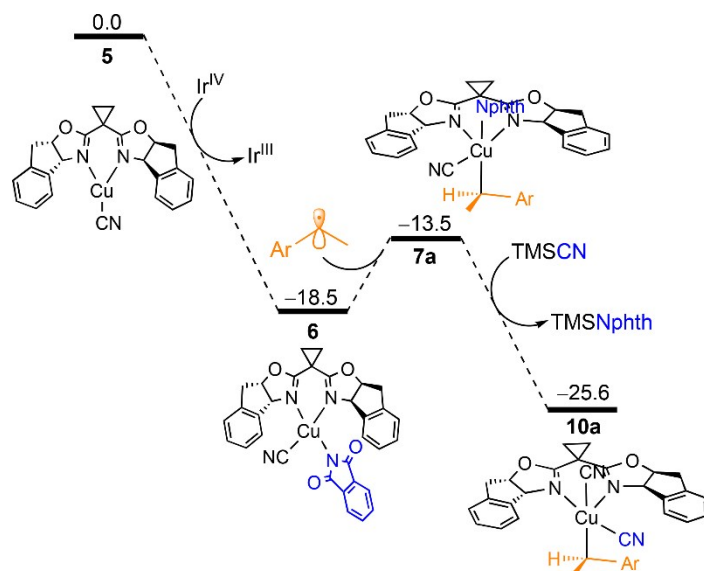


Fig. S4 Gibbs energy profile ($\Delta G^\circ_{298,15}$) of the radical capture from **6**.

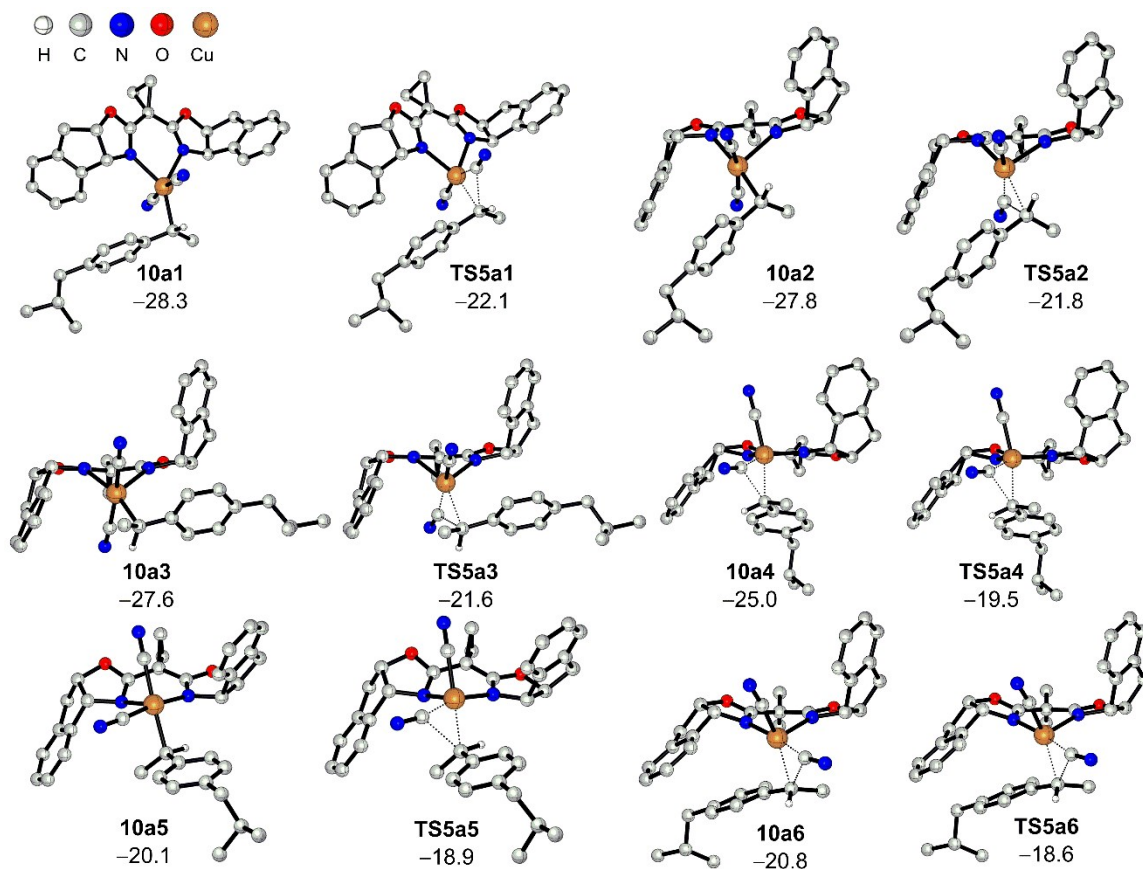


Fig. S5 Optimized structures for selected important stationary points leading to *R-pro* in Fig. 3.

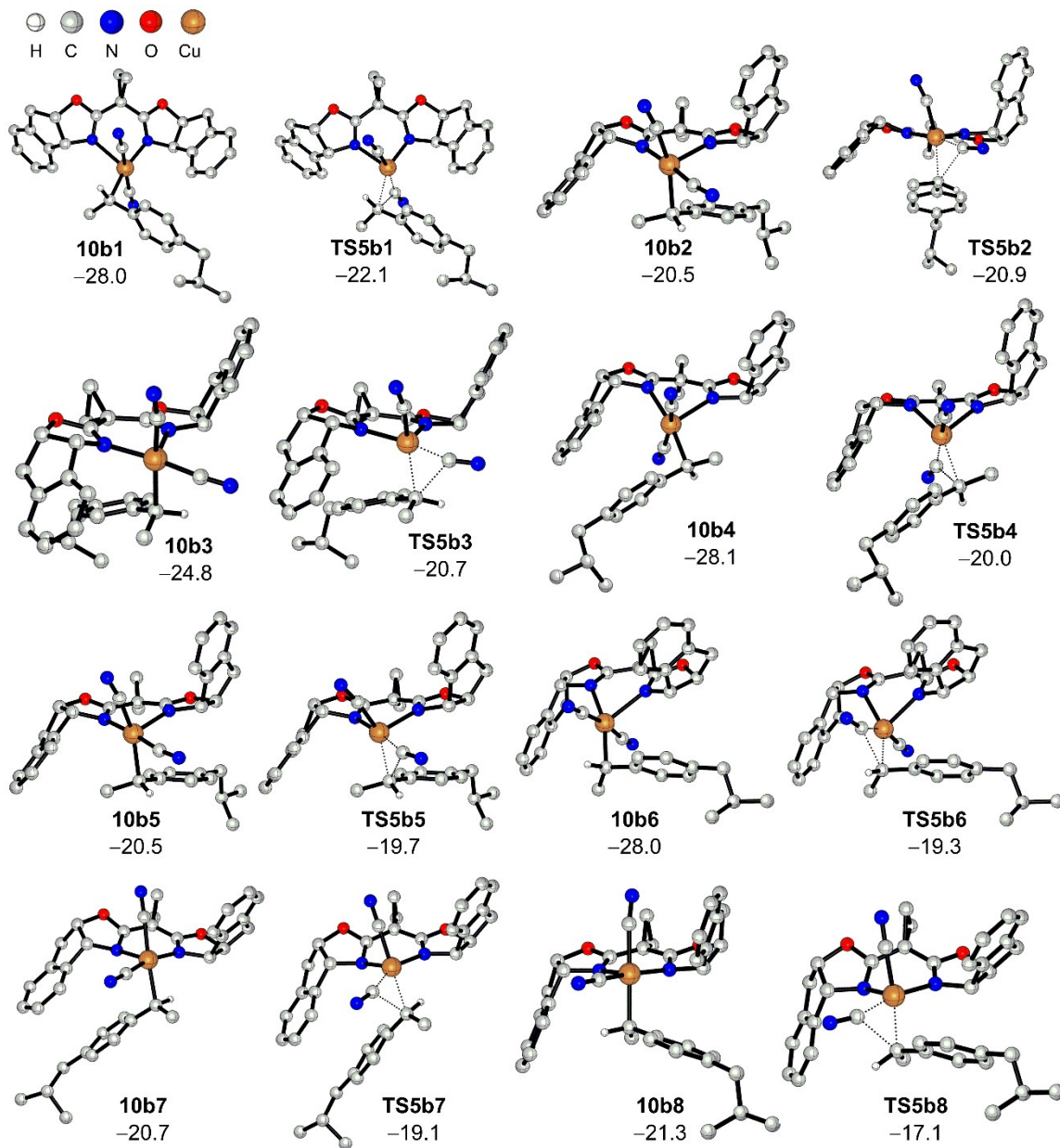


Fig. S6 Optimized structures for selected important stationary points leading to *S-pro* in Fig. 3.

4. Fragment Molecular Orbital (FMO) Analysis

Generally, MOs of a total system AB can be represented by a linear combination of MOs of fragments A and B;^{S3} see eqn (S8):

$$\varphi_i^{AB} = \sum_m C_{im}^A \varphi_m^A + \sum_{n} C_{in}^B \varphi_n^B \quad (\text{S8})$$

where φ_i^{AB} represents the *i*th MO of complex AB and φ_m^A and φ_n^B are the *m*th and *n*th MOs of fragments A and B, respectively. C_{im}^A and C_{in}^B are expansion coefficients of φ_m^A and φ_n^B , respectively. Electron populations of φ_m^A and φ_n^B can be obtained from these coefficients.

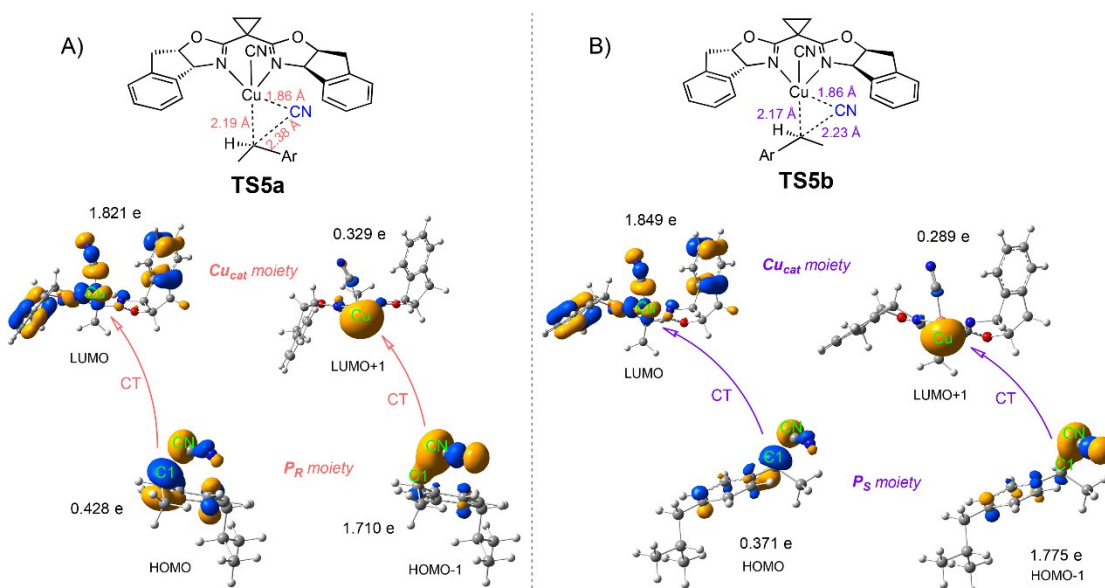


Fig. S7 Important Kohn–Sham orbitals and their electron populations of Cu_{cat} and P moieties in **TS5a** (or **TS5b**).

As shown in Fig. S7A, **TS5a** is divided into two fragments as copper catalyst (Cu_{cat}) and product (P_R) moieties. Specifically, the electron population of the lowest unoccupied molecular orbital (LUMO) of the Cu_{cat} moiety highly increases to 1.821e in **TS5a**. Consistent with this increase in population, the population of the highest occupied molecular orbital (HOMO) of the P_R moiety decreases to 0.428e. The substantial CT occurs from the σ^* anti-bonding orbital (HOMO of P_R moiety) consisting of the p orbitals of the C1 and C(\equiv N) atoms (pC1 and pC(\equiv N)) to the Cu 3d $_{\pi}$ orbital (LUMO), indicating that the C1–C(\equiv N) bond formation is under progress. In addition, the electron population of LUMO+1 of the Cu_{cat} moiety moderately increases to 0.329e in **TS5a**, where the empty orbital mainly consists of 4p

and 3d orbitals of the Cu center. Correspondingly, the population of the HOMO-1 of the P_R moiety decreases to 1.710e. These results clearly indicate that the CT occurs from the pC1 and pC(≡N) orbitals to the LUMO and LUMO+1 of the Cu_{cat} moiety. These CTs contribute to the change of the Cu^{III} to the Cu^I and the formation of a new C1–C(≡N) bond. As shown in Fig. S7B, **TS5b** is divided into Cu_{cat} and P_S moieties in the same way. The LUMO and LUMO+1 populations of the Cu_{cat} moiety increase to 1.849e and 0.289e, respectively, and the populations of the HOMO and HOMO-1 of the P_S moiety correspondingly decreases to 0.371e and 1.775e. This means that a CT similar to that in **TS5a** from σ* to 3d_π and from lone pair to 4p and 3d orbitals of the Cu center is formed in **TS5b**.

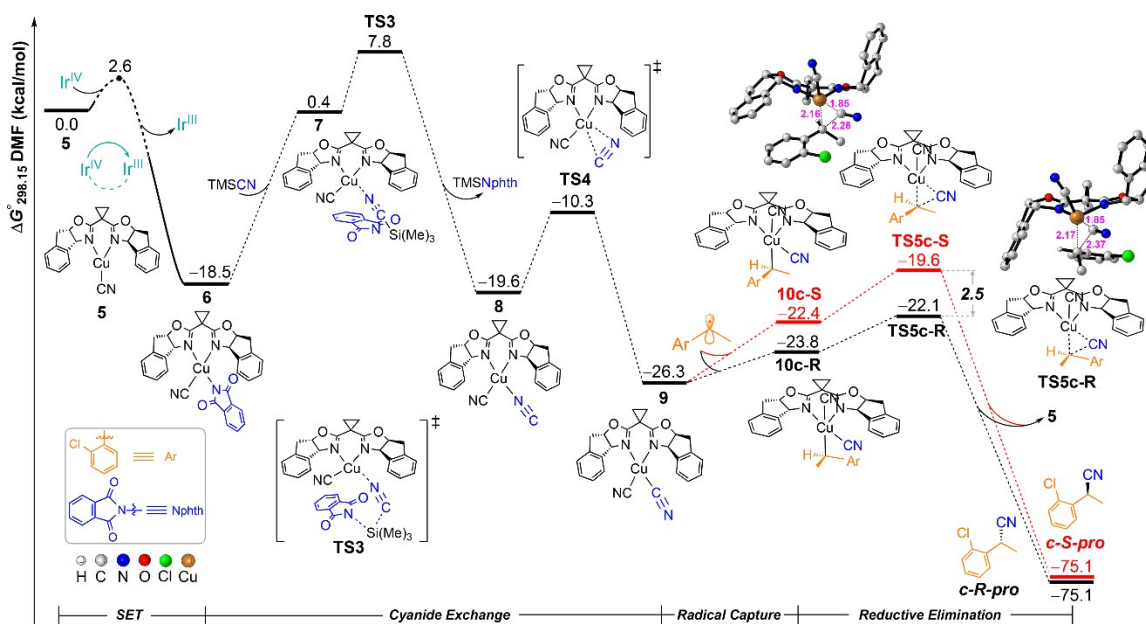


Fig. S8 Gibbs energy profiles ($\Delta G^{\circ}_{298.15}$) of copper catalytic cycle (Cu^I–Cu^{II}–Cu^{III}–Cu^I) providing R-type (black line) and S-type (red line) products with the substrate **S1** (Table 2, entry 1).

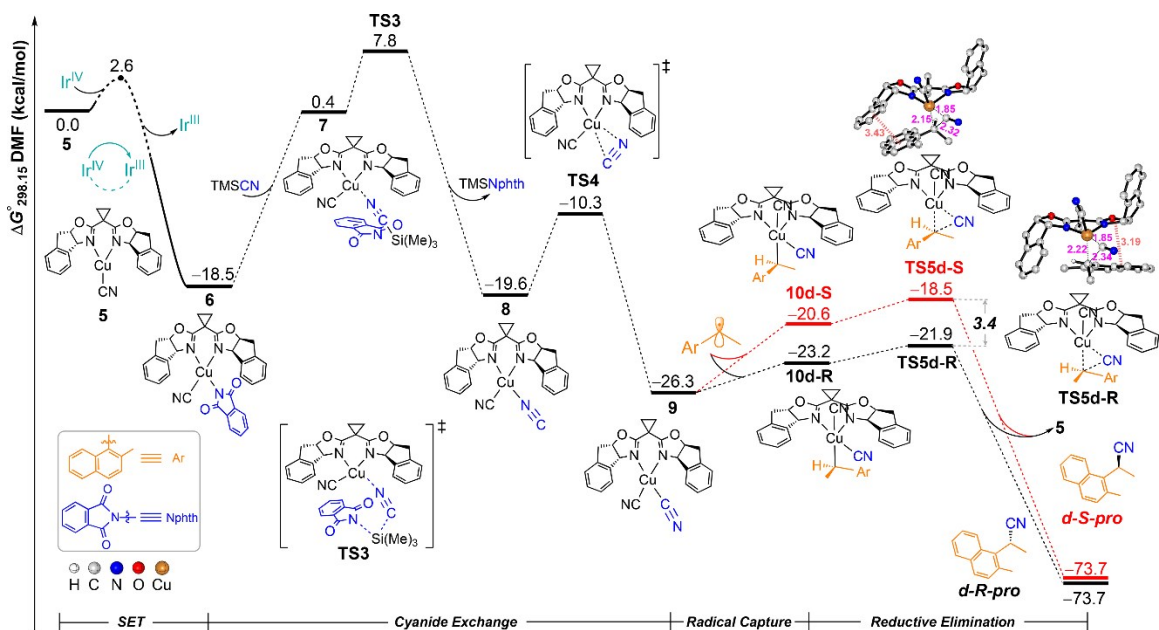


Fig. S9 Gibbs energy profiles ($\Delta G^{\circ}_{298.15}$) of copper catalytic cycle ($\text{Cu}^{\text{I}}-\text{Cu}^{\text{II}}-\text{Cu}^{\text{III}}-\text{Cu}^{\text{I}}$) providing R-type (black line) and S-type (red line) products with the substrate **S2** (Table 2, entry 2).

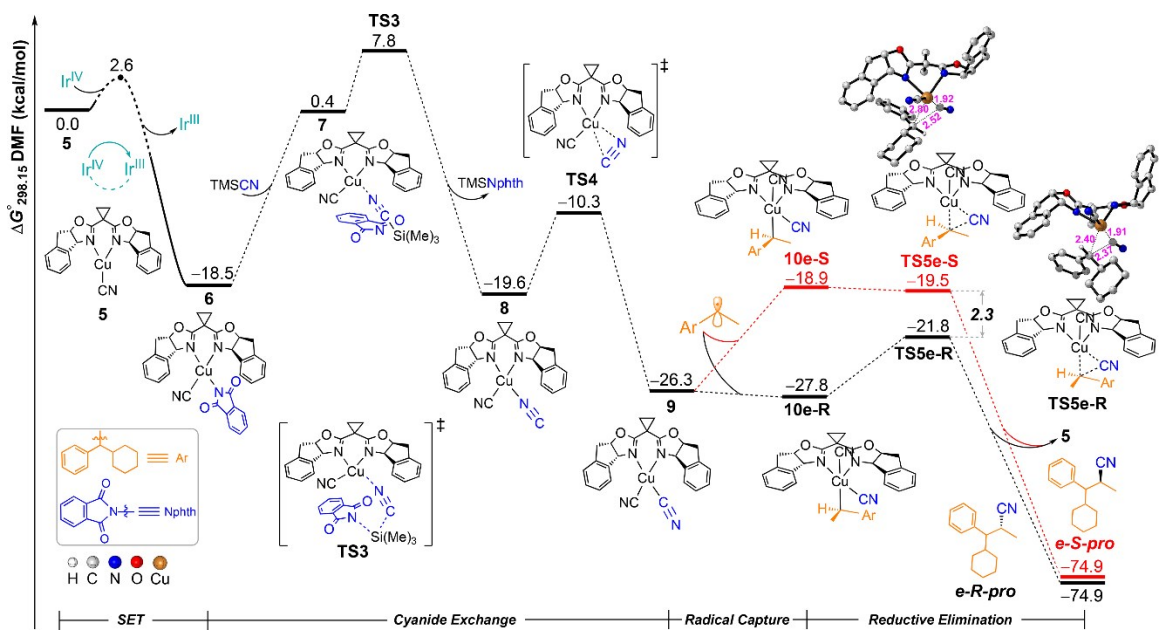


Fig. S10 Gibbs energy profiles ($\Delta G^{\circ}_{298.15}$) of copper catalytic cycle ($\text{Cu}^{\text{I}}-\text{Cu}^{\text{II}}-\text{Cu}^{\text{III}}-\text{Cu}^{\text{I}}$) providing R-type (black line) and S-type (red line) products with the substrate **S3** (Table 2, entry 3).

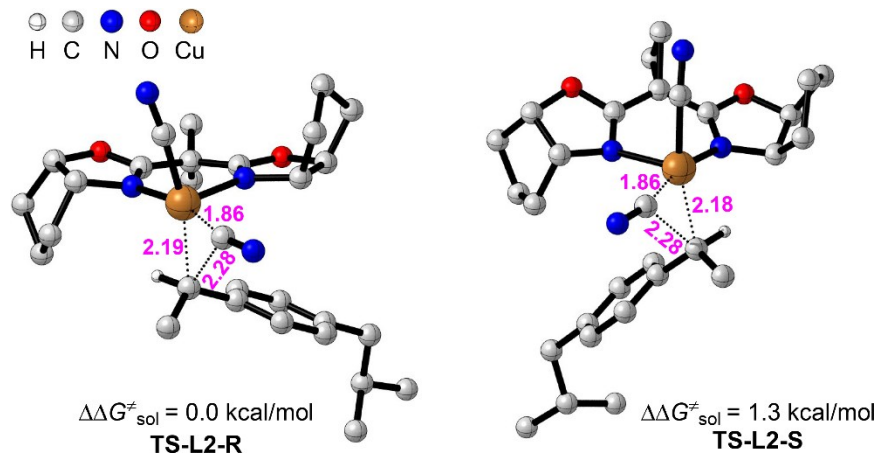


Fig. S11 Relative Gibbs energies ($\Delta G^{\circ}_{298.15}$) of transition states **TS-L2-R** and **TS-L2-S** calculated with the chiral ligand **L2** (Table 2, entry 4).

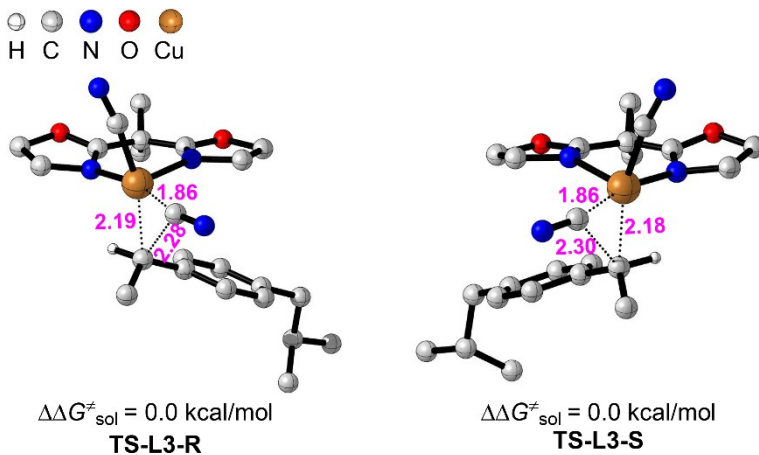


Fig. S12 Relative Gibbs energies ($\Delta G^{\circ}_{298.15}$) of transition states **TS-L3-R** and **TS-L3-S** calculated with the chiral ligand **L3** (Table 2, entry 5).

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CARTESIAN COORDINATES OF OPTIMIZED STRUCTURES

1

C	4.48456400	-0.39277100	-0.27454100
C	3.49132800	-0.32336500	-1.25503800
C	2.21200600	-0.80740700	-1.02211900
C	1.88483900	-1.37390500	0.21257500
C	2.87076800	-1.44350200	1.19435000
C	4.15264300	-0.96120900	0.95388100
H	3.73208800	0.11667800	-2.22439700
H	1.45327000	-0.73035100	-1.79887400
H	2.63224700	-1.88357500	2.16356000
H	4.91099300	-1.02269400	1.73594000
C	5.85276900	0.16737400	-0.53879300
C	0.52134800	-1.95805900	0.48392700
H	0.46592700	-2.27260200	1.53547200
C	-0.60613300	-0.99184100	0.24549000
C	5.91532400	1.70034100	-0.48881800
H	5.18863600	2.08869400	-1.22419200
O	-1.60779100	-1.25342400	1.17806300
N	-2.76508600	-0.59013400	0.88722100
O	-0.73913200	-0.18431800	-0.62646900
C	-2.91995000	0.78198800	1.19079600
C	-3.56064100	-1.01792500	-0.19703000
O	-3.44269300	-2.06512200	-0.77878100
O	-2.21537700	1.42724300	1.91935300
C	-4.50470600	0.10681200	-0.40243600
C	-4.12562400	1.16977100	0.41580700
C	-4.82238200	2.36290200	0.41896800
C	-5.92379300	2.46423300	-0.43258700
C	-6.30286000	1.40009600	-1.25231100
C	-5.59348400	0.19797600	-1.24844000

H	-4.51116300	3.18571200	1.05933400
H	-6.49603600	3.38936600	-0.46264100
H	-7.16429900	1.51334400	-1.90751100
H	-5.87363400	-0.63844600	-1.88555200
C	0.21764500	-3.17973900	-0.40098300
H	-0.78286800	-3.57788300	-0.19111400
H	0.25932600	-2.90313100	-1.46165800
H	0.96308900	-3.96184800	-0.21890400
H	6.57090200	-0.23363300	0.19643600
H	6.20361200	-0.16557400	-1.52906200
C	5.53339000	2.22772200	0.88644600
H	5.59751100	3.32321100	0.92266000
H	4.51284600	1.93920000	1.16782600
H	6.21761000	1.82974900	1.65262300
C	7.30605200	2.17736200	-0.88082700
H	8.05606900	1.80173700	-0.16811000
H	7.59144600	1.82333800	-1.88072300
H	7.36935900	3.27350000	-0.87889200

2

C	4.59156700	-0.44666100	-0.28535100
C	3.57322900	-0.27835400	-1.22708900
C	2.26448600	-0.65040800	-0.95299900
C	1.92841300	-1.20071200	0.28808600
C	2.94297900	-1.36943800	1.22909700
C	4.25435000	-0.99996600	0.94824100
H	3.81668400	0.15330400	-2.20047800
H	1.47990100	-0.49343300	-1.69013200
H	2.69847700	-1.79793400	2.20238800
H	5.03203500	-1.13672500	1.70264200
C	5.99329800	-0.00062200	-0.59210800
C	0.53363900	-1.67350800	0.60270100
H	0.46366500	-1.89418000	1.67707400

C	-0.56458700	-0.68663000	0.26961500
C	6.18963800	1.52005700	-0.53082100
H	5.47305000	1.97674800	-1.23585600
O	-1.53039500	-0.80507900	1.22418200
N	-2.74629200	-0.29507100	0.83722200
O	-0.63830900	0.00251200	-0.70966600
C	-3.12168100	1.05803600	1.05959200
C	-3.53303100	-1.01950500	-0.10029700
O	-3.24573800	-2.15262200	-0.50323000
O	-2.48678200	1.86092300	1.74142100
C	-4.60188400	-0.09967500	-0.36780700
C	-4.35961900	1.13567400	0.32382500
C	-5.26411600	2.19535600	0.20276000
C	-6.38803300	2.03838400	-0.58552900
C	-6.62781300	0.81468900	-1.27236000
C	-5.74511500	-0.24101800	-1.16589000
H	-5.06571000	3.12953100	0.73034200
H	-7.10058500	2.85773200	-0.68855500
H	-7.52052000	0.71651100	-1.89161500
H	-5.91839000	-1.18109600	-1.69169600
C	0.17109200	-2.94984800	-0.17629900
H	-0.87339500	-3.22788700	0.01408300
H	0.27365800	-2.77054700	-1.25428100
H	0.84151600	-3.77174900	0.10584400
H	6.70043400	-0.46923600	0.11467600
H	6.28362500	-0.34881000	-1.59743600
C	5.90025700	2.06170700	0.86105900
H	6.05372100	3.14844600	0.90507800
H	4.87011000	1.85096200	1.17297300
H	6.57515700	1.59917600	1.59935200
C	7.60128300	1.88429300	-0.96737900
H	8.34104000	1.43774600	-0.28466700
H	7.82118300	1.51841700	-1.97994700

H	7.75806900	2.97152600	-0.95828100
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TS1

C	4.25907800	0.34825200	0.60128400
C	3.18146600	1.02924600	0.02848100
C	1.96040500	0.40518400	-0.18589000
C	1.77193400	-0.93306300	0.17796900
C	2.84613700	-1.61216100	0.75292000
C	4.07043200	-0.98464300	0.96072100
H	3.30433700	2.07934700	-0.24724000
H	1.11980100	0.95491900	-0.60347500
H	2.71678500	-2.65537300	1.04645300
H	4.89654800	-1.53792900	1.41319800
C	5.58323400	1.03423600	0.78666300
C	0.48364500	-1.66329300	-0.09101900
H	0.50557200	-2.62520800	0.44089200
C	-0.78422700	-0.92603200	0.34198600
C	6.38613900	1.20060100	-0.51006000
H	5.75526500	1.76147000	-1.22198800
O	-1.66542100	-1.79468100	0.80929100
N	-3.18733500	-1.31012900	0.54331700
O	-0.97155800	0.26067000	0.15965200
C	-3.54672500	-0.25850400	1.43747900
C	-3.43996600	-0.93374300	-0.80225700
O	-3.05219000	-1.56463100	-1.79381400
O	-3.23591800	-0.18123400	2.60586400
C	-4.27141400	0.24660300	-0.71146300
C	-4.38422400	0.65396800	0.63461200
C	-5.14648400	1.73482400	1.01899500
C	-5.87528700	2.41641100	0.03380500
C	-5.80358500	1.99044900	-1.30374100
C	-5.01955100	0.91426600	-1.69513100
H	-5.18511200	2.02785500	2.06852200

H	-6.50840300	3.26158800	0.30159300
H	-6.37825300	2.53127000	-2.05833900
H	-4.96092600	0.59605500	-2.73519400
C	0.29785300	-1.94819400	-1.58925300
H	-0.66227300	-2.44957200	-1.76247400
H	0.27811200	-1.00438000	-2.14958300
H	1.12390000	-2.56485800	-1.96981700
H	5.42827800	2.03203000	1.22997000
H	6.20225100	0.46900200	1.50552000
C	7.65262900	2.00209000	-0.24602200
H	8.23362300	2.15537400	-1.16592200
H	7.42695100	2.98892300	0.18126100
H	8.29982300	1.47094700	0.46936800
C	6.72293400	-0.14722800	-1.13034300
H	7.32750300	-0.74841900	-0.43210900
H	5.81810400	-0.72126500	-1.36484500
H	7.30362700	-0.02746100	-2.05538100

3

C	4.14998200	0.20543000	0.64900800
C	3.02420200	0.90551600	0.20588400
C	1.83764400	0.25394900	-0.09967200
C	1.73246700	-1.13604500	0.03655200
C	2.85506000	-1.83395700	0.48387600
C	4.04452700	-1.17739300	0.78426400
H	3.08139000	1.99260900	0.10882100
H	0.95244600	0.80786400	-0.40550100
H	2.79113800	-2.91709900	0.60219100
H	4.90901300	-1.74730000	1.13314300
C	5.43506500	0.93039500	0.93476700
C	0.48154300	-1.88499600	-0.33130300
H	0.57643000	-2.92120200	0.02251300
C	-0.83398500	-1.30220300	0.25818800

C	6.20717600	1.35077000	-0.32261500
H	5.53189100	1.97583100	-0.93318900
O	-1.57133900	-2.23356000	0.72000300
N	-3.63002300	-1.45245200	0.53959100
O	-1.07284400	-0.10158600	0.13268500
C	-3.81397900	-0.41753400	1.44325500
C	-3.65753600	-0.95178300	-0.75025900
O	-3.38687300	-1.54103400	-1.78247800
O	-3.72616600	-0.46445500	2.65541200
C	-4.14579000	0.46899100	-0.68015300
C	-4.23440100	0.79873900	0.66198200
C	-4.66257100	2.04617900	1.07406600
C	-5.00238700	2.97087600	0.08371800
C	-4.91246700	2.63839500	-1.27005200
C	-4.47969900	1.37230200	-1.67114800
H	-4.72238400	2.28729400	2.13495900
H	-5.34065800	3.96829400	0.36601200
H	-5.18211000	3.38216000	-2.02047300
H	-4.39864400	1.09549900	-2.72183800
C	0.25546400	-1.90696000	-1.84663200
H	-0.67616300	-2.43914300	-2.08026300
H	0.15427600	-0.88239300	-2.22625200
H	1.09487800	-2.39279700	-2.36404200
H	5.22927400	1.83337300	1.53366900
H	6.09741400	0.29560300	1.54967000
C	7.42565300	2.17916000	0.05828600
H	7.98161200	2.51316600	-0.82875400
H	7.14591500	3.06927100	0.63867600
H	8.11574800	1.58362300	0.67630500
C	6.61702700	0.14203100	-1.15071200
H	7.27053800	-0.52084100	-0.56070600
H	5.74558100	-0.44545200	-1.46483700
H	7.17236400	0.44272000	-2.05000400

TS2

C	4.19380600	0.01949300	0.58751900
C	3.31249900	1.08198800	0.37288400
C	2.06705200	0.88020500	-0.20450600
C	1.66097700	-0.39913300	-0.60263300
C	2.53624400	-1.46632700	-0.36746200
C	3.77993000	-1.26021100	0.21186500
H	3.61038600	2.08804000	0.67714200
H	1.39158800	1.72235600	-0.34355700
H	2.21373800	-2.47295300	-0.63590600
H	4.44875800	-2.10678100	0.38082800
C	5.55373000	0.26634200	1.17567800
C	0.33226700	-0.66244400	-1.20696800
H	0.34585700	-1.59839700	-1.77431900
C	-0.70744800	-0.99321800	0.09289900
C	6.56006000	0.86898900	0.18598100
O	-0.81334000	-2.21499800	0.18397100
N	-3.62281400	-1.83334700	0.23468000
O	-1.12517600	0.01574800	0.63249600
C	-4.14509900	-1.10085800	1.28235100
C	-3.53429900	-1.01665400	-0.86205400
O	-3.07386600	-1.29830800	-1.96755700
O	-4.35387300	-1.48454800	2.42362500
C	-4.11371700	0.33692000	-0.53524400
C	-4.49079200	0.28689100	0.79507800
C	-5.07185700	1.37061300	1.42342000
C	-5.26381800	2.52987500	0.66572500
C	-4.88166400	2.58098100	-0.67640900
C	-4.29785600	1.47341000	-1.29869000
H	-5.36071500	1.31244400	2.47275200
H	-5.71588900	3.40992100	1.12486200
H	-5.04259300	3.49952400	-1.24206600

H	-3.99466600	1.49351700	-2.34589400
C	-0.32180800	0.44233300	-2.00017800
H	-1.31077800	0.10918600	-2.34319700
H	-0.46988400	1.33941700	-1.38893700
H	0.29264700	0.69632200	-2.87751700
H	5.46770600	0.94484600	2.04059100
H	5.97346100	-0.67826900	1.56325200
C	7.86458900	1.19853200	0.89702600
H	8.59367800	1.65448700	0.21308600
H	7.70647600	1.89076900	1.73550600
H	8.32075200	0.28285000	1.30432200
H	6.12316700	1.80596000	-0.20266700
C	6.80999800	-0.06480200	-0.98895200
H	7.22063200	-1.02366200	-0.63394400
H	5.88499100	-0.28290200	-1.53681700
H	7.53366600	0.36605000	-1.69453500

Ir^{IV+} Npht⁻

C	0.55933400	2.24909700	3.74216900
C	1.20154600	1.68150600	2.64139600
C	0.51818600	0.77229100	1.83053800
C	-0.78975700	0.39692900	2.16555000
C	-1.43650200	0.99386300	3.25266300
C	-0.75858600	1.91572800	4.03763100
H	1.09242300	2.97215600	4.35927500
H	2.22736200	1.97081300	2.40948700
H	-2.48787900	0.79027900	3.44328200
H	-1.26787900	2.38598100	4.87634000
C	-3.20009300	-2.08135000	0.65494400
C	-2.65970600	-1.19404200	1.56783800
C	-2.48053300	-2.39086500	-0.49498000
C	-1.42031500	-0.60490100	1.31050100
H	-3.22524100	-0.89608600	2.44610600

C	-1.23928200	-1.80849000	-0.67078600
H	-2.87831000	-3.05796500	-1.25470400
N	-0.70521800	-0.94950900	0.21124100
H	-0.64375000	-2.02587400	-1.55505600
H	-4.18852200	-2.50637000	0.82335500
C	1.59131600	-1.94783700	-3.84735900
C	1.32999500	-0.99047700	-2.87038300
C	1.64414100	-1.24426000	-1.53534400
C	2.19533000	-2.49245700	-1.18682000
C	2.44780100	-3.45295700	-2.17131900
C	2.14573000	-3.17884700	-3.49742900
H	1.35373600	-1.73724500	-4.88912700
H	0.87193800	-0.04221600	-3.15424900
H	2.87732600	-4.42041400	-1.91151200
H	2.33710700	-3.92861400	-4.26250600
C	3.25197000	-3.91691900	2.15285800
C	3.01924200	-3.84883700	0.79028100
C	2.93034400	-2.82470300	2.95256200
C	2.46974300	-2.69392000	0.23226600
H	3.26461700	-4.69016500	0.14744200
C	2.38242300	-1.70520300	2.35219800
H	3.09553500	-2.83353100	4.02610600
N	2.15666700	-1.63767700	1.03100800
H	2.10837500	-0.81965300	2.92302700
H	3.68258300	-4.81560400	2.58960200
C	5.43922800	1.42753800	0.18368900
C	4.32718500	0.61414700	0.35366300
C	3.06202000	1.01239500	-0.10959200
C	2.95774200	2.26588300	-0.77438100
C	4.07896000	3.07497100	-0.94077500
C	5.31595900	2.65917300	-0.46111700
H	6.41172900	1.10463400	0.55233300
H	4.44123000	-0.34791900	0.85436600

H	3.99765300	4.03766600	-1.44467800
H	6.18872500	3.29581500	-0.59326100
C	-0.05050300	3.95779300	-2.34463000
C	1.26962100	3.77000200	-1.94055400
C	-0.99905100	2.99361600	-2.04797900
C	1.62161700	2.61899700	-1.25151500
H	2.02690400	4.51763100	-2.16457700
C	-0.59852600	1.86298300	-1.34778500
H	-2.04621500	3.04981600	-2.33264700
N	0.67220700	1.68248500	-0.97171300
H	-1.32966100	1.10377000	-1.08490500
H	-0.32685500	4.85862100	-2.88906100
Ir	1.34783600	0.03377700	0.06083500
N	-3.47511500	1.49710300	-0.10979600
C	-3.89303400	0.91801400	-1.27122600
C	-4.35862700	1.16328700	0.87862600
O	-4.28976600	1.43276600	2.07686300
O	-3.32552000	0.96783000	-2.36695000
C	-5.45600100	0.29495400	0.30796500
C	-5.15573700	0.12812400	-1.03301600
C	-5.90958900	-0.69488300	-1.84742300
C	-6.99658300	-1.35583600	-1.26534500
C	-7.30107000	-1.18564700	0.08686400
C	-6.52503700	-0.35110200	0.89869600
H	-5.65464400	-0.82288300	-2.89921000
H	-7.61751700	-2.01524500	-1.87147800
H	-8.15506900	-1.71362100	0.51075600
H	-6.74198200	-0.21277300	1.95790200

