

Supporting Information

Ligand-Dependent Multi-State Reactivity in Cobalt(III)-Catalyzed C-H Activations

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1. Calculated Energies and Reaction Profiles

1.1 Calculated absolute electronic energies for all species (in Hartree)

Table S1. Calculated absolute energies for all species in C(sp²)-H activation of non-Cp-Co(III) system a

Energy \ Species	E(B3LYP/TZVP) ^[a]	Thermal Gibbs free energy correction ^[b] (ΔG_{therma})	Solvent effect correction (ΔG_{Solv})	E(DLPNO-CCSD(T)/VDZ)	E(DLPNO-CCSD(T)/VTZ)	E(DLPNO-CCSD(T)/CBS) (E_{DLCC})
¹ A	-2641.49986890	0.268135	-0.02379279	-2636.50431710	-2637.74869671	-2638.18661184
³ A	-2641.49057944	0.262711	-0.02752367	-2636.49473609	-2637.73784321	-2638.17531053
⁵ A	-2641.48607054	0.254558	-0.03704371	-2636.50377566	-2637.74077379	-2638.17609126
¹ TS _{AB}	-2641.47583090	0.264276	-0.02261785	-2636.47604937	-2637.72331865	-2638.16225068
³ TS _{AB}	-2641.46303390	0.258420	-0.02506573	-2636.46667888	-2637.70892497	-2638.14608927
⁵ TS _{AB}	-2641.44274644	0.253990	-0.02636632	-2636.45732145	-2637.69475264	-2638.13022251
¹ B	-2641.49638766	0.267665	-0.02319345	-2636.50786497	-2637.75158310	-2638.18926544
³ B	-2641.49239647	0.261359	-0.02489268	-2636.50764127	-2637.74791273	-2638.18438213
⁵ B	-2641.45032814	0.257052	-0.02655186	-2636.46749235	-2637.70500128	-2638.14049851

[a] Results in gas phase including DFT-D3 empirical dispersion correction. [b] Calculated at the experimental temperature of 353.15K.

Table S2. Calculated absolute energies for all species in C(sp³)-H activation of non-Cp-Co(III) system b

Energy \ Species	E(B3LYP/TZVP) ^[a]	Thermal Gibbs free energy correction ^[b] (ΔG_{therma})	Solvent effect correction (ΔG_{Solv})	E(DLPNO-CCSD(T)/VDZ)	E(DLPNO-CCSD(T)/VTZ)	E(DLPNO-CCSD(T)/CBS) (E_{DLCC})
¹ C	-2567.67967270	0.275541	-0.02826964	-2562.90022975	-2564.09747519	-2564.51880311
³ C	-2567.67175272	0.269083	-0.02991775	-2562.89590473	-2564.08780278	-2564.50724889
⁵ C	-2567.66647597	0.260670	-0.03351889	-2562.90478079	-2564.09149407	-2564.50911558
¹ TS _{CD}	-2567.64732270	0.272668	-0.02959887	-2562.86905906	-2564.06537466	-2564.48637536
³ TS _{CD}	-2567.63828269	0.266258	-0.02915393	-2562.86060488	-2564.05416003	-2564.47418929
⁵ TS _{CD}	-2567.61554637	0.260789	-0.02853579	-2562.84563618	-2564.03544214	-2564.45415200
¹ D	-2567.67371165	0.276788	-0.02995807	-2562.90109287	-2564.09819741	-2564.51947575
³ D	-2567.68032767	0.267684	-0.02845095	-2562.91403652	-2564.10462818	-2564.52361454
⁵ D	-2567.64535403	0.258027	-0.02862523	-2562.88295560	-2564.07162343	-2564.48993278

[a] Results in gas phase including DFT-D3 empirical dispersion correction. [b] Calculated at the experimental temperature of 423.15K.

Table S3. Calculated absolute energies for all species in C(sp²)-H activation of Cp-Co(III) system c

Energy \ Species	E(B3LYP/TZVP) ^[a]	Thermal Gibbs free energy correction ^[b] (ΔG_{therma})	Solvent effect correction (ΔG_{Solv})	E(DLPNO-CCSD(T)/VDZ)	E(DLPNO-CCSD(T)/VTZ)	E(DLPNO-CCSD(T)/CBS) (E_{DLCC})
¹ E	-2459.01245056	0.361053	-0.07501447	-2454.47631856	-2455.56205146	-2455.94413652
³ E	-2459.00414351	0.352209	-0.07927922	-2454.46514521	-2455.54681608	-2455.92747165
⁵ E	-2458.98299340	0.349561	-0.08131277	-2454.44141217	-2455.52206033	-2455.90235599
¹ TS _{EF}	-2458.97315757	0.357433	-0.07742997	-2454.43601592	-2455.52266517	-2455.90507270
³ TS _{EF}	-2458.95715231	0.350295	-0.07767601	-2454.41646981	-2455.49878027	-2455.87966092
⁵ TS _{EF}	-2458.93744564	0.344701	-0.08081985	-2454.39405808	-2455.47476417	-2455.85508022
¹ F	-2458.99408593	0.361536	-0.07458811	-2454.46315429	-2455.54941571	-2455.93168676
³ F	-2458.97879298	0.354045	-0.07521845	-2454.44242916	-2455.52536496	-2455.90646568
⁵ F	-2458.94803260	0.348855	-0.07962493	-2454.40675181	-2455.48711018	-2455.86730387

[a] Results in gas phase including DFT-D3 empirical dispersion correction. [b] Calculated at the experimental temperature of 333.15K.

1.2 Reaction energy profiles

- $\Delta E(\text{B3LYP/TZVP})$: Electronic energy calculated in gas phase at the UB3LYP/def2-TZVP level including the DFT-D3 empirical dispersion correction.
- $\Delta E_{\text{solv}}(\text{B3LYP/TZVP})$: Electronic energy calculated in solvent at the UB3LYP/def2-TZVP level, i.e., $\Delta E(\text{B3LYP/TZVP})$ with the solvent effect correction.
- $\Delta G(\text{B3LYP/TZVP})$: Gibbs free energy calculated in solvent at the UB3LYP/def2-TZVP level, i.e., $\Delta E_{\text{solv}}(\text{B3LYP/TZVP})$ with the thermal Gibbs free energy correction.
- $\Delta G(\text{DLCC/CBS})$: Gibbs free energy calculated in solvent with the DLPNO-CCSD(T)/CBS electronic energy calculated in gas phase to replace $\Delta E(\text{B3LYP/TZVP})$ in $\Delta G(\text{B3LYP/TZVP})$.

With these energy definitions from (a) to (d) used in Figures S1-S3, change from (a) to (b) is caused by solvent effect; change from (b) to (c) is caused by thermal Gibbs free energy correction; difference between (a) and (d) represents the difference between B3LYP and DLPNO-CCSD(T) methods.

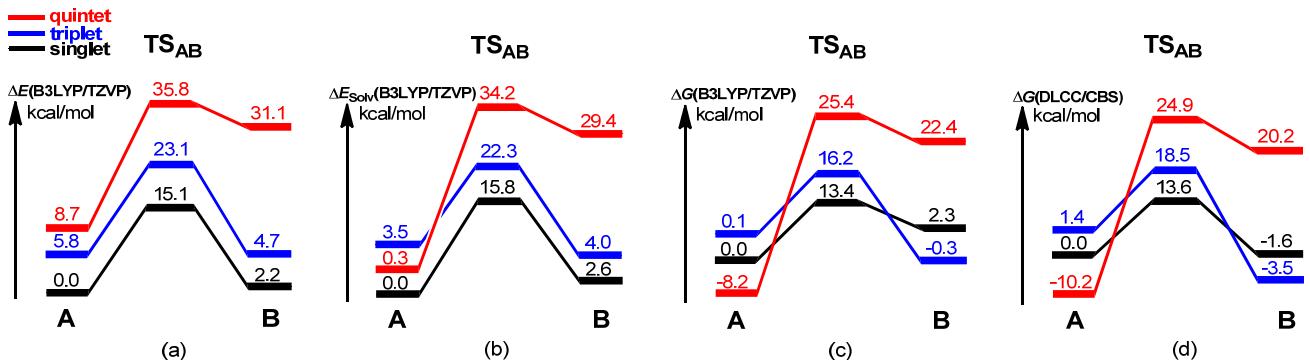


Figure S1. Reaction energy profiles at different levels in $\text{C}(\text{sp}^2)\text{-H}$ activation of non-Cp-Co(III) system a.