***Ir^{III}**

C	0.11782700	3.71388100	2.41762600
C	0.47032200	2.48290000	1.87128700
C	-0.33698600	1.86244800	0.91029700

C	-1.50389500	2.52979900	0.49581600
C	-1.84929200	3.77196900	1.04368700
C	-1.04465500	4.36220300	2.00455500
H	0.75779200	4.17299900	3.17102400
H	1.38473600	1.99345100	2.20979700
H	-2.75068900	4.29024400	0.71650900
H	-1.31732600	5.32754300	2.42717900
C	-4.23399400	1.61028600	-1.95429200
C	-3.55233900	2.32453900	-0.98346200
C	-3.67225200	0.44295600	-2.45914100
C	-2.31449700	1.86384300	-0.52465300
H	-3.98148800	3.23384200	-0.57040800
C	-2.44361300	0.03902100	-1.96069100
H	-4.17289400	-0.15099600	-3.21902900
N	-1.77982000	0.72711700	-1.02655800
H	-1.95450800	-0.86821900	-2.31650800
H	-5.20093300	1.96040000	-2.31152200
C	0.39890200	-3.03284800	-3.07916700
C	0.54747200	-1.82543000	-2.39949700
C	-0.02513000	-1.63577400	-1.14411400
C	-0.82420600	-2.66918600	-0.54935700
C	-0.93624700	-3.89817300	-1.24400600
C	-0.34763800	-4.06332600	-2.48119700
H	0.86144400	-3.18157500	-4.05338700
H	1.13473900	-1.02463600	-2.85535600
H	-1.50361500	-4.72110000	-0.80816000
H	-0.46853400	-5.01171700	-3.00462000
C	-2.79175400	-2.84971200	2.65728700
C	-2.25057200	-3.24659100	1.46179000
C	-2.52143800	-1.53785400	3.13673500
C	-1.43617600	-2.37896800	0.70396800
H	-2.44339200	-4.24764500	1.07872200
C	-1.71787800	-0.71954500	2.38326600

H	-2.93016400	-1.17795900	4.07674000
N	-1.17419800	-1.09862900	1.20776600
H	-1.46008500	0.28737700	2.71191300
H	-3.41681400	-3.52986100	3.23229400
C	3.05115800	-1.75915200	2.72941700
C	1.82988300	-1.39533800	2.17816700
C	1.77417500	-0.58658800	1.03196200
C	3.00029200	-0.16383100	0.44647700
C	4.22288900	-0.54642400	1.00365800
C	4.24772100	-1.33709800	2.14336500
H	3.07819000	-2.38443200	3.62081200
H	0.90367000	-1.74806100	2.63175900
H	5.16303700	-0.23047000	0.55106900
H	5.20162700	-1.63182500	2.57712900
C	3.65234100	2.05098000	-2.54900100
C	3.92226400	1.22984300	-1.46969400
C	2.32555200	2.33195400	-2.87962700
C	2.87235100	0.68303900	-0.72747100
H	4.94902200	1.00477000	-1.19113500
C	1.32396700	1.76116300	-2.11686000
H	2.06991800	2.97730500	-3.71524600
N	1.58392700	0.95010200	-1.08247600
H	0.26879200	1.92950900	-2.32733500
H	4.46808500	2.47554500	-3.13053700
Ir	0.14574900	-0.00369500	0.08083600
+Ir^{IV}			
C	-0.80416100	3.45698900	-2.59849600
C	-0.93852300	2.21338000	-1.98349500
C	-0.04737600	1.81950900	-0.98098100
C	0.97235400	2.70433700	-0.59501100
C	1.09752800	3.95273100	-1.21787200
C	0.21495300	4.32656000	-2.21829000
H	-1.50390300	3.74735300	-3.38094800

H	-1.74170700	1.54829000	-2.30164500
H	1.88665200	4.64353700	-0.92416900
H	0.31673700	5.29682700	-2.69920200
C	3.69369700	2.49457100	2.01841300
C	2.92885900	2.99985900	0.98212600
C	3.38042500	1.24519800	2.54414300
C	1.85932200	2.25572700	0.47635800
H	3.15728500	3.97479900	0.56047800
C	2.31515400	0.55225300	1.99662000
H	3.94764100	0.81004500	3.36196900
N	1.57042000	1.03318400	0.98966700
H	2.03504600	-0.42887000	2.37640400
H	4.52644100	3.07124100	2.41536400
C	0.39623700	-3.12950100	3.03607600
C	-0.08783100	-2.00455700	2.37186500
C	0.40010100	-1.66643800	1.11073800
C	1.41558100	-2.45693100	0.53106700
C	1.89935100	-3.58133300	1.20496400
C	1.39182200	-3.91287100	2.45432000
H	-0.00269500	-3.39829100	4.01275500
H	-0.85945500	-1.39431700	2.84379800
H	2.67469900	-4.20699100	0.76441700
H	1.77475200	-4.78555100	2.97868800
C	3.26347500	-2.17776200	-2.76026300
C	2.89536500	-2.67190400	-1.51982000
C	2.63594000	-1.03830900	-3.25448100
C	1.90332100	-2.02991200	-0.77952400
H	3.37351500	-3.56232300	-1.12051000
C	1.66166000	-0.43383300	-2.48091600
H	2.89234300	-0.62015900	-4.22343800
N	1.30475900	-0.91436300	-1.27892300
H	1.13060600	0.45660200	-2.81236600
H	4.03414200	-2.67998800	-3.34066800

C	-2.82591200	-2.32604900	-2.57077600
C	-1.65601600	-1.79115500	-2.05092700
C	-1.68909100	-0.93605800	-0.93489900
C	-2.95466500	-0.64878800	-0.34679300
C	-4.12220700	-1.19118600	-0.87552900
C	-4.05832600	-2.02658000	-1.98646600
H	-2.78498700	-2.98519500	-3.43579800
H	-0.70217700	-2.04294800	-2.51340700
H	-5.09181800	-0.97149100	-0.43072400
H	-4.97269000	-2.44936900	-2.39674500
C	-3.83449000	1.50433100	2.63904100
C	-4.01899400	0.65712800	1.55799900
C	-2.54843900	1.92451600	2.96526600
C	-2.92029400	0.23407100	0.81318500
H	-5.01633300	0.32078100	1.28708700
C	-1.49146700	1.47624000	2.19304900
H	-2.36193100	2.59205900	3.80136800
N	-1.67126700	0.65042100	1.15250000
H	-0.46325200	1.77003300	2.39477400
H	-4.68897300	1.83768300	3.22336700
Ir	-0.15521400	-0.06095900	-0.06399600

Ar-radical

C	0.54494600	0.02707000	-0.62921000
C	-0.23841000	-1.10364500	-0.35546900
C	-1.58718400	-0.99946600	-0.07789500
C	-2.23532600	0.26408400	-0.05842500
C	-1.43230700	1.40085200	-0.33656900
C	-0.08529100	1.27939900	-0.61265800
H	0.23415800	-2.08790000	-0.36969600
H	-2.16643000	-1.89965500	0.12516400
H	-1.90261000	2.38492400	-0.33069400
H	0.50769900	2.17163000	-0.82167000

C	2.01554900	-0.11155200	-0.89167400
C	-3.60860700	0.40695600	0.21808400
H	-4.01850900	1.41812000	0.20944500
C	2.85118300	-0.37497500	0.36969300
H	2.45689900	-1.29014100	0.84604100
C	-4.52394700	-0.72662900	0.51826000
H	-5.54581500	-0.37912900	0.70207300
H	-4.56786300	-1.45379300	-0.30886900
H	-4.20416600	-1.29279700	1.40821800
H	2.39820900	0.80320400	-1.37562500
H	2.19002700	-0.93527500	-1.60338800
C	2.73238000	0.77131000	1.36318100
H	1.69535600	0.92644500	1.68671900
H	3.34328400	0.58712400	2.25686200
H	3.08491400	1.71038500	0.90782800
C	4.30600400	-0.61140900	-0.00830500
H	4.92020900	-0.82989900	0.87529400
H	4.41318100	-1.44887900	-0.71098000
H	4.72752200	0.28366000	-0.49079100

CO₂

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16414500
O	0.00000000	0.00000000	-1.16414500

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C	3.06968400	1.30292700	-1.71711300
O	2.12180100	2.19373500	-1.07381500
C	2.52715500	-0.09894000	-1.35115600
H	2.39249900	-0.76967200	-2.20959400
C	1.11291700	1.43355000	-0.60874900
N	1.21269300	0.16837600	-0.75070500
C	-0.00005800	2.18730800	0.00024300
C	0.34782900	3.52701800	0.64886200

C	-0.34822000	3.52691600	-0.64854400
H	1.40509400	3.77535700	0.67366300
H	-0.22001700	3.77417000	1.54170200
H	0.21957000	3.77401300	-1.54143100
H	-1.40554800	3.77497800	-0.67332600
C	-3.06983800	1.30255000	1.71735000
O	-2.12205500	2.19348700	1.07404100
C	-2.52722400	-0.09921400	1.35123200
H	-2.39272200	-0.77012200	2.20955900
C	-1.11301300	1.43340100	0.60910500
N	-1.21264300	0.16823200	0.75105100
C	5.57199300	-0.01280400	0.75510800
C	5.49718600	-1.19007000	1.49349100
C	4.43827900	-2.07992700	1.31072100
C	3.43306000	-1.80633100	0.38810700
C	3.51153100	-0.62435700	-0.34049900
C	4.56900300	0.26609400	-0.16599700
H	6.40307600	0.67781500	0.89769700
H	6.27477400	-1.42021500	2.22014100
H	4.39540200	-2.99790000	1.89364700
H	2.59928700	-2.49649800	0.24629000
C	4.45696800	1.44516400	-1.09404900
H	4.55810600	2.41656900	-0.59144500
H	5.22939000	1.41589400	-1.87642300
C	-3.43278800	-1.80620500	-0.38860800
C	-3.51141700	-0.62442200	0.34028100
C	-4.56891400	0.26603500	0.16584800
C	-5.57169900	-0.01262900	-0.75554000
C	-5.49670600	-1.18968600	-1.49425100
C	-4.43782900	-2.07956800	-1.31149600
H	-2.59906600	-2.49643500	-0.24678400
H	-6.40278200	0.67799700	-0.89810200
H	-6.27413800	-1.41963100	-2.22113000

H	-4.39482700	-2.99740500	-1.89463000
C	-4.45717000	1.44472000	1.09441000
H	-4.55871200	2.41636100	0.59234900
H	-3.04156000	1.54011000	2.78655000
H	-5.22949400	1.41477500	1.87686500
H	3.04145600	1.54053400	-2.78630300
C	-0.00048000	-3.20374100	0.00040900
N	-0.00114200	-4.37479600	0.00086800
Cu	0.00029000	-1.32785800	-0.00015900

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C	1.92751200	2.49095400	-2.07764300
O	0.59303600	3.05114100	-1.92563800
C	1.97501200	1.41733900	-0.97014400
H	2.31645900	0.43131400	-1.30549100
C	-0.07393900	2.26489800	-1.07285700
N	0.57456600	1.30517000	-0.52889000
C	-1.48534200	2.62437200	-0.86850800
C	-1.83858000	4.10980000	-0.95588400
C	-2.22506700	3.22478800	-2.06523700
H	-0.99616700	4.78212200	-1.09324000
H	-2.60755000	4.44496300	-0.26513300
H	-1.65344600	3.26576800	-2.98832200
H	-3.26683600	2.93254800	-2.16284200
C	-4.15664900	1.31184800	1.20010400
O	-3.55973400	2.17318600	0.18734200
C	-3.09274000	0.21091500	1.37484000
H	-2.84373900	-0.03552000	2.41346000
C	-2.28279100	1.79931000	0.05129600
N	-1.89802400	0.77402400	0.71497500
C	4.16252200	4.00687100	0.52170500
C	4.42521800	3.52311200	1.80006800
C	3.90761100	2.29703200	2.21736700

C	3.11029000	1.53397100	1.36878900
C	2.84459700	2.02978300	0.09684300
C	3.36638200	3.25038200	-0.32971600
H	4.57445500	4.96167800	0.19519800
H	5.04538100	4.10583000	2.47939300
H	4.13013500	1.92679300	3.21616700
H	2.73049900	0.56290200	1.69573400
C	2.98402900	3.54257900	-1.75508500
H	2.58810900	4.55455600	-1.91453800
H	3.84344600	3.43207500	-2.43252000
C	-3.02700100	-2.15715500	0.29166000
C	-3.65233600	-0.95508100	0.60059000
C	-4.94482300	-0.67984800	0.15594900
C	-5.63258000	-1.60721800	-0.61696800
C	-5.00652500	-2.80750800	-0.93948500
C	-3.71560300	-3.08086800	-0.48775600
H	-2.02392000	-2.37205100	0.65923000
H	-6.64333700	-1.39827600	-0.96710200
H	-5.53025200	-3.54132000	-1.54996800
H	-3.23914800	-4.02374700	-0.74831800
C	-5.42000300	0.65731600	0.65499800
H	-5.88653400	1.28523000	-0.11580900
H	-4.32048100	1.94167400	2.08155700
H	-6.15982400	0.54638600	1.46142600
H	1.98157700	2.10075400	-3.09960600
C	-0.49259800	-1.09540000	2.39633900
N	-0.89691900	-1.64537400	3.34533600
Cu	-0.06063000	-0.14520000	0.75208200
N	1.31231800	-1.42420000	0.17229600
C	2.32333900	-2.05160900	0.88079400
C	0.98246800	-2.14681600	-0.95620600
O	0.09037400	-1.86339200	-1.74128300
O	2.82165600	-1.67234300	1.92316800

C	1.90978400	-3.31787500	-1.02989900
C	2.72164200	-3.26316000	0.09561100
C	3.69683800	-4.21191000	0.33401900
C	3.83328800	-5.23825800	-0.60330000
C	3.01689500	-5.29485200	-1.73447100
C	2.03642000	-4.32708200	-1.96567100
H	4.32354700	-4.15414200	1.22222500
H	4.58611300	-6.01021200	-0.45170600
H	3.14817100	-6.10932900	-2.44518500
H	1.39174200	-4.35905300	-2.84255500

Ir^{III}

C	0.57676300	-3.52441100	2.64328300
C	0.01205400	-2.38949000	2.07164400
C	0.61315400	-1.71903300	0.99574600
C	1.83318500	-2.26087600	0.51636900
C	2.40242800	-3.40695600	1.09172100
C	1.77823700	-4.03880600	2.15395700
H	0.07937300	-4.01778200	3.47902600
H	-0.92793600	-2.00657600	2.47596000
H	3.33994700	-3.81694500	0.71410600
H	2.22140300	-4.92853400	2.59845900
C	4.19664700	-1.20141200	-2.24977100
C	3.68526100	-1.93163400	-1.19247700
C	3.49439000	-0.09460400	-2.72126500
C	2.46991100	-1.56092500	-0.60221600
H	4.22709900	-2.79533400	-0.81582600
C	2.30080700	0.22902500	-2.09945100
H	3.86034600	0.50669300	-3.54918800
N	1.80126100	-0.47779100	-1.07704800
H	1.69900300	1.08182200	-2.41600500
H	5.14117900	-1.49229200	-2.70644800
C	-1.28367000	3.24604200	-2.77305000

C	-1.18886600	1.99061300	-2.18184400
C	-0.43237100	1.77585100	-1.02210900
C	0.22704100	2.90373200	-0.47678500
C	0.13490900	4.16985500	-1.07020000
C	-0.61862500	4.34195100	-2.21976600
H	-1.88293100	3.37964500	-3.67435000
H	-1.72603000	1.15343900	-2.63636300
H	0.65227400	5.02953100	-0.64193500
H	-0.69304900	5.32411800	-2.68353700
C	2.36827300	3.27212700	2.62307000
C	1.68152700	3.62143500	1.47525900
C	2.37580300	1.94084400	3.03190000
C	1.00100100	2.65021300	0.73375000
H	1.65659100	4.65689400	1.14532800
C	1.69163600	1.01514300	2.26646200
H	2.89782200	1.61957500	3.92898900
N	1.02274200	1.35101500	1.15055600
H	1.64895900	-0.03845400	2.53656000
H	2.89180200	4.03227900	3.19997000
C	-3.19779900	0.95827600	2.85849400
C	-1.96321600	0.94347700	2.22391500
C	-1.75845300	0.21408900	1.04269400
C	-2.87226700	-0.49428100	0.52412000
C	-4.11621000	-0.47477800	1.16809500
C	-4.28221700	0.24780000	2.33596500
H	-3.32406100	1.53216600	3.77688800
H	-1.13918300	1.51150200	2.65927100
H	-4.96025900	-1.03108400	0.75826900
H	-5.24659200	0.26349400	2.84034600
C	-3.16948100	-2.62092800	-2.58857400
C	-3.54625700	-1.97442800	-1.42719800
C	-1.84702800	-2.52663700	-3.02117600
C	-2.61219800	-1.23239400	-0.69687100

H	-4.57271600	-2.03118700	-1.07309300
C	-0.96014000	-1.78638800	-2.26447900
H	-1.50532600	-3.01882100	-3.92755600
N	-1.32349400	-1.15306100	-1.13733600
H	0.08436000	-1.67556400	-2.54993800
H	-3.89817800	-3.19534800	-3.15720000
Ir	-0.06484200	0.00286600	0.00350400

TMSCN

Si	0.31236900	0.00008200	-0.00000500
C	0.85302400	-0.75445400	1.62344200
H	0.48236300	-0.17362900	2.47645600
H	0.48271500	-1.78113700	1.72912500
H	1.94846500	-0.78378800	1.68698200
C	0.85305300	-1.02883900	-1.46502500
H	0.48266900	-2.05804400	-1.38803900
H	0.48260600	-0.60757600	-2.40720700
H	1.94850400	-1.06900800	-1.52222000
C	0.85307100	1.78320600	-0.15840400
H	0.48204200	2.23161100	-1.08774100
H	0.48321200	2.38810900	0.67805100
H	1.94852300	1.85273000	-0.16530500
C	-1.56341100	0.00007400	0.00003400
N	-2.72695500	-0.00004900	-0.00004600

TMSNPhth

N	0.56802900	0.07247100	-0.00012500
C	-0.26868800	1.20649100	-0.00005000
C	-0.20540600	-1.10146700	-0.00014300
O	0.23546700	-2.23060700	-0.00019900
O	0.08737700	2.36213300	-0.00003400
C	-1.63029200	-0.68451300	-0.00007600
C	-1.66833500	0.70141800	-0.00003500

C	-2.86454800	1.39497500	0.00004500
C	-4.03790400	0.63966300	0.00009100
C	-3.99900300	-0.75717500	0.00006500
C	-2.78523800	-1.44501700	-0.00002300
H	-2.87777600	2.48324000	0.00008000
H	-5.00239300	1.14420500	0.00016800
H	-4.93387100	-1.31459600	0.00008900
H	-2.73747600	-2.53228400	-0.00008000
Si	2.38055200	-0.00282300	0.00012000
C	2.88270100	-0.92321000	1.54688000
H	3.97496000	-1.02253600	1.59951100
H	2.55208800	-0.39392200	2.44942900
H	2.44673700	-1.92875000	1.55800100
C	3.04740400	1.73900500	0.00025300
H	4.14555400	1.69682000	0.00092100
H	2.72503900	2.30246600	-0.88210600
H	2.72388900	2.30311700	0.88174900
C	2.88298000	-0.92263900	-1.54690100
H	2.44697500	-1.92815600	-1.55856100
H	2.55233600	-0.39283800	-2.44915400
H	3.97522300	-1.02193400	-1.59962100

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C	2.41597700	-1.74278700	1.52487100
O	1.15375500	-2.47465400	1.50209400
C	2.34575700	-0.94119400	0.21429400
H	2.64079300	0.10540600	0.34531800
C	0.38433100	-1.90903800	0.57295400
N	0.91456100	-0.99730600	-0.16132900
C	-0.98123700	-2.44496000	0.50072100
C	-1.14830900	-3.92127400	0.87320700
C	-1.61720300	-2.89769100	1.81737300
H	-0.22494300	-4.45079800	1.09045200

H	-1.88398900	-4.46530600	0.28729000
H	-1.03294500	-2.67982100	2.70851600
H	-2.68458300	-2.71056800	1.89979200
C	-3.80447100	-1.92672500	-1.69856100
O	-3.08604000	-2.50243400	-0.57198700
C	-2.97769500	-0.66597900	-2.01371400
H	-2.76879300	-0.50632700	-3.07743200
C	-1.89631500	-1.89662800	-0.50744400
N	-1.69978400	-0.91319300	-1.30700400
C	4.71019800	-3.62576200	-0.75062300
C	4.85574300	-3.47283600	-2.12609400
C	4.18006500	-2.45718900	-2.80165200
C	3.34976900	-1.57812100	-2.11239300
C	3.20784400	-1.73285100	-0.73768600
C	3.87985500	-2.75115300	-0.06044600
H	5.23560300	-4.42233200	-0.22400100
H	5.50000400	-4.15370800	-2.67997600
H	4.30021900	-2.35118400	-3.87831300
H	2.81976300	-0.78534500	-2.63868800
C	3.58516000	-2.71065000	1.41361700
H	3.33388000	-3.68818600	1.84626400
H	4.44019500	-2.32263800	1.98591200
C	-3.43994600	1.79016600	-1.25772800
C	-3.78312700	0.44934300	-1.39162300
C	-5.00411400	-0.03005000	-0.91457600
C	-5.89123700	0.82086400	-0.26634800
C	-5.54232600	2.15918900	-0.11102700
C	-4.33104600	2.63945700	-0.60860900
H	-2.49060700	2.16136400	-1.63457400
H	-6.84418300	0.44820100	0.10906800
H	-6.22393900	2.83871500	0.39816000
H	-4.07481100	3.68983000	-0.48530400
C	-5.18958100	-1.48285300	-1.25265400

H	-5.55061300	-2.09994700	-0.41905400
H	-3.80498500	-2.68806200	-2.48707200
H	-5.90710500	-1.61284200	-2.07615100
H	2.41325700	-1.13221900	2.43477000
C	-0.67275200	0.94138400	-3.21707100
N	-1.15899700	1.33337400	-4.20462900
Cu	0.00348500	0.20582400	-1.54960500
N	1.09426100	1.75036200	1.48009600
C	-0.17994600	1.55167900	1.07620700
C	1.23498500	1.20615200	2.73436700
O	2.28061600	1.09503400	3.36538300
O	-0.64474100	1.80855100	-0.04849500
C	-0.09598700	0.66754400	3.20136600
C	-0.98207200	0.88591100	2.15750900
C	-2.30708600	0.49701000	2.22780000
C	-2.72614800	-0.11702600	3.41396500
C	-1.83468200	-0.34164600	4.46504100
C	-0.49229100	0.04371400	4.36853600
H	-2.99155600	0.67514100	1.39569200
H	-3.76632700	-0.42309000	3.52364100
H	-2.19478000	-0.82010400	5.37507300
H	0.21450500	-0.12514200	5.18008100
Si	2.96527400	3.64771800	-0.17508400
C	4.15867900	2.93507100	1.06723000
H	4.71750800	3.75241400	1.54324200
H	3.64259000	2.36096000	1.84822700
H	4.89240500	2.28616400	0.57033600
C	3.90411800	4.59747900	-1.49727000
H	4.38062300	5.48183800	-1.05288100
H	4.69442500	3.98986100	-1.95542400
H	3.23771100	4.94563200	-2.29619200
C	1.53405600	4.66195900	0.47007100
H	0.58805000	4.28004300	0.06773400

H	1.47580000	4.58819600	1.56100600
H	1.64410000	5.71494000	0.18114000
C	2.23561900	2.19243500	-1.16788900
N	1.78161600	1.29995000	-1.75959300

TS3

C	2.79748700	-1.24067800	1.74997300
O	1.65449000	-2.13973000	1.92038200
C	2.51677400	-0.60273700	0.37703300
H	2.62281300	0.48786700	0.37871100
C	0.77003600	-1.84478700	0.97434100
N	1.10769300	-0.96244100	0.10237500
C	-0.47809300	-2.62222600	1.02136500
C	-0.31888600	-4.11922300	1.34800000
C	-0.89594000	-3.22058400	2.35615200
H	0.70627600	-4.45901600	1.46954200
H	-0.97822000	-4.78658900	0.79879900
H	-0.28316900	-2.92477000	3.20338100
H	-1.96766200	-3.25331500	2.53300800
C	-3.54470900	-2.63694200	-0.90574800
O	-2.69098300	-2.93812300	0.23648800
C	-2.76849900	-1.52194000	-1.63669000
H	-2.60669000	-1.70343700	-2.70577200
C	-1.53614900	-2.29687600	0.05653500
N	-1.45460600	-1.51977700	-0.96154100
C	5.23454500	-2.94819700	-0.52794300
C	5.29757600	-2.87163100	-1.91620900
C	4.45217800	-2.01456500	-2.62026100
C	3.52631900	-1.22348200	-1.94642900
C	3.45969600	-1.31204700	-0.56003500
C	4.30797800	-2.16340100	0.14791900
H	5.90139000	-3.61407400	0.01942900
H	6.01612400	-3.48433600	-2.45795600

H	4.51669400	-1.96094700	-3.70527900
H	2.87474200	-0.54272400	-2.49516000
C	4.08352200	-2.04854600	1.63146300
H	3.99269900	-3.01430700	2.14638200
H	4.90719100	-1.50835100	2.11989900
C	-3.24340000	1.03354400	-1.70143300
C	-3.56435700	-0.27498800	-1.36364800
C	-4.73223000	-0.57624800	-0.66246900
C	-5.60506200	0.43864500	-0.29025100
C	-5.28737800	1.75367600	-0.62550900
C	-4.11527100	2.04987800	-1.32095400
H	-2.32700500	1.26715800	-2.24363800
H	-6.52222700	0.21242300	0.25341900
H	-5.95875000	2.56000000	-0.33515200
H	-3.86290300	3.08170600	-1.55215300
C	-4.87836400	-2.05723700	-0.44378100
H	-5.07984000	-2.33499800	0.59990200
H	-3.63868400	-3.57238700	-1.46750900
H	-5.69981800	-2.47535500	-1.04316800
H	2.75972100	-0.52981700	2.58162400
C	-0.50358800	-0.41733300	-3.40726300
N	-0.95315900	-0.49027700	-4.48321700
Cu	0.11212800	-0.40943800	-1.56578100
N	0.64565700	2.62442100	1.11491500
C	-0.68430900	2.45159300	0.77477800
C	0.96471000	1.79689200	2.16643000
O	2.05982700	1.63825100	2.69119300
O	-1.25285100	3.00939500	-0.15089700
C	-0.27434200	1.04503800	2.56082400
C	-1.28479000	1.43864300	1.69757800
C	-2.56078100	0.91378100	1.78285100
C	-2.79600700	-0.03584800	2.78161500
C	-1.78394600	-0.41679900	3.66539800

C	-0.49585300	0.11905600	3.56281100
H	-3.34866500	1.24164900	1.10622000
H	-3.79127900	-0.46927600	2.88383900
H	-2.00644900	-1.13893900	4.45103900
H	0.30152500	-0.16397100	4.25013600
Si	1.76866900	3.95965000	-0.14868600
C	3.47550900	3.57801600	0.53354100
H	4.00163800	4.53412100	0.66492900
H	3.44222100	3.05553200	1.49526200
H	4.06198300	2.98073400	-0.17839200
C	2.08400200	4.89953700	-1.78639800
H	2.55586500	5.87363200	-1.58964700
H	2.73564300	4.33481500	-2.46921600
H	1.14354500	5.09692800	-2.32103500
C	0.88009300	5.32731800	0.81590200
H	-0.18637600	5.35853400	0.56062500
H	0.96400600	5.16708000	1.89799700
H	1.31483700	6.30362100	0.56006300
C	1.40447800	2.28464900	-1.24550900
N	1.20358100	1.24483600	-1.73854300

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C	3.04545000	1.36258000	-1.71515500
O	2.09904900	2.26473900	-1.07156400
C	2.53146300	-0.03331800	-1.30103300
H	2.38853600	-0.74181400	-2.12497200
C	1.10810000	1.51492200	-0.57748000
N	1.21745000	0.24544400	-0.69165400
C	0.00085400	2.26480200	0.03774500
C	0.35530700	3.58944600	0.71650000
C	-0.33963200	3.62229000	-0.57909700
H	1.41494800	3.82750100	0.74765600
H	-0.20983100	3.81613700	1.61654600

H	0.22882600	3.88287600	-1.46768100
H	-1.39616900	3.87431500	-0.59872200
C	-3.07500600	1.32235700	1.71524300
O	-2.11525400	2.23664700	1.10959800
C	-2.55346200	-0.06387500	1.28223900
H	-2.43169800	-0.79064400	2.09435500
C	-1.11386600	1.49969900	0.61888000
N	-1.22535300	0.22707000	0.70796000
C	5.58359200	0.18766300	0.78684500
C	5.53165900	-0.95952500	1.57324200
C	4.49063700	-1.87633600	1.42722400
C	3.47948900	-1.65787500	0.49688200
C	3.52987100	-0.50271400	-0.27576500
C	4.57328100	0.41156900	-0.14110600
H	6.40380500	0.89685700	0.89698200
H	6.31481300	-1.14571500	2.30626800
H	4.46849700	-2.77296000	2.04345100
H	2.67302700	-2.37864000	0.36387500
C	4.44073900	1.54349900	-1.12335300
H	4.54660200	2.54039500	-0.67466500
H	5.19806300	1.47562000	-1.91784800
C	-3.45478700	-1.64193500	-0.57974100
C	-3.52636300	-0.50805800	0.22205000
C	-4.56700100	0.40898100	0.08543300
C	-5.55394100	0.20842600	-0.87253200
C	-5.48092000	-0.91779000	-1.68704600
C	-4.44207400	-1.83695700	-1.54024700
H	-2.65041400	-2.36658700	-0.45187300
H	-6.37196900	0.91976400	-0.98468600
H	-6.24542800	-1.08534700	-2.44381500
H	-4.40237700	-2.71630800	-2.17989800
C	-4.45777100	1.51610800	1.09850700
H	-4.55653100	2.52379400	0.67302000

H	-3.03778500	1.51197800	2.79310400
H	-5.23121400	1.42673500	1.87515000
H	2.98666400	1.57477900	-2.78791200
C	1.14840800	-3.19594400	-2.10551200
N	0.68920700	-2.50375700	-1.26480900
Cu	0.00373200	-1.24338400	0.01636800
C	-0.67563400	-2.52901900	1.31734900
N	-1.18691700	-3.19728000	2.12883200

TS4

C	-3.01204300	1.23749900	1.78722500
O	-2.08771300	2.14142800	1.11561600
C	-2.56906500	-0.14579800	1.26992600
H	-2.43227200	-0.90762800	2.04546800
C	-1.12800900	1.39238100	0.56394100
N	-1.26113400	0.12039000	0.63966900
C	-0.03849800	2.15077900	-0.07183300
C	-0.41931500	3.47645700	-0.73430400
C	0.31048000	3.50827300	0.54177100
H	-1.48071200	3.70879300	-0.73541900
H	0.11974600	3.70859500	-1.64885000
H	-0.23436200	3.76066600	1.44721200
H	1.36616400	3.76469400	0.53378800
C	2.99052200	1.22621600	-1.84042000
O	2.04003400	2.14200800	-1.21839200
C	2.55072800	-0.14237500	-1.28510000
H	2.46734600	-0.94171600	-2.03070200
C	1.07203000	1.39802000	-0.67356100
N	1.21679800	0.12689500	-0.71746500
C	-5.68595900	0.33569100	-0.67274300
C	-5.69590000	-0.73672400	-1.55943900
C	-4.67749900	-1.68986500	-1.53492900
C	-3.62634500	-1.58330100	-0.62882500

C	-3.61572700	-0.50167900	0.24539200
C	-4.63703300	0.44729700	0.23166200
H	-6.48712700	1.07439100	-0.68842100
H	-6.50909600	-0.83553000	-2.27666100
H	-4.70488900	-2.52774600	-2.22895200
H	-2.83783900	-2.33556700	-0.58422200
C	-4.43537100	1.48441400	1.30222100
H	-4.55717500	2.51902600	0.95459300
H	-5.14296300	1.34652200	2.13283700
C	3.53221400	-1.45660200	0.73763400
C	3.55753100	-0.43247100	-0.20216100
C	4.57406300	0.52160300	-0.20486400
C	5.58976400	0.46550300	0.74139100
C	5.56831900	-0.55430700	1.68814200
C	4.54928100	-1.50689900	1.68621900
H	2.73585600	-2.20094600	0.73427300
H	6.38779600	1.20773700	0.74512100
H	6.35488100	-0.60899000	2.43897300
H	4.54524400	-2.29727100	2.43401400
C	4.39993700	1.50254300	-1.33223700
H	4.51198100	2.55366700	-1.03442900
H	2.86984600	1.34791200	-2.92243800
H	5.12731900	1.32433100	-2.13782300
H	-2.86936500	1.39613900	2.86160800
C	-1.03825700	-2.92786100	1.27325400
N	-0.13430600	-2.45254900	1.88023500
Cu	-0.01510800	-1.34360500	0.00554500
C	0.78010100	-2.67948100	-1.13718600
N	1.35199800	-3.37986400	-1.87752800
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C	3.06574500	1.35213700	-1.70994400
O	2.10889000	2.25757900	-1.08809500

C	2.54953400	-0.04051700	-1.28886100
H	2.41825800	-0.75674100	-2.10916400
C	1.11402600	1.51115000	-0.59538800
N	1.22868400	0.24045400	-0.69502100
C	0.00016400	2.26764800	0.00009200
C	0.34588300	3.60930200	0.64872500
C	-0.34579100	3.60905000	-0.64908900
H	1.40386500	3.85463400	0.67670100
H	-0.22312000	3.85343800	1.54165100
H	0.22318500	3.85292400	-1.54210600
H	-1.40382200	3.85417400	-0.67715700
C	-3.06557000	1.35214500	1.70995300
O	-2.10806100	2.25767700	1.08926400
C	-2.54952700	-0.04050400	1.28853400
H	-2.41782900	-0.75674600	2.10875400
C	-1.11372000	1.51119400	0.59559500
N	-1.22894700	0.24047000	0.69410300
C	5.57537000	0.20364000	0.83395800
C	5.51529700	-0.93665500	1.62968900
C	4.47739700	-1.85635700	1.47927600
C	3.47806300	-1.64722700	0.53434600
C	3.53648900	-0.49929200	-0.24814900
C	4.57640700	0.41795900	-0.10849800
H	6.39298800	0.91510900	0.94837500
H	6.28943800	-1.11515200	2.37407000
H	4.44832000	-2.74714300	2.10353000
H	2.67442200	-2.37168900	0.40155700
C	4.45303900	1.54160300	-1.10151200
H	4.55033100	2.54220600	-0.65925100
H	5.22078100	1.46970800	-1.88556500
C	-3.47879400	-1.64751500	-0.53393500
C	-3.53680100	-0.49930400	0.24818500
C	-4.57640200	0.41825500	0.10832000

C	-5.57553000	0.20393300	-0.83396700
C	-5.51591000	-0.93665800	-1.62930700
C	-4.47828500	-1.85664400	-1.47869800
H	-2.67533700	-2.37216600	-0.40101900
H	-6.39292800	0.91562900	-0.94854800
H	-6.29018900	-1.11516300	-2.37354300
H	-4.44956100	-2.74764700	-2.10265900
C	-4.45252800	1.54229000	1.10083700
H	-4.54882400	2.54271800	0.65795300
H	-3.02162900	1.55273600	2.78560200
H	-5.22068200	1.47150000	1.88458000
H	3.02115900	1.55330900	-2.78546800
C	-0.65593400	-2.52980300	1.32018000
N	-1.16063800	-3.19368700	2.13975500
Cu	-0.00009200	-1.25128500	-0.00024600
C	0.65621800	-2.53012100	-1.32007000
N	1.16149800	-3.19418900	-2.13914500

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C	3.07712500	-1.14505400	0.47918800
O	2.31208100	-0.79254800	1.66289900
C	1.97865900	-1.59208000	-0.51166800
H	2.06820200	-1.15156100	-1.51464800
C	1.01707000	-0.76662600	1.28455100
N	0.72759800	-1.13455800	0.10322600
C	0.07342300	-0.31513200	2.32671200
C	0.43553100	-0.66723300	3.76953800
C	0.57392200	0.72917500	3.32320700
H	1.33512000	-1.26584600	3.88133600
H	-0.39491500	-0.93088800	4.41762800
H	1.56975700	1.11625100	3.12265300
H	-0.16299500	1.45774100	3.65575000
C	-3.48964700	0.15342100	2.53320200

O	-2.16507400	-0.04971100	3.06755000
C	-3.41059100	-0.46183600	1.13122600
H	-3.73332300	-1.50883000	1.04242900
C	-1.36490600	-0.27841400	2.00747600
N	-1.95328800	-0.43043800	0.87783900
C	3.43315800	-4.87610400	0.39185100
C	2.56891000	-5.79335800	-0.19904900
C	1.46839500	-5.36133600	-0.93976200
C	1.21420800	-4.00361700	-1.10435500
C	2.08102800	-3.09386100	-0.51146400
C	3.17986500	-3.51875800	0.23307200
H	4.28991400	-5.21771300	0.97298700
H	2.75114600	-6.86014000	-0.07785000
H	0.79521100	-6.09045700	-1.38618000
H	0.34739200	-3.66012800	-1.66770400
C	3.97181700	-2.34988900	0.75483500
H	4.21670600	-2.41972800	1.82335900
H	4.92711500	-2.23855700	0.22035700
C	-4.59736900	0.29737400	-1.04565000
C	-4.16665600	0.48990300	0.25980800
C	-4.36573200	1.69984600	0.92564800
C	-4.99316500	2.75396100	0.27483900
C	-5.41553300	2.57448900	-1.04145100
C	-5.22690200	1.35715000	-1.69505600
H	-4.43908800	-0.66016600	-1.54401100
H	-5.15781000	3.70449900	0.78157800
H	-5.91027000	3.39246200	-1.56233500
H	-5.57550000	1.23350200	-2.71880800
C	-3.80670300	1.64558700	2.32355400
H	-2.87437500	2.22827800	2.41022100
H	-4.18710100	-0.34571900	3.21050500
H	-4.49385600	2.04184600	3.08179900
H	3.62069700	-0.23960100	0.17834100

C	-0.64955000	-1.05072000	-2.70085200
N	-0.11618100	-1.26981200	-3.71739300
Cu	-1.28255100	-0.87517600	-0.96143700
C	-2.07597100	-2.69803500	-0.78619000
N	-2.69500800	-3.66680200	-0.56842800
C	2.75460900	2.53182800	-0.35931100
C	2.55140500	1.96249500	-1.62064700
C	1.29754800	1.52925100	-2.02470700
C	0.19290200	1.63979200	-1.16675500
C	0.39607300	2.21989800	0.09450500
C	1.64937400	2.66416700	0.48651400
H	3.40221100	1.85453700	-2.29566400
H	1.17405900	1.04857700	-2.99481900
H	-0.45573700	2.32132900	0.77156400
H	1.78265000	3.11971700	1.47015300
C	4.10762000	3.01365300	0.07691400
C	-1.14528200	1.18822800	-1.54918500
H	-1.88779500	1.41022000	-0.77221300
C	4.27352400	4.53935700	0.02103100
H	3.48310600	4.98431500	0.65138500
C	-1.67620700	1.54744300	-2.90913900
H	-0.96935900	1.34779600	-3.71885400
H	-2.60517800	1.01038500	-3.13152200
H	-1.90824400	2.62591900	-2.90650900
H	4.88876100	2.55569100	-0.55368700
H	4.30323200	2.67621700	1.10838600
C	4.10837400	5.06341200	-1.39786000
H	4.86083400	4.61193500	-2.06333700
H	3.11778100	4.83217900	-1.80955100
H	4.24460300	6.15205500	-1.43568300
C	5.62870000	4.93550800	0.58815200
H	5.76074000	6.02531000	0.58484000
H	5.75840900	4.58191000	1.61996600