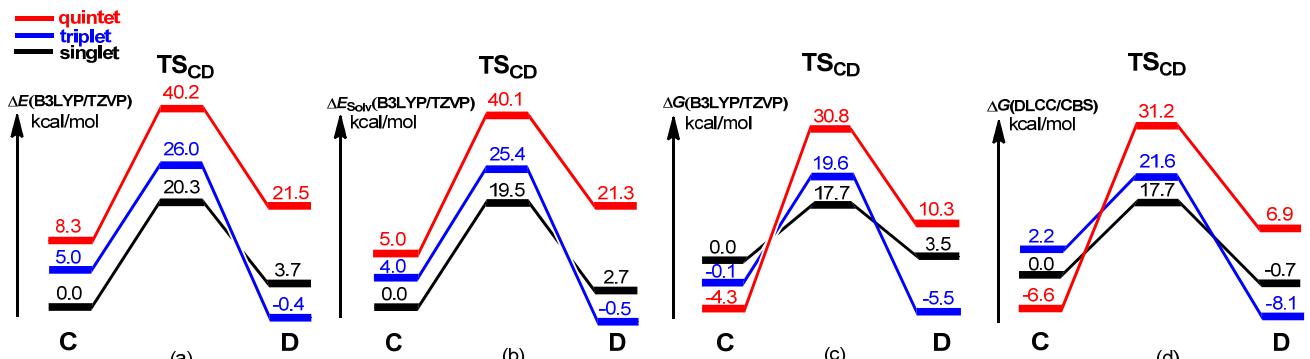


Figure S2. Reaction energy profiles at different levels in $\text{C}(\text{sp}^3)\text{-H}$ activation of non-Cp-Co(III) system b.

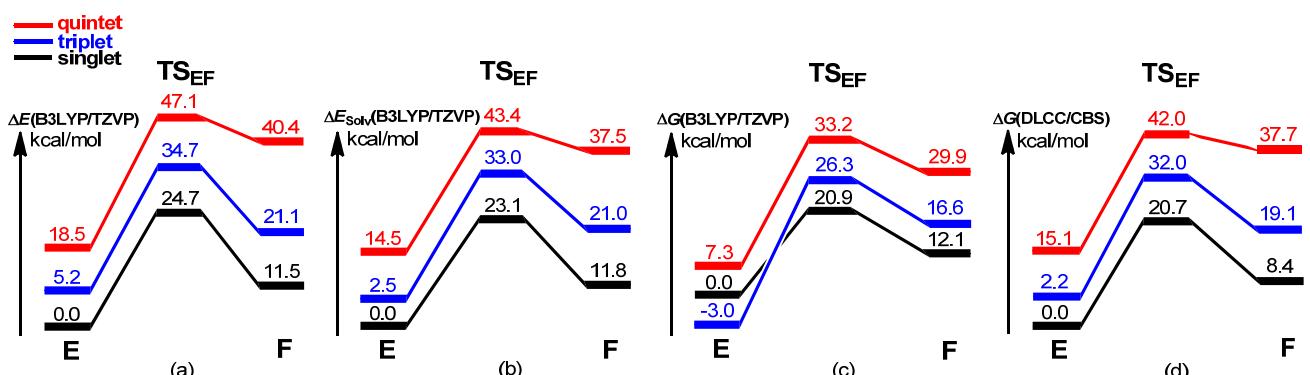


Figure S3. Reaction energy profiles at different levels in $\text{C}(\text{sp}^2)\text{-H}$ activation of Cp-Co(III) system c.

Various factors that affect the relative energies (relative to singlet state) are outlined below:

Solvent effect. The sizes of solvent effect are usually not large (below ~4 kcal/mol), except for the quintet-singlet spin gap (reduced by 8.4 kcal/mol for **A**, Figure S1a,b) in C(sp²)-H activation of non-Cp-Co(III) system a.

Thermal free energy correction. The sizes of thermal free energy correction are usually quite large for quintet states of the three systems (energy lowering by ~7-10 kcal/mol, Figures S1b,c, S2b,c, S3b,c), but much smaller for the triplet states (energy lowering by ~3-6 kcal/mol, Figures S1b,c, S2b,c, S3b,c).

DLPNO-CCSD(T) correction. The sizes of differences between DLPNO-CCSD(T) and B3LYP are quite system-dependent. For C(sp²)-H activation of Cp-Co(III) system c, the differences are very large, up to 7.8 kcal/mol for quintet-singlet spin gap of **E** (Figure S3c,d). For C(sp³)-H activation of non-Cp-Co(III) system b and C(sp²)-H activation of non-Cp-Co(III) system a, the differences between DLPNO-CCSD(T) and B3LYP are relatively smaller (Figure S2c,d; S1c,d).

1.3 Effects of basis set extrapolation and perturbative triples contribution (T) in DLPNO-CCSD(T)

- $\Delta E(\text{DLCC/VDZ})$: Electronic energy calculated in gas phase at the DLPNO-CCSD(T)/cc-pVDZ level.
- $\Delta E(\text{DLCC/VTZ})$: Electronic energy calculated in gas phase at the DLPNO-CCSD(T)/cc-pVTZ level.
- $\Delta E(\text{DLCC/CBS})$: Electronic energy calculated in gas phase at the DLPNO-CCSD(T)/CBS level.
- $\Delta E(\text{DLPNO-CCSD/VDZ})$: Electronic energy calculated in gas phase at the DLPNO-CCSD/cc-pVDZ level.

With these energy definitions from (a) to (d) used in Figures S4-S6, changes from (a) via (b) to (c) are caused by basis set enlargement and extrapolation; change from (a) to (d) is caused by perturbative triples contribution (T) in DLPNO-CCSD(T).

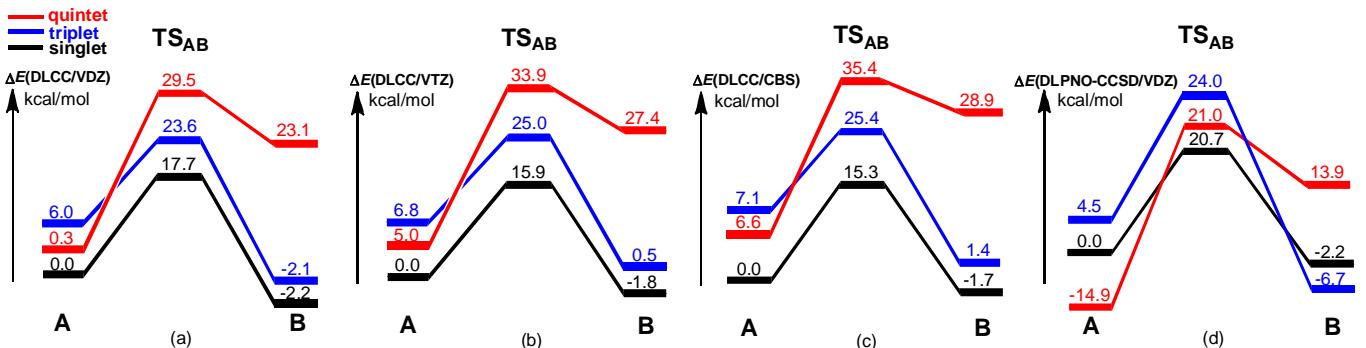


Figure S4. Reaction energy profiles at different levels in $\text{C}(\text{sp}^2)\text{-H}$ activation of non-Cp-Co(III) system a.

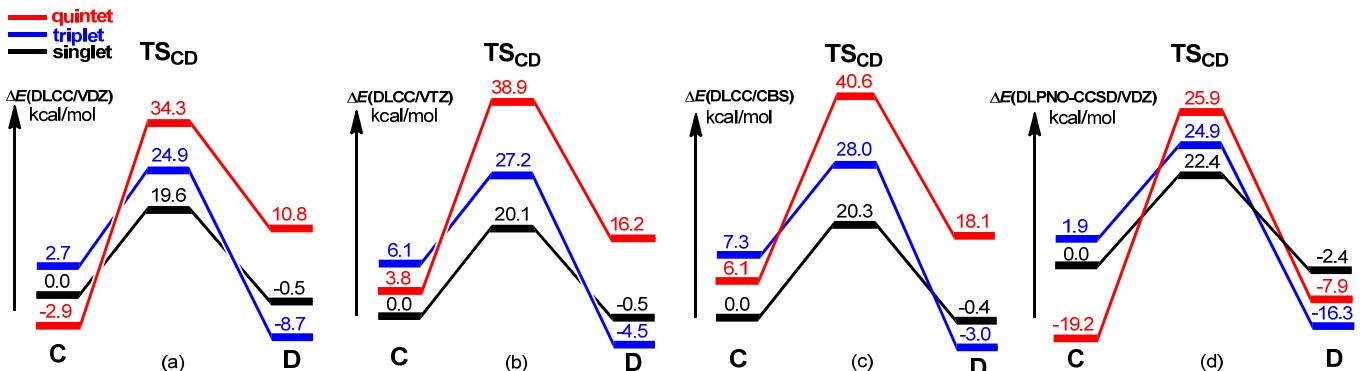


Figure S5. Reaction energy profiles at different levels in $\text{C}(\text{sp}^2)\text{-H}$ activation of non-Cp-Co(III) system b.

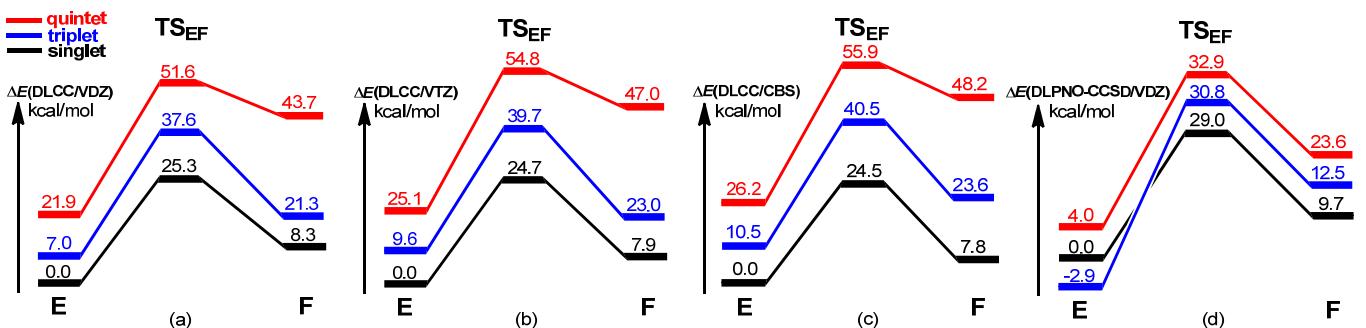


Figure S6. Reaction energy profiles at different levels in $\text{C}(\text{sp}^2)\text{-H}$ activation of Cp-Co(III) system c.

Two factors that affect the relative energies (relative to singlet state) in DLPNO-CCSD(T) are outlined below:

Basis set extrapolation. The sizes of basis set extrapolation effect are below ~9 kcal/mol, with the quintet-singlet spin gap being the largest (increased by 9.0 kcal/mol for **C**, Figure S5a,c).

Perturbative triples contribution (T). The sizes of perturbative triples contribution (T) are usually quite large for quintet states in three systems (up to 20.1 kcal/mol for **F**, Figure S6a,d), but the sizes of this effect for singlet and triplet states are relatively smaller (below ~10 kcal/mol).

1.4 Test of Co 3s3p core-valence correlation and scalar relativistic effects

Table S4. Calculated absolute energies considering Co 3s3p core-valence correlation and scalar relativistic effect for C and TS_{CD} in system b

Species \ Energy	E(DLPNO-CCSD(T)/wDZ)	E(DLPNO-CCSD(T)/wDZ)	E(DLPNO-CCSD(T) /CBS)
¹ C	-2574.28039681	-2575.55776318	-2576.00728681
³ C	-2574.27071592	-2575.54737266	-2575.99664656
⁵ C	-2574.26926753	-2575.54446365	-2575.99322354
¹ TS_{CD}	-2574.24589085	-2575.52508157	-2575.97524723
³ TS_{CD}	-2574.23457995	-2575.51344606	-2575.96349748
⁵ TS_{CD}	-2574.21719646	-2575.49451231	-2575.94401817

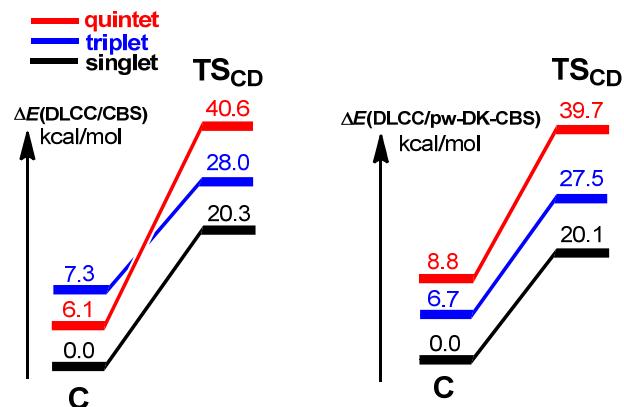


Figure S7. The comparison of relative energies with (right) and without (left) Co 3s3p core-valence correlation and scalar relativistic effects in system b.

2. Mulliken Spin Density Populations

Table S5. Mulliken spin density populations^[a]

Spin density Species \	Co	Directing group ^[b]	Substrate ^[c]	Cp ligand
¹ A	0.0000	0.0000	0.0000	-
³ A	1.6372	0.2180	0.0272	-
⁵ A	2.8041	0.9425	0.0401	-
¹ B	0.0000	0.0000	0.0000	-
³ B	2.0099	0.0513	-0.1687	-
⁵ B	2.9501	0.5413	0.3090	-
¹ TS _{AB}	0.0000	0.0000	0.0000	-
³ TS _{AB}	1.8571	0.0329	-0.0585	-
⁵ TS _{AB}	2.8667	0.7043	0.2104	-
¹ C	0.0000	0.0000	0.0000	-
³ C	1.5851	0.2779	0.0144	-
⁵ C	2.7543	0.9701	0.0468	-
¹ D	0.0000	0.0000	0.0000	-
³ D	2.2001	0.0308	-0.3266	-
⁵ D	2.7943	0.1662	0.9196	-
¹ TS _{CD}	0.0000	0.0000	0.0000	-
³ TS _{CD}	1.8484	0.0497	-0.0629	-
⁵ TS _{CD}	2.8980	0.5255	0.2768	-
¹ E	0.0000	0.0000	0.0000	0.0000
³ E	2.2218	0.0081	0.0058	-0.3492
⁵ E	2.7152	0.0648	0.0085	1.0383
¹ F	0.0000	0.0000	0.0000	0.0000
³ F	2.0474	0.0281	-0.0818	-0.0277
⁵ F	2.7295	0.0624	0.1390	1.0255
¹ TS _{EF}	0.0000	0.0000	0.0000	0.0000
³ TS _{EF}	2.2150	0.0580	0.0102	-0.3247
⁵ TS _{EF}	2.6868	0.0639	0.1003	1.0648

[a] Results at UB3LYP/TZVP level with solvent effect. [b] Refer to (a) aminoquinoline bidentate directing group in systems a and b, (b) pyrazole directing group in system c. [c] Refer to (a) PhCO group of substrate in system a, (b) (CH₃)₃CCO group of substrate in system b, (c) phenyl group of substrate in system c.