H	6.43979900	4.50279100	-0.01683100
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TS5a

C	3.19122300	-0.95725300	0.31681400
O	2.47028300	-0.54996300	1.51025700
C	2.06896700	-1.53479900	-0.57396700
H	2.08182800	-1.17249400	-1.61129500
C	1.15682900	-0.62555400	1.20872400
N	0.82778700	-1.09730200	0.07461100
C	0.24840200	-0.15911500	2.27518600
C	0.70583900	-0.40996100	3.71291100
C	0.75014300	0.96251000	3.18097600
H	1.63896400	-0.95815200	3.80772000
H	-0.07507500	-0.67368800	4.42006300
H	1.71456800	1.38104800	2.90259700
H	-0.00155200	1.67616000	3.51282200
C	-3.32106300	0.14613800	2.64808500
O	-1.95977000	0.06167400	3.11976600
C	-3.27730600	-0.56748600	1.29059800
H	-3.56149700	-1.62919900	1.29063200
C	-1.20520900	-0.21694100	2.03722300
N	-1.83834900	-0.49634800	0.95861000
C	3.74116700	-4.66226000	0.49176900
C	2.89603800	-5.66382100	0.02245200
C	1.73559000	-5.34537200	-0.68367800
C	1.40148400	-4.01868500	-0.93568500
C	2.25092200	-3.02474200	-0.46541200
C	3.40850300	-3.33542400	0.24554100
H	4.64436500	-4.91548500	1.04721200
H	3.14068600	-6.70770800	0.21315100
H	1.07880100	-6.13924800	-1.03365300
H	0.48792100	-3.76202600	-1.47120700
C	4.16247400	-2.09129700	0.63237300

H	4.46603800	-2.06504100	1.68770300
H	5.08131700	-1.97473200	0.03841200
C	-4.55930900	-0.01113300	-0.89179500
C	-4.10469600	0.28912200	0.38558800
C	-4.32844900	1.53600300	0.96930800
C	-5.00614400	2.52018100	0.26071800
C	-5.45221600	2.23346200	-1.02845400
C	-5.23842600	0.97855200	-1.59879500
H	-4.37572800	-0.99628600	-1.32362000
H	-5.19098400	3.49913200	0.70234600
H	-5.98529700	2.99623100	-1.59349300
H	-5.60636700	0.77093500	-2.60201700
C	-3.74058100	1.59933800	2.35527500
H	-2.85049900	2.24858600	2.39510100
H	-3.94814100	-0.34125700	3.39878100
H	-4.44308100	1.99106400	3.10207300
H	3.66998100	-0.05258000	-0.08091500
C	-0.62380200	-1.21274700	-2.63838800
N	-0.07299200	-1.47861500	-3.63517700
Cu	-1.22726900	-1.08797500	-0.88832200
C	-2.00807100	-2.89596400	-0.60407800
N	-2.63556200	-3.84184900	-0.31901600
C	2.40585900	2.70690300	-0.45076600
C	2.34386800	2.04683500	-1.68212300
C	1.16399900	1.47720900	-2.13764900
C	0.00038600	1.53326300	-1.35837000
C	0.05594400	2.21624400	-0.13470200
C	1.23266800	2.80313000	0.30266600
H	3.24814600	1.97314900	-2.28913100
H	1.14898500	0.92810400	-3.07895800
H	-0.84818400	2.28055800	0.47503900
H	1.25309000	3.33473400	1.25628800
C	3.68378400	3.31014400	0.05512600

C	-1.25793800	0.91596500	-1.78120700
H	-2.05677400	1.05691400	-1.04166400
C	3.73704100	4.84093100	-0.04764200
H	2.87626200	5.24451300	0.51464300
C	-1.77975900	1.18473400	-3.16471600
H	-1.03027900	1.04600100	-3.94837100
H	-2.63961600	0.54706300	-3.39842200
H	-2.12204300	2.23278900	-3.18905100
H	4.53967800	2.89414400	-0.50352300
H	3.83188100	3.01985300	1.10938400
C	3.62429200	5.30128300	-1.49365700
H	4.44891800	4.88567700	-2.09381600
H	2.68172900	4.98053800	-1.95514200
H	3.68138300	6.39513400	-1.56633400
C	5.01880600	5.36057300	0.58626600
H	5.06703100	6.45666600	0.55039700
H	5.10890500	5.05186700	1.63652600
H	5.89759800	4.97362700	0.04859700

R-pro

C	3.95135200	-0.58606600	-0.16337100
N	4.62595900	-1.52866200	-0.22563500
C	-1.11116600	-0.21790000	-0.64048800
C	-0.27322800	-1.18427800	-0.08398600
C	1.08473500	-0.94464700	0.09275400
C	1.63899700	0.27441400	-0.28981600
C	0.80854800	1.24696300	-0.84564300
C	-0.54700300	1.00317000	-1.01735000
H	-0.69475000	-2.14528800	0.21406200
H	1.72334200	-1.71963500	0.51834500
H	1.23268000	2.20491800	-1.15189000
H	-1.18295100	1.76911200	-1.46422700
C	-2.58475100	-0.45624400	-0.80677600

C	3.09908400	0.59880900	-0.04447300
H	3.43283400	1.31332500	-0.81364200
C	-3.45039800	0.26163400	0.23814400
H	-3.22159200	1.34059000	0.17791000
C	3.29569100	1.23955300	1.33672600
H	2.68739200	2.14883400	1.40809100
H	2.97009100	0.54778600	2.12313700
H	4.34585300	1.49926000	1.51285800
H	-2.79805500	-1.53698200	-0.75221000
H	-2.90101600	-0.12805000	-1.80999900
C	-4.92454400	0.05922800	-0.07993100
H	-5.18431500	-1.00926800	-0.03368400
H	-5.56572900	0.58583600	0.63905800
H	-5.17734700	0.41930800	-1.08629900
C	-3.13353600	-0.21782400	1.64714200
H	-3.31805900	-1.30023300	1.73386800
H	-2.08572500	-0.03570000	1.91752000
H	-3.76706000	0.28594300	2.38895500

10b

C	-4.33902200	-1.02075800	1.95279900
O	-3.63489100	0.17687600	2.38576400
C	-3.75169400	-1.26904400	0.54252800
H	-3.41738300	-2.30103700	0.36188700
C	-2.66156700	0.39643100	1.47818200
N	-2.59930700	-0.36948500	0.46478600
C	-1.75511900	1.52788700	1.77166000
C	-2.26632000	2.59879800	2.71792800
C	-1.23217400	1.66561100	3.20407200
H	-3.28560100	2.46013800	3.06612400
H	-1.97899000	3.61924800	2.48434400
H	-1.51583100	0.87178600	3.89155000
H	-0.20781400	2.02434200	3.29871300

C	0.48436100	3.43462000	-0.33869400
O	-0.49356600	3.24915600	0.70999300
C	0.40390000	2.13159200	-1.15176700
H	-0.19956100	2.18793400	-2.06813300
C	-0.82781700	1.94805900	0.69628400
N	-0.31099100	1.22503600	-0.22730300
C	-7.12432300	-0.04570000	-0.36801600
C	-7.06045600	0.08803200	-1.75213200
C	-5.89388900	-0.23151500	-2.44822400
C	-4.77096200	-0.69688700	-1.77146300
C	-4.84699200	-0.83423900	-0.39110500
C	-6.00384700	-0.50787600	0.31259300
H	-8.03588500	0.21236300	0.17105400
H	-7.92958600	0.45240700	-2.29769200
H	-5.85684300	-0.10914400	-3.52887100
H	-3.84667700	-0.92442400	-2.30391400
C	-5.83252500	-0.74570500	1.78935900
H	-6.14322900	0.10271700	2.41386900
H	-6.41417200	-1.61516100	2.12968900
C	2.31884900	0.82026700	-2.31002500
C	1.83318600	1.77639200	-1.42762100
C	2.69237200	2.60318700	-0.70334100
C	4.06707000	2.49527200	-0.86927300
C	4.56209300	1.53916300	-1.75415200
C	3.69787900	0.70368800	-2.46206800
H	1.62872800	0.19520500	-2.87817600
H	4.74882800	3.14712200	-0.32225600
H	5.63901800	1.44767300	-1.89927600
H	4.10398200	-0.03762700	-3.14851800
C	1.91981900	3.53026500	0.19787700
H	1.93892200	3.18182200	1.24445400
H	0.18049500	4.32537000	-0.89525500
H	2.30176000	4.55896800	0.20299800

H	-4.11099700	-1.79866400	2.69143600
C	-0.73959000	-2.53532600	-1.13985200
N	-0.85878700	-3.65979200	-1.43355700
Cu	-0.67510600	-0.71165500	-0.73493100
C	-1.21054800	-0.13424300	-2.55348900
N	-1.46890500	0.32411700	-3.59839200
C	4.44554200	-1.47870000	0.24887700
C	3.64523800	-2.55734400	-0.14622600
C	2.27847700	-2.56690700	0.07212600
C	1.65236300	-1.48275800	0.70668400
C	2.45386800	-0.40350900	1.10201900
C	3.82364400	-0.40675500	0.89155800
H	4.11165200	-3.40265100	-0.65381900
H	1.67495500	-3.40085300	-0.28433500
H	1.98515300	0.44956400	1.59824600
H	4.41022700	0.45127500	1.21649300
C	5.90676900	-1.46729500	-0.11142500
C	0.21854800	-1.45890300	1.01393700
C	6.84483000	-0.66775700	0.79109400
H	6.48211500	0.37436600	0.83886400
C	-0.39953000	-2.65808000	1.67701100
H	-0.19684900	-3.59711200	1.15593500
H	0.01219500	-2.73417200	2.69733500
H	-1.48770900	-2.54878100	1.76441500
H	-0.04842300	-0.54238200	1.55179300
H	6.27331800	-2.50728000	-0.16182600
H	5.99843300	-1.07922700	-1.14223500
C	8.24155200	-0.64181300	0.18590700
H	8.64258500	-1.66256900	0.09520700
H	8.24027000	-0.19553600	-0.81839800
H	8.93833500	-0.06735200	0.81022500
C	6.88252300	-1.24044500	2.20133300
H	7.54859400	-0.65787100	2.85144800

H	5.88804900	-1.26218800	2.66503200
H	7.26055000	-2.27390700	2.18007200

TS5b

C	4.16393000	-1.61174500	-1.75056300
O	3.56160400	-0.45024800	-2.38639300
C	3.61340200	-1.52632900	-0.30841600
H	3.21919700	-2.47364500	0.08695200
C	2.62966200	0.01573500	-1.52984700
N	2.52785800	-0.54660000	-0.39208000
C	1.82099000	1.15175000	-2.02376000
C	2.40148500	1.96974900	-3.16315100
C	1.27357700	1.06336300	-3.45107800
H	3.39387300	1.67314700	-3.48932200
H	2.21340500	3.03821700	-3.12448300
H	1.46614300	0.13159900	-3.97813200
H	0.28460000	1.49358700	-3.60333600
C	-0.19981000	3.61849200	-0.30773700
O	0.72650600	3.15115600	-1.31593100
C	-0.19262400	2.49678700	0.74720700
H	0.42553000	2.69017600	1.63511800
C	0.96766800	1.85700300	-1.03962600
N	0.43881900	1.37687300	0.02190700
C	7.10254600	-0.42466200	0.25246400
C	7.09980400	0.01311400	1.57373600
C	5.93702000	-0.04462200	2.34323400
C	4.75639000	-0.54858700	1.80636500
C	4.77144500	-0.99206000	0.48976000
C	5.92499100	-0.92673700	-0.28883300
H	8.01103900	-0.36837900	-0.34716300
H	8.01415200	0.41252800	2.00985700
H	5.94829600	0.31494300	3.37023500
H	3.83679200	-0.57017200	2.39270900

C	5.68085300	-1.46159100	-1.67475300
H	6.05009400	-0.80633300	-2.47507700
H	6.16179200	-2.43993200	-1.82253700
C	-2.17059800	1.53696200	2.12417100
C	-1.63767600	2.29174200	1.08686300
C	-2.45392300	3.01847400	0.22065200
C	-3.83153300	3.01965400	0.39873900
C	-4.37359600	2.26588300	1.43752400
C	-3.55313900	1.52334400	2.28679600
H	-1.51232000	0.98702100	2.79799000
H	-4.47853600	3.60096800	-0.25863000
H	-5.45201200	2.25969800	1.59191300
H	-3.99655800	0.93738900	3.09015000
C	-1.63933700	3.72103900	-0.83345300
H	-1.70711900	3.20411900	-1.80543600
H	0.18896300	4.57435300	0.05375400
H	-1.95098900	4.75863300	-1.00900600
H	3.83215900	-2.48733900	-2.32206700
C	0.43460500	-2.20997100	1.49233800
N	0.42363900	-3.25187000	2.02363100
Cu	0.69857200	-0.45139300	0.95653600
C	1.27558600	0.38541400	2.63926900
N	1.57574900	1.00901000	3.58267800
C	-4.58324500	-1.06263900	0.01553900
C	-3.92632900	-2.10468700	0.67925500
C	-2.56127700	-2.29752100	0.54487900
C	-1.80061300	-1.43714900	-0.25850900
C	-2.45478900	-0.38422000	-0.90872800
C	-3.82596900	-0.21227100	-0.78887600
H	-4.50167700	-2.76931400	1.32571800
H	-2.06212500	-3.09468800	1.09442700
H	-1.87155000	0.30208700	-1.52697300
H	-4.31797900	0.61077000	-1.30884400

C	-6.06454000	-0.87870800	0.17002200
C	-0.36238700	-1.63890200	-0.51028100
C	-6.90335600	-1.91958500	-0.58405700
H	-6.60002600	-2.91872700	-0.22494000
C	0.08147100	-2.97249400	-1.05214900
H	-0.26671300	-3.81774900	-0.45302300
H	-0.33112400	-3.07116000	-2.06920500
H	1.17448700	-3.03098300	-1.12415700
H	0.02654600	-0.84214200	-1.15426300
H	-6.32878900	-0.91893000	1.23997700
H	-6.35436900	0.12564500	-0.18430800
C	-6.64952200	-1.85120400	-2.08293400
H	-5.59673700	-2.03973000	-2.32896300
H	-7.26088600	-2.58600600	-2.62301100
H	-6.91033800	-0.85342300	-2.47012200
C	-8.38025800	-1.72077400	-0.27755900
H	-8.99977800	-2.47036100	-0.78710300
H	-8.58506500	-1.78804000	0.79936300
H	-8.71370300	-0.72887500	-0.61898200

S-pro

C	3.55907600	1.11046000	0.35319700
N	3.86278400	2.10824700	0.86304500
C	-1.14179700	-0.39516400	-0.62749700
C	-0.42622600	0.69169300	-1.13944000
C	0.95228900	0.75947000	-1.01849900
C	1.66530100	-0.25895700	-0.38028100
C	0.95978000	-1.34199100	0.13372900
C	-0.42580700	-1.40591500	0.00853600
H	-0.96503000	1.49480300	-1.64472200
H	1.49099700	1.61894600	-1.42042800
H	1.48249400	-2.15228000	0.63867900
H	-0.96379500	-2.26161900	0.41916600

C	-2.63894900	-0.43683600	-0.73481000
C	3.18144800	-0.15219400	-0.29302700
C	-3.35675200	0.49882000	0.24813000
H	-2.98358700	1.52274700	0.06909500
C	3.88055700	-1.31524700	0.40773400
H	3.54740400	-1.40735400	1.44829700
H	3.66960500	-2.25669800	-0.11227900
H	4.96469100	-1.16122500	0.41296400
H	3.57200000	-0.09310000	-1.32358800
H	-2.94313900	-0.16950300	-1.75968600
H	-2.99882500	-1.46508900	-0.56180100
C	-3.05590900	0.12474200	1.69204900
H	-3.38265500	-0.90723200	1.89628100
H	-1.98396500	0.18692900	1.91807600
H	-3.58724100	0.78416600	2.39069000
C	-4.85560600	0.47510900	-0.01300900
H	-5.39032500	1.15797800	0.66006800
H	-5.09390200	0.76244200	-1.04601000
H	-5.25864300	-0.53558300	0.15301300

10a1

C	4.53204900	0.01113200	-1.90467700
O	4.17565500	1.31846700	-1.38924600
C	3.60789000	-0.92793700	-1.09900100
H	3.06321900	-1.65271800	-1.72175700
C	3.05419300	1.15664500	-0.65502500
N	2.64353600	-0.03285700	-0.45805400
C	2.46676700	2.40291100	-0.13029900
C	3.45538100	3.43435100	0.40269600
C	2.76915500	3.69892900	-0.87599100
H	4.50011000	3.13590400	0.37657200
H	3.13899900	3.97724100	1.28863200
H	3.32560800	3.58992000	-1.80264100

H	1.96333800	4.42824000	-0.88995500
C	-0.47457600	3.12686700	1.85517000
O	0.77367300	3.43420600	1.18669700
C	-0.89532800	1.80759500	1.17465200
H	-1.21032100	1.02509100	1.87997100
C	1.14139500	2.32266900	0.51387700
N	0.30929600	1.35740500	0.47118100
C	6.85723900	-1.67086400	0.51423000
C	6.51274400	-2.47083600	1.59993700
C	5.18035600	-2.80409300	1.84530100
C	4.17304100	-2.34993400	1.00019500
C	4.52491600	-1.56422200	-0.09014300
C	5.85200800	-1.21378500	-0.33002200
H	7.89805100	-1.40102800	0.33543400
H	7.29010600	-2.83089200	2.27201500
H	4.92499600	-3.41213800	2.71102800
H	3.12557400	-2.57173100	1.20898400
C	5.97479800	-0.34453300	-1.55279100
H	6.57271600	0.56230100	-1.39049400
H	6.44429200	-0.88478600	-2.38806600
C	-2.57894500	1.46430600	-0.77386900
C	-1.98278400	2.22602900	0.22227100
C	-2.33355000	3.56050500	0.41750900
C	-3.31460600	4.14715600	-0.37351700
C	-3.93026300	3.38258200	-1.36086900
C	-3.56221700	2.05199500	-1.56306000
H	-2.26689700	0.43440700	-0.94781200
H	-3.59410900	5.19074700	-0.22888600
H	-4.69825500	3.83133200	-1.98907600
H	-4.03691600	1.46851100	-2.35108400
C	-1.53908700	4.17395400	1.53897600
H	-1.07719600	5.13557400	1.27781400
H	-0.24467800	3.03586200	2.92291700

H	-2.16330100	4.35610900	2.42626300
H	4.33068300	0.03359700	-2.98144600
C	0.24613300	-0.79957700	-1.85061000
N	0.09354100	-0.77455600	-3.00988500
Cu	0.60836500	-0.80925200	0.03679600
C	0.84984500	-1.08810400	1.91586400
N	0.92730200	-1.19283500	3.07817700
C	-4.54492300	-1.31702300	-0.09116600
C	-3.89982900	-1.79830000	-1.23443500
C	-2.58398500	-2.23094800	-1.19050800
C	-1.87410900	-2.21897900	0.02041400
C	-2.53006500	-1.75677300	1.17639600
C	-3.83842900	-1.31181500	1.11753200
H	-4.44039600	-1.81125700	-2.18189400
H	-2.09051500	-2.55032300	-2.10599000
H	-1.97748900	-1.73015800	2.11716800
H	-4.32560400	-0.93710200	2.01882000
C	-5.95841400	-0.81947400	-0.14299700
C	-0.49883600	-2.68394000	0.13805300
H	-0.23681400	-2.93724000	1.16402300
C	-6.97504600	-1.76759700	0.50875200
H	-6.66611800	-1.92364600	1.55737000
C	0.13141500	-3.61031600	-0.85257800
H	-0.29435700	-4.61559800	-0.69120800
H	-0.02724900	-3.32053900	-1.89397900
H	1.21195500	-3.68673000	-0.67957700
H	-6.25798000	-0.65533900	-1.19182200
H	-6.01464800	0.16336700	0.35295900
C	-6.99673700	-3.11855100	-0.19175100
H	-7.26392100	-2.99560600	-1.25315500
H	-6.02088800	-3.61913100	-0.14984900
H	-7.73968200	-3.78796600	0.26118300
C	-8.35736600	-1.13221400	0.49902500

H	-9.09876700	-1.78010200	0.98463200
H	-8.36371300	-0.16311200	1.01569900
H	-8.69414600	-0.96110700	-0.53465900

TS5a1

C	4.32184400	-0.13772000	-1.98178200
O	4.02218800	1.19877100	-1.50085400
C	3.53032700	-1.02255100	-0.99806100
H	2.94892400	-1.81332300	-1.49366900
C	2.98020600	1.07656700	-0.65248900
N	2.61158200	-0.10005200	-0.32840400
C	2.41777900	2.34976200	-0.16395100
C	3.42988600	3.41059200	0.25349500
C	2.66919600	3.60353600	-0.99582400
H	4.47271500	3.11203600	0.18237200
H	3.16414300	4.00139600	1.12552200
H	3.17003100	3.44293500	-1.94624000
H	1.86083200	4.33007800	-1.00262900
C	-0.44203300	3.18706100	1.90010800
O	0.79156400	3.44823400	1.18523800
C	-0.90250500	1.85406000	1.27681900
H	-1.23677400	1.10832200	2.01240700
C	1.12628500	2.30608800	0.54835300
N	0.28273800	1.34917000	0.57993400
C	6.97367600	-1.56263400	0.25222800
C	6.78848300	-2.24786200	1.44965000
C	5.50573600	-2.56215200	1.89949800
C	4.38858400	-2.20575800	1.15060400
C	4.58109400	-1.53926300	-0.05285200
C	5.85904800	-1.20464100	-0.49712700
H	7.97694100	-1.30368100	-0.08616800
H	7.65318800	-2.53048900	2.04807500
H	5.37734300	-3.07911000	2.84876300

H	3.38113800	-2.40941100	1.51578100
C	5.80228000	-0.46213800	-1.80577400
H	6.41091000	0.45186700	-1.82125800
H	6.15096500	-1.08679400	-2.64140300
C	-2.58255100	1.49325500	-0.67228300
C	-1.98092100	2.26765700	0.31072200
C	-2.30150400	3.61492900	0.46622700
C	-3.26081800	4.20251200	-0.35019200
C	-3.88256600	3.42612100	-1.32447200
C	-3.54236500	2.08289500	-1.48840100
H	-2.29031000	0.45311800	-0.81792700
H	-3.51638900	5.25610100	-0.23752600
H	-4.63187600	3.87575900	-1.97419700
H	-4.01785600	1.49191800	-2.27028100
C	-1.49591200	4.24059200	1.57293400
H	-1.02601600	5.19313100	1.29375100
H	-0.18352900	3.13106900	2.96391400
H	-2.11271000	4.44249100	2.46130700
H	3.96832900	-0.18499900	-3.01803900
C	0.22378800	-0.81871600	-1.96432100
N	0.18169800	-0.96360000	-3.12520800
Cu	0.49922200	-0.72774500	-0.02457300
C	0.65233300	-1.29000800	1.78010100
N	0.92039300	-1.25952400	2.91979400
C	-4.52404800	-1.33049400	-0.08584500
C	-3.75643600	-1.84523100	-1.13299100
C	-2.44236100	-2.24726100	-0.93748300
C	-1.86488500	-2.16912300	0.33585400
C	-2.64044600	-1.67282200	1.39522900
C	-3.94227600	-1.25235100	1.18439000
H	-4.19478800	-1.91401800	-2.12946600
H	-1.85396600	-2.59292100	-1.78450400
H	-2.19295800	-1.60300900	2.38844200

H	-4.52410100	-0.84958500	2.01471900
C	-5.93959400	-0.88127800	-0.29803700
C	-0.50231800	-2.65111400	0.62741500
H	-0.45893100	-3.04428300	1.64221100
C	-6.98830600	-1.83753200	0.28724500
H	-6.77954700	-1.94644200	1.36625300
C	0.24581800	-3.56212200	-0.30440000
H	-0.22712500	-4.55664100	-0.24641000
H	0.24922100	-3.22855500	-1.34531600
H	1.28453100	-3.67798800	0.02730900
H	-6.13729600	-0.76692700	-1.37715600
H	-6.07590600	0.11659700	0.15006000
C	-6.90383500	-3.21261300	-0.35926600
H	-7.06982000	-3.13611400	-1.44536100
H	-5.92292000	-3.67994300	-0.20463700
H	-7.66819000	-3.88873300	0.04564700
C	-8.38052200	-1.24723600	0.11931800
H	-9.14758500	-1.90071900	0.55508100
H	-8.46484600	-0.26110000	0.59541200
H	-8.61905500	-1.12346200	-0.94792900

10a2

C	-4.41855100	-1.20530100	1.85353900
O	-4.39843600	0.22711700	1.64277700
C	-3.33634300	-1.69112500	0.86511500
H	-2.66401100	-2.45720600	1.27919100
C	-3.27124600	0.49904400	0.94587000
N	-2.56977500	-0.48539400	0.53953300
C	-2.98610000	1.93507100	0.76504800
C	-4.11611000	2.92148000	1.03817400
C	-3.03801300	2.79401300	2.03215400
H	-5.08166500	2.47401400	1.25503000
H	-4.13303000	3.80151900	0.40163000

H	-3.22768900	2.24528300	2.95118600
H	-2.27621300	3.56622900	2.10188400
C	-0.67831800	3.85211400	-1.20248100
O	-1.90942300	3.65622000	-0.47301700
C	-0.35581500	2.44994600	-1.75156300
H	-0.66611200	2.27258800	-2.79146300
C	-1.98239500	2.33162300	-0.23783900
N	-1.16641600	1.58040700	-0.87896000
C	-6.41161300	-2.64409300	-0.96871500
C	-5.94609900	-3.01854700	-2.22583100
C	-4.58347000	-2.97582400	-2.52195400
C	-3.66143700	-2.56230300	-1.56504000
C	-4.13336100	-2.19832200	-0.30969900
C	-5.49439300	-2.23085300	-0.00991400
H	-7.47777900	-2.66897100	-0.74317400
H	-6.65364000	-3.34138100	-2.98813700
H	-4.23578600	-3.26080100	-3.51322800
H	-2.59824200	-2.50243300	-1.80175600
C	-5.75206500	-1.79383400	1.40662500
H	-6.55982500	-1.05625000	1.50390500
H	-6.02205700	-2.64436800	2.05040400
C	1.97266800	1.33566900	-2.06664900
C	1.12342200	2.30602800	-1.54868200
C	1.60212600	3.32373800	-0.72407600
C	2.95036000	3.38016300	-0.39834500
C	3.80784500	2.41230000	-0.91612700
C	3.32587100	1.40177600	-1.74635500
H	1.58459900	0.53694100	-2.69954900
H	3.33172400	4.16743000	0.25116900
H	4.86957700	2.44663200	-0.67183800
H	4.01057300	0.65302000	-2.14201300
C	0.48714900	4.22403700	-0.27108200
H	0.21283800	3.98609600	0.77017700

H	-0.87895000	4.60559800	-1.96912000
H	0.73806300	5.29161200	-0.30971800
H	-4.18811700	-1.37603600	2.91270500
C	0.12185100	0.96569200	1.54257800
N	0.28525300	1.75145700	2.39432600
Cu	-0.28281700	-0.13700000	0.00944600
C	-0.26101400	-1.22406700	-1.57668700
N	-0.22643800	-1.87730900	-2.54668400
C	4.93917000	-1.04730100	0.12726300
C	4.33604500	-0.45777800	1.24197800
C	2.99069900	-0.64278200	1.51198500
C	2.19920100	-1.43688700	0.66770500
C	2.80023600	-2.01378900	-0.46517900
C	4.14823000	-1.83213100	-0.71861500
H	4.93754000	0.17018900	1.90071300
H	2.53766200	-0.13749000	2.36284700
H	2.18245300	-2.58876400	-1.15536300
H	4.59930500	-2.28628800	-1.60258700
C	6.39611000	-0.84907100	-0.16903100
C	0.79590600	-1.72141200	0.94318100
H	0.39498300	-2.50920400	0.30291600
C	7.26634500	-2.07311300	0.15224700
H	6.86700600	-2.92739800	-0.42226600
C	0.28966900	-1.83027700	2.35024100
H	0.58864700	-2.82031900	2.73436300
H	0.68128000	-1.06152800	3.02038900
H	-0.80483700	-1.77892500	2.38892900
H	6.78156100	0.01178900	0.40322900
H	6.52307800	-0.59776700	-1.23561300
C	7.20677200	-2.41923800	1.63289600
H	7.56449600	-1.57208100	2.23912500
H	6.18570700	-2.65457000	1.95907600
H	7.84346900	-3.28342100	1.86336200

C	8.70133400	-1.82014400	-0.28542800
H	9.33887900	-2.69214200	-0.08933200
H	8.76560300	-1.58796000	-1.35699200
H	9.12710500	-0.96846900	0.26655500

TS5a2

C	4.37250500	-1.21905800	-1.87116400
O	4.37281600	0.21512200	-1.66860200
C	3.29948300	-1.69041200	-0.86497700
H	2.60092100	-2.43655300	-1.27126800
C	3.26622900	0.50627400	-0.94896900
N	2.56424500	-0.46970000	-0.52214600
C	2.99471700	1.94709800	-0.78336400
C	4.12333100	2.92141400	-1.09986200
C	3.02537400	2.77677200	-2.07040400
H	5.08360400	2.46735100	-1.32633800
H	4.15441400	3.81534800	-0.48338800
H	3.20000500	2.20892700	-2.98079300
H	2.26771800	3.55275300	-2.14226300
C	0.70039500	3.91391800	1.15337300
O	1.90455500	3.70837900	0.38360600
C	0.43486700	2.53315700	1.78588100
H	0.76461800	2.42998100	2.82959400
C	2.01468700	2.37216400	0.23354100
N	1.25614000	1.63580000	0.95407000
C	6.38881900	-2.69687900	0.91511700
C	5.93638300	-3.08187600	2.17373500
C	4.57795000	-3.03256300	2.48762500
C	3.64640800	-2.59906400	1.54885400
C	4.10609700	-2.22080200	0.29282300
C	5.46257200	-2.26386900	-0.02608800
H	7.45141700	-2.73031700	0.67429800
H	6.65084900	-3.42070400	2.92254000

H	4.24007900	-3.33011000	3.47857100
H	2.58584600	-2.54108300	1.79864300
C	5.70644400	-1.82029600	-1.44291600
H	6.51797000	-1.08762700	-1.54614700
H	5.96303800	-2.66913500	-2.09432900
C	-1.83701700	1.32718800	2.16690300
C	-1.04064500	2.32245500	1.61315500
C	-1.57459400	3.28641500	0.75902500
C	-2.92674100	3.26807300	0.44472200
C	-3.73206500	2.27635100	0.99953900
C	-3.19411900	1.31657500	1.85561500
H	-1.40623000	0.56478100	2.81631800
H	-3.35009400	4.01370900	-0.22767200
H	-4.79577900	2.24814400	0.76249500
H	-3.83895800	0.54835600	2.27985000
C	-0.50772900	4.21531800	0.25159800
H	-0.25388200	3.96173800	-0.79109500
H	0.91424800	4.70953200	1.87254600
H	-0.79819000	5.27357200	0.27089600
H	4.12421900	-1.39136400	-2.92615400
C	-0.16190400	0.73054100	-1.36267700
N	-0.32222200	1.58096200	-2.15281100
Cu	0.42798000	-0.18871100	0.20246900
C	0.25697700	-1.43157100	1.70369100
N	0.09455100	-2.21424500	2.55957300
C	-4.98855900	-0.96114700	-0.20700600
C	-4.48672100	-0.33091100	-1.34956700
C	-3.15155900	-0.44293700	-1.69964100
C	-2.27369100	-1.19633100	-0.90840600
C	-2.77049200	-1.82141500	0.24678600
C	-4.11117000	-1.71652100	0.57638800
H	-5.15957000	0.26985200	-1.96316800
H	-2.77399100	0.08915400	-2.57114500

H	-2.08374800	-2.36377400	0.89773500
H	-4.48395700	-2.20273600	1.47946600
C	-6.43021700	-0.83104100	0.18703700
C	-0.87548200	-1.39716400	-1.27314500
H	-0.37214100	-2.11642300	-0.62214100
C	-7.26677200	-2.08843100	-0.09020100
H	-6.79245800	-2.93008400	0.44438000
C	-0.45937100	-1.56186800	-2.70319000
H	-0.77194600	-2.57147600	-3.01563100
H	-0.91023300	-0.83114900	-3.37914800
H	0.62978800	-1.49863900	-2.80898400
H	-6.88981200	0.01837800	-0.34652100
H	-6.49412800	-0.59532200	1.26278400
C	-7.29388400	-2.41639700	-1.57591500
H	-7.72927700	-1.57991300	-2.14508600
H	-6.28820500	-2.60285000	-1.97377100
H	-7.90632800	-3.30575500	-1.77395400
C	-8.67794400	-1.90326500	0.44739700
H	-9.28921900	-2.80035500	0.28365200
H	-8.67844700	-1.68530400	1.52381600
H	-9.17689800	-1.06539800	-0.06289400

10a3

C	1.95451900	2.40757100	-1.29016800
O	0.64013100	2.94250000	-1.57502500
C	1.65793000	1.39452900	-0.16696400
H	2.17369800	0.43615700	-0.29575900
C	-0.24865300	2.11917500	-0.97173900
N	0.20694300	1.18713700	-0.23045200
C	-1.66129000	2.40950000	-1.28273000
C	-1.98790300	3.76469400	-1.89939500
C	-2.00531800	2.57433700	-2.76556800
H	-1.15216800	4.45379200	-1.97658900

H	-2.93624500	4.20053000	-1.59837800
H	-1.17850100	2.40419100	-3.45032500
H	-2.95767500	2.15010500	-3.07350900
C	-4.82380500	1.29146100	-0.01742500
O	-3.95301400	2.24130300	-0.66580300
C	-3.89510400	0.56570100	0.97449500
H	-3.92816900	0.93968600	2.00801100
C	-2.70158900	1.78648700	-0.44916900
N	-2.56082100	0.85947700	0.42219600
C	3.20920900	4.13028700	1.79104000
C	3.00137800	3.75120900	3.11418300
C	2.33517000	2.56353400	3.41765200
C	1.86930300	1.73183100	2.40348600
C	2.08541800	2.11426700	1.08511200
C	2.74435600	3.30311000	0.77540500
H	3.72254300	5.06310200	1.55694800
H	3.35621100	4.39175400	3.92036000
H	2.16943800	2.28638200	4.45722200
H	1.32342000	0.81617100	2.63613100
C	2.86414100	3.48787400	-0.71357700
H	2.56331300	4.48463600	-1.06322600
H	3.89766200	3.33156100	-1.05793800
C	-3.92954400	-1.93654800	1.68325300
C	-4.28822000	-0.87752900	0.85870900
C	-5.10339900	-1.07147200	-0.25579900
C	-5.56796700	-2.34170900	-0.56823500
C	-5.20829900	-3.40963000	0.25017700
C	-4.39948700	-3.21008000	1.36856300
H	-3.28546200	-1.77323900	2.54804200
H	-6.20096900	-2.50238100	-1.44023800
H	-5.56931300	-4.41042300	0.01849100
H	-4.13981500	-4.05386200	2.00662500
C	-5.32266700	0.21672000	-0.99775400

H	-4.70104100	0.23971300	-1.90798400
H	-5.63125300	1.86280600	0.44871800
H	-6.36305400	0.37395600	-1.30916300
H	2.32752400	1.95967200	-2.22072300
C	-1.69859600	-0.94075700	-1.59003200
N	-2.09527800	-0.93420200	-2.69074000
Cu	-1.12254400	-0.72880200	0.23049200
C	-0.71269100	-0.83798600	2.10273200
N	-0.47785800	-0.88007700	3.24802300
C	3.96920200	-1.49495300	-0.51783500
C	3.43896900	-1.70628300	0.76012500
C	2.10575800	-2.03955400	0.94002800
C	1.25381800	-2.18090900	-0.16745700
C	1.77866300	-1.94231100	-1.44989900
C	3.11394400	-1.61602700	-1.61965800
H	4.08927400	-1.59652100	1.62874500
H	1.70679500	-2.16025000	1.94607800
H	1.11390800	-2.01349700	-2.31178000
H	3.50766300	-1.44170700	-2.62242900
C	5.41835800	-1.16388900	-0.71889100
C	-0.13444000	-2.61528000	-0.05440000
C	6.25585200	-2.34781000	-1.22619200
H	5.80349700	-2.69701900	-2.17120800
C	-0.58544600	-3.56671300	1.00789900
H	-0.22213800	-4.56945900	0.72464500
H	-0.21790500	-3.32648700	2.00810900
H	-1.68040400	-3.61454200	1.04339900
H	-0.56082400	-2.86760000	-1.02458100
H	5.51057600	-0.33550600	-1.44025300
H	5.85665600	-0.80569200	0.22724500
C	7.67972600	-1.89143400	-1.50769300
H	8.15769800	-1.53140200	-0.58413400
H	8.29315600	-2.71409900	-1.89763300

H	7.70832500	-1.07206200	-2.23855600
C	6.24535900	-3.50074400	-0.23316700
H	6.65560400	-3.17613000	0.73594300
H	5.23181900	-3.88225900	-0.05525000
H	6.86215500	-4.33557800	-0.59057800

TS5a3

C	1.95564100	2.49970500	-1.25780400
O	0.63378600	2.98586200	-1.59493400
C	1.65602900	1.46140200	-0.15731800
H	2.20114400	0.51777000	-0.28252500
C	-0.24903200	2.13378300	-1.02852500
N	0.21457700	1.21393900	-0.27535800
C	-1.65819700	2.36587700	-1.39994000
C	-2.00593600	3.67389500	-2.10018500
C	-1.94396300	2.44020800	-2.90194400
H	-1.19476900	4.39137900	-2.18142900
H	-2.98192300	4.08625700	-1.86035900
H	-1.08232100	2.27188800	-3.54327400
H	-2.86407400	1.95953200	-3.22388100
C	-4.82442900	1.18002500	-0.19837900
O	-3.97140600	2.10176400	-0.90816700
C	-3.91099700	0.62147400	0.91021800
H	-4.02890200	1.10014800	1.89303900
C	-2.71101400	1.75623500	-0.56915100
N	-2.56462900	0.93943700	0.40415800
C	3.04036900	4.22042400	1.88996000
C	2.81508400	3.80683800	3.19981700
C	2.19521800	2.58511700	3.46378400
C	1.79104500	1.75397400	2.42304100
C	2.02065900	2.17365900	1.11824100
C	2.63735000	3.39427400	0.84748500
H	3.52040900	5.17785100	1.68661600

H	3.12163400	4.44583600	4.02673500
H	2.01802100	2.27883900	4.49315300
H	1.28483900	0.80892600	2.62667300
C	2.79395700	3.61115700	-0.63369400
H	2.45447800	4.59784300	-0.97656000
H	3.84410600	3.51313900	-0.94742400
C	-3.85448100	-1.78398800	1.89590500
C	-4.22024100	-0.84640900	0.93804400
C	-4.97394000	-1.20598200	-0.17939400
C	-5.37211600	-2.52447200	-0.35581100
C	-5.01371400	-3.46998200	0.60309100
C	-4.26292200	-3.10440200	1.72053500
H	-3.24526900	-1.49547700	2.75223700
H	-5.96001000	-2.81520000	-1.22596200
H	-5.32872500	-4.50537000	0.48102300
H	-3.99189500	-3.85481400	2.46155800
C	-5.22024200	-0.02186600	-1.07207700
H	-4.55647700	-0.06257100	-1.95154100
H	-5.68267900	1.75246400	0.16470600
H	-6.25151300	0.04181300	-1.44191200
H	2.38481000	2.07851000	-2.17650600
C	-1.54054100	-1.03508500	-1.42404200
N	-2.04989200	-0.92711400	-2.47404000
Cu	-1.00256800	-0.58057300	0.35027300
C	-0.59211700	-0.88832300	2.23796000
N	-0.34369400	-1.14306700	3.35378800
C	3.92476400	-1.51881600	-0.52483200
C	3.27394600	-1.85616200	0.66619600
C	1.92021200	-2.15691100	0.69065500
C	1.17257200	-2.13783100	-0.49578400
C	1.82004000	-1.78722000	-1.69134200
C	3.17194200	-1.48545600	-1.70458900
H	3.84348200	-1.87450800	1.59594200