3. T1 Diagnostics

Table S6. T1 diagnostics of the DLPNO-CCSD(T) calculations (VDZ) in this work

Species	Value	T1 diagnostics
¹ A		0.0105
³ A		0.0130
⁵ A		0.0204
¹ B		0.0110
³ B		0.0153
⁵ B		0.0139
¹ TS _{AB}		0.0107
³ TS _{AB}		0.0138
⁵ TS _{AB}		0.0166
¹ C		0.0104
³ C		0.0130
⁵ C		0.0201
¹ D		0.0112
³ D		0.0176
⁵ D		0.0147
¹ TS _{CD}		0.0104
³ TS _{CD}		0.0139
⁵ TS _{CD}		0.0144
¹ E		0.0109
³ E		0.0195
⁵ E		0.0148
¹ F		0.0105
³ F		0.0151
⁵ F		0.0158
¹ TS _{EF}		0.0111
³ TS _{EF}		0.0197
⁵ TS _{EF}		0.0160

4. Cartesian Coordinates of the Optimized Structures

¹A

C	3.72756600	0.93800900	4.23494200	C	2.86627400	-1.17809900	2.66781600
C	4.45782100	-0.22635200	4.37730900	C	1.66591200	0.56360900	3.65648100
C	4.05178300	-1.41472300	3.71506300	H	5.91861100	-1.79135500	4.12016400
C	2.87848400	-1.32716900	2.90693500	H	2.59182700	1.58709300	5.32720300
C	2.55658100	0.92824100	3.44703300	H	4.65173400	0.16337300	5.25753000
H	5.61315300	-2.76074600	4.41538800	C	5.07173700	-1.89238900	3.43780000
H	4.02864100	1.86206300	4.73144200	C	2.87122200	-2.17333900	1.63738200
H	5.35621100	-0.24484400	5.00047100	H	0.75754700	1.17068600	3.64124900
C	4.71799700	-2.66267300	3.79773600	C	3.97998000	-3.01868900	1.54967500
C	2.38148200	-2.42420600	2.13374400	C	5.05952200	-2.86133000	2.44988400
H	1.92104800	1.80896600	3.33622400	H	3.99049900	-3.79476200	0.78769000
C	3.05571900	-3.64473200	2.27805200	H	5.91406600	-3.53651100	2.35294300
C	4.20415700	-3.73891900	3.09446400	N	1.73061300	-2.16785000	0.86220800
H	2.68652500	-4.52381900	1.75655300	C	1.32459800	-3.18919200	0.03940100
H	4.70240200	-4.70975600	3.16497100	O	1.97599000	-4.18645500	-0.24620400
N	1.34669400	-2.09742900	1.27087600	C	-0.08820300	-2.96055300	-0.40993400
C	0.70050400	-3.09555700	0.54964200	C	-0.62870200	-1.65839000	-0.27721600
O	0.64002800	-4.26149700	0.91592500	C	-0.87113500	-4.02714700	-0.85678100
C	0.15632200	-2.73549300	-0.80622400	C	-1.99597400	-1.47167500	-0.56590900
C	0.87725100	-1.91087600	-1.68271000	C	-2.22058400	-3.81243400	-1.14971900
C	-1.00108300	-3.38211000	-1.26656600	H	-0.41226900	-5.01431200	-0.94864600
C	0.43740900	-1.72627800	-2.99791900	C	-2.78641700	-2.53773500	-0.99878200
C	-1.45434100	-3.17548300	-2.56944000	H	-2.42714400	-0.46921400	-0.48816700
H	-1.53356700	-4.05118300	-0.58767500	H	-2.84148000	-4.64386500	-1.49457800
C	-0.73308800	-2.34957500	-3.44096300	H	-3.84194800	-2.37848000	-1.23531000
H	1.01554500	-1.09799600	-3.68107100	N	1.75322900	-0.39298100	2.74974200
H	-2.36608500	-3.67036400	-2.91434300	Co	0.50048700	-0.78689800	1.28611100
H	-1.07815800	-2.20227700	-4.46795800	O	1.51176500	0.56550600	0.36753700
N	2.16485000	-0.17143400	2.82187900	O	0.61498000	0.20903700	-1.63922400
Co	0.54437500	-0.39761700	1.81789500	C	1.39660100	0.81889400	-0.87202800
O	0.89841300	0.68191500	0.23950700	C	2.28429100	1.90358400	-1.43760900
O	-0.97154200	-0.33255800	0.58922000	H	1.75242400	2.44890400	-2.22886600
C	-0.30412300	0.47658400	-0.12764800	H	2.62099900	2.58514500	-0.64648900
C	-0.91101800	1.18555700	-1.29602900	H	3.16762900	1.42552800	-1.89163600
H	-1.49929900	2.03857800	-0.91962000	O	-0.99318300	0.33342500	2.00274900
H	-0.12720600	1.56035100	-1.96604600	O	-0.69959900	-1.74660200	2.51711400
H	-1.58878600	0.50812400	-1.83211300	C	-1.39099400	-0.69053500	2.64384900
O	-0.38804400	1.00535600	2.87540200	C	-2.63513000	-0.66983800	3.48155300
O	-0.39395300	-1.09433300	3.38348500	H	-3.45496300	-1.12419200	2.90161100
C	-0.81487600	0.07677200	3.63374700	H	-2.49294700	-1.27464400	4.38806200
C	-1.79078900	0.34111700	4.73894300	H	-2.91198000	0.36119700	3.73710600
H	-2.81058000	0.20251700	4.34403900	H	0.02278900	-0.70899400	-0.82778600
H	-1.64148500	-0.37466300	5.55846800				
H	-1.69467500	1.37523400	5.09557900				
H	1.78842100	-1.42355300	-1.33159700				

¹B

C	2.81457600	0.97044900	4.51850600
C	3.92080300	0.14444800	4.50684700
C	3.97620500	-0.96316800	3.61920600
C	2.84699800	-1.15980800	2.76756900
C	1.74109400	0.69507400	3.64123800
H	5.93331500	-1.73614900	4.17607700

¹TS_{AB}

C	2.70261500	0.79073200	4.58906400
C	3.83730200	0.00452300	4.54531600
C	3.95889200	-1.02021000	3.56986200

H	2.75345200	1.82822900	5.19110600	H	4.64343300	-4.85291500	2.97420000
H	4.76398000	0.33288100	5.17745200	N	1.26571100	-2.09804300	1.33210100
C	5.06332600	-1.87143500	3.52947000	C	0.57956600	-3.08208800	0.57870700
C	2.79514100	-2.24406900	1.82430600	O	0.32967600	-4.17998400	1.03795000
H	0.84595800	1.32331900	3.61716300	C	0.24771600	-2.74630000	-0.84259900
C	3.88774000	-3.11684000	1.77299400	C	0.99003800	-1.81037600	-1.57946700
C	4.99798100	-2.91550600	2.62348800	C	-0.75375900	-3.49390700	-1.48521100
H	3.85878300	-3.94714600	1.07102700	C	0.72652100	-1.61942500	-2.93900200
H	5.83344500	-3.61791300	2.55554900	C	-1.02750200	-3.28853900	-2.83651300
N	1.64094800	-2.28591400	1.07475000	H	-1.30550200	-4.23498200	-0.90388700
C	1.29609500	-3.26714800	0.17468800	C	-0.28468000	-2.35226100	-3.56764900
O	1.98254700	-4.22924300	-0.15029700	H	1.31419800	-0.89480400	-3.50828400
C	-0.07188300	-2.98866800	-0.36953800	H	-1.81636600	-3.86460500	-3.32698800
C	-0.70874700	-1.82311400	0.10706500	H	-0.49202500	-2.19883700	-4.63011800
C	-0.69217200	-3.83495400	-1.29324000	N	2.21560100	-0.23814700	2.84850500
C	-1.99313200	-1.52094200	-0.36684900	Co	0.54928800	-0.42429000	1.85080400
C	-1.97352400	-3.52115500	-1.75808900	O	0.52398200	0.88152700	0.12323900
H	-0.15704000	-4.72710800	-1.62899600	O	-1.04418900	-0.49196300	0.75343200
C	-2.61942800	-2.36815100	-1.29783600	C	-0.63712900	0.43396300	-0.03626600
H	-2.51259800	-0.62422500	-0.01587500	C	-1.56027000	0.93217100	-1.11223600
H	-2.47072600	-4.17339300	-2.48086100	H	-2.52293300	1.22433100	-0.66677600
H	-3.62100200	-2.12293700	-1.66328500	H	-1.10955600	1.78243200	-1.63882400
N	1.76446600	-0.33036100	2.80896900	H	-1.75719000	0.11513500	-1.82324600
Co	0.36880500	-0.92224600	1.43827600	O	-0.26365200	1.09927500	2.85551400
O	1.26124700	0.36349400	0.22080100	O	-0.56655200	-0.89081300	3.69266100
O	0.43985700	0.01692300	-1.84336100	C	-0.79689900	0.33618100	3.73952000
C	1.22526400	0.61630700	-0.98395000	C	-1.70561200	0.94153200	4.77833300
C	2.11322200	1.66317900	-1.59013300	H	-2.71328500	1.04298000	4.34325200
H	1.50702200	2.37491300	-2.17015000	H	-1.77025800	0.28646500	5.65689800
H	2.67568700	2.18186800	-0.80601500	H	-1.36004000	1.94555200	5.06135500
H	2.80924000	1.17755200	-2.29235900	H	1.77049200	-1.23016700	-1.08648700
O	-1.11220600	0.22999900	2.14038000	³T_{SAB}			
O	-0.68174900	-1.77166300	2.83442700	C	2.81750200	0.71593900	4.53958900
C	-1.40692600	-0.73230500	2.91616700	C	3.92763200	-0.10697400	4.52520000
C	-2.57028600	-0.67025700	3.86127000	C	4.02706200	-1.15244000	3.56999900
H	-3.41818100	-1.21222200	3.41150200	C	2.94109700	-1.29233900	2.66180800
H	-2.31917600	-1.17011500	4.80722500	C	1.78339100	0.50436000	3.60050700
H	-2.86875500	0.37151700	4.03620400	H	5.95941500	-1.97712300	4.14422500
H	-0.11318400	-0.65963400	-1.37367000	H	2.72417700	1.52911700	5.26148000
³A				H	4.73794900	0.03984900	5.24455600
C	3.83719600	0.77910700	4.26775300	C	5.11412700	-2.06230600	3.45763600
C	4.54248500	-0.40719200	4.35665300	C	2.92293100	-2.30042800	1.64921100
C	4.08833100	-1.56006900	3.66517900	H	0.88988800	1.13239900	3.56090100
C	2.90090900	-1.41324100	2.89611100	C	4.00167000	-3.17902900	1.57639900
C	2.65311500	0.82813300	3.50122900	C	5.08192400	-3.04254300	2.48389100
H	5.63017700	-2.97634500	4.27029400	H	3.99940800	-3.96296400	0.82260200
H	4.17218100	1.67765500	4.78867600	H	5.91664700	-3.74341700	2.40104500
H	5.45365100	-0.46778500	4.95806000	N	1.78000500	-2.25579500	0.85754500
C	4.72141800	-2.83226100	3.68213300	C	1.35368700	-3.28349100	0.03046800
C	2.34969500	-2.47578100	2.11609700	O	1.98625100	-4.29410200	-0.22713100
H	2.03895600	1.72841100	3.42538800	C	-0.04398100	-3.02152800	-0.43773600
C	2.99463000	-3.71358700	2.17716700	C	-0.53654100	-1.69721400	-0.35429700
C	4.16607800	-3.86980100	2.95517000	C	-0.86690500	-4.07378200	-0.84307400
H	2.58903500	-4.56517400	1.63419100	C	-1.89819500	-1.46786000	-0.63659400

C	-2.20877300	-3.81786100	-1.13819900	O	1.23285800	0.50756000	0.21565500
H	-0.44942400	-5.08177300	-0.89768200	O	0.24992700	0.24289000	-1.78591200
C	-2.72765500	-2.51881600	-1.02805000	C	1.08573800	0.83731700	-0.95266000
H	-2.28792800	-0.44759800	-0.58637400	C	1.84653200	1.96883100	-1.58589800
H	-2.86228900	-4.63761300	-1.44852200	H	2.41516400	1.59083100	-2.44952100
H	-3.77876600	-2.33087100	-1.26222500	H	1.13839400	2.72079800	-1.96679900
N	1.85163800	-0.47267800	2.71465900	H	2.52428300	2.42176700	-0.85372000
Co	0.59420200	-0.84216200	1.23630200	O	-1.00585600	0.17955200	2.17597200
O	1.41500300	0.81243800	0.37222800	O	-0.98925600	-1.80956300	3.08035600
O	0.70552500	0.25661100	-1.66524100	C	-1.49975300	-0.67104400	2.99937300
C	1.31146900	1.02228400	-0.87552400	C	-2.70376300	-0.28810800	3.82548700
C	1.95785300	2.27870300	-1.42234000	H	-3.60526700	-0.69588300	3.33940100
H	1.87092500	2.32011600	-2.51502100	H	-2.63539500	-0.73850400	4.82550100
H	1.46789100	3.15752800	-0.97450700	H	-2.80696200	0.80273300	3.89438000
H	3.01582900	2.30709600	-1.12105100	H	-0.22248500	-0.48484200	-1.31849600
O	-0.90240000	0.19907000	2.03878100				
O	-0.86149200	-1.89841600	2.65097300	5A			
C	-1.40764300	-0.78001500	2.70355800	C	3.94647800	0.81132000	4.15632400
C	-2.66999200	-0.54020700	3.49549800	C	4.66277800	-0.37184300	4.11499600
H	-3.53538400	-0.70690300	2.83306300	C	4.13296700	-1.49456100	3.42882100
H	-2.73623800	-1.25113000	4.32986000	C	2.86878100	-1.32266200	2.80149800
H	-2.71697000	0.49573800	3.85814700	C	2.69022100	0.87708900	3.51780200
H	0.14176400	-0.76890500	-0.84695200	H	5.75140700	-2.90428000	3.80869100
H				H	4.33247200	1.68826000	4.67914700
H				H	5.63478200	-0.45374200	4.60906500
3B				C	4.77895900	-2.76103500	3.33192700
C	2.92210400	0.75714300	4.57918400	C	2.24242700	-2.39926300	2.05995900
C	4.04199600	-0.04958200	4.51323500	H	2.06681100	1.77520200	3.54629900
C	4.08795200	-1.13285100	3.59733400	C	2.92381300	-3.63724000	2.00816100
C	2.93734600	-1.33089700	2.77970700	C	4.16963100	-3.79754000	2.63773800
C	1.82720600	0.48510100	3.72974700	H	2.47014400	-4.47822000	1.48397700
H	6.07928500	-1.88093200	4.06510300	H	4.66807900	-4.76784100	2.57452000
H	2.86833700	1.59767200	5.27354500	N	1.06947800	-2.09685400	1.46060600
H	4.90235200	0.13806200	5.16178200	C	0.32946100	-3.12464800	0.80702500
C	5.19034400	-2.01732800	3.44501800	O	-0.08021500	-4.08057500	1.43147400
C	2.87344400	-2.38997900	1.81207200	C	0.11005900	-2.95757400	-0.65966100
H	0.92211100	1.09914200	3.74012000	C	0.75530100	-1.96122700	-1.41002600
C	3.97789700	-3.23551900	1.69595400	C	-0.72325000	-3.88499800	-1.30836500
C	5.11641700	-3.03542400	2.51375700	C	0.57240700	-1.90004000	-2.79320400
H	3.94424100	-4.04610900	0.97157800	C	-0.91379500	-3.81331700	-2.68705200
H	5.96264300	-3.71758400	2.39588400	H	-1.21115500	-4.65478600	-0.70752100
N	1.68341700	-2.43273100	1.10132800	C	-0.26309600	-2.82226900	-3.43204200
C	1.35459500	-3.38177500	0.14215000	H	1.08093000	-1.12668300	-3.37433800
O	2.06182000	-4.30672100	-0.22628500	H	-1.56912100	-4.53165600	-3.18589300
C	-0.01239800	-3.09056500	-0.38698300	H	-0.40835800	-2.76889400	-4.51430600
C	-0.65804100	-1.96529000	0.15815900	N	2.18707300	-0.16001400	2.86326400
C	-0.62793500	-3.87792400	-1.36455400	Co	0.27950900	-0.25558700	1.92884600
C	-1.94066800	-1.62977000	-0.29007900	O	0.76482800	1.12857300	0.37988700
C	-1.90870700	-3.53682200	-1.80967000	O	-1.11479000	0.00980600	0.39394800
H	-0.09036500	-4.74463700	-1.75838700	C	-0.37932900	0.90900400	-0.11609200
C	-2.55923300	-2.41743400	-1.27662700	C	-0.86508600	1.68317500	-1.31562100
H	-2.46034700	-0.76010000	0.12147900	H	-1.87136000	2.08004400	-1.11484000
H	-2.40338400	-4.14164100	-2.57397400	H	-0.17445600	2.49897900	-1.56356000
H	-3.56127900	-2.15325600	-1.62696400	H	-0.95257400	0.99615700	-2.17229900
N	1.84135400	-0.52220800	2.87446900	O	-0.47410200	1.23083600	3.32861800
Co	0.41442200	-1.09101000	1.52581100				