H	1.43192000	-2.37513000	1.63850400
H	1.23854500	-1.74768300	-2.61385100
H	3.66088100	-1.21728500	-2.64274300
C	5.39554100	-1.22453000	-0.55632600
C	-0.23744400	-2.54245300	-0.56588800
C	6.24523100	-2.38593000	-1.09438900
H	5.87660700	-2.62916500	-2.10674700
C	-0.87290000	-3.47747000	0.41710700
H	-0.48863900	-4.48786500	0.19724100
H	-0.67034000	-3.23625300	1.46359200
H	-1.95988700	-3.49886200	0.27258600
H	-0.48934000	-2.84059500	-1.58263800
H	5.58112800	-0.33652600	-1.18208700
H	5.74941000	-0.97300800	0.45706600
C	7.70141200	-1.95667800	-1.19668200
H	8.09740900	-1.70135900	-0.20220100
H	8.32744700	-2.76094700	-1.60455700
H	7.82239300	-1.07436500	-1.83952300
C	6.10927500	-3.62541000	-0.22220300
H	6.43397700	-3.40761300	0.80730200
H	5.07373600	-3.98578700	-0.17571900
H	6.73493700	-4.44458500	-0.59992400

10a4

C	2.53532900	2.77903400	0.05272000
O	1.64692200	2.46093600	1.14779600
C	2.61491600	1.45038400	-0.72981600
H	2.36433100	1.56182200	-1.79411100
C	1.16658400	1.22359900	0.94468500
N	1.59668100	0.60332600	-0.09000200
C	0.19260300	0.78607000	1.96185000
C	0.32220000	1.42449100	3.34116900
C	-0.78291400	1.85405800	2.46772600

H	1.16913400	2.09119200	3.47115400
H	0.10328500	0.76693500	4.17697300
H	-0.72380700	2.82038500	1.97157200
H	-1.78885800	1.49445700	2.67752500
C	-1.58579600	-2.25168300	2.70820300
O	-0.97565400	-0.98719200	3.03584400
C	-0.88955900	-2.66902300	1.39484000
H	-0.07518100	-3.40039100	1.50821700
C	-0.34162400	-0.58819100	1.91222500
N	-0.28913400	-1.40556700	0.93803600
C	6.07544600	1.61573100	0.56502300
C	6.64773900	0.42431900	0.13064500
C	5.91374300	-0.48577100	-0.63011200
C	4.59175100	-0.21795400	-0.96508000
C	4.02160600	0.96713300	-0.51760000
C	4.75181300	1.88291200	0.23571700
H	6.65511100	2.32459400	1.15584500
H	7.68052100	0.19783900	0.38974200
H	6.37264200	-1.41782900	-0.95221600
H	4.00857700	-0.93777500	-1.54079300
C	3.94037400	3.10825300	0.55917900
H	3.91316000	3.34618700	1.63112400
H	4.33290300	4.00050700	0.05041500
C	-1.92071200	-3.79382600	-0.71038000
C	-2.00878300	-3.14119100	0.51336200
C	-3.24362100	-2.79240400	1.06031800
C	-4.41801500	-3.08051400	0.37592200
C	-4.33684200	-3.72166600	-0.85834900
C	-3.10004300	-4.07792700	-1.39583600
H	-0.95046200	-4.06404500	-1.12985200
H	-5.38739200	-2.81364800	0.79708000
H	-5.24919300	-3.95438000	-1.40519800
H	-3.05383400	-4.58819500	-2.35607900

C	-3.07791900	-2.08393000	2.37669900
H	-3.30273900	-1.00814500	2.28573600
H	-1.40268400	-2.92287200	3.55136700
H	-3.73310700	-2.47667800	3.16512300
H	2.06258600	3.60009800	-0.49931900
C	2.47556100	-2.05382200	0.63777000
N	3.09154800	-2.45232200	1.54842000
Cu	1.20916000	-1.28875900	-0.69735600
C	1.28420900	-2.82678800	-1.76641600
N	1.31104000	-3.80129000	-2.41032700
C	-2.60864700	2.32536700	-0.48124800
C	-1.44714700	2.68738300	-1.17011400
C	-0.63678600	1.73023300	-1.76442300
C	-0.94877600	0.36354800	-1.68357800
C	-2.13629300	0.00947000	-1.01988600
C	-2.94380400	0.96776200	-0.43050000
H	-1.18441900	3.74450000	-1.24707700
H	0.25383800	2.04869900	-2.30711700
H	-2.41423800	-1.04322600	-0.96815900
H	-3.86168500	0.66081000	0.07717300
C	-3.50381600	3.35515000	0.14360600
C	-0.11136300	-0.68493400	-2.26916500
H	-0.67538300	-1.61001000	-2.40705200
C	-4.77295800	3.65227200	-0.66896700
H	-5.31481400	2.69909500	-0.80038600
C	0.76583500	-0.35605700	-3.44773000
H	0.17029400	0.14059400	-4.23144300
H	1.59600900	0.32044100	-3.20347300
H	1.20206200	-1.26762900	-3.86682500
H	-3.80550600	3.02080900	1.15043000
H	-2.95059000	4.30021400	0.28187200
C	-4.43501700	4.20571100	-2.04541200
H	-3.85887000	5.13995400	-1.95244200

H	-3.83674600	3.50097700	-2.63662800
H	-5.34592800	4.43479400	-2.61356600
C	-5.66512400	4.61845600	0.09625800
H	-6.59380700	4.82450700	-0.45153100
H	-5.93617300	4.22692600	1.08603000
H	-5.15065400	5.57960900	0.24737200

TS5a4

C	-2.76009800	-2.54909500	-0.43148300
O	-1.91736500	-2.42172900	0.73826200
C	-2.87928600	-1.08617800	-0.89944000
H	-2.78209100	-0.96390300	-1.98766000
C	-1.36403300	-1.19462200	0.70236900
N	-1.76120100	-0.40442100	-0.22476000
C	-0.39185000	-0.94743400	1.78273600
C	-0.66594000	-1.67237400	3.10052800
C	0.44922500	-2.13229700	2.25615100
H	-1.57494400	-2.26589800	3.12590400
H	-0.44446700	-1.10363400	3.99848400
H	0.33574200	-3.05099400	1.68562600
H	1.46680300	-1.88472000	2.55353100
C	1.59619700	1.84300900	2.87391500
O	0.86100300	0.61818900	3.06245200
C	0.99201100	2.44093800	1.58691400
H	0.23354000	3.22284100	1.74042800
C	0.25266200	0.37556800	1.87962600
N	0.31282300	1.27959000	0.98518900
C	-6.19723300	-1.58152000	0.67239500
C	-6.74433900	-0.30226500	0.70820300
C	-6.03815100	0.78830500	0.20146100
C	-4.77439800	0.61821200	-0.35455400
C	-4.23192100	-0.66026200	-0.38512800
C	-4.93267300	-1.75366600	0.12351400

H	-6.74823800	-2.43155600	1.07461100
H	-7.73069900	-0.15047600	1.14363100
H	-6.46805300	1.78639400	0.25309500
H	-4.20964900	1.47660500	-0.71406400
C	-4.15127200	-3.02820000	-0.03841200
H	-4.11169400	-3.64672200	0.86814600
H	-4.56789500	-3.66245300	-0.83513800
C	2.19760900	3.69335900	-0.34222200
C	2.18159900	2.90212100	0.79905100
C	3.35969700	2.39249200	1.34466500
C	4.58117700	2.65500100	0.73653200
C	4.60319400	3.43094200	-0.42109700
C	3.42282300	3.94884800	-0.95485100
H	1.27214100	4.09281600	-0.75641500
H	5.50818700	2.26549200	1.15783800
H	5.55366200	3.64474200	-0.90753900
H	3.45653000	4.56398300	-1.85210800
C	3.07950700	1.56881600	2.57173000
H	3.20782200	0.49123100	2.37257500
H	1.44384900	2.44953400	3.77064700
H	3.73600200	1.81342100	3.41687400
H	-2.23707900	-3.21833200	-1.12749000
C	-2.19842000	2.66286500	0.21582900
N	-2.84542700	3.34410900	0.91318800
Cu	-0.98501600	1.46695400	-0.78492400
C	-0.49837600	2.68888900	-2.10894700
N	-0.39863800	3.66640000	-2.74553200
C	2.48345400	-2.26724600	-0.43466600
C	1.28915500	-2.55560900	-1.09929400
C	0.57487700	-1.56303700	-1.75712800
C	1.03353300	-0.23918200	-1.77844500
C	2.24232100	0.04455700	-1.12542600
C	2.94575600	-0.94714300	-0.46179300

H	0.91867900	-3.58333600	-1.10594200
H	-0.34512900	-1.82429700	-2.27971500
H	2.62292400	1.06664300	-1.13827000
H	3.88732000	-0.69807000	0.03305600
C	3.28699300	-3.33935200	0.24220100
C	0.36017700	0.82458200	-2.55294600
H	1.11140500	1.54038700	-2.88782000
C	4.50882700	-3.80189400	-0.56557900
H	5.13383900	-2.91285500	-0.76138400
C	-0.57078000	0.41850500	-3.66520500
H	-0.05259400	-0.28510900	-4.33479800
H	-1.47963200	-0.07837500	-3.30431100
H	-0.88061600	1.29195300	-4.24514700
H	3.63689300	-2.97611300	1.22319800
H	2.65053800	-4.21859200	0.44339900
C	4.09782300	-4.40327600	-1.90141600
H	3.44246600	-5.27466600	-1.74458500
H	3.55418900	-3.68379700	-2.52669800
H	4.97423100	-4.74685400	-2.46608400
C	5.32104100	-4.79928300	0.24716600
H	6.21691000	-5.12369100	-0.29795200
H	5.64452900	-4.37577000	1.20756100
H	4.72269400	-5.69739200	0.46330200

10a5

C	-0.19847400	3.52383200	-2.08076600
O	-1.59201800	3.31815900	-1.75869300
C	0.50343000	2.41743200	-1.26920500
H	1.19878500	1.82111600	-1.87635700
C	-1.69766100	2.17774900	-1.06112800
N	-0.59852800	1.56018800	-0.80490600
C	-3.06740100	1.85651000	-0.63713000
C	-3.80590000	3.04171900	-0.00152500

C	-4.21599100	2.57958600	-1.33691200
H	-3.22386100	3.95497300	0.08479500
H	-4.40466300	2.78775300	0.86763800
H	-3.94882100	3.17554900	-2.20495300
H	-5.13266900	2.00184400	-1.42336400
C	-4.74196500	-0.92754000	0.88477900
O	-4.59878800	0.44534300	0.48219300
C	-3.29924300	-1.46138400	0.87604800
H	-2.79674700	-1.43883200	1.85509200
C	-3.36509100	0.53221900	-0.05881700
N	-2.59881700	-0.48675300	0.00723900
C	1.52423200	5.39430700	0.67855000
C	2.18109600	4.86134300	1.78316400
C	2.33299500	3.48245900	1.92576500
C	1.83092400	2.61481100	0.96257500
C	1.17330600	3.15174800	-0.13833600
C	1.01677100	4.52875500	-0.28282000
H	1.40307200	6.47218500	0.57431200
H	2.57395700	5.52751700	2.54918100
H	2.83580400	3.08010200	2.80243600
H	1.93848600	1.53571600	1.08485500
C	0.29195800	4.87129900	-1.55556800
H	-0.55224400	5.55865700	-1.41123400
H	0.96065000	5.34478800	-2.28922500
C	-2.52980400	-3.89702000	0.39143300
C	-3.43504000	-2.84655200	0.31822400
C	-4.68753600	-3.01373500	-0.27432200
C	-5.03523000	-4.23202600	-0.84293300
C	-4.11741800	-5.27943700	-0.80208000
C	-2.87892300	-5.11685600	-0.18269500
H	-1.58155100	-3.76337000	0.91412600
H	-6.01446500	-4.37326200	-1.30049800
H	-4.37920400	-6.24185300	-1.23937100

H	-2.18671700	-5.95568700	-0.13217300
C	-5.51158400	-1.76038200	-0.15397800
H	-5.55010700	-1.20560000	-1.10495200
H	-5.21581500	-0.92744000	1.87014300
H	-6.55094400	-1.95339600	0.14129700
H	-0.11194500	3.41679200	-3.16795900
C	-1.16273600	1.18231800	1.99614500
N	-1.82580600	1.86967800	2.67230500
Cu	-0.34828300	0.07215800	0.53209100
C	0.00885900	-1.42295000	1.59112600
N	0.07918000	-2.37704600	2.26266800
C	4.94439800	-1.40560400	0.23696300
C	4.03727100	-2.41765900	0.56707500
C	2.69597100	-2.32290100	0.23782500
C	2.20098800	-1.20217600	-0.44836000
C	3.11713700	-0.19216400	-0.78256700
C	4.45824800	-0.28945300	-0.44663800
H	4.39694700	-3.29611700	1.10437900
H	2.01240100	-3.10804300	0.55183400
H	2.76973800	0.68820900	-1.32402900
H	5.14491100	0.51427500	-0.71705000
C	6.40347800	-1.52092400	0.56592300
C	0.79629700	-1.07971700	-0.85783800
H	0.66168800	-0.27513600	-1.58802700
C	7.27944200	-1.90205900	-0.63695700
H	7.11876500	-1.14135400	-1.42156100
C	0.02771900	-2.30268900	-1.25706700
H	0.43248500	-2.67602400	-2.21264900
H	0.09993400	-3.11141500	-0.52404100
H	-1.03382500	-2.07315200	-1.40458500
H	6.76666400	-0.56429200	0.97453200
H	6.55110200	-2.27476000	1.35709100
C	6.89130300	-3.26151900	-1.19977600

H	7.00574500	-4.04151700	-0.43066500
H	5.84893200	-3.28233000	-1.54239500
H	7.53218700	-3.53663900	-2.04774000
C	8.74713100	-1.88474600	-0.23600100
H	9.39760900	-2.12784700	-1.08644300
H	9.05136700	-0.90409700	0.15397700
H	8.93906900	-2.62995300	0.55073700

TS5a5

C	-0.13650300	3.40095000	-2.18691300
O	-1.52195800	3.28997100	-1.78755400
C	0.54792300	2.36649600	-1.27521700
H	1.26610800	1.73115900	-1.81462700
C	-1.64388800	2.18288800	-1.03659000
N	-0.56081000	1.54653800	-0.76673600
C	-3.00682100	1.91683200	-0.55624400
C	-3.65265900	3.12338000	0.13629800
C	-4.15254900	2.70366800	-1.18370100
H	-3.02274200	4.00645500	0.20474800
H	-4.21743700	2.88482600	1.03233000
H	-3.90183100	3.30104400	-2.05567200
H	-5.10050700	2.17386800	-1.22957000
C	-4.74320700	-0.83013300	0.96288200
O	-4.54711800	0.54569800	0.59567200
C	-3.33210300	-1.43769100	0.86592400
H	-2.79377000	-1.49395500	1.82406600
C	-3.33402700	0.59355800	0.00874500
N	-2.61183900	-0.46096100	0.01576300
C	1.57937200	5.51437700	0.38043600
C	2.16158700	5.09243100	1.57181000
C	2.24671900	3.73556200	1.88141200
C	1.75705700	2.77839700	0.99940100
C	1.18352700	3.20344200	-0.19351700

C	1.08626200	4.56007200	-0.50059200
H	1.50229900	6.57626900	0.14818600
H	2.54280000	5.82979500	2.27603700
H	2.68330200	3.42147700	2.82698100
H	1.79834600	1.72007000	1.26034100
C	0.42308500	4.77408100	-1.83360400
H	-0.37492300	5.52808700	-1.81562500
H	1.14338000	5.09529000	-2.60054700
C	-2.70475500	-3.87402400	0.20328500
C	-3.56215100	-2.78218200	0.24098600
C	-4.84853400	-2.85889500	-0.29489800
C	-5.28070000	-4.02366100	-0.91535200
C	-4.41244000	-5.11056900	-0.98527900
C	-3.13840200	-5.03995300	-0.42325700
H	-1.72715900	-3.81633600	0.68369000
H	-6.28691700	-4.09304600	-1.32880300
H	-4.74007200	-6.03186700	-1.46470600
H	-2.48417800	-5.90955300	-0.45886300
C	-5.60808800	-1.58135700	-0.06289300
H	-5.68306500	-0.97902500	-0.98214500
H	-5.16731700	-0.83764000	1.97055400
H	-6.63439600	-1.74853100	0.28876000
H	-0.09839900	3.16670700	-3.25746300
C	-1.12530400	1.08722000	2.12782200
N	-1.76812800	1.75951700	2.83794700
Cu	-0.38391400	0.02609600	0.61985900
C	0.02572800	-1.61745900	1.38928800
N	0.04566000	-2.60672300	2.01381600
C	4.98750500	-1.60415300	0.35650500
C	4.13077200	-2.70159600	0.48393500
C	2.78450100	-2.60702600	0.17111900
C	2.24329800	-1.40283500	-0.29755700
C	3.10395800	-0.30450000	-0.42653700

C	4.44847700	-0.40117300	-0.10402500
H	4.53312300	-3.64753200	0.84864400
H	2.13623600	-3.46700200	0.32535800
H	2.70907600	0.64820800	-0.78166900
H	5.09498500	0.47168000	-0.20672600
C	6.45120200	-1.71052300	0.66856700
C	0.82955400	-1.26781100	-0.68241900
H	0.67804100	-0.37208400	-1.29424000
C	7.34310200	-1.80713700	-0.57805100
H	7.14305100	-0.91778100	-1.20185300
C	0.08896200	-2.42935400	-1.27363300
H	0.50352400	-2.62838900	-2.27494500
H	0.17950600	-3.34320200	-0.67954600
H	-0.97662300	-2.19719500	-1.38587500
H	6.76669300	-0.83520300	1.25854500
H	6.63689000	-2.59561200	1.29954600
C	7.02320900	-3.04956000	-1.39641100
H	7.17817400	-3.95688900	-0.79164500
H	5.98278600	-3.05582000	-1.74558500
H	7.67598400	-3.12314700	-2.27613200
C	8.80876100	-1.79476200	-0.16955400
H	9.46908500	-1.83542000	-1.04577400
H	9.06376300	-0.89450200	0.40554700
H	9.03956400	-2.66795700	0.45926600

10a6

C	4.36760900	-0.72180700	-2.07294500
O	3.85221100	0.63234400	-2.18308700
C	3.59792100	-1.29165200	-0.85504800
H	3.05934900	-2.23044600	-1.05278800
C	2.86298600	0.74196000	-1.27061800
N	2.62173600	-0.25226500	-0.51849700
C	2.14745200	2.03279400	-1.26817800

C	2.96194300	3.25808400	-1.66214700
C	1.95825800	2.74135400	-2.60989700
H	4.01011500	3.06236200	-1.86964200
H	2.74779700	4.17315900	-1.11930900
H	2.29018100	2.18991700	-3.48657400
H	1.02328700	3.28810300	-2.72294000
C	-0.31593800	3.51589000	0.90015000
O	0.81963700	3.51175500	0.01455200
C	-0.39244300	2.06980700	1.39647600
H	0.13815400	1.87033700	2.33731000
C	1.06853000	2.22185300	-0.27437900
N	0.35447400	1.34231200	0.33439400
C	6.99647400	-1.08392500	0.59485500
C	6.80723300	-1.45425600	1.92311900
C	5.54136500	-1.80608700	2.39370000
C	4.44196600	-1.79598400	1.54168500
C	4.64119800	-1.42787700	0.21690300
C	5.89965700	-1.06944000	-0.25933900
H	7.98705300	-0.80723200	0.23367200
H	7.65673600	-1.46629100	2.60434100
H	5.40984300	-2.08485500	3.43730900
H	3.44637100	-2.05614500	1.90108900
C	5.85726200	-0.72356900	-1.72408400
H	6.30900500	0.24976000	-1.95964700
H	6.38972000	-1.46967500	-2.33189000
C	-2.50133500	0.81914100	2.23858800
C	-1.86230300	1.81114600	1.50863100
C	-2.58124300	2.82546900	0.87124100
C	-3.96532600	2.86397800	0.96484300
C	-4.61377100	1.86943700	1.69538200
C	-3.89123200	0.85284500	2.31903600
H	-1.91889800	0.05308200	2.75133800
H	-4.53498500	3.66448500	0.49281600

H	-5.69909100	1.89143700	1.78868500
H	-4.41673400	0.08895300	2.89030800
C	-1.64572400	3.78506900	0.18337100
H	-1.53500600	3.53832700	-0.88705200
H	-0.10713100	4.24601000	1.68709400
H	-1.96145000	4.83398800	0.23919300
H	4.14353600	-1.21360800	-3.02664500
C	0.80738500	-2.54426500	0.55065400
N	1.05087600	-3.68615700	0.60370600
Cu	0.58946800	-0.67865700	0.48097500
C	0.99576900	-0.47883600	2.41482300
N	1.14580600	-0.25801900	3.55392800
C	-4.54742400	-1.13827500	-0.26147700
C	-3.95799700	-0.07182500	-0.94152200
C	-2.60244600	-0.06728700	-1.23258700
C	-1.79083500	-1.15873400	-0.88831400
C	-2.38320000	-2.22444900	-0.18581100
C	-3.73203600	-2.21033400	0.11879200
H	-4.57682700	0.77690800	-1.23591100
H	-2.17373700	0.78350400	-1.76234300
H	-1.75793100	-3.06406000	0.11951000
H	-4.17046900	-3.04719300	0.66468100
C	-6.01619500	-1.15672200	0.04229900
C	-0.39344100	-1.26058700	-1.32153800
C	-6.82212800	-2.11627800	-0.84485700
H	-6.39369000	-3.12641400	-0.72180800
C	0.08221800	-0.38790500	-2.44716700
H	-0.51467900	-0.62323900	-3.34428800
H	-0.02886400	0.68583700	-2.25528300
H	1.13044100	-0.59123100	-2.69540900
H	-0.10016700	-2.29660800	-1.48587900
H	-6.17040900	-1.43998900	1.09698100
H	-6.43467100	-0.14216300	-0.07319800

C	-6.72128400	-1.72774700	-2.31269700
H	-7.10711100	-0.70738200	-2.46616300
H	-5.68462200	-1.75001800	-2.67215300
H	-7.31327500	-2.40396900	-2.94323000
C	-8.27478800	-2.14584100	-0.39352800
H	-8.86722500	-2.84662400	-0.99616300
H	-8.36805900	-2.44284200	0.65974200
H	-8.73095400	-1.14988600	-0.50095700

TS5a6

C	3.81523200	-2.41311500	0.47154300
O	2.84126500	-2.61134100	-0.58955200
C	3.54010700	-0.95811800	0.91519000
H	3.44953800	-0.82021700	2.00132800
C	2.01643700	-1.54361700	-0.56477700
N	2.26718900	-0.61684900	0.27196000
C	0.91816100	-1.57097200	-1.55139900
C	1.17915200	-2.38757700	-2.81401900
C	0.22501300	-2.90549300	-1.81840100
H	2.16196400	-2.84554900	-2.87298800
H	0.79210400	-1.96738100	-3.73686400
H	0.52714900	-3.73491600	-1.18218400
H	-0.83961300	-2.83947500	-2.03603300
C	-1.27767200	0.97938200	-2.85807800
O	-0.51675800	-0.24484100	-2.89989300
C	-0.71297900	1.71844700	-1.63571900
H	0.05870900	2.46857500	-1.85750700
C	0.10637400	-0.34320000	-1.70845800
N	-0.03720500	0.63105100	-0.89017100
C	6.72757600	-0.49025200	-0.90769400
C	6.88220100	0.89257900	-0.94713400
C	5.93773200	1.73445500	-0.35851300
C	4.82213100	1.20725500	0.28428400

C	4.67801200	-0.17416100	0.32140900
C	5.61275800	-1.02122200	-0.26952800
H	7.46618300	-1.14300800	-1.37304400
H	7.74837700	1.32271900	-1.44764200
H	6.06786600	2.81367500	-0.40745200
H	4.07009400	1.85884600	0.73016000
C	5.23787600	-2.46696500	-0.08093400
H	5.27593600	-3.06051800	-1.00430500
H	5.90184600	-2.96614400	0.64034700
C	-1.95959600	3.32046200	-0.01941500
C	-1.91856600	2.32908400	-0.99062500
C	-3.08595000	1.82634500	-1.56712500
C	-4.32319000	2.32951700	-1.18716800
C	-4.37389000	3.32125900	-0.20808500
C	-3.20456100	3.80682500	0.37650300
H	-1.03221200	3.71765900	0.39555000
H	-5.23967400	1.96702100	-1.65477500
H	-5.33682500	3.73190800	0.09246700
H	-3.26242900	4.59209600	1.12816800
C	-2.76831300	0.75361700	-2.57374700
H	-2.90107500	-0.24867600	-2.12905100
H	-1.10298400	1.49267800	-3.80816300
H	-3.38931100	0.79322600	-3.47753900
H	3.60700700	-3.17551500	1.23218300
C	1.51388100	1.23026700	2.68146600
N	2.17452800	1.45767400	3.61957900
Cu	0.88023800	1.01565100	0.94370300
C	1.52976000	2.76037100	0.25818000
N	1.79469900	3.78605600	-0.23958300
C	-3.74466000	-1.03826300	0.40808200
C	-2.65213100	-1.90167900	0.28564900
C	-1.45737900	-1.64785300	0.94270400
C	-1.31277000	-0.51049600	1.75007300

C	-2.40706400	0.36084000	1.86405500
C	-3.59849400	0.09746700	1.21062200
H	-2.75723800	-2.80479600	-0.32011700
H	-0.62960500	-2.34976700	0.84217300
H	-2.30888900	1.25488300	2.48170500
H	-4.43484500	0.78932100	1.31469500
C	-5.05494600	-1.33014500	-0.26203500
C	-0.11555900	-0.27194900	2.56924200
C	-6.13633800	-1.86027500	0.69062000
H	-6.26812100	-1.11348500	1.49321300
C	0.71262400	-1.46171800	2.96269300
H	0.05815800	-2.19554300	3.45904100
H	1.17124500	-1.96263000	2.10140700
H	1.50294600	-1.17288400	3.66069900
H	-0.36633900	0.35955400	3.42129200
H	-5.43112700	-0.41119500	-0.74221600
H	-4.90922000	-2.06926100	-1.06895900
C	-7.45453300	-2.01343000	-0.05352700
H	-7.35449400	-2.74929000	-0.86589300
H	-8.25201200	-2.36551500	0.61362100
H	-7.78222200	-1.06561900	-0.50136900
C	-5.71912100	-3.17904700	1.32479900
H	-5.54289000	-3.93947600	0.54752800
H	-4.79663400	-3.07983600	1.91100200
H	-6.50265800	-3.56318900	1.99081100

10b1

C	-0.56131900	3.81676500	-1.64339800
O	-1.69965600	3.67379000	-0.75825600
C	0.14519200	2.44393600	-1.54245600
H	0.27006100	1.92107600	-2.50048000
C	-1.70412000	2.40654900	-0.30834100
N	-0.74945500	1.65116000	-0.69323100

C	-2.79120800	2.07359400	0.63011400
C	-2.86620900	2.96908200	1.86761400
C	-3.90882100	3.08538600	0.83084900
H	-2.10238500	3.74057800	1.92883700
H	-3.08685000	2.45485000	2.79878800
H	-3.89535200	3.94667400	0.16911400
H	-4.88801800	2.66029100	1.03425200
C	-4.12091000	-1.01621300	1.94474100
O	-4.06992100	0.41704000	1.75747100
C	-3.27201800	-1.53502000	0.76241900
H	-2.49962400	-2.25485300	1.07503600
C	-3.12975100	0.65045900	0.81694000
N	-2.62109300	-0.34807300	0.20862000
C	2.69539800	4.58168500	0.08231900
C	3.67982100	3.68084600	0.47772900
C	3.54957200	2.31907300	0.20556900
C	2.42999300	1.83794500	-0.46554700
C	1.44830100	2.74178900	-0.85368300
C	1.57444900	4.10282100	-0.58567000
H	2.80274400	5.64517900	0.29534200
H	4.56104600	4.04311100	1.00474400
H	4.32610600	1.62279800	0.52099400
H	2.32625900	0.77251400	-0.68400900
C	0.40848000	4.88342600	-1.12923600
H	-0.08307400	5.51571700	-0.37732800
H	0.71621500	5.55171900	-1.94632500
C	-4.05518100	-2.57178500	-1.48361500
C	-4.27755300	-2.11949800	-0.18902200
C	-5.55599100	-2.10526400	0.36429600
C	-6.63798200	-2.57291800	-0.37291100
C	-6.42019800	-3.04428700	-1.66431200
C	-5.13954600	-3.04027200	-2.21870200
H	-3.05554800	-2.53104900	-1.91878400

H	-7.64283400	-2.56520600	0.04936400
H	-7.25998000	-3.41100500	-2.25252300
H	-4.98998600	-3.39703800	-3.23615300
C	-5.54089400	-1.55261600	1.76506600
H	-6.28103500	-0.75807700	1.93011200
H	-3.69033000	-1.21618900	2.93236200
H	-5.74901800	-2.33423200	2.51030600
H	-0.97001100	4.04257100	-2.63370700
C	-0.22101900	0.06581500	1.77902000
N	-0.34895700	0.28111800	2.92180900
Cu	-0.25371900	-0.30680800	-0.11465900
C	-0.04551800	-0.79825300	-1.95349900
N	0.09544000	-1.00698300	-3.09527400
C	4.85341000	-1.33061900	0.08012200
C	4.15161900	-1.83186800	-1.02257400
C	2.79456600	-2.09684800	-0.95062200
C	2.08763900	-1.87021800	0.24225700
C	2.78907200	-1.35806400	1.34626300
C	4.14841600	-1.10384600	1.26573500
H	4.68411300	-1.99947400	-1.95981400
H	2.26533300	-2.44238600	-1.83653300
H	2.24236300	-1.13700700	2.26333600
H	4.67816500	-0.70860100	2.13392200
C	6.32539500	-1.05964900	-0.01811200
C	0.66403400	-2.16836700	0.38543800
C	7.19234400	-2.32665800	0.03605100
H	6.86470400	-2.99010400	-0.78367900
C	0.01775400	-3.26932400	-0.40079700
H	0.27605600	-3.26831600	-1.46207400
H	0.33960300	-4.22686400	0.04267500
H	-1.07589300	-3.22869200	-0.32424900
H	0.34928300	-2.17796400	1.42984400
H	6.63846200	-0.38809700	0.79966400

H	6.53877400	-0.52760500	-0.95918200
C	7.01353600	-3.06597600	1.35394800
H	5.97470200	-3.38303600	1.51084400
H	7.64945700	-3.95994300	1.39516200
H	7.29675600	-2.41822600	2.19851500
C	8.65358800	-1.96484900	-0.18492000
H	9.29196100	-2.85798900	-0.17820000
H	8.80510600	-1.44743000	-1.14172000
H	9.00956400	-1.29800200	0.61502000

TS5b1

C	-0.64210700	3.86336900	-1.63992400
O	-1.76718600	3.69847400	-0.74161600
C	0.07131600	2.48982800	-1.57944100
H	0.17024300	1.98133100	-2.54841400
C	-1.74537600	2.42686600	-0.30249900
N	-0.79263300	1.68460400	-0.71474200
C	-2.79852900	2.06509200	0.66506300
C	-2.82016300	2.91908500	1.93426000
C	-3.90491800	3.06868200	0.94591900
H	-2.05262500	3.68763800	1.98777000
H	-2.99878500	2.37321100	2.85643600
H	-3.91828100	3.95097100	0.31220100
H	-4.87551400	2.63763700	1.17656700
C	-4.04881700	-1.07230000	1.94806800
O	-4.03334000	0.36638500	1.78252900
C	-3.23728400	-1.55301100	0.72428900
H	-2.44483800	-2.27164600	0.98674500
C	-3.12422900	0.63507200	0.82489700
N	-2.62042900	-0.34415200	0.17872900
C	2.65785400	4.60491400	0.01710500
C	3.65766900	3.70074900	0.36328400
C	3.52641100	2.34485100	0.06355800

C	2.39047900	1.87351000	-0.58659600
C	1.39377600	2.78056100	-0.92574300
C	1.52023700	4.13548100	-0.62936400
H	2.76604300	5.66372700	0.25193200
H	4.55172800	4.05580600	0.87330400
H	4.31501300	1.64587600	0.34108700
H	2.28653100	0.81285600	-0.82637300
C	0.33374900	4.92184000	-1.11798300
H	-0.14277700	5.52475500	-0.33296400
H	0.61427900	5.61953800	-1.92016800
C	-4.09066700	-2.54245100	-1.51662500
C	-4.27073300	-2.12552200	-0.20396400
C	-5.52737200	-2.14442200	0.39683100
C	-6.62952400	-2.60861400	-0.31232800
C	-6.45387000	-3.04314800	-1.62300800
C	-5.19483000	-3.00721100	-2.22395700
H	-3.10696000	-2.47739900	-1.98444000
H	-7.61791800	-2.62684800	0.14684400
H	-7.31004500	-3.40677400	-2.18908800
H	-5.07869300	-3.33688500	-3.25489000
C	-5.46501500	-1.62974700	1.81079100
H	-6.21222900	-0.85479500	2.02828700
H	-3.57515800	-1.27780500	2.91402600
H	-5.62778800	-2.43571500	2.54122200
H	-1.06566700	4.11019600	-2.61885700
C	-0.27921200	0.02616800	1.96647800
N	-0.45948900	0.10301600	3.12110800
Cu	-0.32616700	-0.22164300	0.00717700
C	0.02099800	-0.94476300	-1.69944900
N	0.12990400	-1.03380000	-2.86193400
C	4.90297000	-1.31467100	0.04474400
C	4.32679900	-1.82341400	-1.12491700
C	2.97446700	-2.11545600	-1.18895200

C	2.15068700	-1.90469900	-0.07438100
C	2.72121500	-1.38693300	1.09661400
C	4.07886400	-1.10918500	1.15364000
H	4.95452200	-1.97579400	-2.00408200
H	2.54184800	-2.47277600	-2.12201700
H	2.08189000	-1.17727200	1.95501600
H	4.50965200	-0.70872600	2.07247300
C	6.37196100	-1.01292800	0.09514100
C	0.71819900	-2.22678300	-0.08887100
C	7.25740600	-2.26237300	0.21056300
H	7.02623600	-2.91609100	-0.64904500
C	0.21163700	-3.43821200	-0.81772000
H	0.57572400	-3.51978700	-1.84482900
H	0.54907300	-4.32034700	-0.25066900
H	-0.88446000	-3.45560500	-0.84153500
H	0.28031700	-2.16964200	0.91101600
H	6.58899000	-0.35156600	0.95134200
H	6.66392200	-0.45743200	-0.81082600
C	6.96774900	-3.03147400	1.49125400
H	5.92581000	-3.37249100	1.54029100
H	7.61626100	-3.91298200	1.57847600
H	7.15274300	-2.39508600	2.37089700
C	8.72482500	-1.86655500	0.13962000
H	9.37929100	-2.74637800	0.19275000
H	8.95699200	-1.32723900	-0.78854800
H	8.98649300	-1.20854700	0.98210900

10b2

C	-3.06320700	1.36708300	0.31898300
O	-2.41713800	0.66957600	1.41571600
C	-1.86828000	1.80961400	-0.55948500
H	-1.96211700	1.53796600	-1.62035300
C	-1.10920400	0.57419900	1.09518900

N	-0.71245400	1.11276800	0.01455000
C	-0.27223200	-0.11332500	2.09940600
C	-0.67333700	0.13391800	3.56026900
C	-0.92108900	-1.18754800	2.96286900
H	-1.51652700	0.80588400	3.69162000
H	0.14312400	0.24938200	4.26605200
H	-1.93969800	-1.44777500	2.68483600
H	-0.27793800	-2.01841100	3.24678400
C	3.26769400	-0.64701600	2.51737200
O	1.89280300	-0.56799100	2.94174300
C	3.28062100	0.12991900	1.20171700
H	3.50468200	1.20256200	1.28229400
C	1.17953600	-0.21649100	1.85268400
N	1.85289000	0.03313500	0.78647300
C	-2.89401000	5.08596300	0.82916100
C	-1.90659100	5.95702500	0.37756400
C	-0.86232500	5.49734800	-0.42555200
C	-0.78896000	4.15769300	-0.79233500
C	-1.77734500	3.29422200	-0.33606700
C	-2.82089800	3.74521700	0.46902600
H	-3.70695500	5.44948200	1.45801400
H	-1.94766100	7.00864300	0.65748100
H	-0.09192100	6.18819500	-0.76210000
H	0.03152200	3.78836800	-1.40683800
C	-3.76969100	2.62869600	0.81399700
H	-3.99300600	2.55308400	1.88695700
H	-4.73602200	2.74741300	0.30165600
C	4.88889400	-0.17748200	-0.80517300
C	4.25863900	-0.61243700	0.35213300
C	4.51153100	-1.87220700	0.89762400
C	5.38905600	-2.73910100	0.26035900
C	6.01029800	-2.31921700	-0.91544900
C	5.77116300	-1.04911000	-1.44015400

H	4.69029700	0.82147300	-1.19541900
H	5.59907800	-3.72574900	0.67261900
H	6.70522800	-2.98694900	-1.42205700
H	6.28248200	-0.73485500	-2.34804400
C	3.71843800	-2.07425800	2.16399800
H	2.82966700	-2.70407800	1.98923200
H	3.87236700	-0.19715600	3.30958900
H	4.28991600	-2.55254700	2.96905100
H	-3.73325800	0.64021700	-0.15770300
C	0.81519000	1.21720200	-2.76448700
N	0.38481000	1.63536300	-3.76746500
Cu	1.29511400	0.71774100	-1.03384100
C	2.27948800	2.41735500	-0.65386500
N	2.98652800	3.29649800	-0.34245300
C	-3.04144300	-2.24332500	-0.49151200
C	-2.89244100	-1.48424700	-1.65676100
C	-1.63672700	-1.15515300	-2.13978700
C	-0.47391300	-1.56840600	-1.46961000
C	-0.62332800	-2.36342800	-0.32391300
C	-1.88407500	-2.69939400	0.14528700
H	-3.78421200	-1.14335700	-2.18671000
H	-1.53220800	-0.54191600	-3.03632500
H	0.25901900	-2.71999100	0.20874700
H	-1.97976300	-3.32041800	1.03855500
C	-4.39514000	-2.57703100	0.06329600
C	0.82884800	-1.18999300	-2.00800300
C	-4.82080300	-4.03600600	-0.15169700
H	-4.05075900	-4.68150100	0.30680900
C	2.04271400	-2.01182700	-1.69119500
H	2.20266000	-2.17960500	-0.62105900
H	1.92336400	-2.99835600	-2.17102000
H	2.95389800	-1.55998700	-2.09902600
H	0.76987700	-0.97637600	-3.07343100

H	-5.15707000	-1.92241300	-0.39384700
H	-4.40872900	-2.35696000	1.14479700
C	-6.14998400	-4.29793200	0.54063900
H	-6.46312700	-5.34345100	0.42284200
H	-6.10034100	-4.07834400	1.61571100
H	-6.93996700	-3.66587500	0.10753700
C	-4.90782800	-4.37095800	-1.63359000
H	-5.64291800	-3.71919100	-2.13137300
H	-3.94491200	-4.23707600	-2.14278500
H	-5.22968800	-5.40922400	-1.78676100