O	-0.95396500	-0.90233100	3.47342100
C	-1.10540700	0.28997200	3.88681400
C	-2.06190300	0.56493700	5.02176400
H	-3.08843600	0.56717500	4.62005500
H	-2.00360700	-0.23553400	5.77271300
H	-1.85878300	1.54391000	5.47492100
H	1.39067600	-1.22805600	-0.91044900

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C	3.01897600	0.61249400	4.73327000
C	4.09436400	-0.24957500	4.63411600
C	4.11089700	-1.24800300	3.62639200
C	2.98765600	-1.30487100	2.75161700
C	1.94995300	0.47631000	3.82162700
H	6.02895600	-2.15276100	4.12099100
H	2.98278600	1.39054900	5.49797200
H	4.93749500	-0.17408600	5.32634200
C	5.16478700	-2.18876900	3.45327300
C	2.90891200	-2.29631800	1.69888600
H	1.08225400	1.14249300	3.85429100
C	3.97278600	-3.20761900	1.57852300
C	5.07946900	-3.13782400	2.45016900
H	3.92706700	-3.95929800	0.79454500
H	5.89042800	-3.85894400	2.32042400
N	1.77763300	-2.22337200	0.93017900
C	1.38992800	-3.20859800	0.00573100
O	2.07784500	-4.16227400	-0.32251600
C	-0.00909400	-2.99723300	-0.48134600
C	-0.61600400	-1.71910600	-0.38598300
C	-0.71455500	-4.11322300	-0.95830300
C	-1.97924200	-1.63225200	-0.72900200
C	-2.05786200	-3.98486800	-1.30803500
H	-0.19945200	-5.07453000	-1.02298400
C	-2.69574100	-2.74248900	-1.18350200
H	-2.48090000	-0.66008300	-0.67433700
H	-2.61507100	-4.85348200	-1.66898300
H	-3.75051800	-2.64208300	-1.45560500
N	1.94137100	-0.45275500	2.88120000
Co	0.48937900	-0.74594800	1.29915600
O	1.39695700	0.82493200	0.33983400
O	0.43573800	0.35088600	-1.61284800
C	1.16652500	1.08171000	-0.86592300
C	1.75434500	2.32483400	-1.48688400
H	2.10665700	2.10826200	-2.50510400
H	0.95984700	3.08481500	-1.56523100
H	2.56713600	2.71986200	-0.86521800
O	-1.03576200	0.48655500	2.03895300
O	-0.85632200	-1.58033200	2.71859000
C	-1.47448600	-0.48085500	2.73917800
C	-2.73544600	-0.32392300	3.55221600
H	-3.58256300	-0.70710100	2.95969300
H	-2.67583500	-0.92091400	4.47279800
H	-2.92384600	0.73328200	3.78157300
H	0.01363600	-0.56012800	-0.96272000

⁵B

C	3.06682300	0.69782700	4.66338600
C	4.11223100	-0.20437600	4.62438600
C	4.09959300	-1.26369600	3.68059900
C	2.97680100	-1.33768200	2.80421300
C	1.99671800	0.53978600	3.75612900
H	5.98953500	-2.19263100	4.23507000
H	3.05348400	1.52228000	5.37879100
H	4.95491900	-0.11463700	5.31559000
C	5.12608100	-2.24182400	3.56728500
C	2.86802200	-2.38412200	1.81035500
H	1.14828100	1.23126200	3.74821800
C	3.90885400	-3.32480800	1.74341900
C	5.01467300	-3.23942300	2.61644400
H	3.84847700	-4.11398900	0.99856400
H	5.80403600	-3.99057900	2.52911400
N	1.73194700	-2.32621500	1.04173600
C	1.40135400	-3.27931500	0.06643300
O	2.13018600	-4.19194100	-0.29424300
C	0.02818100	-3.06334800	-0.48769400
C	-0.70486500	-1.94114600	-0.04762400
C	-0.51368800	-3.99869900	-1.38119700
C	-2.02466200	-1.80532200	-0.50880100
C	-1.81841200	-3.82570200	-1.84638600
H	0.09387000	-4.85513200	-1.68431400
C	-2.57419000	-2.73024400	-1.40936900
H	-2.63465800	-0.95593600	-0.18148500
H	-2.25330000	-4.54781900	-2.54258200
H	-3.59835100	-2.59709800	-1.77115400
N	1.96111900	-0.44221500	2.87206700
Co	0.39360500	-0.86467800	1.40038600
O	1.20803600	0.69842500	0.19735100
O	0.15669600	0.34197400	-1.74959400
C	0.96396000	1.01652900	-0.96432700
C	1.57384500	2.22639400	-1.61259300
H	2.10141700	1.92665400	-2.53085900
H	0.77298900	2.92144200	-1.90944100
H	2.26303100	2.71954800	-0.91810300
O	-1.01214600	0.45752800	2.16050800
O	-0.83650900	-1.53203600	3.05172100
C	-1.41617700	-0.41958100	2.99939200
C	-2.60165100	-0.11957700	3.88446100
H	-3.51637400	-0.46285000	3.37343300
H	-2.52091300	-0.66723800	4.83328800
H	-2.69449400	0.96058700	4.06089700
H	-0.21288800	-0.44081100	-1.25645800
¹C			
C	-7.25786900	4.49627900	-0.27834300
C	-5.01019300	3.88871200	-0.52304500
C	-4.77146100	4.93728700	-1.46379400
C	-5.86945900	5.78343900	-1.76919500
C	-7.10100600	5.56712100	-1.18350600
H	-8.22014700	4.26302500	0.18015400