TS5b2

C	-2.51104800	-2.78866900	-0.19838300
O	-1.60482900	-2.56898500	0.91396000
C	-2.68260400	-1.36830200	-0.78368900
H	-2.55092800	-1.30059700	-1.87269700
C	-1.15874900	-1.30022600	0.80487500
N	-1.64481400	-0.57365300	-0.11954600
C	-0.16816100	-0.89723500	1.82068200
C	-0.34910400	-1.53339000	3.20333700
C	0.77563200	-1.96760800	2.35981500
H	-1.21041300	-2.18881000	3.29557000
H	-0.14977900	-0.88636500	4.05198100
H	0.71832900	-2.93293300	1.86197300
H	1.77747900	-1.62220400	2.60798600
C	1.48870300	2.16973800	2.70025300
O	0.98850800	0.84047400	2.93492400
C	0.62123700	2.68259400	1.54902800
H	-0.29100000	3.22356800	1.83558900
C	0.32727200	0.49298700	1.81092200
N	0.18545500	1.40698600	0.92076300
C	-5.98348200	-1.80695300	0.83302900
C	-6.57802600	-0.55445200	0.70866800

C	-5.91348100	0.49135100	0.06673300
C	-4.64165400	0.30191900	-0.46426600
C	-4.05680700	-0.95202100	-0.33707800
C	-4.71188800	-1.99973800	0.30602000
H	-6.50570500	-2.61943000	1.33846200
H	-7.57211400	-0.38758400	1.12074300
H	-6.38920400	1.46670200	-0.01424000
H	-4.10797100	1.11552900	-0.95576200
C	-3.87888500	-3.25365600	0.29725400
H	-3.79388800	-3.73800400	1.27946100
H	-4.29168900	-4.00747200	-0.38955100
C	1.25387900	4.47987700	-0.21171700
C	1.56182300	3.50802400	0.73087900
C	2.88350700	3.20357900	1.06594200
C	3.92913900	3.84468500	0.41439000
C	3.62867500	4.80352600	-0.55297900
C	2.30635900	5.12815900	-0.85481900
H	0.21133200	4.70979700	-0.43653400
H	4.96577300	3.61985800	0.66460600
H	4.43906300	5.31943900	-1.06552500
H	2.09494800	5.89553700	-1.59712300
C	2.93240500	2.17578100	2.16718400
H	3.17382400	1.17109500	1.78110700
H	1.37655700	2.72634800	3.63467100
H	3.67309100	2.40420200	2.94362900
H	-2.01545300	-3.50458400	-0.86603100
C	-1.53022400	1.17533600	-2.57443800
N	-2.24388100	1.01767000	-3.48821600
Cu	-0.85660700	1.39340500	-0.84799000
C	-1.96443300	2.93249200	-0.25239700
N	-2.41711900	3.91498200	0.19542300
C	2.51462600	-2.63821000	-0.36952100
C	1.39550700	-2.82065600	-1.18765400

C	0.78245500	-1.74296000	-1.80702000
C	1.25250700	-0.43393200	-1.62073400
C	2.36399200	-0.24868900	-0.78360600
C	2.98500600	-1.33479300	-0.18376500
H	1.01565100	-3.83080100	-1.35155300
H	-0.07794100	-1.90070200	-2.46052400
H	2.76214500	0.75404900	-0.62504000
H	3.86419000	-1.17426200	0.44494500
C	3.22561000	-3.80014900	0.26069600
C	0.64437100	0.66073900	-2.38543500
C	4.51469900	-4.20917800	-0.46787700
H	5.17266200	-3.32276900	-0.50206800
C	1.38773100	1.94996800	-2.57250300
H	1.73273000	2.39494600	-1.63406700
H	2.27681600	1.75846200	-3.19577000
H	0.76599600	2.69041100	-3.08752200
H	0.24739400	0.28258100	-3.32533600
H	3.48013900	-3.55695800	1.30598300
H	2.55470700	-4.67564200	0.29876400
C	4.23161400	-4.65267900	-1.89554900
H	3.54804500	-5.51631700	-1.90080000
H	3.76810600	-3.85571000	-2.49067400
H	5.15484900	-4.95972200	-2.40379800
C	5.22106300	-5.31089900	0.30823900
H	6.16219500	-5.60086300	-0.17665200
H	5.45156500	-5.00234300	1.33684600
H	4.58762400	-6.20916200	0.36352300

10b3

C	-2.38521400	-2.96154600	-0.33607000
O	-1.47341600	-2.73278700	0.76885500
C	-2.63747500	-1.53195200	-0.87618800
H	-2.49315900	-1.42203900	-1.96158200

C	-1.11376800	-1.43336900	0.71263300
N	-1.65397900	-0.70165500	-0.17593100
C	-0.13620600	-1.01244200	1.73499000
C	-0.27268300	-1.69318900	3.10178400
C	0.86371200	-2.04977500	2.23794800
H	-1.10140100	-2.39106100	3.18166700
H	-0.09949800	-1.06025800	3.96671200
H	0.84697900	-3.00282400	1.71481900
H	1.85097200	-1.66386900	2.48429700
C	1.39042100	2.10815100	2.68868500
O	0.97965000	0.73887700	2.87075500
C	0.47574500	2.61134200	1.56904400
H	-0.45133200	3.10303300	1.89573600
C	0.29416500	0.39812600	1.76230700
N	0.07793100	1.33980900	0.91639600
C	-5.91153300	-2.21125800	0.71492700
C	-6.58544900	-0.99810000	0.60887800
C	-5.99018600	0.09683200	-0.01825100
C	-4.70906700	-0.00273800	-0.55045900
C	-4.04118700	-1.21567000	-0.43655900
C	-4.62896000	-2.31320200	0.18860000
H	-6.38045800	-3.06377000	1.20647100
H	-7.58786300	-0.90157300	1.02316500
H	-6.52576700	1.04161100	-0.08446700
H	-4.23379600	0.85197300	-1.03091100
C	-3.72017200	-3.51253500	0.16252500
H	-3.59797300	-3.99833300	1.14008600
H	-4.09141700	-4.28533200	-0.52680900
C	0.98071900	4.43064500	-0.20622600
C	1.35690600	3.48818700	0.74034900
C	2.69806000	3.26368200	1.05847200
C	3.69405300	3.96812100	0.39433700
C	3.32478700	4.90428400	-0.57139300

C	1.98231800	5.14245000	-0.86343400
H	-0.07404200	4.60138200	-0.42517000
H	4.74540200	3.80743800	0.63191600
H	4.09599800	5.46846900	-1.09313100
H	1.71530500	5.88853600	-1.60928200
C	2.82653800	2.23413300	2.15181800
H	3.14695600	1.25583300	1.75746400
H	1.24714000	2.61378300	3.64737400
H	3.54682900	2.51568700	2.93007300
H	-1.86652500	-3.63240000	-1.03225100
C	-1.90091100	1.65414800	-2.38932000
N	-2.53271300	1.75562400	-3.36656900
Cu	-1.01568300	1.38354000	-0.76602500
C	-2.35428400	2.47023000	0.22869300
N	-3.00974900	3.16505600	0.90395000
C	2.90366200	-2.33651200	-0.35692900
C	1.74346600	-2.65487300	-1.06749600
C	0.95717900	-1.66082300	-1.62882300
C	1.29093000	-0.30305600	-1.50233700
C	2.46076300	0.01302900	-0.79076500
C	3.24859600	-0.98597500	-0.23777800
H	1.46107000	-3.70326100	-1.18443800
H	0.06444800	-1.92768000	-2.19693200
H	2.75979400	1.05676500	-0.68226100
H	4.16077400	-0.71876200	0.30126500
C	3.77804100	-3.40131400	0.23787000
C	0.47033500	0.70492500	-2.17688100
C	5.04762600	-3.69232200	-0.57604100
H	5.60487200	-2.74385800	-0.67447400
C	1.14660600	1.95883300	-2.65987200
H	1.60936300	2.54189800	-1.85441500
H	1.95126300	1.68521800	-3.36301200
H	0.44031000	2.61039500	-3.18419400

H	-0.15303900	0.24397400	-2.94484200
H	4.07691400	-3.10684300	1.25795600
H	3.20761800	-4.34071400	0.34021200
C	4.70969400	-4.19776700	-1.97088000
H	4.12045900	-5.12637000	-1.90995000
H	4.12425200	-3.46724600	-2.54338700
H	5.62043900	-4.42170700	-2.54127600
C	5.92009800	-4.69546800	0.16391300
H	6.84845300	-4.89934500	-0.38519700
H	6.19155800	-4.33890100	1.16669300
H	5.38967300	-5.65245500	0.28256000

TS5b3

C	2.83293200	2.67060200	-0.45938500
O	1.87986700	2.64018500	0.63427900
C	2.92984100	1.18276800	-0.87264600
H	2.79976300	0.99563100	-1.94831900
C	1.37868500	1.38818300	0.68012100
N	1.84576500	0.52740500	-0.13288900
C	0.35519600	1.16494900	1.71708600
C	0.56147000	1.92600800	3.02861100
C	-0.52105300	2.34623900	2.12308900
H	1.46327400	2.53034000	3.07005700
H	0.30880900	1.38605300	3.93594800
H	-0.39272500	3.25097400	1.53410100
H	-1.54697800	2.09507800	2.38578400
C	-1.62734700	-1.61878500	2.83026900
O	-0.96103600	-0.35046100	2.96398800
C	-0.87425100	-2.30493900	1.68236600
H	-0.07700000	-2.99968900	1.98047300
C	-0.26225100	-0.17123400	1.82435400
N	-0.22125500	-1.15778600	1.00707400
C	6.23144200	1.61942400	0.74395000

C	6.76244700	0.33292600	0.75712100
C	6.05308100	-0.73812400	0.21223900
C	4.79884100	-0.54110900	-0.35634300
C	4.27688500	0.74679700	-0.36572900
C	4.97753800	1.82045700	0.17885500
H	6.78878000	2.45244200	1.17252500
H	7.74196000	0.15970200	1.20023800
H	6.48054300	-1.73856700	0.23620500
H	4.23326000	-1.37139200	-0.77908700
C	4.21326700	3.10829900	0.02844900
H	4.13078600	3.68694600	0.95849100
H	4.68279800	3.77202500	-0.71260900
C	-1.81835200	-3.93099600	-0.10360500
C	-1.95374500	-2.95824400	0.87719200
C	-3.20722300	-2.47276100	1.25385100
C	-4.35219800	-2.93442700	0.61765700
C	-4.22235900	-3.89061900	-0.38919700
C	-2.96947700	-4.39185000	-0.74145400
H	-0.83077700	-4.32301100	-0.35199100
H	-5.33714300	-2.56603400	0.90492500
H	-5.11200100	-4.26453600	-0.89330900
H	-2.89060900	-5.15581100	-1.51291200
C	-3.08315600	-1.46050600	2.36037900
H	-3.22649100	-0.43279600	1.98449200
H	-1.54165600	-2.12938700	3.79332500
H	-3.80959100	-1.60947700	3.16928500
H	2.40842400	3.33508200	-1.22210200
C	1.82261300	-1.56336000	-2.32086300
N	2.63074400	-1.63637400	-3.16392800
Cu	0.95577600	-1.45794600	-0.67204700
C	1.80502600	-3.02917800	0.19556900
N	2.08697600	-4.00020500	0.78547700
C	-2.72430600	2.13808200	-0.48151200

C	-1.51614300	2.51423600	-1.07573200
C	-0.71078000	1.57819700	-1.70540100
C	-1.07337400	0.22356600	-1.75609800
C	-2.29147900	-0.15198500	-1.16782700
C	-3.09774500	0.79136500	-0.55064500
H	-1.21191800	3.56280500	-1.05041700
H	0.21929300	1.89080700	-2.18310900
H	-2.61077400	-1.19381800	-1.19335700
H	-4.04972200	0.47819800	-0.11472200
C	-3.62567700	3.14223500	0.17549300
C	-0.23552100	-0.72167400	-2.50226600
C	-4.83647000	3.54563400	-0.67902400
H	-5.39510200	2.62430200	-0.92113700
C	-0.86431700	-1.97206300	-3.04883800
H	-1.20151500	-2.65798300	-2.26168100
H	-1.74972300	-1.70159300	-3.64626900
H	-0.15948600	-2.51285000	-3.68631500
H	0.37931200	-0.19411500	-3.23104600
H	-3.99435300	2.73521500	1.13253600
H	-3.05572700	4.05444300	0.42340400
C	-4.40313800	4.20096000	-1.98208300
H	-3.81025900	5.10645400	-1.77768600
H	-3.78872600	3.53032500	-2.59602400
H	-5.27253600	4.50381200	-2.57986400
C	-5.74572600	4.47249600	0.11423400
H	-6.63433700	4.75322700	-0.46581700
H	-6.08541800	4.00847500	1.05001100
H	-5.21524200	5.40067400	0.37563200

10b4

C	4.62477500	-0.95375500	-1.85519200
O	4.53021200	0.45565400	-1.54847500
C	3.46062600	-1.54525700	-1.03115100

H	2.84965000	-2.26037000	-1.60059600
C	3.34145700	0.64138900	-0.92843000
N	2.64259300	-0.38941500	-0.65408000
C	2.99686800	2.05570700	-0.68356200
C	4.09568800	3.09636200	-0.86096000
C	3.06409300	2.97884200	-1.90467200
H	5.08601500	2.69793400	-1.05993700
H	4.05276000	3.94352900	-0.18262900
H	3.30857600	2.48449700	-2.84151000
H	2.27458100	3.72359300	-1.96846900
C	0.57567400	3.79087300	1.31025200
O	1.84029800	3.66794800	0.62706500
C	0.25835200	2.35126500	1.75086300
H	0.55583800	2.09799400	2.77893300
C	1.93820000	2.36610800	0.29086800
N	1.09932300	1.56304200	0.83045400
C	6.34677000	-2.65064100	1.00979100
C	5.76068600	-3.16645000	2.16205500
C	4.37392800	-3.17189300	2.31423200
C	3.54900100	-2.67040500	1.31202300
C	4.14104000	-2.17059300	0.15822500
C	5.52645300	-2.14792300	0.00677700
H	7.43120400	-2.63434100	0.90058200
H	6.39176200	-3.55955400	2.95773000
H	3.93046600	-3.56055500	3.22901800
H	2.46696200	-2.63809400	1.44742900
C	5.92336700	-1.54559200	-1.31388700
H	6.70031900	-0.77381500	-1.23097900
H	6.30895900	-2.30725000	-2.00789700
C	-2.08543900	1.25416100	2.02153100
C	-1.21966600	2.22214500	1.52726500
C	-1.68733500	3.28760300	0.75690500
C	-3.03991100	3.39526300	0.46322200

C	-3.91380100	2.43153300	0.96147400
C	-3.44273700	1.37313300	1.73614300
H	-1.70666700	0.42072700	2.61381100
H	-3.41325200	4.22403600	-0.13764700
H	-4.97964900	2.50733700	0.74602400
H	-4.14023400	0.62922600	2.11854800
C	-0.55780400	4.19411500	0.35343500
H	-0.24795300	3.98081000	-0.68315300
H	0.72108600	4.49753300	2.13200900
H	-0.80504200	5.26160500	0.40866100
H	4.51453800	-1.05191200	-2.94203100
C	0.02310600	0.93118900	-1.70545700
N	-0.09653900	1.68836900	-2.58976400
Cu	0.31959300	-0.15078500	-0.12844700
C	0.21432000	-1.20012300	1.47318700
N	0.14252200	-1.79279800	2.47919200
C	-4.90979300	-1.03935400	-0.17006500
C	-4.28530600	-0.35483100	-1.21587500
C	-2.94221600	-0.54621800	-1.48935700
C	-2.17703400	-1.44880200	-0.73190200
C	-2.80042100	-2.12693700	0.32907800
C	-4.14443600	-1.92828600	0.59334900
H	-4.86439000	0.35274300	-1.81090400
H	-2.45674500	0.02156400	-2.28348400
H	-2.21918100	-2.79294400	0.96376500
H	-4.61488100	-2.45699500	1.42415100
C	-6.36315300	-0.83455600	0.13897000
C	-0.78889700	-1.68981700	-1.10789900
C	-7.26507000	-1.98869900	-0.32295100
H	-6.89589800	-2.91290300	0.15556200
C	-0.12405400	-3.00060500	-0.81587500
H	-0.27895200	-3.35925800	0.20439200
H	-0.53087800	-3.74623500	-1.51995000

H	0.95687700	-2.94573700	-0.99005700
H	-0.56269000	-1.33284800	-2.11332800
H	-6.49282200	-0.70214300	1.22635000
H	-6.71866300	0.09664000	-0.33413600
C	-7.20134500	-2.17028900	-1.83244000
H	-7.52910700	-1.25127300	-2.34338700
H	-6.18435000	-2.39774100	-2.17630100
H	-7.86014000	-2.98464900	-2.16122900
C	-8.69637600	-1.74351300	0.13097400
H	-9.35677800	-2.56906300	-0.16497200
H	-8.76437600	-1.62976100	1.22126400
H	-9.09215900	-0.82364300	-0.32567800

TS5b4

C	4.64489700	-1.03004800	-1.78048200
O	4.55127900	0.38678700	-1.50218600
C	3.47145900	-1.60118500	-0.95541900
H	2.87506000	-2.35190400	-1.49257400
C	3.35028800	0.59163600	-0.91641000
N	2.63794600	-0.43323100	-0.64730100
C	3.01015900	2.00992300	-0.68956000
C	4.11401600	3.04415700	-0.87709900
C	3.08053600	2.91984600	-1.91850700
H	5.10378600	2.64243600	-1.07213500
H	4.07188100	3.89740400	-0.20621200
H	3.32819200	2.41763600	-2.85063400
H	2.29320600	3.66597700	-1.98870300
C	0.59908500	3.75831500	1.31668400
O	1.82668200	3.64522200	0.56825300
C	0.33756800	2.31971000	1.80341000
H	0.66014000	2.11760200	2.83524500
C	1.96377600	2.33025100	0.29702600
N	1.18110300	1.51865600	0.90129700

C	6.34011600	-2.60138400	1.16512800
C	5.74240100	-3.08146400	2.32680600
C	4.35350000	-3.10141200	2.45680700
C	3.53650000	-2.64354200	1.42729900
C	4.14137700	-2.16966200	0.26927700
C	5.52862800	-2.14322700	0.13418800
H	7.42570900	-2.58122000	1.06840300
H	6.36581500	-3.44085500	3.14426400
H	3.90046600	-3.47294000	3.37407000
H	2.45062800	-2.63934700	1.53470600
C	5.93740300	-1.60320800	-1.20914400
H	6.71914100	-0.83344900	-1.15971800
H	6.31931800	-2.39892000	-1.86622500
C	-1.94937300	1.12465900	2.12776900
C	-1.14021200	2.13495400	1.62168400
C	-1.67489200	3.18908700	0.88004200
C	-3.04305500	3.25680100	0.65067400
C	-3.86162200	2.25966700	1.17551200
C	-3.32080900	1.20090100	1.90346000
H	-1.51762000	0.29058600	2.68127300
H	-3.46990200	4.08106700	0.07964200
H	-4.93878000	2.30347700	1.01283000
H	-3.97486000	0.42375000	2.29648600
C	-0.59434400	4.12949100	0.42283000
H	-0.33423400	3.92690600	-0.62988400
H	0.77752400	4.48185200	2.11736900
H	-0.86960400	5.18923100	0.49610700
H	4.54808900	-1.14956400	-2.86682300
C	-0.01350200	0.83328600	-1.62471500
N	-0.05810100	1.78327600	-2.31037400
Cu	0.39950100	-0.22910600	-0.09212100
C	0.12306900	-1.56734700	1.30021600
N	-0.06169000	-2.40821500	2.09416500

C	-4.92963800	-0.96303000	-0.16509200
C	-4.50547600	-0.05070000	-1.13358500
C	-3.20885900	-0.08329900	-1.61704500
C	-2.29441000	-1.03850500	-1.15053500
C	-2.71341300	-1.95242100	-0.17197100
C	-4.01443400	-1.91311400	0.30067700
H	-5.20441500	0.70235100	-1.50071000
H	-2.87886900	0.64973900	-2.35427600
H	-2.00989700	-2.67023100	0.24384300
H	-4.32668200	-2.62205700	1.06895300
C	-6.32917600	-0.93411800	0.37450600
C	-0.97732100	-1.09648100	-1.78438400
C	-7.22889100	-2.05347500	-0.16924000
H	-6.74146100	-3.01631200	0.06441500
C	-0.16131600	-2.35535800	-1.83587900
H	-0.04132600	-2.85787300	-0.87227000
H	-0.67260800	-3.04082900	-2.53315800
H	0.82994100	-2.14849300	-2.25540800
H	-1.00200300	-0.63140500	-2.76885400
H	-6.29919900	-1.01140200	1.47419300
H	-6.80106900	0.03606400	0.14177700
C	-7.38942900	-1.94920500	-1.67884200
H	-7.84205000	-0.98234900	-1.95010400
H	-6.42683900	-2.02474000	-2.20050100
H	-8.04571800	-2.74107100	-2.06295600
C	-8.58395600	-2.01328900	0.52135400
H	-9.23757700	-2.82111400	0.16714400
H	-8.48860800	-2.10841100	1.61131500
H	-9.09350200	-1.06023700	0.31292400

10b5

C	-3.06387800	1.36689600	0.31894200
O	-2.41762700	0.66943700	1.41565800

C	-1.86909400	1.80923000	-0.55978800
H	-1.96323000	1.53767900	-1.62064700
C	-1.10976000	0.57399600	1.09485700
N	-0.71323900	1.11227300	0.01399200
C	-0.27259000	-0.11335600	2.09902300
C	-0.67397100	0.13317400	3.55991700
C	-0.92111300	-1.18818400	2.96204400
H	-1.51745700	0.80473200	3.69142400
H	0.14235300	0.24879400	4.26582900
H	-1.93959600	-1.44862700	2.68378200
H	-0.27767500	-2.01891700	3.24571700
C	3.26747000	-0.64566700	2.51735600
O	1.89258700	-0.56665400	2.94167600
C	3.28028700	0.13062100	1.20134600
H	3.50406600	1.20336400	1.28144200
C	1.17924500	-0.21593000	1.85242500
N	1.85257600	0.03326500	0.78609000
C	-2.89377700	5.08565300	0.82950100
C	-1.90631100	5.95657300	0.37771200
C	-0.86246600	5.49680500	-0.42589300
C	-0.78953200	4.15719500	-0.79292100
C	-1.77787600	3.29384700	-0.33636300
C	-2.82108500	3.74495500	0.46912100
H	-3.70642900	5.44922800	1.45870100
H	-1.94701000	7.00814300	0.65785700
H	-0.09200600	6.18751200	-0.76260000
H	0.03065200	3.78780900	-1.40778200
C	-3.77012800	2.62859100	0.81396900
H	-3.99382900	2.55299300	1.88683700
H	-4.73626600	2.74754800	0.30128800
C	4.88874700	-0.17734200	-0.80526800
C	4.25849400	-0.61190800	0.35217600
C	4.51159100	-1.87139700	0.89823800

C	5.38930800	-2.73839600	0.26139200
C	6.01055600	-2.31889600	-0.91455900
C	5.77123500	-1.04906000	-1.43982300
H	4.69004900	0.82139800	-1.19600100
H	5.59948200	-3.72483400	0.67407500
H	6.70563300	-2.98672500	-1.42083500
H	6.28255700	-0.73509600	-2.34780900
C	3.71844100	-2.07300600	2.16465700
H	2.82976200	-2.70302400	1.99008800
H	3.87204500	-0.19529400	3.30935900
H	4.28992900	-2.55086100	2.96995400
H	-3.73408800	0.64002500	-0.15752800
C	0.81635400	1.21780300	-2.76496600
N	0.38681100	1.63597200	-3.76829200
Cu	1.29500000	0.71738800	-1.03428900
C	2.27697600	2.41813000	-0.65290400
N	2.98211900	3.29848900	-0.34064400
C	-3.04062900	-2.24374700	-0.49152000
C	-2.89155000	-1.48443200	-1.65660400
C	-1.63581100	-1.15528100	-2.13952000
C	-0.47303900	-1.56865900	-1.46936200
C	-0.62251800	-2.36399100	-0.32391300
C	-1.88329300	-2.70007100	0.14515100
H	-3.78327600	-1.14334500	-2.18650000
H	-1.53126000	-0.54193000	-3.03597900
H	0.25982700	-2.72061500	0.20873500
H	-1.97898200	-3.32123500	1.03831700
C	-4.39437100	-2.57734800	0.06325500
C	0.82982800	-1.19008400	-2.00750600
C	-4.81996500	-4.03636300	-0.15157300
H	-4.05007600	-4.68185300	0.30716000
C	2.04336800	-2.01243200	-1.69064500
H	2.20327600	-2.18000400	-0.62046800

H	1.92350800	-2.99905700	-2.17013700
H	2.95473400	-1.56113600	-2.09865100
H	0.77098400	-0.97652600	-3.07297000
H	-4.40811800	-2.35699800	1.14470000
H	-5.15624800	-1.92289300	-0.39417300
C	-4.90662400	-4.37151100	-1.63345800
H	-5.64172400	-3.71996400	-2.13148400
H	-3.94362400	-4.23745100	-2.14243100
H	-5.22821900	-5.40985100	-1.78659000
C	-6.14932000	-4.29823000	0.54045400
H	-6.46243600	-5.34374700	0.42262100
H	-6.09987600	-4.07863200	1.61552000
H	-6.93917400	-3.66617300	0.10716000

TS5b5

C	-3.06338300	1.54052100	0.27683600
O	-2.45222600	0.85497700	1.40135600
C	-1.84025100	1.94858500	-0.57467600
H	-1.92909500	1.70803200	-1.64290900
C	-1.15151400	0.68159900	1.08628200
N	-0.72435500	1.19145100	0.00200700
C	-0.36188200	-0.05606300	2.09140800
C	-0.80409900	0.13418700	3.54636000
C	-1.06243700	-1.15428700	2.88410400
H	-1.63634800	0.81841200	3.68353500
H	-0.00773200	0.19779700	4.28111300
H	-2.07628300	-1.38184100	2.56291200
H	-0.44400100	-2.01052600	3.14755300
C	3.13644000	-0.74689600	2.56631900
O	1.76685900	-0.58508000	2.97940300
C	3.21462500	0.04915600	1.26382100
H	3.49754000	1.10619100	1.36150500
C	1.09157300	-0.19873100	1.87659400

N	1.79046200	0.03263100	0.82401700
C	-2.77934600	5.23982800	0.83705500
C	-1.73716300	6.07479100	0.44377200
C	-0.67963500	5.58428400	-0.32304100
C	-0.64700600	4.24903300	-0.71210700
C	-1.69183800	3.42298300	-0.31644700
C	-2.74880900	3.90425600	0.45313200
H	-3.60124900	5.62709200	1.43948300
H	-1.74509900	7.12210000	0.74209200
H	0.13256200	6.24761400	-0.61363300
H	0.18313700	3.85354800	-1.29741300
C	-3.75632600	2.82159100	0.73517500
H	-4.04972400	2.75133300	1.79137600
H	-4.68296900	2.97353700	0.16175500
C	4.86570800	-0.31787500	-0.70162900
C	4.16704500	-0.73665200	0.42197100
C	4.31820100	-2.02375200	0.94256800
C	5.15212300	-2.93504100	0.30904300
C	5.83696500	-2.53141100	-0.83663900
C	5.70515600	-1.23402600	-1.33175400
H	4.74648700	0.70238300	-1.06883900
H	5.28146700	-3.94295400	0.70283200
H	6.49909200	-3.23372400	-1.34059600
H	6.26797100	-0.93356500	-2.21366400
C	3.48364600	-2.19601800	2.18557700
H	2.55130700	-2.74705300	1.97431600
H	3.76464700	-0.35753200	3.37218400
H	3.99668800	-2.73911100	2.98891300
H	-3.73240400	0.81359100	-0.20251600
C	0.68773800	1.21530000	-2.73792500
N	0.21230200	1.72655000	-3.67688200
Cu	1.26123200	0.81285800	-1.01014100
C	2.46962100	2.36875000	-0.71700300

N	3.31456600	3.13346500	-0.44875500
C	-2.93570000	-2.36092400	-0.43408900
C	-2.92922500	-1.51846900	-1.55063400
C	-1.73957000	-1.08870100	-2.11462500
C	-0.50367600	-1.47009600	-1.56981500
C	-0.50790700	-2.32778000	-0.46145100
C	-1.70423900	-2.77308000	0.08216200
H	-3.88047300	-1.20660500	-1.98633500
H	-1.74624000	-0.42762200	-2.98264100
H	0.43601600	-2.65664200	-0.02625900
H	-1.68888900	-3.45057900	0.93869600
C	-4.21820400	-2.84161500	0.17887800
C	0.72538700	-1.01288000	-2.21915000
C	-4.58397900	-4.28605400	-0.19358800
H	-3.74190100	-4.93240000	0.11158400
C	2.02842600	-1.72486500	-2.00748900
H	2.28596600	-1.89898800	-0.95768700
H	1.96691400	-2.70522300	-2.50951500
H	2.85714300	-1.17535600	-2.46829900
H	0.55903800	-0.83894100	-3.28003300
H	-4.15242600	-2.76906200	1.27747600
H	-5.04846500	-2.18172800	-0.12565400
C	-4.78681900	-4.43808500	-1.69393800
H	-5.59902900	-3.77961100	-2.03995400
H	-3.88315700	-4.17977000	-2.26045900
H	-5.06432000	-5.46814200	-1.95274900
C	-5.82973200	-4.71868400	0.56530800
H	-6.09628900	-5.75864300	0.33634600
H	-5.69508300	-4.63528000	1.65220000
H	-6.68791500	-4.08872900	0.28641400

10b6

C	-4.83528300	1.17564400	-0.21430500
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O	-3.98753400	2.12592600	-0.89218400
C	-3.93198500	0.61457400	0.89967900
H	-4.05907800	1.08199000	1.88686600
C	-2.72651300	1.77666600	-0.56132200
N	-2.58527600	0.94699800	0.40255900
C	-1.67383600	2.38547100	-1.38889000
C	-1.97166700	2.46715500	-2.88871300
C	-2.01572800	3.69896800	-2.08354500
H	-2.90090700	2.00069100	-3.20538000
H	-1.11730700	2.28766700	-3.53591100
H	-2.98547100	4.12106200	-1.83486500
H	-1.19743900	4.40801600	-2.16831000
C	1.93911300	2.41778000	-1.37580700
O	0.62158400	2.92809700	-1.68562700
C	1.65299200	1.45106600	-0.20790400
H	2.15069300	0.47857700	-0.31284900
C	-0.26291500	2.13902100	-1.03236700
N	0.19867600	1.26002800	-0.23237600
C	-5.31626300	-2.53514400	-0.44117400
C	-4.96744200	-3.48912300	0.51225700
C	-4.25312100	-3.12837800	1.65517500
C	-3.87347700	-1.80365500	1.86107300
C	-4.22578100	-0.85769500	0.90569600
C	-4.94393800	-1.21326500	-0.23564900
H	-5.87555600	-2.82223400	-1.33094600
H	-5.26105500	-4.52755500	0.36617500
H	-3.99673600	-3.88478800	2.39520100
H	-3.30724800	-1.51312100	2.74586400
C	-5.18618500	-0.01989300	-1.11675700
H	-4.49834600	-0.03788200	-1.97821700
H	-6.20735200	0.03191700	-1.51497600
C	1.93428200	1.86769500	2.34363300
C	2.11757700	2.20691200	1.00851200

C	2.76760600	3.38539600	0.64532800
C	3.25894300	4.24300000	1.62265300
C	3.08576600	3.90569400	2.96191100
C	2.42594600	2.72963800	3.31944900
H	1.38643000	0.96624400	2.62084300
H	3.76550100	5.16792300	1.34628700
H	3.46129800	4.57089900	3.73813300
H	2.28364100	2.48662900	4.37090300
C	2.84515700	3.52829700	-0.85086600
H	2.51610300	4.50944400	-1.21896000
H	2.31480700	1.93305900	-2.28569900
H	3.87210000	3.38288800	-1.21823800
H	-5.71214000	1.72373600	0.14124700
C	-1.51170700	-0.96173000	-1.43823200
N	-1.82651600	-1.02374900	-2.56348800
Cu	-1.09004600	-0.60668400	0.40646000
C	-0.78861500	-0.54005800	2.29922300
N	-0.59720200	-0.51571000	3.45304900
C	3.87837700	-1.60345400	-0.49412500
C	2.95668700	-1.92387600	-1.49976200
C	1.63452800	-2.20634000	-1.20027500
C	1.18896900	-2.18797500	0.13202700
C	2.10692100	-1.84456300	1.13895800
C	3.42864800	-1.56563800	0.82926800
H	3.29011200	-1.94067900	-2.53866000
H	0.92844600	-2.41716900	-2.00197700
H	1.75794700	-1.78342300	2.17064100
H	4.12753400	-1.30149800	1.62392300
C	5.31192300	-1.33171000	-0.84238500
C	-0.17515400	-2.54186000	0.51243200
C	6.11916700	-2.59955800	-1.16072600
H	5.61030800	-3.12017600	-1.99115500
C	-0.97566600	-3.54529000	-0.25726800

H	-0.90688700	-3.43606900	-1.34191400
H	-0.59973900	-4.54427500	0.02366900
H	-2.03566400	-3.50251700	0.02221900
H	-0.28449100	-2.68002900	1.58816800
H	5.80693800	-0.80276200	-0.01111000
H	5.35888400	-0.65951700	-1.71463300
C	6.17245100	-3.53867500	0.03542300
H	5.17279500	-3.86897800	0.34521700
H	6.76831500	-4.43260900	-0.19029100
H	6.64064800	-3.03656100	0.89661500
C	7.52224400	-2.22017500	-1.61077700
H	8.11224700	-3.10858500	-1.87100100
H	7.50447000	-1.55739400	-2.48643600
H	8.05525200	-1.69375400	-0.80459200

TS5b6

C	-4.76792200	1.06067000	-0.63967700
O	-3.87407600	1.93912000	-1.35180500
C	-3.98121400	0.70589700	0.63539200
H	-4.22662800	1.31701100	1.51618500
C	-2.65079800	1.68853100	-0.83846500
N	-2.59088700	1.00342500	0.24197500
C	-1.53155400	2.22636200	-1.62998000
C	-1.67437300	2.11701000	-3.15116200
C	-1.82752700	3.43423700	-2.51184800
H	-2.55205500	1.57751500	-3.49667000
H	-0.75380800	1.89014100	-3.68261500
H	-2.82719500	3.84829400	-2.41297400
H	-1.02180800	4.15706200	-2.60138000
C	2.05855200	2.39183400	-1.25518600
O	0.76490200	2.84369200	-1.71926800
C	1.68242400	1.49434900	-0.05961000
H	2.22215000	0.53928900	-0.04261100

C	-0.15909800	2.06205200	-1.11677400
N	0.24730600	1.24305600	-0.22535800
C	-5.19435900	-2.64416100	-0.32935900
C	-4.97871800	-3.42036500	0.80738400
C	-4.41541800	-2.86379000	1.95607400
C	-4.04754000	-1.51983200	1.98001500
C	-4.26486900	-0.75240800	0.84253000
C	-4.84270500	-1.30112500	-0.30271800
H	-5.64072700	-3.08240100	-1.22128000
H	-5.26207900	-4.47186900	0.80194600
H	-4.26721600	-3.48114600	2.84084400
H	-3.59536700	-1.07778200	2.86739500
C	-4.98554900	-0.26755800	-1.38429900
H	-4.19214100	-0.39904200	-2.13902900
H	-5.94953900	-0.31106700	-1.90651300
C	1.65410400	2.10564900	2.46798100
C	1.98431200	2.35149700	1.14099700
C	2.64207200	3.52166500	0.76530700
C	2.99627500	4.46337000	1.72425400
C	2.67831300	4.21837000	3.05701900
C	2.00924600	3.05098300	3.42554700
H	1.09916100	1.20914900	2.74722300
H	3.50769000	5.38247400	1.43784300
H	2.94581700	4.94974800	3.81825400
H	1.75255100	2.88122200	4.46969000
C	2.88249600	3.55932700	-0.71999600
H	2.57969700	4.50317200	-1.19295300
H	2.53054300	1.86079200	-2.09177100
H	3.94573800	3.41247500	-0.96201200
H	-5.69356000	1.61643600	-0.46455700
C	-1.43472300	-1.09599400	-1.59835100
N	-1.75296300	-1.31429300	-2.70455400
Cu	-1.03403400	-0.54957100	0.26082800

C	-0.80588700	-0.69261700	2.13473300
N	-0.82494600	-0.39511800	3.26762400
C	3.88339600	-1.64149800	-0.42451200
C	2.84358700	-2.02377100	-1.28020300
C	1.55957200	-2.24135000	-0.80566600
C	1.27831600	-2.09090500	0.55980900
C	2.31511200	-1.69962300	1.41822600
C	3.59617700	-1.48019800	0.93362200
H	3.04852600	-2.14416900	-2.34504000
H	0.76234700	-2.49940000	-1.50059800
H	2.10023300	-1.55691000	2.47851100
H	4.39090300	-1.17726100	1.61641700
C	5.27080100	-1.44517400	-0.96159100
C	-0.04395300	-2.37847800	1.14816700
C	6.00765300	-2.75989300	-1.25867500
H	5.39283700	-3.33285000	-1.97495600
C	-0.99007000	-3.37968300	0.54521800
H	-1.09133100	-3.30456600	-0.53943600
H	-0.60836900	-4.38077100	0.80651200
H	-1.99058700	-3.28419000	0.98468500
H	0.06613200	-2.58430600	2.21220800
H	5.87315200	-0.86267700	-0.24452200
H	5.22674900	-0.85190500	-1.88938300
C	6.18232200	-3.59538100	0.00105800
H	5.21943200	-3.86640300	0.45250800
H	6.72767700	-4.52375300	-0.21291500
H	6.76025500	-3.03726000	0.75449100
C	7.35515800	-2.46486900	-1.90073600
H	7.89079700	-3.39041600	-2.14875800
H	7.24761500	-1.87877200	-2.82335200
H	7.99156800	-1.88907400	-1.21174900

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C	3.92260500	-0.64031600	-2.42138300
O	3.46318200	0.73125100	-2.33617600
C	3.27142400	-1.28935000	-1.18345600
H	2.76494000	-2.24131900	-1.40213600
C	2.51457300	0.79106600	-1.38861400
N	2.27999500	-0.29589500	-0.74802000
C	1.92867500	2.12488400	-1.18625700
C	2.96492300	3.25423500	-1.13231800
C	2.08295000	3.14936800	-2.30640400
H	3.99998600	2.93810100	-1.22531800
H	2.77110400	4.01515300	-0.38269200
H	2.49563700	2.77860700	-3.24068200
H	1.26082500	3.85481500	-2.39764000
C	-0.70361500	3.49923800	0.84095900
O	0.47634000	3.55919400	0.01793000
C	-0.78616400	2.01912100	1.25304000
H	-0.33199900	1.79724300	2.23124800
C	0.76586400	2.27670600	-0.28813200
N	0.05951900	1.35450800	0.23932200
C	6.79395600	-1.11684700	-0.05792500
C	6.73617600	-1.50099400	1.27799900
C	5.52122000	-1.84721700	1.86889400
C	4.34451200	-1.81839400	1.12932200
C	4.40719400	-1.43488700	-0.20480100
C	5.61796600	-1.08284000	-0.79762700
H	7.74450800	-0.84014400	-0.51326300
H	7.64810300	-1.52265700	1.87200700
H	5.48945000	-2.12631700	2.91974300
H	3.39122800	-2.05626700	1.60327200
C	5.43617800	-0.71937500	-2.24611200
H	5.90917400	0.23091800	-2.52736000
H	5.85346900	-1.48775600	-2.91341800
C	-2.92900700	0.66194000	1.80956400

C	-2.25397700	1.71795100	1.21435700
C	-2.94290800	2.74042400	0.55762000
C	-4.32861000	2.71193300	0.47780600
C	-5.01315800	1.65463300	1.07683100
C	-4.31987800	0.63916500	1.73349800
H	-2.37946400	-0.11958900	2.33751600
H	-4.87481200	3.51472900	-0.01774100
H	-6.10295700	1.62980500	1.04534100
H	-4.87057400	-0.17338900	2.20627900
C	-1.99011400	3.79159300	0.05376000
H	-1.78883900	3.67164300	-1.02306300
H	-0.54894800	4.18850600	1.67562000
H	-2.35532300	4.81657700	0.19656200
H	3.56694700	-1.02748000	-3.38320300
C	2.24294100	0.65185200	1.99027000
N	2.84451100	1.55694500	2.42431500
Cu	1.11210100	-0.58348200	0.87473200
C	0.09657100	-1.31356400	2.26378900
N	-0.55826700	-1.69293200	3.15446900
C	-4.06471900	-1.20123500	-1.01959900
C	-3.72789100	-2.13321500	-0.03408600
C	-2.40401300	-2.40639100	0.27954600
C	-1.36004900	-1.76274700	-0.39680900
C	-1.70038800	-0.80874900	-1.37196700
C	-3.02045400	-0.53832300	-1.67485100
H	-4.51246600	-2.65344000	0.51378000
H	-2.17824000	-3.11898300	1.07077500
H	-0.89857600	-0.28298500	-1.89230500
H	-3.26265200	0.20660000	-2.43481200
C	-5.47933200	-0.82601100	-1.37467400
C	0.04589800	-2.09510100	-0.19830300
C	-6.61262900	-1.65339800	-0.77613500
H	-6.45200800	-1.72960700	0.31391900

C	0.43961800	-3.45391500	0.30917800
H	-0.04411200	-3.71260500	1.25537900
H	0.16102200	-4.21266700	-0.44112800
H	1.52361800	-3.52626500	0.46741400
H	0.62422700	-1.79721900	-1.07735600
H	-5.58491200	-0.83673000	-2.47477000
H	-5.61669200	0.23049000	-1.08484200
C	-6.66227900	-3.05523500	-1.37227200
H	-5.71212400	-3.59286700	-1.26186600
H	-7.45073600	-3.66049200	-0.90580400
H	-6.88352500	-2.99654100	-2.44892100
C	-7.94096500	-0.94302400	-1.00034800
H	-8.77926700	-1.52184700	-0.59101000
H	-7.95431700	0.05038200	-0.53120600
H	-8.12765900	-0.80527400	-2.07633300

TS5b7

C	-3.86060400	-0.68942900	2.48441900
O	-3.45141300	0.69613600	2.37739600
C	-3.22714300	-1.32031200	1.22738700
H	-2.69676000	-2.26393400	1.42802800
C	-2.52649500	0.77469700	1.40568100
N	-2.27241600	-0.30517000	0.76300100
C	-1.98867000	2.12353200	1.16993000
C	-3.06938100	3.20766900	1.06757000
C	-2.19640400	3.17651800	2.25298600
H	-4.09145500	2.85087200	1.15980700
H	-2.89983100	3.94891800	0.29255400
H	-2.60446300	2.81888800	3.19435600
H	-1.40593600	3.91863300	2.32984900
C	0.63529700	3.55022500	-0.83075500
O	-0.55511000	3.58262800	-0.02246900
C	0.74987400	2.07493500	-1.25178300

H	0.31704000	1.85109000	-2.23929000
C	-0.82514600	2.29431800	0.27583700
N	-0.09896200	1.38729800	-0.25451800
C	-6.78542800	-1.23578500	0.20531400
C	-6.75544500	-1.60351300	-1.13617000
C	-5.54850100	-1.90735500	-1.76559300
C	-4.35260300	-1.85322800	-1.05885100
C	-4.38742200	-1.48831600	0.28114200
C	-5.59011900	-1.17665700	0.91189600
H	-7.72981600	-0.99015600	0.69041600
H	-7.68305100	-1.64418200	-1.70437000
H	-5.53876600	-2.17205000	-2.82063000
H	-3.40621100	-2.05404400	-1.56292500
C	-5.37519000	-0.82016300	2.35762300
H	-5.87244800	0.10993800	2.66340000
H	-5.74301800	-1.60924700	3.03002000
C	2.92410700	0.74873600	-1.76295900
C	2.22086600	1.79465500	-1.18203000
C	2.87916600	2.81624600	-0.49415500
C	4.26104200	2.79087700	-0.35892100
C	4.97287300	1.73937800	-0.93535500
C	4.31058900	0.72885500	-1.63093600
H	2.39927300	-0.03043000	-2.31852300
H	4.78412400	3.59159200	0.16419200
H	6.06043300	1.71638800	-0.85756800
H	4.88256400	-0.07833000	-2.08734500
C	1.90429800	3.86138700	-0.02106700
H	1.68252000	3.75428200	1.05278900
H	0.47856100	4.24285400	-1.66214400
H	2.26283700	4.88808700	-0.16913500
H	-3.46162900	-1.05978900	3.43600500
C	-2.30037700	0.69808100	-2.07035500
N	-2.91408600	1.60337500	-2.48717500

Cu	-1.15093400	-0.49804700	-0.97224100
C	-0.02358900	-1.35318600	-2.18569200
N	0.62966500	-1.68359800	-3.09873600
C	4.10396100	-1.26203900	1.00534200
C	3.83548400	-2.18311800	-0.01084100
C	2.53452200	-2.45852500	-0.40836700
C	1.45096700	-1.82522600	0.20835500
C	1.71929500	-0.89228400	1.22224500
C	3.01751500	-0.62263700	1.61217800
H	4.65556500	-2.68741200	-0.51991400
H	2.35981700	-3.15531700	-1.22644600
H	0.88415100	-0.37391000	1.69474900
H	3.20776800	0.11061300	2.39761100
C	5.49182700	-0.86908600	1.43995100
C	0.05753200	-2.14649500	-0.10431900
C	6.67301700	-1.62133600	0.83467500
H	6.54119700	-1.65313900	-0.26153100
C	-0.32261200	-3.52712500	-0.56123100
H	0.23514600	-3.85706500	-1.44191300
H	-0.12555500	-4.23244000	0.26200300
H	-1.39079500	-3.58291700	-0.80523700
H	-0.58369100	-1.81067300	0.71535600
H	5.55725200	-0.94514600	2.54058500
H	5.60351700	0.20737400	1.22141500
C	6.76773500	-3.04600900	1.36852300
H	5.84185500	-3.61527500	1.21773800
H	7.58721700	-3.59861600	0.89035000
H	6.96863500	-3.02735800	2.45054500
C	7.96505900	-0.86909400	1.12489000
H	8.83657200	-1.39663000	0.71566600
H	7.95015100	0.14285200	0.69732600
H	8.11770400	-0.76954200	2.21038400

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C	0.36372800	3.42570300	-1.73285800
O	-0.97758800	3.07250600	-2.12920200
C	0.89258500	2.14797500	-1.05633200
H	1.55357400	1.53412400	-1.68308100
C	-1.31643800	1.99985700	-1.39266500
N	-0.35435500	1.38382800	-0.80429800
C	-2.76986200	1.75189600	-1.34678800
C	-3.62935300	3.02321300	-1.29261600
C	-3.59280000	2.23847900	-2.53692900
H	-3.07724800	3.95707000	-1.24044400
H	-4.50306100	2.95616800	-0.65129000
H	-3.02370400	2.62457200	-3.37815000
H	-4.45256300	1.62322700	-2.78788700
C	-4.95406900	-0.68343500	0.17182300
O	-4.65169100	0.50803400	-0.58347200
C	-3.62688100	-1.01226000	0.89209400
H	-3.58375600	-0.71248200	1.95037600
C	-3.30442300	0.62452500	-0.56147900
N	-2.64987400	-0.18983800	0.16364700
C	1.73193300	4.63117500	1.54508700
C	2.49993600	3.91484300	2.45794800
C	2.80063400	2.57198300	2.23693800
C	2.33513500	1.92297100	1.09815700
C	1.55695800	2.63888900	0.19757200
C	1.25746800	3.98167300	0.41441200
H	1.49177300	5.67830000	1.72514200
H	2.86738000	4.40801200	3.35616800
H	3.40076400	2.02419100	2.96078100
H	2.56829000	0.87243500	0.92884800
C	0.35571700	4.52213700	-0.65685200
H	-0.66753300	4.63824500	-0.26444700
H	0.66747500	5.49924800	-1.04764600

C	-2.51635400	-3.33049900	1.28726800
C	-3.44288200	-2.48751400	0.68489200
C	-4.34397000	-2.96472400	-0.26623900
C	-4.31182000	-4.29956200	-0.65092100
C	-3.36961000	-5.14436300	-0.07013400
C	-2.48291600	-4.66609400	0.89466900
H	-1.83249400	-2.94872400	2.04747600
H	-5.01474400	-4.68195900	-1.39098200
H	-3.33370400	-6.19265400	-0.36252700
H	-1.76552400	-5.34432800	1.35327200
C	-5.26205600	-1.87531200	-0.75008600
H	-5.04999200	-1.59205200	-1.79233300
H	-5.78137500	-0.43355700	0.84160400
H	-6.32035400	-2.16599600	-0.71546000
H	0.90026400	3.70986600	-2.64227500
C	-1.18483900	1.81107900	1.79817000
N	-1.67692800	2.83552700	2.07893100
Cu	-0.52334200	0.18606600	0.81491600
C	-0.24815900	-0.84218600	2.36321500
N	-0.12062500	-1.50495700	3.31750900
C	4.52597800	-1.13633000	-0.34520200
C	3.72336400	-0.82087700	-1.44462000
C	2.34255300	-0.94356900	-1.38405400
C	1.70426700	-1.38105200	-0.21232800
C	2.51522600	-1.70401200	0.88949000
C	3.89384300	-1.58563000	0.81896000
H	4.19605000	-0.47833400	-2.36697800
H	1.74777800	-0.71146800	-2.26749600
H	2.03797700	-2.02315000	1.81630300
H	4.50172800	-1.84434800	1.68711600
C	6.01989200	-1.03455500	-0.43951800
C	0.25016700	-1.56763200	-0.13945100
C	6.66913600	-2.18277500	-1.22661100

H	6.21919800	-2.19275600	-2.23535800
C	-0.51754400	-1.72099500	-1.42311700
H	-0.47559700	-0.83920600	-2.07378500
H	-0.08667400	-2.56990900	-1.98095700
H	-1.56948800	-1.95332100	-1.23048400
H	-0.02625700	-2.33908900	0.58049600
H	6.29620100	-0.08128700	-0.91821700
H	6.45888400	-1.01452200	0.57193200
C	6.40263600	-3.52877100	-0.56882100
H	5.32985200	-3.75145100	-0.50691500
H	6.88570200	-4.34325600	-1.12437200
H	6.80624700	-3.54131600	0.45585500
C	8.16451500	-1.93707200	-1.36342400
H	8.64882500	-2.73063700	-1.94741000
H	8.37683800	-0.97758600	-1.85404700
H	8.64271400	-1.91729400	-0.37240500

TS5b8

C	0.83581700	2.83511900	-2.14788900
O	-0.47839700	3.19555900	-1.66814800
C	1.18069300	1.62394200	-1.26588500
H	1.62994700	0.79158200	-1.82047800
C	-0.93247200	2.17784200	-0.91739400
N	-0.11772300	1.20469300	-0.70715300
C	-2.28438900	2.39958100	-0.37472900
C	-2.40739300	3.69295600	0.44226400
C	-3.06571400	3.60902500	-0.87269300
H	-1.48594300	4.26116200	0.54295600
H	-2.99326700	3.60378900	1.35245400
H	-2.63319600	4.14578200	-1.71167800
H	-4.14418400	3.47924000	-0.89885300
C	-4.91075800	0.33398200	0.95693500
O	-4.26989000	1.58219100	0.63236000

C	-3.76383400	-0.69393100	0.88440500
H	-3.34641500	-0.98124800	1.86082500
C	-3.06387000	1.25340800	0.12219300
N	-2.71146900	0.02724100	0.14328600
C	3.30543100	4.23056700	0.29123100
C	3.79087900	3.62323500	1.44499700
C	3.43755700	2.31146400	1.76011400
C	2.59300000	1.58800300	0.92598500
C	2.11136400	2.19617400	-0.22611200
C	2.46132500	3.50784400	-0.54326200
H	3.57770800	5.25788100	0.04994000
H	4.44643700	4.17998400	2.11248100
H	3.81267400	1.85338300	2.67317000
H	2.30411100	0.56901800	1.18256800
C	1.84038400	3.93962600	-1.84293200
H	1.34289400	4.91752700	-1.79606400
H	2.58665900	4.00347100	-2.64879400
C	-3.82876200	-3.13150000	-0.01594200
C	-4.34974100	-1.85230800	0.13334600
C	-5.57312500	-1.50121800	-0.43673100
C	-6.28702800	-2.42873300	-1.18493600
C	-5.76057400	-3.70701100	-1.35413700
C	-4.54329800	-4.05802100	-0.77139900
H	-2.89453500	-3.40145600	0.47876500
H	-7.24820000	-2.16522300	-1.62643100
H	-6.31245800	-4.44436200	-1.93512400
H	-4.15744700	-5.06859800	-0.89456600
C	-5.94013000	-0.07904000	-0.10866300
H	-5.84071900	0.58030000	-0.98455900
H	-5.34806900	0.44916500	1.95238400
H	-6.97439100	0.02400000	0.24503200
H	0.73004200	2.61159700	-3.21670300
C	-0.62464200	1.04139300	2.19812100

N	-0.85998600	1.93124200	2.92039600
Cu	-0.45916900	-0.26805800	0.71897600
C	-0.79957700	-1.85491100	1.63660000
N	-1.18859700	-2.65932600	2.39286300
C	4.36865400	-1.55793100	-0.07481000
C	3.68812200	-1.36105500	-1.27744800
C	2.31064800	-1.52155900	-1.36009900
C	1.56056500	-1.88287100	-0.23396500
C	2.24898600	-2.11193400	0.96735000
C	3.62367500	-1.95051300	1.04067100
H	4.25104000	-1.07320500	-2.16715400
H	1.81326800	-1.38594600	-2.32031900
H	1.68455700	-2.39616200	1.85578700
H	4.13532300	-2.12275300	1.98847700
C	5.85744000	-1.38323000	-0.00437600
C	0.09475200	-2.10242400	-0.31377300
C	6.64738600	-2.53271000	-0.64640200
H	6.31827400	-2.61984900	-1.69726500
C	-0.64656600	-1.87249400	-1.60294100
H	-0.44895300	-0.89476000	-2.05566100
H	-0.35823700	-2.66087000	-2.31838500
H	-1.72801600	-1.95117600	-1.44401900
H	-0.15789100	-3.08871300	0.07579700
H	6.17276500	-1.28896200	1.04811700
H	6.14007800	-0.43965100	-0.49825800
C	6.37099000	-3.85496600	0.05425500
H	5.30969000	-4.13082700	0.00940100
H	6.95138200	-4.67080300	-0.39606300
H	6.65545300	-3.79264700	1.11638900
C	8.13503200	-2.21391100	-0.62822900
H	8.72081400	-3.00974500	-1.10651300
H	8.35627900	-1.27151600	-1.14715300
H	8.49419500	-2.11601300	0.40739900

6c

C	-2.31240100	-3.15312800	-2.16039800
O	-1.23233800	-3.74991000	-1.39671800
C	-2.64907100	-1.87351500	-1.35814300
H	-2.59685000	-0.93790400	-1.93076500
C	-0.92625100	-2.89606700	-0.40283400
N	-1.61868300	-1.82644400	-0.30459500
C	0.21687100	-3.31920000	0.43389500
C	0.43428400	-4.82306700	0.59263700
C	1.34379300	-4.06566600	-0.28373800
H	-0.32152600	-5.45553800	0.13565900
H	0.79855800	-5.14168600	1.56551800
H	1.22750900	-4.16394500	-1.36002500
H	2.35026100	-3.85401100	0.06824500
C	1.82570700	-2.03299400	3.42144000
O	1.68869500	-2.89820100	2.26067400
C	0.82364200	-0.89765200	3.11505700
H	0.14128300	-0.66226100	3.94236500
C	0.60584200	-2.47380800	1.57932300
N	0.03373600	-1.40767500	1.98633700
C	-5.74825300	-3.81627700	-0.77898800
C	-6.49292900	-3.00381300	0.07098100
C	-6.00652900	-1.75995000	0.47445300
C	-4.76493900	-1.30829700	0.03833000
C	-4.02105200	-2.13151300	-0.79990400
C	-4.50477400	-3.37138600	-1.21286500
H	-6.13505100	-4.78391100	-1.09889000
H	-7.46736800	-3.34106200	0.42123900
H	-6.60180900	-1.13428000	1.13683900
H	-4.37902400	-0.33842800	0.35357700
C	-3.55062300	-4.05168300	-2.15669300
H	-3.28263800	-5.07294700	-1.85278500

H	-3.97171400	-4.12832100	-3.16955900
C	1.30044300	1.48262800	2.18637000
C	1.69681400	0.26372500	2.72318000
C	3.04276900	-0.03425900	2.92694200
C	4.01895300	0.90328100	2.61284000
C	3.62972200	2.12308900	2.06739900
C	2.28203700	2.40992000	1.84823900
H	0.24586200	1.70998900	2.02362300
H	5.07516800	0.67893600	2.76959600
H	4.38871800	2.85555300	1.79449700
H	1.97812000	3.35694700	1.40787400
C	3.22257500	-1.41916600	3.48738200
H	3.94015000	-2.03120900	2.92147900
H	1.57197300	-2.64617100	4.29374200
H	3.58002800	-1.40071300	4.52738800
H	-1.91218100	-2.97009700	-3.16425900
C	-2.65973000	1.04589500	1.80699400
N	-3.30477500	1.98805100	2.07264000
Cu	-1.62415800	-0.41477200	1.22119100
C	5.22471200	0.74822900	-1.02231600
C	4.46577400	1.54411100	-1.87975500
C	3.10619900	1.31593300	-2.06201700
C	2.46667900	0.28713500	-1.37171900
C	3.22215700	-0.51816700	-0.51896100
C	4.58097700	-0.29509200	-0.35437400
H	4.95112000	2.36298500	-2.41313300
H	2.53319800	1.94910600	-2.73894200
H	2.73002200	-1.31399500	0.04660400
H	5.15312200	-0.92150100	0.33391600
C	6.69277200	0.98763400	-0.81493300
C	1.00200100	-0.03525600	-1.57626700
H	0.63264100	-0.54996400	-0.67820000
C	0.16489200	1.20581900	-1.75713800

C	7.59838400	-0.02880900	-1.52264100
H	7.31295100	-1.03546900	-1.16833400
O	-0.49667400	1.48001500	-0.57508200
N	-1.38184400	2.51659000	-0.67599600
O	0.04324500	1.86086600	-2.75106700
C	-2.69918300	2.27598500	-1.10352300
C	-1.23523600	3.67930000	0.10388500
O	-0.24234500	4.01537100	0.69659200
O	-3.08027100	1.27360300	-1.65664600
C	-2.55217700	4.34620800	-0.02878900
C	-3.41533800	3.52037200	-0.74559500
C	-4.72126100	3.88628100	-0.99918600
C	-5.14689100	5.12166200	-0.50680200
C	-4.28305600	5.94800900	0.21102000
C	-2.96279500	5.56836600	0.46151700
H	-5.38720400	3.22599600	-1.55075400
H	-6.17217000	5.44363900	-0.67865400
H	-4.64837500	6.90121500	0.58829800
H	-2.28065500	6.19651900	1.03043300
C	0.81065200	-0.93232200	-2.79960800
H	-0.24719200	-1.19566400	-2.94078700
H	1.15493800	-0.41836900	-3.70502800
H	1.39471400	-1.85416000	-2.68073400
H	6.91773100	0.96865600	0.26508400
H	6.96111600	1.99757700	-1.16828800
C	7.40859900	0.01992500	-3.03168900
H	6.37391400	-0.20260600	-3.32170800
H	7.65458200	1.02244900	-3.41581700
H	8.06592900	-0.69900200	-3.53834000
C	9.05331200	0.22145500	-1.15433300
H	9.21347800	0.16931200	-0.06884900
H	9.71971200	-0.50986000	-1.63043800
H	9.36757700	1.22174300	-1.48899600

TS5c

C	3.27483400	-0.08588000	2.95060400
O	2.89950300	-1.46059500	2.66511300
C	3.19508700	0.57592400	1.56298500
H	2.66563400	1.53456100	1.55313300
C	2.41510200	-1.48006800	1.40406600
N	2.45815000	-0.39356600	0.73507300
C	1.91223400	-2.80121100	0.97257000
C	2.59599400	-4.01729300	1.59392900
C	1.23317800	-3.67075600	2.03298800
H	3.42574900	-3.79619400	2.25877500
H	2.72771500	-4.86832400	0.93224100
H	1.10293000	-3.20912800	3.00884300
H	0.40233600	-4.27705000	1.68103200
C	0.75293200	-4.21365700	-2.15919900
O	1.11646100	-4.22741600	-0.75547500
C	0.67502000	-2.70252700	-2.47680400
H	1.24873400	-2.38910900	-3.35937800
C	1.42053400	-2.95954100	-0.41045300
N	1.24567800	-2.05394200	-1.29111300
C	6.86613700	0.30241000	1.96374900
C	7.36369700	0.64833500	0.71067200
C	6.49921800	0.99987100	-0.32644600
C	5.12192400	1.01786900	-0.12801500
C	4.63282400	0.67724500	1.12779000
C	5.49109800	0.31510400	2.16519400
H	7.54362200	0.01970900	2.76969300
H	8.43859700	0.63736700	0.53603800
H	6.90262500	1.25599600	-1.30435100
H	4.44125300	1.27510000	-0.93918300
C	4.72448100	-0.00942300	3.41933700
H	5.03346000	-0.94740700	3.90021600

H	4.83113300	0.78209700	4.17608100
C	-1.42598000	-1.20186300	-2.75744900
C	-0.80055000	-2.43125000	-2.59883700
C	-1.53892300	-3.60894900	-2.49084400
C	-2.92733100	-3.56937700	-2.54907000
C	-3.55903600	-2.33909100	-2.71441700
C	-2.81583500	-1.16206500	-2.81271700
H	-0.84456200	-0.28205800	-2.82237000
H	-3.51288200	-4.48533500	-2.47006100
H	-4.64657800	-2.29560600	-2.76387000
H	-3.31569900	-0.20040800	-2.90915900
C	-0.63906700	-4.80838500	-2.36424100
H	-0.90240200	-5.47690800	-1.53354600
H	1.54470300	-4.75282100	-2.69093400
H	-0.65799200	-5.42110100	-3.27744100
H	2.54695900	0.29507300	3.67829600
C	2.53220200	0.42525500	-2.82605300
N	3.14124700	0.58945400	-3.81136900
Cu	1.53087700	0.07357200	-1.23283200
C	-5.25671700	0.52585100	1.29541000
C	-4.54761800	1.07787300	2.36211200
C	-3.20753800	0.77096700	2.56970900
C	-2.54690400	-0.11397000	1.71859500
C	-3.24686900	-0.65950100	0.64088000
C	-4.58143000	-0.34543200	0.43658600
H	-5.05643300	1.76531800	3.03977200
H	-2.67266800	1.23245400	3.39923700
H	-2.73092800	-1.32769600	-0.05169700
H	-5.11159900	-0.77744500	-0.41454600
C	-6.71247900	0.82552100	1.08098500
C	-1.07801200	-0.42686000	1.88290500
H	-0.86958400	-1.36767400	1.35120300
C	-0.32146100	0.69604800	1.14361300

C	-7.64956000	-0.31199800	1.51020700
H	-7.35219700	-1.21776100	0.95238600
O	-0.23836800	0.35854500	-0.12425800
N	0.22531700	1.84101100	-1.15030500
O	0.05783200	1.71864600	1.66669300
C	1.12039100	2.85012100	-0.73571300
C	-1.06655700	2.36830300	-1.40624600
O	-2.07452200	1.74629300	-1.62808000
O	2.26071800	2.68651600	-0.37578500
C	-0.89298700	3.84293100	-1.37684800
C	0.40332100	4.12862700	-0.96648700
C	0.86659100	5.42708500	-0.86752500
C	-0.03653200	6.44595600	-1.17360600
C	-1.34233600	6.15976100	-1.58007400
C	-1.79075000	4.84360900	-1.69745900
H	1.88881900	5.63349700	-0.55813300
H	0.27972900	7.48433800	-1.09504500
H	-2.01876400	6.98060900	-1.81050900
H	-2.80082000	4.60288600	-2.02221900
C	-0.58044600	-0.51897800	3.31642600
H	0.46192500	-0.86697600	3.34368100
H	-0.61223700	0.45852400	3.81006900
H	-1.19553300	-1.22602100	3.88678200
H	-6.89089000	1.04362700	0.01563500
H	-6.99451600	1.73604900	1.63645500
C	-7.52469800	-0.60333200	2.99849400
H	-6.50468500	-0.90011000	3.27353000
H	-7.78234700	0.29173100	3.58662300
H	-8.20689900	-1.40763400	3.30415900
C	-9.08696200	0.03194800	1.14847300
H	-9.20095100	0.22599100	0.07338400
H	-9.77487500	-0.77930800	1.42104400
H	-9.41239800	0.93571000	1.68591600

7c

C	3.34045900	2.10147300	2.27656400
O	3.94598100	0.77696800	2.19820100
C	2.64572100	2.23121900	0.90833900
H	1.62260200	2.61695400	0.94898700
C	3.39330700	0.17518600	1.13084000
N	2.62234400	0.85731000	0.38218900
C	3.80364800	-1.22832900	0.92890600
C	5.23891900	-1.57215400	1.30887200
C	4.14403100	-2.06026700	2.16636200
H	5.83399300	-0.73338000	1.65886200
H	5.74759000	-2.27863600	0.65940900
H	3.96088400	-1.56700800	3.11709800
H	3.87320100	-3.11213800	2.11759800
C	3.16306200	-3.64806200	-1.69978200
O	3.83190600	-3.10655800	-0.52495200
C	1.83108100	-2.87444000	-1.70631400
H	1.52637300	-2.50235500	-2.69334300
C	3.20044300	-1.97954200	-0.18273200
N	2.12227400	-1.72616000	-0.83060600
C	5.58693200	4.41808900	0.37250800
C	5.53951000	4.70979900	-0.98781900
C	4.51831500	4.19921300	-1.78993400
C	3.52637100	3.38966100	-1.24462300
C	3.57990700	3.10224900	0.11349400
C	4.59936600	3.60709600	0.91909100
H	6.38787700	4.81619700	0.99596700
H	6.30908200	5.34022900	-1.43112400
H	4.49869300	4.43323000	-2.85296100
H	2.72881000	2.97855300	-1.86287300
C	4.42291800	3.17308700	2.34998000
H	5.33828500	2.78124200	2.81394800

H	4.08082800	4.00532600	2.98308200
C	-0.46104900	-3.62419600	-0.69880900
C	0.85410500	-3.84990100	-1.09165900
C	1.44818700	-5.10219000	-0.93269400
C	0.73924200	-6.15196000	-0.36161300
C	-0.57287100	-5.93078400	0.04275800
C	-1.16644400	-4.68016700	-0.12972600
H	-0.92845900	-2.64904700	-0.83536500
H	1.20232500	-7.13027300	-0.23462400
H	-1.14324700	-6.74184500	0.49274200
H	-2.20063700	-4.53068400	0.17821400
C	2.84699200	-5.11927000	-1.48284200
H	3.58676300	-5.58703600	-0.81981300
H	3.82045700	-3.44216400	-2.55188300
H	2.89629700	-5.65680600	-2.44128800
H	2.65631400	2.08075000	3.13157100
C	1.44629300	0.39670300	-2.38357300
N	1.82761300	0.69642700	-3.44501200
Cu	0.91315100	-0.16960400	-0.68053200
C	-5.08682900	0.20081400	0.57616400
C	-4.38048900	1.15960600	1.30521200
C	-3.19342600	0.83947000	1.95249400
C	-2.68217900	-0.46052000	1.90254300
C	-3.35974000	-1.40622800	1.13209700
C	-4.54439100	-1.08275100	0.48301600
H	-4.77017400	2.17800000	1.35936100
H	-2.65121100	1.60925000	2.50113700
H	-2.94466800	-2.41174500	1.04440800
H	-5.06192000	-1.83932200	-0.10999500
C	-6.41151500	0.51563000	-0.05770900
C	-1.40163600	-0.82590900	2.61926600
H	-1.26829300	-1.91406400	2.53870400
C	-0.26979600	-0.16032400	1.81796800

C	-7.61719800	-0.01840300	0.72806500
H	-7.48717400	-1.10980700	0.83653300
O	0.11940600	-0.92751500	0.84559000
N	-0.59258500	0.90260500	-0.99157800
O	0.11983100	0.96587700	2.08251500
C	-0.71515100	2.28695900	-0.94233200
C	-1.68087400	0.29535600	-1.60310700
O	-1.76786200	-0.87706000	-1.90687600
O	0.13033800	3.08904200	-0.61593900
C	-2.68259600	1.37646600	-1.81401900
C	-2.10926500	2.57279500	-1.39928500
C	-2.80256300	3.76582900	-1.45348500
C	-4.10742200	3.72189000	-1.95114400
C	-4.67862500	2.52168500	-2.37790100
C	-3.96913400	1.32049300	-2.31063500
H	-2.34071300	4.69529300	-1.12625900
H	-4.68821500	4.64030400	-2.01718600
H	-5.69644100	2.52329700	-2.76545500
H	-4.40146800	0.37327300	-2.62988200
C	-1.37354600	-0.39845000	4.07817500
H	-0.45358300	-0.74384000	4.56642200
H	-1.39807200	0.69287600	4.16763900
H	-2.23098100	-0.81611300	4.62023200
H	-6.44806000	0.09473500	-1.07696400
H	-6.52383200	1.60823000	-0.16824300
C	-7.69301000	0.59635500	2.11789800
H	-6.79649500	0.37855500	2.71171800
H	-7.78871800	1.69147600	2.04713500
H	-8.56584100	0.22274600	2.66959700
C	-8.90080000	0.24413200	-0.04591100
H	-8.87426100	-0.21124700	-1.04528900
H	-9.77738300	-0.15239400	0.48323900
H	-9.05578700	1.32612900	-0.17670100

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C	3.56771700	-3.00932700	1.70849200
O	2.21774800	-3.45817000	2.00060000
C	3.33402200	-1.89635000	0.66018500
H	3.87920500	-0.96307500	0.85572600
C	1.38839600	-2.53970000	1.46597700
N	1.88834400	-1.61854800	0.73581900
C	-0.04465600	-2.73504200	1.78518800
C	-0.61790300	-4.11779500	1.48647900
C	-0.39986900	-3.71999600	2.89132100
H	0.07728000	-4.82168900	1.03455400
H	-1.63435100	-4.14301400	1.10133700
H	0.44158700	-4.14533100	3.42993800
H	-1.26828700	-3.46069200	3.49148900
C	-2.92582500	-0.56573100	1.91467200
O	-2.25625600	-1.84537800	1.81990200
C	-1.86176800	0.43961000	1.42918700
H	-2.01455700	0.81530500	0.40720200
C	-0.94771900	-1.57642300	1.64619100
N	-0.62209400	-0.35785000	1.43369500
C	4.65051800	-4.61250200	-1.49930000
C	4.50950500	-4.11345800	-2.79042300
C	3.99057900	-2.83591400	-3.00229500
C	3.59583700	-2.04360300	-1.92823100
C	3.72299800	-2.55235700	-0.64095500
C	4.25611700	-3.82257700	-0.42523500
H	5.06629100	-5.60638000	-1.33285300
H	4.81336800	-4.72162800	-3.64114000
H	3.89766500	-2.45275500	-4.01768100
H	3.20091600	-1.03880900	-2.07609100
C	4.36332900	-4.12636300	1.04342500
H	3.96995000	-5.11195000	1.32668200

H	5.41008200	-4.09634200	1.37995900
C	-1.14857600	2.71207500	2.45318100
C	-1.85091000	1.51404400	2.47333700
C	-2.63659900	1.15242100	3.56546700
C	-2.74665400	2.00510100	4.65692700
C	-2.04793300	3.20950800	4.64168700
C	-1.25148400	3.55990800	3.55156400
H	-0.52321400	2.97272700	1.59870300
H	-3.36469300	1.73619400	5.51349500
H	-2.12203000	3.88506500	5.49237200
H	-0.70458400	4.50052100	3.56096700
C	-3.26179900	-0.20281700	3.36978900
H	-2.82549600	-0.95395500	4.04653900
H	-3.80612100	-0.62440800	1.26766600
H	-4.34401200	-0.20619500	3.55716700
H	3.99268500	-2.66077800	2.65647500
C	2.64779700	1.48785200	2.02004300
N	3.60302100	2.06494900	2.37638800
Cu	1.19767300	0.44623700	1.43976800
C	-4.76776400	-0.38619200	-1.41081600
C	-4.00098200	-1.52060400	-1.14622700
C	-2.66154100	-1.59019100	-1.51770000
C	-2.05311000	-0.52850100	-2.18294600
C	-2.81947900	0.60874300	-2.45491500
C	-4.15036700	0.68076500	-2.06947500
H	-4.45592100	-2.36270000	-0.61943000
H	-2.09182600	-2.48723600	-1.27833500
H	-2.35678200	1.45588600	-2.96540700
H	-4.72907200	1.57960800	-2.28660100
C	-6.21631000	-0.33706400	-1.01600100
C	-0.61594300	-0.56909400	-2.65152100
H	-0.60533200	-0.42897400	-3.74421000
C	-7.14029500	-1.14164200	-1.94089000

H	-6.77426900	-2.18370000	-1.95369900
C	0.14282500	-1.85690100	-2.33398400
H	1.13047000	-1.84800400	-2.80629500
H	0.30075500	-1.97097000	-1.25207700
H	-0.40409000	-2.72643900	-2.71665100
H	-6.33264000	-0.71960300	0.01221600
H	-6.56536100	0.70906300	-0.99886800
C	-7.10686100	-0.60329600	-3.36369800
H	-6.09969200	-0.64812500	-3.79699700
H	-7.78181800	-1.17090600	-4.01753600
H	-7.43319100	0.44845100	-3.38316300
C	-8.56046000	-1.13098200	-1.39471500
H	-9.23679900	-1.72211300	-2.02585400
H	-8.60832800	-1.53653500	-0.37501200
H	-8.95230000	-0.10300900	-1.36300400
C	0.15451600	0.59539300	-2.07703800
O	1.18493100	0.92768300	-2.94054400
N	1.85378800	2.05215800	-2.53309200
O	-0.03821300	1.18562000	-1.05115000
C	2.77582400	1.98869000	-1.45510500
C	1.20568000	3.30694000	-2.62777400
O	0.21557800	3.52905900	-3.27696800
O	3.28124100	0.97642500	-1.04524600
C	2.01402700	4.18184200	-1.75169400
C	2.92828300	3.40072100	-1.04173000
C	3.77617000	3.95118700	-0.09823400
C	3.68806800	5.33048100	0.10187200
C	2.78529200	6.11492400	-0.61715500
C	1.92412100	5.54701100	-1.55761100
H	4.42866300	3.31989500	0.50140300
H	4.32630400	5.79995300	0.84750800
H	2.74289000	7.18628800	-0.42933100
H	1.20158500	6.14185100	-2.11276800

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C	3.97980300	-2.70369600	-0.09825500
O	2.98150200	-3.74148400	-0.08837800
C	3.17072500	-1.42381600	-0.42448000
H	3.19377500	-0.67991700	0.38351800
C	1.79060800	-3.14538400	-0.31306300
N	1.77659700	-1.89458900	-0.55355300
C	0.64755300	-4.08048800	-0.20472900
C	0.81996300	-5.45408600	-0.85356700
C	0.92248000	-5.34982900	0.61127700
H	1.73188700	-5.58153700	-1.43149200
H	-0.07677300	-5.89113300	-1.28543000
H	1.90205500	-5.39291900	1.07496400
H	0.09440000	-5.70832100	1.21427100
C	-2.79136600	-3.90666400	0.71478400
O	-1.64553200	-4.54696700	0.12313200
C	-2.59000800	-2.41848300	0.37532800
H	-3.20723500	-2.04973600	-0.45424000
C	-0.73098300	-3.57290700	-0.06747000
N	-1.16387900	-2.36634500	-0.02611000
C	5.46872100	-1.50631100	-3.33759600
C	5.16107100	-0.35541600	-4.05504700
C	4.18224000	0.52163600	-3.59047000
C	3.49089200	0.25404800	-2.41252500
C	3.78060400	-0.91208400	-1.70711200
C	4.77691400	-1.77651100	-2.16251700
H	6.24787300	-2.18405800	-3.68706900
H	5.69561100	-0.13193400	-4.97702600
H	3.95971600	1.42948700	-4.14863100
H	2.74050700	0.95460100	-2.04765700
C	4.99850900	-2.92506500	-1.21904800
H	4.83649300	-3.90565300	-1.68839500

H	6.02592000	-2.93285700	-0.82883000
C	-2.93539400	-0.33004200	1.89025900
C	-2.84896400	-1.69857400	1.66828400
C	-2.93971600	-2.60470300	2.72192200
C	-3.11933500	-2.15174500	4.02155700
C	-3.19305200	-0.78119700	4.25111100
C	-3.10169900	0.12315000	3.19480100
H	-2.86027000	0.38004700	1.06744300
H	-3.18305500	-2.85561700	4.85074200
H	-3.31844100	-0.41183000	5.26751800
H	-3.15369100	1.19272800	3.38838700
C	-2.75804200	-4.01808700	2.24818500
H	-1.77432900	-4.40411800	2.56064100
H	-3.67990800	-4.35767900	0.26420900
H	-3.51372100	-4.71331800	2.63675000
H	4.42936200	-2.69513400	0.89971800
C	0.52605600	-1.23149000	2.08008900
N	0.84877000	-1.89018000	2.99182100
Cu	-0.06654900	-0.66037700	0.28480100
C	-4.72152700	1.61354800	-1.17154100
C	-4.28534500	0.41078500	-1.73265800
C	-2.93495800	0.09817500	-1.80173300
C	-1.96100900	0.97388300	-1.30339900
C	-2.39881400	2.19704200	-0.77555300
C	-3.75151300	2.50199200	-0.70440100
H	-5.02290400	-0.29219700	-2.12562700
H	-2.62872500	-0.84215000	-2.25933400
H	-1.66268200	2.91071300	-0.41027400
H	-4.06600900	3.45898500	-0.28504300
C	-6.18409100	1.94960400	-1.13116900
C	-0.51005300	0.67596800	-1.39695900
H	0.03670200	1.61413100	-1.55100300
C	-6.76124500	2.37491900	-2.48887800

H	-6.57172700	1.55511600	-3.20447700
C	-0.07912600	-0.28988600	-2.48414500
H	1.00761100	-0.39935600	-2.51804800
H	-0.50071400	-1.29553300	-2.37827100
H	-0.40914300	0.12002400	-3.45299200
H	-6.75315700	1.07965100	-0.76536900
H	-6.36144600	2.76307600	-0.40768600
C	-6.08400800	3.63328800	-3.01155200
H	-5.00460400	3.49175500	-3.14937500
H	-6.51112800	3.94236600	-3.97468800
H	-6.22436000	4.46558400	-2.30385800
C	-8.26442100	2.58123400	-2.37351000
H	-8.70640600	2.85976400	-3.33924900
H	-8.77368000	1.67594600	-2.01622400
H	-8.48738200	3.39094400	-1.66213700
C	0.44387900	1.14998500	0.45507900
O	1.79032400	1.20958000	0.04200700
N	2.40942000	2.36098100	0.44620400
O	-0.05869600	2.01264000	1.10805900
C	2.90870200	2.48469300	1.76469200
C	2.06477800	3.58814100	-0.14218100
O	1.45460200	3.72229000	-1.17544700
O	3.10751000	1.57651400	2.52419800
C	2.63044700	4.59818900	0.78529600
C	3.12554200	3.94648700	1.91447800
C	3.70570000	4.64539100	2.95542500
C	3.77356600	6.03459700	2.83573300
C	3.27827700	6.68693700	1.70565500
C	2.69718600	5.97248900	0.65665600
H	4.08317100	4.12245000	3.83179900
H	4.21681300	6.62168700	3.63771300
H	3.34437700	7.77151000	1.64512100
H	2.30380500	6.46740100	-0.22900700