C	-3.99519300	2.95919300	-0.12505800	H	-3.60968000	5.68689500	-3.10598500
C	-3.48003000	5.05166800	-2.03438700	H	-1.51830100	4.71288200	-2.18012900
H	-5.72899300	6.60142500	-2.48113800	H	-1.56151800	3.12999100	-0.26094800
H	-7.96007100	6.19934000	-1.41444000	N	-3.90634900	2.31343300	1.01412300
C	-2.50841400	4.13421700	-1.67146100	C	-2.91136000	1.63096500	1.66751900
C	-2.74581300	3.09528800	-0.74738300	O	-1.71755900	1.73264500	1.41246300
H	-3.27481500	5.84299000	-2.75819600	C	-3.42189400	0.65780400	2.74830300
H	-1.51334700	4.20378800	-2.11952800	C	-4.86929200	1.00495200	3.13778900
H	-1.95332300	2.38607900	-0.52135700	H	-5.24561400	0.25857200	3.86532100
N	-4.36228800	2.10369900	0.89786200	H	-4.89755000	1.94656400	3.69783000
C	-3.52457600	1.02816300	1.23486900	C	-3.29493000	-0.76424100	2.15591200
O	-2.82674700	0.47891300	0.39650100	H	-3.68555200	-1.51715400	2.85942500
C	-3.32989400	0.62960300	2.72335500	H	-3.84400900	-0.86182400	1.20784200
C	-4.27490100	1.29401800	3.72926600	C	-2.50437300	0.76948500	3.98057000
H	-3.93602100	1.05564900	4.75128300	H	-1.45562200	0.61851500	3.68587600
H	-4.28797900	2.38687800	3.62107500	H	-2.58383500	1.76407000	4.44821200
C	-3.41332700	-0.90399000	2.84283500	H	-2.77605600	0.01362200	4.73554100
H	-3.12086400	-1.22376400	3.85622300	N	-6.05989000	3.38821400	0.03680800
H	-4.44149300	-1.25125800	2.66007700	Co	-5.73134100	2.14087100	1.51201200
C	-1.88073500	1.08633400	3.03817200	O	-5.93112900	3.66152100	2.79096500
H	-1.16171200	0.61392600	2.35386800	C	-7.14923400	3.34089500	2.94270000
H	-1.77961600	2.18040800	2.94627200	O	-7.56744800	2.34491200	2.27150600
H	-1.61841200	0.81107900	4.07251100	C	-8.04094800	4.07959800	3.89698200
N	-6.24070400	3.70844200	0.03554900	H	-7.95092600	3.61642000	4.89336100
Co	-6.30068400	2.10052600	1.08544200	H	-7.72737400	5.12897300	3.97893100
O	-6.60900000	3.03961900	2.79276000	H	-9.08939900	4.00528200	3.57882900
C	-7.85482000	2.85764100	2.64528000	H	-2.23776500	-0.98956400	1.95127400
O	-8.22147100	2.31393500	1.55441600	O	-6.55107100	-0.60785300	1.90624200
C	-8.83657900	3.23236400	3.71400800	C	-6.53887600	-0.33851500	0.67422800
H	-8.87902300	2.41389400	4.45109300	O	-6.08400400	0.75492100	0.22383900
H	-8.50265800	4.13962200	4.23589900	C	-7.07362400	-1.35202100	-0.30387800
H	-9.83871900	3.36918600	3.28699700	H	-8.13168700	-1.54803200	-0.07144200
H	-2.74335700	-1.38675000	2.11677500	H	-6.97433100	-0.99513500	-1.33574100
O	-6.38730100	0.20072100	1.62319900	H	-6.53053800	-2.30020900	-0.17384200
C	-6.50388000	-0.09097100	0.39113200	H	-5.85895700	0.34542600	2.43100900
O	-6.48781400	0.89389800	-0.41272900				
C	-6.60132300	-1.50227500	-0.09196800	¹D			
H	-7.05575800	-2.13977800	0.67777800	C	-7.22199300	3.78769700	-0.40042600
H	-7.17252800	-1.54613300	-1.02883300	C	-4.90216900	3.72968000	-0.59496700
H	-5.57968100	-1.86520500	-0.29176600	C	-4.92008700	4.59916200	-1.72994200
H	-5.30446700	0.93224500	3.62729300	C	-6.19243500	5.04908900	-2.17202200
			C	-7.33863900	4.64802700	-1.51512800	
¹TS_{CD}			H	-8.10598500	3.44976600	0.14952100	
C	-7.22500500	3.83315500	-0.40134300	C	-3.66984700	3.21048900	-0.06327100
C	-4.89638800	3.75419600	-0.57150900	C	-3.68906300	4.95643800	-2.33759500
C	-4.88846900	4.65264800	-1.68038500	H	-6.25006500	5.71589200	-3.03705500
C	-6.14913200	5.13050300	-2.12443100	H	-8.32635200	4.98220300	-1.83878200
C	-7.30896300	4.72154000	-1.49558200	C	-2.51077000	4.45350000	-1.81529700
H	-8.11346000	3.47899000	0.12645900	C	-2.48062100	3.59302900	-0.69555400
C	-3.69475800	3.18046300	-0.04392600	H	-3.68803000	5.62191700	-3.20389500
C	-3.63987100	4.99776300	-2.25915500	H	-1.55916400	4.72752000	-2.27947400
H	-6.18949900	5.82034800	-2.97195800	H	-1.54006900	3.21305600	-0.30457500
H	-8.28864200	5.07050400	-1.82684900	N	-3.81858600	2.37335900	1.02502300
C	-2.48244800	4.44910400	-1.73681200	C	-2.79818600	1.71610700	1.66564200
C	-2.48716500	3.54897500	-0.64627000	O	-1.60778200	1.83008200	1.40240300

C	-3.31412700	0.73932700	2.74484200	H	-4.40833800	-1.13900500	2.80689300	
C	-4.78823100	1.05461200	3.06544400	C	-1.72560200	1.08465000	2.67769900	
H	-5.38841600	0.13902400	3.20779200	H	-1.10617600	0.50629400	1.97620500	
H	-4.86989300	1.66383300	3.97846300	H	-1.58515000	2.15753300	2.46567300	
C	-3.15396000	-0.68129600	2.15814000	H	-1.36306900	0.89764600	3.70097900	
H	-3.46240400	-1.43816100	2.89893100	N	-6.19116100	3.74431400	-0.01923500	
H	-3.76826800	-0.80975800	1.25395600	Co	-6.26935600	2.07457000	1.00445100	
C	-2.42502500	0.87041400	3.99475000	O	-6.81597600	2.93763700	2.97326600	
H	-1.36894700	0.71136300	3.72906400	C	-7.99424500	2.75638100	2.59768800	
H	-2.51273900	1.87439200	4.44043800	O	-8.20175400	2.32684300	1.40689600	
H	-2.71744500	0.13068100	4.75815300	C	-9.17064100	2.99316800	3.50978100	
N	-6.05248500	3.35290600	0.03467700	H	-9.39021900	2.05421100	4.04402100	
Co	-5.58126000	2.13555600	1.64162300	H	-8.92596800	3.76189900	4.25489000	
O	-5.81157500	3.66522600	2.88688900	H	-10.06435500	3.27243200	2.93536400	
C	-6.98623700	3.29149000	3.13137500	H	-2.78478000	-1.42054200	2.11504200	
O	-7.40258700	2.24488900	2.51482300	O	-6.32108300	0.22602100	1.64355000	
C	-7.86978900	4.00975700	4.10750100	C	-6.70021800	-0.23744200	0.50335500	
H	-7.95441200	3.40256700	5.02340600	O	-6.85074300	0.56254100	-0.44501500	
H	-7.44520600	4.98853500	4.36304600	C	-6.90458300	-1.71986300	0.35019000	
H	-8.88119600	4.12217600	3.69083800	H	-7.31834400	-2.15042300	1.27246700	
H	-2.10380200	-0.86825000	1.88621200	H	-7.55997100	-1.92569000	-0.50580600	
O	-7.84002600	-0.09695300	1.41969700	H	-5.92426600	-2.18833300	0.16460000	
C	-6.82816500	-0.23855800	0.59914200	H	-5.09547900	1.20926900	3.57848800	
O	-5.87137200	0.53937500	0.52924100					
C	-6.89408200	-1.46448900	-0.26237600	³TS_{CD}				
H	-7.90969600	-1.59616400	-0.66168600	C	-7.18931300	3.76712200	-0.42450000	
H	-6.15808000	-1.39659100	-1.07152800	C	-4.86017400	3.80151100	-0.59453100	
H	-6.66656600	-2.34408800	0.36195100	C	-4.88982800	4.74820200	-1.65737800	
H	-7.76140300	0.73803700	1.95647600	C	-6.16937400	5.19072000	-2.08295500	
³C								
C	-7.18871700	4.55404600	-0.34206700	C	-7.31057600	4.70082300	-1.47693200	
C	-4.93630900	3.97376600	-0.49629000	H	-8.05721900	3.34752300	0.08973900	
C	-4.63605900	5.07899600	-1.33799200	C	-3.64029000	3.25531600	-0.08946400	
C	-5.71458200	5.94469200	-1.65534700	C	-3.65144800	5.16963300	-2.21272200	
C	-6.98027400	5.68205200	-1.16436800	H	-6.24022500	5.91724700	-2.89704200	
H	-8.17169900	4.28969400	0.05405000	C	-8.30415900	5.02170800	-1.79447800	
C	-3.95152400	3.01079600	-0.11244600	C	-2.47482500	4.64650400	-1.71306700	
C	-3.30240100	5.21815000	-1.81185700	C	-2.44762600	3.69442900	-0.66326500	
H	-5.53625000	6.81132100	-2.29771800	H	-3.64618800	5.89740900	-3.02724600	
H	-7.82616500	6.32797300	-1.40574200	H	-1.52099600	4.96856500	-2.13901800	
C	-2.35568300	4.27448800	-1.45405100	H	-1.50519800	3.29589200	-0.29805800	
C	-2.65961800	3.17340900	-0.62039000	N	-3.83517100	2.32428800	0.93561700	
H	-3.04554500	6.05613800	-2.46321700	C	-2.79692200	1.67854700	1.59294500	
H	-1.33371700	4.37166400	-1.82919000	O	-1.61826900	1.83963500	1.32386800	
H	-1.88454000	2.44446800	-0.38679300	C	-3.25653000	0.69229900	2.68052300	
N	-4.41304800	2.05312800	0.77089800	C	-4.71662600	0.97474000	3.05810100	
C	-3.58169900	0.93448100	1.09445300	H	-5.07126300	0.25389700	3.81861700	
O	-3.09797000	0.26818100	0.20641000	H	-4.81592400	1.95324600	3.54808500	
C	-3.21791600	0.67441300	2.57278700	C	-3.07084400	-0.72954400	2.10368600	
C	-4.03435800	1.48412800	3.58687800	H	-3.39677700	-1.48649600	2.83461500	
H	-3.63953500	1.29590500	4.59877300	H	-3.65880700	-0.87522100	1.18573300	
H	-3.97104900	2.56561900	3.39783800	C	-2.34605500	0.86683900	3.91050700	
C	-3.35265400	-0.83462800	2.85229400	H	-1.29110700	0.75666100	3.61903500	
H	-2.96567200	-1.06649600	3.85746200	H	-2.47095200	1.86386700	4.36243500	
				N	-2.58467200	0.11120200	4.67611800	
				N	-6.00558200	3.35630200	-0.00622300	