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C	4.50992500	-2.10642800	-0.56320800
O	3.73093400	-3.27930000	-0.26496200
C	3.46874100	-0.96089200	-0.55965400
H	3.53294400	-0.29615500	0.31343400
C	2.43388200	-2.89322000	-0.27418800
N	2.17576000	-1.66264400	-0.47426400
C	1.49248300	-3.99202400	0.02187700
C	1.90438000	-5.39978600	-0.40329600
C	2.02665700	-5.03250900	1.01667700
H	2.80782300	-5.45680400	-1.00421600
H	1.09335700	-6.05838800	-0.70203000
H	3.00879800	-4.81266700	1.42324000
H	1.29885000	-5.41808300	1.72427600
C	-1.93639800	-4.35642600	0.95975100
O	-0.67339100	-4.82735000	0.44860100
C	-1.99532200	-2.89021200	0.48949900
H	-2.65670700	-2.70889200	-0.36788000
C	0.04702200	-3.72995200	0.14741700
N	-0.59627900	-2.62233200	0.07544200
C	4.98714700	-0.43263100	-3.89845600
C	4.42170100	0.75876200	-4.34312600
C	3.51322400	1.45233200	-3.54414700
C	3.15548000	0.96180400	-2.29234200
C	3.71007000	-0.23672500	-1.85679500
C	4.62523300	-0.92707500	-2.65046300
H	5.70728300	-0.96738700	-4.51798900
H	4.69780700	1.15620600	-5.31865400
H	3.08222000	2.38900200	-3.89378400
H	2.45106900	1.50797400	-1.66771200
C	5.11982400	-2.17357000	-1.97079400
H	4.77507400	-3.08756400	-2.47654800

H	6.21652700	-2.22796500	-1.94233800
C	-2.70235900	-0.76755700	1.81587000
C	-2.39332300	-2.11795300	1.71493600
C	-2.35160300	-2.93235000	2.84355300
C	-2.62016900	-2.40333800	4.09820600
C	-2.91406300	-1.04718900	4.20705200
C	-2.95448300	-0.23486200	3.07577700
H	-2.73161500	-0.12875500	0.93455200
H	-2.58036900	-3.03346500	4.98609100
H	-3.10868700	-0.61608100	5.18764600
H	-3.17392000	0.82663100	3.17300200
C	-1.93944100	-4.33394400	2.49687900
H	-0.92199500	-4.53942400	2.86543700
H	-2.71142900	-4.99854000	0.53199600
H	-2.59690900	-5.10220800	2.92492700
H	5.26533800	-2.02064100	0.22361600
C	0.77051200	-1.26389500	2.14676300
N	1.11236300	-1.87201300	3.08613700
Cu	0.17858500	-0.74142000	0.31479200
C	-4.69172400	0.80110800	-1.36383700
C	-4.15520800	-0.40079300	-1.83418900
C	-2.78445300	-0.60657000	-1.87780400
C	-1.88301800	0.37728200	-1.43927100
C	-2.42643200	1.59434000	-0.99840000
C	-3.79934600	1.79508200	-0.95790900
H	-4.83103100	-1.18705600	-2.17712400
H	-2.39965500	-1.54887100	-2.26734200
H	-1.75575700	2.38909800	-0.67861000
H	-4.19310100	2.75114600	-0.60896000
C	-6.17644200	1.02177500	-1.35425600
C	-0.42261900	0.17508200	-1.48836900
H	0.09791500	1.13648900	-1.56166400
C	-6.77222600	1.30069600	-2.74160500

H	-6.51323300	0.44809700	-3.39430800
C	0.08587700	-0.78209100	-2.54335400
H	1.17707300	-0.77251300	-2.60110900
H	-0.22542100	-1.82078500	-2.37742900
H	-0.30661300	-0.46598500	-3.52471000
H	-6.67940300	0.13835400	-0.92846200
H	-6.42476900	1.86911100	-0.69305700
C	-6.18902700	2.56612700	-3.35310700
H	-5.10065400	2.49841600	-3.47531200
H	-6.62937100	2.76991700	-4.33816600
H	-6.39970100	3.43471500	-2.70922800
C	-8.28782100	1.39788700	-2.64732800
H	-8.74111900	1.57066000	-3.63240400
H	-8.72926300	0.48424400	-2.22664600
H	-8.57883000	2.23739700	-1.99771500
C	0.35318000	1.08738200	0.79342300
O	1.69530100	1.44240500	0.56511500
N	1.94143300	2.76171200	0.86362200
O	-0.42445100	1.85066700	1.27459100
C	2.09143200	3.19420700	2.20608900
C	1.45288600	3.76615200	0.01161500
O	1.05202500	3.59795800	-1.11560300
O	2.30644700	2.49212500	3.15472600
C	1.56576900	5.00750300	0.81360200
C	1.93966200	4.66912400	2.11246500
C	2.11071000	5.63160800	3.08876300
C	1.89031000	6.96076200	2.72341300
C	1.51551200	7.29963200	1.42215300
C	1.34753400	6.32060800	0.44170100
H	2.39882900	5.35086100	4.09979600
H	2.00879400	7.74834800	3.46507900
H	1.34891400	8.34541500	1.17131300
H	1.05204200	6.56866600	-0.57577300

7a

C	-0.49405600	-3.68574700	0.20803300
O	0.05644600	-2.89568400	1.28007700
C	-0.96181100	-2.62113700	-0.80841600
H	-0.53647200	-2.76802300	-1.81113000
C	0.04677800	-1.60720000	0.89933600
N	-0.45044000	-1.35359100	-0.25625800
C	0.63421600	-0.69765800	1.89625100
C	0.52148600	-1.13921700	3.34565900
C	1.83528300	-1.23369200	2.68188800
H	-0.03868700	-2.05292200	3.51709000
H	0.34135700	-0.33579600	4.05293400
H	2.20905900	-2.20886000	2.37651000
H	2.59751600	-0.49296300	2.91843500
C	1.08718700	2.84200400	2.27429900
O	0.86980200	1.50250200	2.74580400
C	0.62675100	2.79674900	0.79899600
H	-0.36973200	3.22581100	0.61123500
C	0.64848700	0.75617800	1.64633800
N	0.55996400	1.35260900	0.52363400
C	-4.24654300	-3.96559600	0.23881100
C	-5.15959200	-3.19171400	-0.47187000
C	-4.72263500	-2.20739000	-1.35909800
C	-3.36309200	-1.97714600	-1.54085700
C	-2.45938000	-2.73044100	-0.80507800
C	-2.88741700	-3.72865600	0.06648000
H	-4.59283200	-4.74287400	0.91974700
H	-6.22678700	-3.36017800	-0.33717100
H	-5.44169200	-1.60221300	-1.90899700
H	-3.02997500	-1.19294600	-2.22097700
C	-1.72580500	-4.46267700	0.67847400
H	-1.75506200	-4.49844100	1.77585800

H	-1.68118400	-5.50524100	0.33192500
C	1.74496800	3.90151300	-1.28229100
C	1.72886000	3.49303400	0.04685500
C	2.84571500	3.66890700	0.86408300
C	4.01080900	4.22718400	0.35218900
C	4.04085600	4.61539800	-0.98487300
C	2.91450600	4.46133200	-1.79239800
H	0.86410100	3.77626500	-1.91306000
H	4.88515300	4.36706500	0.98829100
H	4.94682700	5.05550300	-1.39890100
H	2.94464500	4.78641900	-2.83086800
C	2.58675300	3.18255100	2.26185700
H	3.16233800	2.27146000	2.49259000
H	0.49814100	3.50731100	2.91139500
H	2.85648700	3.92322100	3.02657200
H	0.31806700	-4.32752400	-0.15459400
C	-0.86066900	1.87231500	-2.37017600
N	-0.95513800	2.81343000	-3.05623500
Cu	-0.65886500	0.45587300	-1.14689500
N	-2.44834100	0.83145500	-0.25235900
C	-3.60135800	1.06415800	-0.98645000
C	-2.73801400	0.86954300	1.09352100
O	-1.97480000	0.67024900	2.03152100
O	-3.72080300	1.00181000	-2.19732800
C	-4.19140400	1.19724900	1.24898800
C	-4.71641500	1.33205200	-0.02510100
C	-6.05016100	1.62403700	-0.23553000
C	-6.85250900	1.79276100	0.89560200
C	-6.32263400	1.66082000	2.18088500
C	-4.97349900	1.35593800	2.37683100
H	-6.44676600	1.72154700	-1.24506500
H	-7.90859400	2.03117400	0.77746800
H	-6.97556100	1.79736300	3.04183100

H	-4.54665400	1.24500900	3.37243000
C	4.08455000	-1.57528300	-0.02585800
C	3.21961400	-2.39967900	-0.75360200
C	2.23076900	-1.86211800	-1.56343500
C	2.06200400	-0.47211900	-1.67369400
C	2.95869400	0.35142600	-0.96946200
C	3.94366000	-0.18997200	-0.16146800
H	3.33721600	-3.48286100	-0.68498400
H	1.58244500	-2.53098300	-2.12971500
H	2.86345400	1.43302600	-1.06203000
H	4.62320900	0.47338300	0.37806900
C	5.16909000	-2.14752500	0.83869900
C	1.03245700	0.14445100	-2.50247200
H	1.28440000	1.17592900	-2.74927500
C	6.56774300	-2.08159800	0.20674100
H	6.77710100	-1.02334600	-0.02888600
C	0.41753400	-0.60452800	-3.64913100
H	-0.26484200	0.04250500	-4.20823700
H	1.21321800	-0.94914200	-4.33042700
H	-0.14723100	-1.49483400	-3.34352200
H	5.19556100	-1.60874400	1.80036200
H	4.94417800	-3.20132300	1.07691800
C	7.60894000	-2.57500900	1.20048100
H	7.42431600	-3.62850400	1.46003700
H	8.62198500	-2.51122600	0.78256300
H	7.59047900	-1.99447800	2.13265600
C	6.63296800	-2.88331000	-1.08480300
H	6.39156900	-3.94075000	-0.89266400
H	5.92687900	-2.51003200	-1.83734200
H	7.63989300	-2.84854800	-1.52059300

10c-R

C	-3.34923100	1.56654800	-0.02390800
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O	-2.48075600	1.73535000	-1.17858700
C	-2.78797600	0.28547300	0.62941200
H	-2.66664700	0.34545300	1.71800700
C	-1.44680300	0.88793300	-1.00450300
N	-1.47276900	0.10733500	-0.00025900
C	-0.41753100	0.93439900	-2.06210000
C	-0.93724300	1.22219500	-3.47449100
C	-0.17356100	2.26373000	-2.76956000
H	-2.01552700	1.32894900	-3.55051500
H	-0.45564400	0.67219800	-4.27740600
H	-0.70325000	3.11501400	-2.34942800
H	0.85421800	2.45052200	-3.07369100
C	2.61162600	-0.88898400	-2.77025900
O	1.47238300	-0.06325800	-3.08821800
C	2.19181500	-1.60411200	-1.47889100
H	1.77443700	-2.61313200	-1.60363300
C	0.72663500	0.01038900	-1.96975700
N	1.09756200	-0.73398400	-0.99241600
C	-5.85621700	-1.05595500	-0.95363600
C	-5.73132800	-2.43386700	-0.79927200
C	-4.62561400	-2.98129800	-0.14800800
C	-3.62540000	-2.15960600	0.36194900
C	-3.75544200	-0.78594800	0.20134000
C	-4.85664100	-0.23243500	-0.44967900
H	-6.72084600	-0.63245900	-1.46496700
H	-6.50370200	-3.09194500	-1.19466200
H	-4.53692600	-4.06082700	-0.04349100
H	-2.75128900	-2.58220100	0.85628800
C	-4.77689800	1.27059900	-0.47097000
H	-4.98270400	1.71594600	-1.45369700
H	-5.49014900	1.72214800	0.23478800
C	3.62668300	-2.21954500	0.59050600
C	3.40430800	-1.54691700	-0.60435400

C	4.32588400	-0.63030800	-1.11081200
C	5.48680100	-0.35117700	-0.39959700
C	5.70656700	-1.00441800	0.81190100
C	4.79070900	-1.93623800	1.30101800
H	2.89598000	-2.93878600	0.96376600
H	6.21676700	0.36272600	-0.78033200
H	6.61167200	-0.79308300	1.37855000
H	4.98779300	-2.44573700	2.24219600
C	3.85518300	-0.05119700	-2.42015500
H	3.56173300	1.00765900	-2.32449700
H	2.76791500	-1.55381600	-3.62355400
H	4.62082500	-0.09166600	-3.20547200
H	-3.24554800	2.47525000	0.58244800
C	-0.31857100	-1.34900100	2.53480700
N	-0.86239300	-1.56385100	3.54539300
Cu	0.29414900	-1.07477500	0.81349300
C	-0.21674400	-2.89329900	0.19519900
N	-0.36659400	-3.95186600	-0.27944400
C	0.81981900	4.18968600	-0.00247200
C	-0.04086400	3.75750600	0.99854200
C	0.15870300	2.52279300	1.60820500
C	1.19610500	1.66030300	1.21674200
C	2.04590900	2.13444600	0.19903600
C	1.87900500	3.37585400	-0.39394600
H	-0.86542400	4.38301400	1.33467900
H	2.88742400	1.50341200	-0.09160000
H	2.57866100	3.71046000	-1.15909800
C	1.51349800	0.35005000	1.81065900
H	2.35188200	-0.10090700	1.26541900
C	1.79794300	0.27931600	3.29038400
H	2.61716800	0.98577900	3.50618700
H	0.94973000	0.53472600	3.92801900
H	2.13333300	-0.72609600	3.56775500

H	0.66780300	5.16447800	-0.46219700
Cl	-0.94708500	2.08351200	2.88531900

TS5c-R

C	-3.37146200	1.56261200	-0.11680300
O	-2.49722900	1.69325400	-1.27244300
C	-2.79665900	0.32094300	0.59698700
H	-2.67656100	0.43300600	1.68179200
C	-1.45460800	0.86606800	-1.05960900
N	-1.47941800	0.12805000	-0.02280300
C	-0.41659700	0.88667000	-2.10965400
C	-0.91894900	1.16021200	-3.53030300
C	-0.15528000	2.20562600	-2.83086500
H	-1.99522400	1.27471500	-3.62106400
H	-0.43165500	0.59671600	-4.32032600
H	-0.68349300	3.06635800	-2.42813200
H	0.87708300	2.38172400	-3.12555400
C	2.59539700	-0.99113100	-2.75562200
O	1.47226800	-0.15379200	-3.10266100
C	2.15602500	-1.66399900	-1.44684500
H	1.73546100	-2.67468700	-1.54298300
C	0.71768500	-0.04791700	-1.99145100
N	1.06505500	-0.77444400	-0.99420700
C	-5.83928600	-1.13600700	-0.93059900
C	-5.69695600	-2.50301500	-0.70915300
C	-4.58689600	-3.00375600	-0.02833400
C	-3.59956700	-2.14517800	0.44507600
C	-3.74838000	-0.78248900	0.21910300
C	-4.85313800	-0.27568400	-0.46278600
H	-6.70690100	-0.74954500	-1.46561600
H	-6.45884300	-3.18972400	-1.07504900
H	-4.48471600	-4.07574400	0.12852000
H	-2.72126500	-2.53148400	0.96197200

C	-4.79206100	1.22538900	-0.55845900
H	-4.99572400	1.61788900	-1.56388700
H	-5.51658000	1.70253500	0.11832500
C	3.55740200	-2.22148800	0.66122400
C	3.35968300	-1.59048500	-0.56068800
C	4.30309100	-0.71084800	-1.09148300
C	5.46316100	-0.42752800	-0.38018000
C	5.65822100	-1.03704600	0.85801900
C	4.71937700	-1.93155900	1.37299100
H	2.81006600	-2.91594600	1.04851900
H	6.21034300	0.25741000	-0.78041500
H	6.56203400	-0.82161800	1.42529100
H	4.89812300	-2.40896200	2.33453800
C	3.85206200	-0.16607700	-2.42205000
H	3.57708800	0.89984300	-2.35841000
H	2.74450800	-1.68084100	-3.59032500
H	4.62210700	-0.24352600	-3.20031200
H	-3.28600600	2.49914300	0.44851300
C	-0.34417300	-1.04915500	2.58890300
N	-0.94813600	-1.17849000	3.58073600
Cu	0.22543200	-1.04828200	0.83346300
C	-0.14504200	-2.94990500	0.40109600
N	-0.18019600	-4.06024200	0.03341700
C	1.04486300	4.09548200	-0.20571300
C	0.11431000	3.79622200	0.78071200
C	0.20610900	2.60242400	1.49025900
C	1.20055400	1.65097500	1.21317800
C	2.12286500	1.98832400	0.20484900
C	2.06359400	3.18905800	-0.48458400
H	-0.68212200	4.49491900	1.02873100
H	2.93013600	1.28379600	-0.00336200
H	2.81687400	3.42040400	-1.23683500
C	1.42603500	0.38333900	1.93539000

H	2.23232300	-0.18342200	1.45124900
C	1.70849500	0.46620600	3.41537800
H	2.57745800	1.13306800	3.54195300
H	0.88081000	0.86378600	4.00656400
H	1.96907500	-0.51835300	3.81678100
H	0.97780700	5.03947800	-0.74348000
Cl	-0.97767200	2.33598500	2.74502900

c-R-pro

C	-2.12283500	-0.57363500	-0.81102800
N	-2.87987400	-0.15992300	-1.58728500
C	2.91914800	0.13951500	-0.21089700
C	1.92378200	1.09623700	-0.06338400
C	0.59536300	0.70131200	0.04882400
C	0.22654700	-0.64690000	0.00985100
C	1.24990800	-1.58540400	-0.13950100
C	2.58180100	-1.20794900	-0.24720100
H	2.16431300	2.15644200	-0.03351000
H	0.98500000	-2.64247500	-0.17344700
H	3.35272700	-1.96655000	-0.36396400
C	-1.19596300	-1.14666600	0.17088500
H	-1.17472200	-2.22621200	-0.04679100
C	-1.72722500	-0.97570000	1.60028000
H	-1.05285700	-1.48292200	2.29985600
H	-1.78579900	0.08168200	1.87773200
H	-2.72738100	-1.41327600	1.69443400
H	3.95761700	0.45214400	-0.29824800
Cl	-0.60370200	1.96210400	0.23576200

10c-S

C	-3.91552400	0.35751600	-1.86191800
O	-3.14339400	-0.84548000	-2.13994200
C	-3.25586600	0.89667400	-0.56991600

H	-2.99078500	1.96325200	-0.59624100
C	-2.09975100	-0.83213800	-1.28595900
N	-2.03391300	0.10166000	-0.42654100
C	-1.12854700	-1.93688900	-1.44225600
C	-1.63904800	-3.20705100	-2.10031200
C	-0.72408900	-2.33737000	-2.86351500
H	-2.69268100	-3.19777600	-2.36311000
H	-1.25728600	-4.14106900	-1.70035200
H	-1.12402600	-1.71857900	-3.66363700
H	0.30966800	-2.65723700	-2.98896200
C	1.39746600	-3.26866000	0.78086700
O	0.33387200	-3.33641800	-0.19434400
C	1.30012000	-1.83713300	1.33200100
H	0.76849600	-1.74262200	2.28869500
C	-0.08523300	-2.07761000	-0.39941100
N	0.46133800	-1.16147500	0.31487000
C	-6.44358600	-0.37354600	0.81697100
C	-6.27542700	-0.24319500	2.19265700
C	-5.09676800	0.28408800	2.72222600
C	-4.06564200	0.69504600	1.88337700
C	-4.24540300	0.56610100	0.51186300
C	-5.41499500	0.03356500	-0.02483700
H	-7.36433900	-0.79121200	0.40955100
H	-7.07159000	-0.56118000	2.86411100
H	-4.97823200	0.36947600	3.80060200
H	-3.13194900	1.08858000	2.28702300
C	-5.36529400	0.00887400	-1.52953000
H	-5.64363500	-0.95950400	-1.96686500
H	-6.04163800	0.75709700	-1.96861200
C	3.22063200	-0.25509900	2.06986100
C	2.72390800	-1.37943500	1.42358600
C	3.57441000	-2.30059500	0.81142300
C	4.95002700	-2.11876900	0.85814000

C	5.45545600	-0.99391200	1.50622300
C	4.59998000	-0.06503400	2.09787100
H	2.54183600	0.44525200	2.55847200
H	5.62389000	-2.84341700	0.40070900
H	6.53254200	-0.84024600	1.55571400
H	5.01330400	0.80704100	2.60115500
C	2.79140800	-3.40551000	0.15431400
H	2.71643800	-3.24809500	-0.93548800
H	1.19097600	-4.04409300	1.52364700
H	3.22570700	-4.40266400	0.29917500
H	-3.80680000	1.00435700	-2.74063100
C	-0.51036200	2.58452500	0.62167400
N	-1.03985000	3.61957600	0.73049200
Cu	-0.03334700	0.79093000	0.51118400
C	-0.38873600	0.51262000	2.43274500
N	-0.53775800	0.23656400	3.55948400
C	4.93004000	1.03561500	-1.33847100
C	4.33580400	2.20561900	-0.89002400
C	2.94989300	2.32844500	-0.86977200
C	2.10978700	1.28384000	-1.29805400
C	2.75511800	0.10743900	-1.72777100
C	4.13158500	-0.02233600	-1.76240600
H	4.93941700	3.04209800	-0.54499600
H	2.12862700	-0.72019200	-2.06393600
H	4.58258900	-0.94988800	-2.11108700
C	0.63896200	1.31603700	-1.39581600
C	-0.02899900	2.42612300	-2.16466500
H	0.16044500	3.42510900	-1.76882400
H	0.33904800	2.39034800	-3.20380800
H	-1.11503700	2.27496300	-2.18924800
H	0.29174700	0.35243500	-1.78442200
H	6.01488700	0.94874700	-1.34716400
Cl	2.30852500	3.82152200	-0.24686300

TS5c-S

C	-3.93277000	0.43722000	-1.81957300
O	-3.18994900	-0.76794700	-2.15608200
C	-3.22435100	0.92831500	-0.53481600
H	-2.93900100	1.98988800	-0.54107700
C	-2.12309200	-0.80263300	-1.33194500
N	-2.01447500	0.10567900	-0.44837100
C	-1.18036500	-1.92074700	-1.55550400
C	-1.70985200	-3.13026800	-2.30333900
C	-0.77305900	-2.22732100	-2.99947200
H	-2.76065100	-3.08428900	-2.57315600
H	-1.34770100	-4.09650200	-1.96658200
H	-1.15717600	-1.54903400	-3.75811600
H	0.25643200	-2.55460500	-3.14060700
C	1.32216600	-3.43747600	0.56797300
O	0.24194900	-3.43382100	-0.39058500
C	1.25017800	-2.04153600	1.20830100
H	0.72940800	-1.99343500	2.17456100
C	-0.14464900	-2.15257600	-0.52176700
N	0.41976800	-1.28990100	0.23992700
C	-6.38885100	-0.32243400	0.91907600
C	-6.17446500	-0.23160300	2.29156800
C	-4.97026200	0.26093100	2.79681400
C	-3.95933000	0.67639500	1.93595700
C	-4.18566400	0.58757500	0.56822400
C	-5.38052500	0.08925300	0.05521500
H	-7.32934400	-0.71380100	0.53116300
H	-6.95437400	-0.55388700	2.97981000
H	-4.81597200	0.31505500	3.87267000
H	-3.00610600	1.04375700	2.31855700
C	-5.37739600	0.10233500	-1.45066600
H	-5.68395300	-0.85057200	-1.90283000

H	-6.05524800	0.87123300	-1.84984500
C	3.20196400	-0.54190400	2.03179800
C	2.68136000	-1.60923600	1.31146300
C	3.50987800	-2.49116700	0.61697300
C	4.88816400	-2.32373900	0.64633900
C	5.41760200	-1.25281000	1.36341700
C	4.58321400	-0.36544600	2.04303200
H	2.53750000	0.11937000	2.58888200
H	5.54569500	-3.01958400	0.12466500
H	6.49698100	-1.11136500	1.40021400
H	5.01569800	0.46194800	2.60259500
C	2.70220900	-3.54231100	-0.09662900
H	2.60416900	-3.31056400	-1.17148300
H	1.12420600	-4.25799100	1.26308600
H	3.13088000	-4.55021500	-0.03054600
H	-3.84166000	1.10805400	-2.68224000
C	-0.40617100	2.51224700	0.51421000
N	-0.93948400	3.54053500	0.67062400
Cu	-0.04338800	0.69614400	0.59684700
C	-0.22623300	0.39457500	2.52934300
N	-0.25034400	0.08650900	3.65778200
C	4.90775600	1.25645400	-1.14834000
C	4.31260300	2.43976800	-0.73722900
C	2.92654300	2.56695300	-0.73399700
C	2.09181400	1.50715000	-1.13045200
C	2.73529200	0.31636900	-1.51684900
C	4.11210600	0.18751000	-1.54661100
H	4.91502700	3.28673400	-0.41693600
H	2.10975800	-0.52602200	-1.81547000
H	4.56327300	-0.75117600	-1.86191100
C	0.62054600	1.54258800	-1.27142800
C	-0.00915100	2.60817200	-2.13293700
H	0.18263400	3.62757900	-1.79457800

H	0.40020800	2.49167200	-3.14962800
H	-1.09491500	2.46623600	-2.18693300
H	0.27271900	0.56686800	-1.62754900
H	5.99263600	1.16859100	-1.14895400
Cl	2.28586000	4.09462600	-0.20127200

c-S-pro

C	2.12211800	-0.57440500	-0.81148100
N	2.87813200	-0.16125800	-1.58904500
C	-2.91903700	0.13921000	-0.21093900
C	-1.92373400	1.09603800	-0.06349000
C	-0.59534000	0.70124500	0.04900200
C	-0.22644200	-0.64701100	0.01062100
C	-1.24969000	-1.58556100	-0.13873600
C	-2.58160500	-1.20820300	-0.24687400
H	-2.16439700	2.15621900	-0.03399200
H	-0.98473100	-2.64263800	-0.17223100
H	-3.35240800	-1.96691400	-0.36364300
C	1.19619300	-1.14645000	0.17197800
C	1.72834500	-0.97378700	1.60077400
H	1.78691400	0.08388700	1.87710900
H	1.05454100	-1.48044100	2.30130400
H	2.72861600	-1.41114500	1.69470600
H	1.17493000	-2.22628400	-0.04436400
H	-3.95748800	0.45181600	-0.29854700
Cl	0.60366200	1.96222700	0.23516700

10d-R

C	-3.31160300	1.82892200	0.05845500
O	-2.34303800	2.06852900	-0.99263700
C	-2.90765300	0.42950700	0.57563500
H	-2.83203300	0.36250200	1.66932900
C	-1.40970000	1.09947200	-0.89021800

N	-1.58644300	0.18886700	-0.01863600
C	-0.30429700	1.20987700	-1.86207500
C	-0.66614200	1.84105800	-3.20849700
C	0.15052700	2.61402200	-2.25979900
H	-1.71407000	2.10176600	-3.32358700
H	-0.18667700	1.40402800	-4.07897100
H	-0.31314800	3.42332500	-1.70063500
H	1.21652300	2.72507200	-2.44686000
C	2.48743700	-0.86654700	-2.83308200
O	1.49915600	0.17179100	-2.99117300
C	1.98443100	-1.66570400	-1.61805500
H	1.48163800	-2.61284100	-1.86109500
C	0.72165900	0.15278700	-1.89469000
N	0.96189500	-0.76987500	-1.03716500
C	-6.00121100	-0.41808800	-1.27621400
C	-6.03241700	-1.80936000	-1.24735100
C	-5.03496600	-2.53166400	-0.59220900
C	-3.98802400	-1.87440200	0.04525300
C	-3.95841900	-0.48594500	0.00537500
C	-4.95285000	0.24162400	-0.64597800
H	-6.78315200	0.14272500	-1.78845600
H	-6.84323700	-2.34002900	-1.74412700
H	-5.06663000	-3.61921900	-0.58647600
H	-3.20146600	-2.43544100	0.54851400
C	-4.72004400	1.72295800	-0.51983400
H	-4.79334200	2.26786100	-1.47072300
H	-5.44494700	2.18822700	0.16481900
C	3.31157100	-2.59077100	0.40780200
C	3.19089000	-1.82513200	-0.74488000
C	4.24339400	-1.03444500	-1.20494500
C	5.43850400	-0.98785300	-0.49633600
C	5.55732600	-1.73387600	0.67469300
C	4.50486200	-2.53204400	1.12393700

H	2.48295400	-3.21747700	0.74399100
H	6.27060500	-0.37741600	-0.84773300
H	6.48673600	-1.70183400	1.24054800
H	4.61987700	-3.11830800	2.03383900
C	3.86741000	-0.29960900	-2.46326600
H	3.77640500	0.78423700	-2.28967800
H	2.49438300	-1.43497800	-3.76691400
H	4.60070100	-0.43289500	-3.26927700
H	-3.18679800	2.63870800	0.78820300
C	-0.81493900	-2.30458000	2.03401200
N	-1.37034800	-2.87514100	2.88920300
Cu	-0.12233200	-1.45612300	0.53335900
C	-0.81786900	-2.86712600	-0.70034900
N	-1.08349800	-3.65374200	-1.52463200
C	-0.16293500	3.63608300	1.70469100
C	-0.82433700	2.77654500	2.53894200
C	-0.41287800	1.43703900	2.72590700
C	0.68241400	0.94541700	2.00396100
C	1.45464500	1.86935100	1.20066500
C	1.01641100	3.21922000	1.04952400
H	-1.70406300	3.12242900	3.08341100
C	1.08468200	-0.46596300	2.03923900
H	1.90068200	-0.68356800	1.34902600
C	1.37207800	-1.14523000	3.35263400
H	2.19733500	-0.59308300	3.83449700
H	0.53579600	-1.18136200	4.05251400
H	1.70550100	-2.17638800	3.19130000
H	-0.50754100	4.66207200	1.57234900
C	-1.21799000	0.61690800	3.68891300
H	-1.42067000	-0.40102400	3.33515300
H	-0.70159700	0.51979600	4.65445800
H	-2.17922000	1.10426400	3.89654800
C	1.77891500	4.13938600	0.28992300

C	2.96835300	3.77105000	-0.28299700
H	1.40729300	5.16051000	0.19552900
C	2.69906000	1.53374000	0.60601600
C	3.43342200	2.45299000	-0.10630700
H	3.55958900	4.49131500	-0.84546400
H	3.12839500	0.54403800	0.74546300
H	4.40329100	2.15955000	-0.50877800

TS5d-R

C	-3.29246200	1.77918700	-0.04542700
O	-2.34112600	1.98826200	-1.11986600
C	-2.86650600	0.40426300	0.51539700
H	-2.78043100	0.37385400	1.61063800
C	-1.39250400	1.03788300	-0.99257600
N	-1.54806900	0.16108900	-0.08149200
C	-0.29527100	1.12790200	-1.97591600
C	-0.67172000	1.70075300	-3.34353100
C	0.13705000	2.52165600	-2.42839000
H	-1.72346200	1.94283600	-3.46537900
H	-0.18835000	1.23718200	-4.19814900
H	-0.33550900	3.34671400	-1.90049300
H	1.20098500	2.63862400	-2.62330700
C	2.53881000	-0.94144900	-2.84276600
O	1.53893100	0.07780800	-3.05613400
C	2.02866200	-1.69787000	-1.60201100
H	1.55602500	-2.66932300	-1.80676000
C	0.74576400	0.08443700	-1.96843300
N	0.97865400	-0.80411700	-1.07745700
C	-5.95950900	-0.54391500	-1.28730700
C	-5.96434700	-1.93450300	-1.22629300
C	-4.94675600	-2.62296800	-0.56564300
C	-3.90678800	-1.93184100	0.04741400
C	-3.90625700	-0.54400400	-0.02067400

C	-4.91871100	0.14963300	-0.68131800
H	-6.75524400	-0.00984100	-1.80681900
H	-6.76914300	-2.49144400	-1.70369100
H	-4.95628800	-3.71059400	-0.53691900
H	-3.10222900	-2.46782600	0.54964500
C	-4.70760600	1.63729100	-0.59829500
H	-4.80452300	2.15504600	-1.56211500
H	-5.42816500	2.11014900	0.08579100
C	3.31983200	-2.47711800	0.50651000
C	3.21615300	-1.78318800	-0.69283800
C	4.26363400	-0.99660500	-1.16993100
C	5.43854900	-0.88452100	-0.43503200
C	5.54148900	-1.55969000	0.77968900
C	4.49278800	-2.35197900	1.24797400
H	2.49565300	-3.10321700	0.85475000
H	6.26734900	-0.27719000	-0.79964300
H	6.45513500	-1.47605500	1.36566400
H	4.59571300	-2.88331900	2.19250600
C	3.90604500	-0.34059500	-2.47684400
H	3.80299100	0.75081900	-2.37071900
H	2.56693200	-1.54537800	-3.75366800
H	4.65746200	-0.51406700	-3.25827900
H	-3.16427200	2.61661600	0.65201600
C	-0.66605500	-2.03666100	2.20820800
N	-1.22092300	-2.56667300	3.09105900
Cu	-0.13209200	-1.44263900	0.53350000
C	-0.66701200	-3.05186400	-0.50080100
N	-0.84103600	-3.96253100	-1.21468400
C	-0.28860700	3.68017500	1.58967400
C	-0.93946100	2.87107200	2.47910000
C	-0.52122400	1.54506400	2.74430200
C	0.56206100	1.01437400	2.03699000
C	1.32889000	1.88950600	1.17671500

C	0.88828500	3.22856800	0.95316300
H	-1.81408300	3.24669100	3.01181000
C	0.99101900	-0.39052000	2.16391200
H	1.76527700	-0.65905600	1.44247800
C	1.39776600	-0.91727900	3.51469700
H	2.26620500	-0.31841500	3.83853600
H	0.62633300	-0.84332100	4.28390700
H	1.70885300	-1.96554600	3.45455900
H	-0.63629200	4.69610200	1.40015500
C	-1.30297700	0.80077200	3.78649900
H	-1.45874200	-0.25789500	3.55540200
H	-0.79216600	0.84454400	4.75953700
H	-2.28633500	1.26642200	3.93069800
C	1.64809900	4.10818600	0.14514000
C	2.83973900	3.71305900	-0.40461800
H	1.27427000	5.12205500	-0.00324400
C	2.57360800	1.52440500	0.59974200
C	3.30702200	2.40742500	-0.15787600
H	3.43088800	4.40404300	-1.00283000
H	3.00562900	0.54413600	0.78909300
H	4.27841700	2.09600800	-0.54230200

d-R-pro

C	1.86108000	-1.80619500	-0.75530600
N	1.86714600	-2.71141000	-1.48253900
C	-1.28832200	2.22602100	-0.19325500
C	-1.63379400	0.86264400	-0.06991600
C	-0.59688700	-0.11366800	0.03298400
C	0.76680700	0.31732000	0.00520600
C	1.07177700	1.66574300	-0.10370100
C	0.02288700	2.61069400	-0.20599300
C	1.90643500	-0.67569000	0.17767600
H	2.84324800	-0.15946600	-0.07258600

C	2.03770300	-1.16111800	1.62934300
H	2.19376500	-0.29471600	2.28362100
H	1.12938500	-1.67394500	1.96373200
H	2.88646600	-1.84543700	1.74204700
H	-2.08575300	2.96500300	-0.27252100
C	2.48490800	2.18318700	-0.10972400
H	3.04181300	1.89535100	0.79331500
H	3.05945900	1.82227600	-0.97435900
H	2.49384400	3.27796600	-0.15480600
C	-0.99080000	-1.47198000	0.16471900
C	-2.98970400	0.45842600	-0.04140500
C	-2.31455700	-1.83312100	0.19163600
H	-0.24047000	-2.25587000	0.22736500
C	-3.33043300	-0.86183000	0.08842900
H	-3.75833600	1.22725800	-0.12433400
H	-2.58030200	-2.88415600	0.28875500
H	-4.37608500	-1.16279000	0.10962600
H	0.28033700	3.66579500	-0.29623200

10d-S

C	-3.99455900	1.56745300	1.35068500
O	-3.11514000	2.35674600	0.50217800
C	-3.49693200	0.12374400	1.10475900
H	-3.32819400	-0.46757900	2.01548000
C	-2.14592500	1.52051900	0.07351400
N	-2.22703400	0.29286600	0.39443600
C	-1.09430600	2.14121800	-0.75979700
C	-1.53473300	3.34978500	-1.58470900
C	-0.65657700	3.56744800	-0.42390700
H	-2.58604200	3.60611400	-1.49292900
H	-1.11017100	3.42562900	-2.58065600
H	-1.07893900	3.98973800	0.48563300
H	0.39618700	3.77992700	-0.60211400

C	1.51495600	0.81925100	-2.87653500
O	0.53246900	1.78589000	-2.44773600
C	1.08848300	-0.46888000	-2.16505900
H	0.42576700	-1.12803700	-2.74308700
C	-0.07740900	1.25703200	-1.37361600
N	0.26866400	0.06330800	-1.04750100
C	-6.67693800	0.04895300	-0.78903500
C	-6.63742600	-1.17725900	-1.44664500
C	-5.55517100	-2.04248600	-1.28079900
C	-4.49398400	-1.69764600	-0.44959200
C	-4.54431600	-0.47377100	0.20597300
C	-5.61729900	0.39873400	0.03980300
H	-7.52220400	0.72334300	-0.92654000
H	-7.45857300	-1.46256700	-2.10248400
H	-5.53502900	-2.99274100	-1.81070700
H	-3.63462700	-2.35820400	-0.33005800
C	-5.43838400	1.64812400	0.86040800
H	-5.60995600	2.57679900	0.29961500
H	-6.12534400	1.66901800	1.71945400
C	2.60548200	-2.46624200	-1.49769300
C	2.38558400	-1.13447800	-1.82349800
C	3.44609100	-0.24618200	-2.01503000
C	4.75561000	-0.68881300	-1.88810200
C	4.98437300	-2.02529700	-1.56598900
C	3.92136400	-2.90469600	-1.36452100
H	1.76150900	-3.14839800	-1.38523800
H	5.59049600	-0.00504800	-2.04621300
H	6.00736300	-2.38825000	-1.47451100
H	4.12028800	-3.94754400	-1.12292200
C	2.93594300	1.12212000	-2.38366200
H	2.88841600	1.77912400	-1.49776800
H	1.45032200	0.76610500	-3.96705300
H	3.54874800	1.63617800	-3.13419100

H	-3.85310700	1.93655900	2.37345200
C	-1.04536100	-2.20841400	1.78978100
N	-1.60405600	-2.84007600	2.59764300
Cu	-0.42696600	-1.15962400	0.38772400
C	-0.94067800	-2.50436900	-0.97470500
N	-1.12733400	-3.25295000	-1.85415300
C	4.72258200	-0.22008200	1.38148500
C	4.03180900	-1.33993500	1.74451300
C	2.62896600	-1.33550900	1.92762600
C	1.91562900	-0.14892600	1.74384500
C	2.63646300	1.05821000	1.41112700
C	4.04801700	1.00654000	1.20702500
H	4.56241500	-2.28275700	1.87508900
C	0.44973300	-0.05272000	1.93978200
C	-0.04420900	-0.12070100	3.36241300
H	0.23663500	-1.03524600	3.89173700
H	0.40637800	0.73012000	3.90346700
H	-1.13391300	-0.02419000	3.41881800
H	0.03843100	0.83953700	1.46639700
H	5.80037100	-0.25721200	1.21992200
C	1.98977900	-2.65299700	2.24863000
H	1.35788300	-2.62794000	3.14269800
H	1.34020100	-3.00064700	1.43248700
H	2.75773400	-3.41967600	2.40400500
C	4.76158300	2.17363500	0.84605500
C	2.02908700	2.33845600	1.31816300
C	2.74832900	3.46340800	0.98569300
C	4.13022200	3.38484800	0.72586800
H	5.83620600	2.08657600	0.68040300
H	0.97245300	2.45874700	1.54818800
H	2.24509800	4.42934700	0.94462500
H	4.68963400	4.27871700	0.45695800

TS5d-S

C	-4.01695500	1.49469200	1.35806500
O	-3.13816600	2.34259500	0.56877900
C	-3.47046600	0.07604200	1.07142500
H	-3.28817200	-0.53738800	1.96506700
C	-2.14376400	1.55051800	0.11460000
N	-2.20080000	0.30725800	0.37819000
C	-1.09413200	2.23556000	-0.66740900
C	-1.53738000	3.49319000	-1.41173900
C	-0.67311200	3.63834000	-0.22881200
H	-2.59140700	3.73577900	-1.31380900
H	-1.10292500	3.64008200	-2.39542700
H	-1.10862000	3.99552700	0.70223400
H	0.37980700	3.86966700	-0.38019500
C	1.54789600	1.08813300	-2.83728900
O	0.54530700	2.00975200	-2.36398300
C	1.13911200	-0.24797000	-2.20642200
H	0.49318200	-0.88356000	-2.82860100
C	-0.06015000	1.40432000	-1.32583100
N	0.29979800	0.20021700	-1.06562800
C	-6.61997500	-0.04307300	-0.86894400
C	-6.53660200	-1.25207000	-1.55359200
C	-5.43189500	-2.08976300	-1.39318800
C	-4.39226500	-1.73456200	-0.53945500
C	-4.48777000	-0.52909000	0.14465900
C	-5.58210200	0.31704800	-0.01730000
H	-7.48217200	0.61020700	-1.00313800
H	-7.34046500	-1.54539800	-2.22706300
H	-5.37724800	-3.02607900	-1.94500600
H	-3.51516700	-2.37229000	-0.42342400
C	-5.45029900	1.55272400	0.83247200
H	-5.62718900	2.48827300	0.28480900
H	-6.15969000	1.54300500	1.67320300

C	2.69664200	-2.25896400	-1.67922800
C	2.44924700	-0.91121500	-1.90616200
C	3.49335500	0.00812800	-2.03325500
C	4.81170600	-0.41671700	-1.93981900
C	5.06724900	-1.76854100	-1.71692300
C	4.02135900	-2.68023000	-1.58131000
H	1.86644900	-2.96400100	-1.62028100
H	5.63269400	0.29255500	-2.05191000
H	6.09728700	-2.11790900	-1.65561900
H	4.24046600	-3.73452600	-1.41982800
C	2.95668500	1.38771500	-2.30896900
H	2.88536400	1.97871700	-1.37860200
H	1.49844500	1.09770500	-3.93000600
H	3.56506500	1.96732100	-3.01408900
H	-3.91634700	1.82654600	2.39805600
C	-0.99448800	-2.15159700	1.73960200
N	-1.60193600	-2.82905300	2.47339900
Cu	-0.43184100	-1.16438500	0.27769900
C	-0.79394200	-2.49900600	-1.12979100
N	-0.88770700	-3.23612700	-2.03372400
C	4.60456300	-0.36871100	1.36529200
C	3.93737100	-1.52494900	1.64771200
C	2.54095900	-1.55327900	1.87502900
C	1.81470300	-0.36445100	1.81035000
C	2.50609300	0.87644900	1.55387900
C	3.91233000	0.85955800	1.31312400
H	4.48147200	-2.46845300	1.68111300
C	0.35678500	-0.29561000	2.08315300
C	-0.03754400	-0.41745200	3.53451000
H	0.29987200	-1.34453800	4.00676200
H	0.44628600	0.42330000	4.06107200
H	-1.12022700	-0.34035700	3.67548000
H	-0.10273700	0.60233100	1.66858800

H	5.67764600	-0.37706300	1.17283000
C	1.92312000	-2.89872100	2.11537000
H	1.29273400	-2.93727400	3.01002200
H	1.27937800	-3.20650400	1.27882600
H	2.70455000	-3.65964100	2.22462600
C	4.60406500	2.06182600	1.03498100
C	1.87845000	2.15033000	1.57012400
C	2.57784500	3.30782400	1.31733500
C	3.95597300	3.27000100	1.02879800
H	5.67520900	2.00258600	0.83745800
H	0.82148000	2.23797600	1.81560400
H	2.06113300	4.26646700	1.35998700
H	4.49863800	4.19070900	0.82373800

d-S-pro

C	2.74413600	-0.94977600	-0.74140500
N	3.71107300	-0.84169400	-1.37497600
C	-1.28142600	2.14799600	-0.00504600
C	0.05819900	2.38600800	0.10783600
C	1.00620800	1.33259600	0.13529500
C	0.56433700	0.02247200	0.02756000
C	-0.83934800	-0.26010700	-0.04444300
C	-1.76793800	0.82397400	-0.07071800
H	0.42515800	3.40984200	0.17918600
C	1.52976600	-1.15339800	0.05242400
C	1.87228800	-1.58857700	1.48428600
H	2.36244800	-0.77841200	2.03645700
H	0.94747000	-1.84514100	2.01457900
H	2.53639200	-2.46072700	1.48724600
H	1.04456700	-2.00419400	-0.44532700
H	-1.99420100	2.97236900	-0.02821000
C	2.45090800	1.72522200	0.27479000
H	2.96469200	1.75394000	-0.69524000

H	2.52592300	2.72565300	0.71719900
H	3.02816200	1.04375200	0.91015300
C	-3.15654400	0.56621800	-0.15016100
C	-1.38063800	-1.57310600	-0.07104000
C	-2.73403000	-1.79431500	-0.13880700
C	-3.63862200	-0.71576500	-0.18616100
H	-3.83674100	1.41791500	-0.17642000
H	-0.72622400	-2.44087000	-0.02106800
H	-3.11000800	-2.81581800	-0.15460600
H	-4.70892300	-0.90310500	-0.24557400

10e-R

C	-4.04229300	-0.16790900	-1.24349200
O	-3.48008900	-1.48827700	-1.42913500
C	-3.01434400	0.49771900	-0.30676800
H	-2.75154800	1.51845100	-0.60253000
C	-2.21663200	-1.44042800	-0.94851400
N	-1.82975000	-0.36387200	-0.38477700
C	-1.42639600	-2.66866800	-1.15492300
C	-2.15176600	-3.90626000	-1.66966000
C	-1.28775000	-3.15922800	-2.59795700
H	-3.22898700	-3.80675400	-1.76367200
H	-1.79564600	-4.85538200	-1.28006400
H	-1.74226800	-2.51514200	-3.34709100
H	-0.30853600	-3.55078000	-2.86287400
C	1.49486100	-4.05465200	0.38735700
O	0.23930000	-4.13938000	-0.31303500
C	1.34101000	-2.79326200	1.25001200
H	0.95997200	-2.96904500	2.26677100
C	-0.26801500	-2.89039300	-0.27429200
N	0.30350800	-2.04802800	0.50665500
C	-5.77632300	-0.12728300	2.08054500
C	-5.22037600	0.18355900	3.31832200

C	-3.89805100	0.61822200	3.41619200
C	-3.10990100	0.75392600	2.27714200
C	-3.67403600	0.44635600	1.04518500
C	-4.99214200	0.00537100	0.94059000
H	-6.80734200	-0.47409200	2.00880600
H	-5.82212500	0.08034300	4.22017700
H	-3.47453300	0.84723100	4.39249100
H	-2.06736000	1.06814900	2.35026800
C	-5.36989600	-0.24832000	-0.49454000
H	-5.85552100	-1.21942300	-0.66008900
H	-6.06292600	0.51870200	-0.87149300
C	3.26003700	-1.28033900	2.13806500
C	2.71512600	-2.19604100	1.24751000
C	3.48290800	-2.76514000	0.22902100
C	4.81388300	-2.40199100	0.07508900
C	5.36763600	-1.48580200	0.96725500
C	4.60173200	-0.93474600	1.99414400
H	2.64657900	-0.83773400	2.92256600
H	5.42157100	-2.84050500	-0.71579500
H	6.41549100	-1.20471300	0.86811500
H	5.05445300	-0.22636400	2.68623800
C	2.67419700	-3.76266400	-0.55445300
H	2.29241900	-3.30852400	-1.48456600
H	1.61438700	-4.98267100	0.95378500
H	3.23496900	-4.66327000	-0.83311900
H	-4.11811400	0.29194700	-2.23764200
C	1.00534100	-0.60146100	-1.86457800
N	1.28515300	-1.10223300	-2.88444800
Cu	0.50573200	0.02602000	-0.12233200
C	0.49318600	0.78383000	1.64386100
N	0.49384700	1.21576600	2.73118300
C	-2.63192400	4.08908300	-1.25334300
C	-1.96396700	4.06237000	-0.02834000

C	-0.79111400	3.33669500	0.11420400
C	-0.25941000	2.62977600	-0.97779600
C	-0.95937200	2.63821900	-2.19575700
C	-2.13152300	3.36888300	-2.33592700
H	-2.36632700	4.60763800	0.82317200
H	-0.56054800	2.06502000	-3.03386800
H	-2.65417900	3.38011300	-3.29088200
C	1.04174200	1.96676400	-0.93806000
H	1.36115800	1.65729000	-1.93576600
H	-3.55033200	4.66412100	-1.35886400
H	-0.28778100	3.29140900	1.07903100
C	4.98763400	3.51497700	-0.11030500
C	4.60045400	2.18307200	0.52024100
C	3.39465700	1.56869900	-0.17478800
C	2.19949600	2.51872500	-0.16351200
C	2.59659700	3.85767300	-0.82401200
C	3.80244800	4.47129100	-0.12052900
H	5.83863600	3.96411600	0.42077000
H	5.44507700	1.47998400	0.49380200
H	3.64680800	1.32454700	-1.22295200
H	2.84045200	3.67569400	-1.88569300
H	3.52401700	4.71755700	0.91774300
H	4.35619000	2.33826000	1.58590500
H	3.11510000	0.61964900	0.30604800
H	1.91523100	2.72165300	0.87986700
H	1.74496800	4.55296200	-0.80852600
H	4.07055400	5.42013500	-0.60663900
H	5.32053400	3.34093400	-1.14784800

TS5e-R

C	4.06278300	0.14123800	1.76417800
O	3.36536000	-1.12919500	1.85751800
C	3.49335400	0.73908400	0.45751400

H	3.13093000	1.77055800	0.56986000
C	2.40298300	-1.11012700	0.92038300
N	2.36079300	-0.12490200	0.10723400
C	1.46005500	-2.24592800	0.96469800
C	1.92652100	-3.53417200	1.60310100
C	0.96249800	-2.68563100	2.33808300
H	2.95874000	-3.55041700	1.94124700
H	1.56864000	-4.44947500	1.13946200
H	1.30249100	-2.08647500	3.17997300
H	-0.08046800	-3.00040600	2.37865100
C	-0.72208200	-3.32508600	-1.70114400
O	0.36609200	-3.49822800	-0.77527800
C	-0.88962800	-1.79585300	-1.79502900
H	-0.37647200	-1.31271100	-2.63905200
C	0.48363100	-2.30682300	-0.14559000
N	-0.23003600	-1.33320400	-0.55850900
C	6.91664400	-0.10565200	-0.67192500
C	6.88834700	0.16208000	-2.03755300
C	5.72936400	0.64733900	-2.64509400
C	4.58130400	0.87351200	-1.89268800
C	4.61858700	0.60915600	-0.52963800
C	5.77028600	0.11951800	0.08210800
H	7.82310700	-0.48960700	-0.20365900
H	7.77903700	-0.01257000	-2.63934700
H	5.72335700	0.84581000	-3.71550900
H	3.66325500	1.23698200	-2.35538000
C	5.56197500	-0.07596400	1.56065300
H	5.86443100	-1.06914800	1.91925300
H	6.13484900	0.65682500	2.14771300
C	-3.07792500	-0.46547000	-2.23616900
C	-2.37506400	-1.59871500	-1.84392700
C	-3.03610000	-2.77252900	-1.47928500
C	-4.42537000	-2.81857400	-1.47134200

C	-5.13787200	-1.68013300	-1.84450500
C	-4.47093400	-0.51526500	-2.22752800
H	-2.53098000	0.42288000	-2.56135000
H	-4.95084000	-3.73236400	-1.19374200
H	-6.22676600	-1.70543500	-1.85243900
H	-5.04502300	0.35629400	-2.54046500
C	-2.05176900	-3.86025200	-1.14240100
H	-1.95455500	-3.98960500	-0.05098000
H	-0.43064500	-3.80869000	-2.63787600
H	-2.32624100	-4.83987900	-1.55367500
H	3.80219800	0.70271400	2.66713500
C	0.50480400	1.18475100	1.82537600
N	0.97352400	1.28093500	2.89680700
Cu	0.32107700	0.86143100	-0.07623400
C	-0.12075000	1.50709000	-1.85940100
N	-0.53763700	1.77387800	-2.92254600
C	-1.85323700	5.42365100	-0.96053700
C	-2.50280000	4.27991900	-1.41940100
C	-2.46980600	3.11868900	-0.66942000
C	-1.80270900	3.09812500	0.57078900
C	-1.15509700	4.26648600	1.02290500
C	-1.17673300	5.41794200	0.26130800
H	-3.00184600	4.28428300	-2.38515200
H	-0.61207100	4.23115300	1.96762100
H	-0.66594800	6.31351100	0.60792200
C	-1.77824300	1.94577200	1.41426600
H	-1.45513500	2.13912600	2.43771200
H	-1.86435000	6.32813100	-1.56609100
H	-2.94791200	2.21492000	-1.04309400
C	-4.54724300	-1.19955800	2.42447200
C	-3.12861300	-1.60286700	2.04471400
C	-2.16673700	-0.42954500	2.14170700
C	-2.61637800	0.73520000	1.25863600

C	-4.05454100	1.16063900	1.67003600
C	-5.01317100	-0.02165500	1.58068400
H	-5.23606700	-2.04764900	2.30323200
H	-2.77896600	-2.42794800	2.68296900
H	-2.09695100	-0.07767700	3.18644500
H	-4.02827400	1.54515400	2.70454900
H	-5.08944500	-0.33758700	0.52727500
H	-3.12547900	-1.97723600	1.00641900
H	-1.15501000	-0.73204400	1.84471500
H	-2.65167300	0.40602100	0.20695600
H	-4.40092900	1.98571900	1.03252400
H	-6.01668800	0.30512300	1.88843200
H	-4.57366000	-0.91968300	3.49152300

e-R-pro

C	-0.15200900	2.30668200	0.28601100
N	-0.16785800	3.43153900	-0.00174500
C	-3.84925100	-1.04365700	-0.37491200
C	-3.22854100	-0.21058400	-1.30109500
C	-2.03415700	0.42264900	-0.98006200
C	-1.44755700	0.22993000	0.27117500
C	-2.07637700	-0.60212700	1.19506700
C	-3.27106100	-1.23810200	0.87462300
H	-3.67982000	-0.04840400	-2.27832100
H	-1.62197400	-0.75524800	2.17499200
H	-3.75284300	-1.88436600	1.60621800
C	-0.11886700	0.87712800	0.60599000
H	0.05115000	0.79037100	1.69360800
H	-4.78632200	-1.53710800	-0.62629600
H	-1.55733100	1.08797300	-1.70116300
C	3.65377500	-1.26171200	-0.05781100
C	3.59229100	0.22157300	-0.39937100
C	2.39774500	0.89272200	0.26799300

C	1.08394500	0.20486100	-0.10115200
C	1.15147900	-1.28370600	0.23258500
C	2.34908800	-1.95344200	-0.43195400
H	4.50358100	-1.74069700	-0.56366700
H	4.52143100	0.72838300	-0.10462300
H	2.51944700	0.84483700	1.36583100
H	1.23207400	-1.39338000	1.33047500
H	2.21972700	-1.91374800	-1.52687900
H	3.50722100	0.33903000	-1.49296600
H	2.35937000	1.95899000	0.00366900
H	0.92728000	0.31088100	-1.19118400
H	0.22019400	-1.78610700	-0.06342900
H	2.38092600	-3.01814900	-0.16226100
H	3.82787800	-1.37731700	1.02569200

10e-S

C	4.26974600	0.26002700	1.58134900
O	3.65276300	-1.05484800	1.49731200
C	3.48348800	1.06342100	0.52076900
H	3.10659100	2.02708000	0.89194400
C	2.55610900	-0.92010800	0.74189800
N	2.34332000	0.20861800	0.17244200
C	1.65001400	-2.08607300	0.70132400
C	2.10874700	-3.40570200	1.26406900
C	1.14275300	-2.59703200	2.04470000
H	3.13840000	-3.45174500	1.60778500
H	1.75034000	-4.28966900	0.74212200
H	1.48096000	-2.04328500	2.91933200
H	0.09227900	-2.88887500	2.06007600
C	-0.30932800	-2.84488000	-2.23207700
O	0.75545600	-3.09714300	-1.29790400
C	-0.62601600	-1.35199200	-2.03732300
H	-0.08938800	-0.66091200	-2.70332100

C	0.69221000	-2.06296700	-0.42587400
N	-0.12058200	-1.11222300	-0.66747800
C	6.72412400	0.70094700	-1.23085700
C	6.47361500	1.22075800	-2.49751000
C	5.21364100	1.72315800	-2.82615400
C	4.18559900	1.71645100	-1.88893900
C	4.44602200	1.20402200	-0.62437600
C	5.69843700	0.69293500	-0.29222100
H	7.70803100	0.30308000	-0.98223100
H	7.26804100	1.23085600	-3.24225600
H	5.03350200	2.11862100	-3.82428800
H	3.19064000	2.08753400	-2.13693800
C	5.72841400	0.20272700	1.13116900
H	6.13002000	-0.81395700	1.23772500
H	6.34627000	0.85245900	1.76819500
C	-2.89822000	-0.16076800	-2.47275500
C	-2.11224300	-1.27681400	-2.20933400
C	-2.67410900	-2.55060300	-2.09966400
C	-4.04946700	-2.71777900	-2.20627600
C	-4.84885400	-1.59743500	-2.43082600
C	-4.27820300	-0.33240300	-2.57446900
H	-2.42872300	0.81751300	-2.59751200
H	-4.49811500	-3.70858200	-2.12796400
H	-5.92775100	-1.71529400	-2.51935100
H	-4.91549100	0.52508600	-2.78660600
C	-1.60724600	-3.58678500	-1.86509200
H	-1.56375500	-3.87893200	-0.80212200
H	0.06075900	-3.10677300	-3.22746900
H	-1.75558700	-4.50722000	-2.44371000
H	4.12258900	0.60177100	2.61089300
C	0.81168700	0.90939300	2.37011600
N	1.29341200	0.81964800	3.43360700
Cu	0.26571800	1.00222000	0.53152100

C	-0.15659400	1.77276600	-1.19112100
N	-0.40987400	2.13242700	-2.27642000
C	-2.84957600	-2.64651300	2.67503900
C	-3.17441700	-2.18015600	1.40281900
C	-2.82385400	-0.89333800	1.02428100
C	-2.13169000	-0.05019100	1.91223100
C	-1.79664500	-0.54475200	3.19031300
C	-2.16305600	-1.82345200	3.56991900
H	-3.71316900	-2.81447800	0.70010600
H	-1.22355700	0.08578700	3.86786400
H	-1.90765200	-2.18710700	4.56312500
C	-1.83363400	1.32502100	1.58537600
H	-1.42703800	1.90731300	2.41634200
H	-3.13274900	-3.65488200	2.97315800
H	-3.08790000	-0.53238800	0.03281300
C	-4.42612400	4.36493300	-0.11395500
C	-4.95076300	2.94995900	0.09007500
C	-4.10478800	2.16252000	1.08533400
C	-2.62816500	2.12584400	0.60947300
C	-2.12249000	3.56146400	0.47710600
C	-2.95832100	4.34703600	-0.52176600
H	-5.03355400	4.89237500	-0.86255100
H	-5.99606800	2.96574600	0.43020000
H	-4.15289800	2.63431000	2.08197400
H	-2.17739800	4.04154500	1.47135800
H	-2.84546600	3.88101600	-1.51536800
H	-4.94088500	2.41409700	-0.87490600
H	-4.49668000	1.14236400	1.19543800
H	-2.62281400	1.63894400	-0.37875700
H	-1.06788800	3.55956500	0.17521600
H	-2.57051400	5.37031900	-0.61490200
H	-4.53369200	4.92715300	0.82955400

TS5e-S

C	4.15487900	0.19409000	1.67816900
O	3.47778900	-1.08759000	1.57592300
C	3.53940200	0.99304500	0.50548400
H	3.15650400	1.97996400	0.80192100
C	2.49478300	-0.93162000	0.67662300
N	2.41686600	0.17311500	0.03713600
C	1.54310800	-2.05551600	0.57030400
C	1.94724800	-3.41228200	1.08860800
C	0.99024000	-2.60196800	1.87920600
H	2.96748600	-3.50421500	1.45076300
H	1.57198700	-4.26433400	0.52700500
H	1.32759300	-2.09438800	2.78135100
H	-0.06718600	-2.86763800	1.86356200
C	-0.44842300	-2.68345800	-2.37679300
O	0.62061400	-2.97740200	-1.45861500
C	-0.74408600	-1.19101900	-2.13767200
H	-0.23584700	-0.48886100	-2.81388300
C	0.60096700	-1.96088200	-0.56750300
N	-0.18561200	-0.98035300	-0.78534400
C	6.95180400	0.44959900	-0.82348200
C	6.88626600	0.95792800	-2.11756200
C	5.70300100	1.51393000	-2.60606000
C	4.56795600	1.57121700	-1.80387400
C	4.64261700	1.06763700	-0.51147500
C	5.81848800	0.50571100	-0.01992400
H	7.87728100	0.01193700	-0.44893300
H	7.76672200	0.91839900	-2.75722600
H	5.66810400	1.90203600	-3.62260900
H	3.63162000	1.98859700	-2.17552900
C	5.65083700	0.04314000	1.40311400
H	5.97421600	-0.99354700	1.56815100
H	6.23026500	0.66671800	2.09955200

C	-3.02378700	0.03745400	-2.38528200
C	-2.23752100	-1.09843100	-2.22640300
C	-2.80786400	-2.37023800	-2.14192300
C	-4.18932600	-2.51946700	-2.17372300
C	-4.98690000	-1.38233100	-2.29617000
C	-4.40960600	-0.11746700	-2.41174100
H	-2.54900900	1.01564800	-2.49651100
H	-4.64428100	-3.50898400	-2.11627000
H	-6.07051800	-1.48540300	-2.32635400
H	-5.04822400	0.75494100	-2.54556300
C	-1.74552900	-3.42869800	-2.01416800
H	-1.66709500	-3.79476100	-0.97637200
H	-0.08840400	-2.92134600	-3.38163800
H	-1.92675100	-4.30671500	-2.64712700
H	3.91264500	0.59003800	2.66961100
C	0.58926000	1.02966300	2.06028500
N	1.05174200	0.93475000	3.13438600
Cu	0.32023000	1.07501200	0.15607800
C	-0.15766500	1.99665500	-1.49997800
N	-0.59735100	2.43404100	-2.49486800
C	-2.83841100	-2.85499500	2.64937900
C	-3.16146600	-2.32122400	1.40262300
C	-2.83135800	-1.00879500	1.10226400
C	-2.17118300	-0.21012800	2.05500300
C	-1.82423800	-0.77526700	3.30057300
C	-2.16605000	-2.08133200	3.59825300
H	-3.68273600	-2.92313700	0.65954200
H	-1.25733500	-0.17259400	4.00932800
H	-1.90306500	-2.50678000	4.56430800
C	-1.91623000	1.18269600	1.84187800
H	-1.55299700	1.72185900	2.71912600
H	-3.10690400	-3.88403200	2.88333800
H	-3.09086000	-0.59317800	0.13067100

C	-4.19887700	4.38811300	0.07491000
C	-4.79882400	2.99170800	0.16137300
C	-4.07441100	2.11794700	1.18019200
C	-2.56219100	2.03462800	0.81864700
C	-1.98007500	3.44770500	0.77799100
C	-2.70885600	4.31815000	-0.23300300
H	-4.72660200	4.98067800	-0.68494500
H	-5.86644800	3.03715100	0.41987900
H	-4.18368100	2.54521700	2.19177800
H	-2.06412600	3.88758700	1.78866400
H	-2.54077300	3.89852500	-1.23882400
H	-4.73066200	2.50410400	-0.82612500
H	-4.51414900	1.11120600	1.20554800
H	-2.49777700	1.57251800	-0.17956800
H	-0.91037400	3.39201800	0.53413400
H	-2.26852400	5.32410600	-0.24170100
H	-4.35134700	4.90501400	1.03819700

e-S-pro

C	0.15224700	2.30665900	0.28601600
N	0.16859000	3.43163800	-0.00124600
C	3.84932800	-1.04370200	-0.37474400
C	3.22890900	-0.21032000	-1.30082600
C	2.03443000	0.42290900	-0.97993000
C	1.44748100	0.22976100	0.27106000
C	2.07599100	-0.60274500	1.19483000
C	3.27075600	-1.23858700	0.87455500
H	3.68030900	-0.04787300	-2.27794000
H	1.62127200	-0.75620600	2.17454700
H	3.75224100	-1.88526400	1.60598800
C	0.11877400	0.87704700	0.60585300
H	-0.05113500	0.79052800	1.69348700
H	4.78638800	-1.53723500	-0.62602100

H	1.55791400	1.08858400	-1.70096400
C	-3.65384900	-1.26153800	-0.05782200
C	-2.34924200	-1.95330900	-0.43213400
C	-1.15157700	-1.28364900	0.23236500
C	-1.08410600	0.20493300	-0.10127200
C	-2.39786100	0.89280500	0.26801800
C	-3.59242000	0.22173400	-0.39934400
H	-4.50375200	-1.74050300	-0.56352100
H	-2.38107500	-3.01803600	-0.16249100
H	-1.23198300	-1.39344500	1.33027200
H	-2.51935900	0.84488800	1.36588300
H	-3.50747600	0.33915100	-1.49295700
H	-2.22011900	-1.91351500	-1.52707800
H	-0.22028900	-1.78600200	-0.06384900
H	-0.92761100	0.31099600	-1.19132900
H	-2.35940300	1.95907100	0.00368300
H	-4.52151000	0.72856400	-0.10446000
H	-3.82771500	-1.37715500	1.02572500

TS-L2-R

C	1.38384400	2.74216700	-0.88530300
O	0.62207100	2.03163300	-1.90098200
C	0.74920000	2.26851600	0.44865200
H	1.43518700	1.72378600	1.11094600
C	-0.30610100	1.30867500	-1.24567000
N	-0.31124600	1.35416700	0.02374300
C	-1.21310100	0.52606400	-2.10956800
C	-1.46716600	1.07769800	-3.50632100
C	-0.59817700	-0.10440900	-3.36241300
H	-0.99992700	2.03571300	-3.71496800
H	-2.47134500	0.94091200	-3.89568700
H	0.47677400	0.02063200	-3.46912200
H	-0.99412500	-1.07764700	-3.64442500

C	-4.23378800	-1.40442100	-1.57518700
O	-3.24564700	-0.66858400	-2.34038000
C	-3.76368000	-1.23503400	-0.11146900
H	-4.41426400	-0.61282100	0.51642200
C	-2.31342200	-0.23222200	-1.47983100
N	-2.47779500	-0.53487800	-0.24633900
C	1.11460600	4.23782800	-0.97217900
H	0.99150600	4.56823700	-2.01063300
H	1.98219300	4.77126600	-0.55552000
C	-4.15299100	-2.89587200	-1.88242900
H	-3.85049900	-3.07688500	-2.92048300
H	-5.20148700	-0.95186700	-1.81014000
H	-5.15144400	-3.33684100	-1.74863800
H	2.43256300	2.46048200	-1.03283800
C	-0.57105700	0.34881000	3.02110200
N	0.00614500	0.69083800	3.97886100
Cu	-1.55227400	0.19601500	1.45152300
C	-3.07540400	1.40775300	1.77964700
N	-4.05410100	2.04734800	1.82155500
C	3.70510500	-0.56496300	0.07932300
C	3.48802200	-0.50540300	1.45889200
C	2.24608400	-0.79048300	2.00864500
C	1.16991600	-1.15132900	1.18711100
C	1.39154900	-1.22127800	-0.19606200
C	2.63336100	-0.93355300	-0.73995100
H	4.31288200	-0.21910900	2.11283600
H	2.08936800	-0.68401900	3.08080900
H	0.56313300	-1.50647500	-0.84921700
H	2.78266500	-0.99056000	-1.82022900
C	5.05147700	-0.27668700	-0.51820500
C	-0.16104500	-1.47840100	1.71417800
H	-0.80275000	-1.85816500	0.91008600
C	5.82505000	-1.53477000	-0.93974700

H	5.19319500	-2.09189400	-1.65418100
C	-0.28246100	-2.34577100	2.93796200
H	0.03257100	-3.36729900	2.67001500
H	0.33430000	-2.00055600	3.77202400
H	-1.31941800	-2.39196900	3.29214900
H	5.66897700	0.28617700	0.20158700
H	4.93234000	0.37223600	-1.40161800
C	6.11146800	-2.43585000	0.25244200
H	6.71258500	-1.89889500	1.00293500
H	5.19028200	-2.77437600	0.74342500
H	6.67941200	-3.32492500	-0.05123000
C	7.11735100	-1.13932800	-1.63882700
H	7.67721400	-2.02207700	-1.97421800
H	6.92925100	-0.50454900	-2.51528500
H	7.76834800	-0.57619400	-0.95313400
C	-0.10564500	4.45561200	-0.07592600
H	-1.02639200	4.14856800	-0.59446000
H	-0.23760400	5.50204600	0.22082100
C	0.16795700	3.52501400	1.10325300
H	-0.71654500	3.28763900	1.70575600
H	0.92110300	3.96787700	1.77110700
C	-3.58256000	-2.65788000	0.41624900
H	-4.54283000	-3.01959100	0.81204200
H	-2.85754100	-2.70595400	1.23873500
C	-3.19759200	-3.45636400	-0.82680100
H	-3.28924700	-4.54035200	-0.69635100
H	-2.15171200	-3.24840400	-1.10674400

TS-L2-S

C	0.25212800	-0.83726400	2.77447400
N	-0.32044400	-0.70440000	3.78531400
Cu	1.26027100	-0.64966600	1.22233000
C	2.97168100	0.20460200	1.82187300

N	3.99972900	0.76251700	1.87757100
C	-3.99295100	-0.41952300	-0.29643100
C	-3.88127100	-0.98233900	0.98024600
C	-2.68910500	-1.53233800	1.42334800
C	-1.56022100	-1.54524200	0.59179100
C	-1.66998300	-0.97734500	-0.68514900
C	-2.86710800	-0.43088300	-1.12238500
H	-4.74749100	-0.96922400	1.64353500
H	-2.61719100	-1.92386300	2.43630000
H	-0.79003200	-0.95865100	-1.32996300
H	-2.93493600	0.00436400	-2.12074100
C	-5.29744000	0.16133100	-0.75728700
C	-0.29211100	-2.15757500	0.99384800
H	0.33565500	-2.34385000	0.11634200
C	-6.34891000	-0.89293000	-1.13220100
H	-6.50413000	-1.53867000	-0.24991300
C	-0.27597900	-3.35499200	1.90338100
H	-0.83928100	-3.20754600	2.82819000
H	-0.71260000	-4.20740100	1.35834700
H	0.75142300	-3.62048400	2.17974400
H	-5.12887900	0.81288300	-1.63157000
H	-5.71271600	0.80483500	0.03520900
C	-5.87458800	-1.76348800	-2.28665900
H	-5.67520900	-1.14503100	-3.17612100
H	-4.95097100	-2.30329100	-2.04157800
H	-6.63627500	-2.50428400	-2.56301600
C	-7.66641800	-0.21370400	-1.47537800
H	-8.44393300	-0.94897900	-1.72045900
H	-8.03445800	0.40407900	-0.64525500
H	-7.54412200	0.44239800	-2.35055800
C	0.12585800	3.65286600	0.90102400
O	1.10480400	3.38973400	-0.13550300
C	-0.24633700	2.24241300	1.42161400

H	0.10680100	2.02247000	2.43818300
C	1.19240300	2.05077300	-0.24846000
N	0.45227500	1.33513000	0.50223200
C	2.21158100	1.58832000	-1.21022100
C	2.58875300	2.52713200	-2.34976500
C	3.51825600	2.39561100	-1.21602300
H	1.98580000	3.42837300	-2.41913200
H	2.84440000	2.05302500	-3.29309700
H	3.57130700	3.18240000	-0.46938000
H	4.42461900	1.80685300	-1.33448500
C	3.46089600	-1.58637100	-2.40012600
O	3.20404600	-0.16201000	-2.45312700
C	2.57044300	-2.07334600	-1.23185200
H	1.76860100	-2.75992500	-1.54100500
C	2.40918700	0.14552300	-1.41948800
N	1.97661500	-0.83475400	-0.71160300
C	-1.15408900	4.24081100	0.31221800
H	-0.94650800	4.83854400	-0.58337300
H	-1.60624400	4.91120300	1.05791200
C	4.90055200	-1.85328700	-1.97865000
H	5.57659000	-1.08007000	-2.36292500
H	3.20011500	-1.98312400	-3.38645100
H	5.21801100	-2.81416900	-2.41064900
H	0.61807600	4.30495500	1.62895400
C	3.53255400	-2.70083800	-0.21848500
H	3.65028900	-3.77105900	-0.44651700
C	4.84370100	-1.95505800	-0.45391800
H	5.71059600	-2.47338300	-0.03008300
C	-2.06901000	3.03430700	0.08384200
H	-1.79109500	2.50895300	-0.84309500
H	-3.12783400	3.30840100	-0.00112000
C	-1.76277300	2.15211400	1.29032800
H	-2.10001600	1.11419700	1.19733800

H	-2.22740800	2.57332100	2.19445400
H	3.15821700	-2.61290800	0.81082000
H	4.79676800	-0.96194500	0.01897800

TS-L3-R

C	0.79841200	1.38055500	2.68388200
O	0.09813800	2.29163700	1.80822800
C	0.12887300	0.02295900	2.42368400
H	0.84090100	-0.75369800	2.11564100
C	-0.75966900	1.53697700	1.08993900
N	-0.80699000	0.29227000	1.33664100
C	-1.55339900	2.28033500	0.09198600
C	-1.91919100	3.71550500	0.45228500
C	-0.88179800	3.48702000	-0.56932700
H	-1.60653900	4.03590400	1.44202800
H	-2.90175200	4.04909300	0.13225400
H	0.16010100	3.64643400	-0.30250800
H	-1.13726600	3.65709300	-1.61248500
C	-4.15344600	1.42522200	-2.26581700
O	-3.37363900	2.30453900	-1.42767700
C	-3.76609400	0.02713500	-1.78267200
H	-4.53623800	-0.45263500	-1.16300500
C	-2.50773300	1.53332600	-0.74982900
N	-2.59483400	0.26903000	-0.93393400
H	-5.20767000	1.67490600	-2.12077500
H	1.85949300	1.40101000	2.40600300
C	-1.02810700	-2.82978400	0.81767400
N	-0.54493700	-3.71098600	1.41542000
Cu	-1.90718100	-1.30438200	0.22683200
C	-3.65320900	-1.38256800	1.14370900
N	-4.76025900	-1.29017300	1.51077300
C	3.42262800	-0.12727000	0.05182500
C	3.16249000	-1.47606600	0.31219600

C	1.96310300	-2.06642700	-0.06041300
C	0.97435700	-1.31950200	-0.71506500
C	1.23992400	0.03134400	-0.98364000
C	2.43900200	0.61641400	-0.60798400
H	3.91830100	-2.07143500	0.82625900
H	1.76536500	-3.10457100	0.20133500
H	0.48269400	0.62617400	-1.49803000
H	2.62131700	1.67118300	-0.82414000
C	4.72715300	0.51012600	0.43250600
C	-0.30657700	-1.89917400	-1.13927400
H	-0.86713900	-1.18680700	-1.75763200
C	5.68473800	0.71491600	-0.75080700
H	5.15872100	1.32821700	-1.50388800
C	-0.33376300	-3.26696900	-1.76531000
H	0.14206200	-3.19960800	-2.75692700
H	0.19574700	-4.02122100	-1.17750700
H	-1.36301300	-3.61631100	-1.90667200
H	5.23846300	-0.10535800	1.19138300
H	4.53722400	1.49009000	0.90142000
C	6.06597900	-0.61119900	-1.39224800
H	6.56138600	-1.26442000	-0.65690000
H	5.19089300	-1.14850200	-1.77925400
H	6.76560400	-0.46079400	-2.22474000
C	6.92472700	1.46715400	-0.29073400
H	7.61371700	1.65077100	-1.12540800
H	6.67061000	2.43696400	0.15799700
H	7.47035600	0.88274900	0.46547100
H	0.68595800	1.74955100	3.70818600
H	-0.42767100	-0.36605400	3.28584200
H	-3.87306000	1.62463400	-3.30719600
H	-3.50758300	-0.65686200	-2.60098700

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C	3.92808800	1.92430200	-2.10072900
O	3.05125500	2.62924100	-1.19621000
C	3.70592000	0.45295300	-1.74862300
H	3.51763300	-0.17721700	-2.62714400
C	2.28614400	1.70651900	-0.59125200
N	2.52213700	0.48144800	-0.88243700
C	1.24859300	2.26087100	0.29931300
C	1.43783800	3.69689700	0.77808700
C	0.43689800	3.42568700	-0.26910800
H	2.37307700	4.17225400	0.49787000
H	1.08693600	3.89577600	1.78687500
H	0.67063600	3.70979000	-1.29251900
H	-0.61629400	3.43442800	-0.00044400
C	-1.00856900	0.84419000	2.73506000
O	-0.42791300	1.91368000	1.95627000
C	-0.04672300	-0.33134300	2.52267400
H	0.56170300	-0.56521000	3.40607400
C	0.56577100	1.34948600	1.23852000
N	0.83599300	0.12656700	1.45204800
H	-1.08678000	1.18792000	3.77062800
H	3.62750600	2.18345300	-3.12306800
C	1.24660400	-2.85655300	0.63608700
N	0.80598900	-3.78318300	1.19693200
Cu	2.01899400	-1.24991800	0.11890900
C	3.80739500	-1.29944100	0.95767200
N	4.92350100	-1.17508700	1.28587700
C	-3.27157100	-0.12391400	-0.03220700
C	-2.97673200	-1.46304700	0.25035900
C	-1.77825000	-2.03791600	-0.14337200
C	-0.82023500	-1.28392000	-0.83763700
C	-1.11781900	0.05535800	-1.12344900
C	-2.32106100	0.62411700	-0.73069700
H	-3.70374900	-2.06079800	0.80271000

H	-1.55147200	-3.06697500	0.13224300
H	-0.38252200	0.65573000	-1.66287100
H	-2.53623800	1.66692700	-0.97137300
C	-4.58473400	0.46976500	0.38780400
C	0.45835200	-1.85205900	-1.28269000
H	1.01663600	-1.13329800	-1.89648300
C	-5.77059400	0.03492300	-0.48582400
H	-5.81921500	-1.06784700	-0.45756800
C	0.47432000	-3.20978800	-1.93131100
H	-0.05902400	-3.97015000	-1.35515200
H	-0.00708700	-3.11939800	-2.91852200
H	1.49940400	-3.56457200	-2.08548500
H	-4.52229000	1.57109200	0.36749000
H	-4.79887400	0.18903600	1.43236700
C	-5.58372700	0.47074800	-1.93169700
H	-5.49395100	1.56689400	-1.99329400
H	-4.68133800	0.03545200	-2.37963700
H	-6.44266200	0.17470200	-2.54779000
C	-7.06627600	0.59429600	0.08269300
H	-7.93358800	0.27382100	-0.50891100
H	-7.22798200	0.27379400	1.12061200
H	-7.04747400	1.69470000	0.07234300
H	4.94630500	2.27974600	-1.92236000
H	4.53087400	0.00669200	-1.17662000
H	-2.01383400	0.65205600	2.33497600
H	-0.55502600	-1.25554600	2.22123900