Co	-5.63537500	2.06120400	1.42428500	H	-8.06642200	4.69255300	4.43937900
O	-6.00065900	3.80209900	2.93717700	H	-9.21264700	3.58556200	3.59945400
C	-7.14160500	3.30178600	3.00648800	H	-2.05559600	-0.82614500	1.64137900
O	-7.42279400	2.27049400	2.29464300	O	-8.13029200	-0.06126500	1.49901500
C	-8.20581200	3.85186000	3.92561500	C	-7.14472900	-0.29087400	0.66428500
H	-8.30097100	3.18583600	4.79855100	O	-6.14108300	0.41557200	0.57157200
H	-7.93120200	4.85664200	4.27098300	C	-7.33122900	-1.52396800	-0.17756200
H	-9.18192300	3.86779700	3.41966800	H	-7.18152500	-2.41240800	0.45744600
H	-2.01108600	-0.90345900	1.86504700	H	-8.35914100	-1.56908600	-0.56517600
O	-6.33008700	-0.76967500	1.87577600	H	-6.60302300	-1.53763800	-0.99676900
C	-6.68739100	-0.46968400	0.70367200	H	-7.92774700	0.75335400	2.05563100
O	-6.42438500	0.64718700	0.16978600				
C	-7.48652800	-1.47396000	-0.09463300	5C			
H	-7.37911200	-2.48126300	0.32700500	C	-7.30593500	3.95295800	-0.97397000
H	-8.54881800	-1.18265900	-0.05308900	C	-5.01391600	3.78618000	-0.67920000
H	-7.17656900	-1.45372800	-1.14866800	C	-4.74507500	4.58519200	-1.82429500
H	-5.60963800	0.29012700	2.34029900	C	-5.86411800	5.05642100	-2.55563700
3D				C	-7.14315100	4.74556400	-2.12812800
C	-7.12025800	3.70752400	-0.39932100	H	-8.29283000	3.69588600	-0.57946700
C	-4.80202700	3.77501900	-0.59285600	C	-3.93936100	3.28515300	0.16016700
C	-4.86657100	4.65871700	-1.71307700	C	-3.39009500	4.88282600	-2.15172000
C	-6.15979100	5.04981500	-2.14910700	H	-5.70540900	5.67116800	-3.44573600
C	-7.28308600	4.57790100	-1.49980900	H	-8.02262500	5.10472300	-2.66559600
H	-7.98640900	3.31146400	0.13997800	C	-2.36007000	4.41085400	-1.34659400
C	-3.54354000	3.31246700	-0.07340400	C	-2.61221000	3.63594500	-0.20615100
C	-3.65448100	5.08774400	-2.31584500	H	-3.17417900	5.49336400	-3.03170500
H	-6.25223400	5.72658900	-3.00317600	H	-1.32510900	4.65096700	-1.60134500
H	-8.28713800	4.86404500	-1.81872900	H	-1.78020600	3.30079100	0.41179100
C	-2.45190800	4.63847400	-1.80578100	N	-4.30191600	2.51647700	1.20347800
C	-2.37825300	3.76086800	-0.69822500	C	-3.34425500	2.24112200	2.22565600
H	-3.68948400	5.76616600	-3.17140700	O	-2.73508500	3.15846000	2.73005800
H	-1.51632400	4.96719700	-2.26642900	C	-3.14826100	0.77405600	2.64374000
H	-1.41777500	3.42181700	-0.31850200	C	-4.26091600	0.37591800	3.64283900
N	-3.65333300	2.44588900	1.00981400	H	-4.03661300	-0.62786300	4.04001400
C	-2.58590600	1.81897900	1.62554900	H	-4.30475100	1.08085200	4.48604400
O	-1.41063700	1.98061000	1.34052900	C	-3.17777900	-0.14383900	1.40510700
C	-3.05618700	0.81066400	2.69644600	H	-3.05701900	-1.19265200	1.72000900
C	-4.46174800	1.20253700	3.15231700	H	-4.12024000	-0.05954200	0.84535400
H	-5.09726000	0.35825900	3.45754700	C	-1.78230100	0.66735000	3.34526300
H	-4.45442800	1.97941100	3.93190200	H	-0.95722800	0.95909600	2.67585100
C	-3.05831700	-0.58077900	2.02356500	H	-1.73823800	1.31721800	4.23005400
H	-3.34922500	-1.35500400	2.75301100	N	-1.61107000	-0.37274800	3.66406500
H	-3.76859700	-0.61405900	1.18349400	Co	-6.26834700	3.48986600	-0.29030600
C	-2.06293200	0.81642700	3.87116000	O	-6.38670000	2.08265000	1.29095800
H	-1.04541700	0.61577700	3.50236300	O	-6.46341100	2.80310300	3.29080000
H	-2.04899400	1.79508100	4.37658100	C	-7.63244200	3.22558800	3.06901300
H	-2.33325600	0.04905000	4.61437400	O	-8.12278900	3.12670000	1.90174600
N	-5.93067600	3.32956000	0.03141500	C	-8.45740500	3.81223400	4.18921700
Co	-5.41012400	2.14910300	1.67546900	H	-9.05722800	3.00451500	4.64035000
O	-6.13526600	3.87681400	2.95785100	H	-7.80873100	4.23419200	4.96839400
C	-7.13592400	3.18682400	3.21123800	H	-9.15009100	4.57217500	3.80228400
O	-7.22270200	2.01154700	2.68411300	H	-2.35187500	0.09051800	0.71258900
C	-8.24449600	3.65899900	4.11842900	O	-7.17323500	0.13239700	1.92489000
H	-8.29895700	3.00071700	4.99981800	C	-6.98642500	-0.26570300	0.74617600
				O	-6.44219300	0.51417600	-0.10475500

C	-7.36121800	-1.66947200	0.33593900
H	-8.21331700	-2.02776600	0.92896100
H	-7.58287700	-1.71481900	-0.73873300
H	-6.50423300	-2.33373000	0.53677000
H	-5.25598800	0.34197000	3.18157700

5TS CD

C	-7.19996300	3.91868000	-0.57361900
C	-4.87372900	3.87235700	-0.63002000
C	-4.83074300	4.82332300	-1.69311700
C	-6.07274600	5.30622500	-2.17977200
C	-7.25601200	4.85568700	-1.62734900
H	-8.10689700	3.52986000	-0.10061700
C	-3.66301800	3.31514900	-0.06753500
C	-3.56718100	5.23464100	-2.19818800
H	-6.07859200	6.03584500	-2.99431600
H	-8.22369900	5.20995800	-1.98728000
C	-2.41397800	4.70567200	-1.65156500
C	-2.44413500	3.76063000	-0.60278200
H	-3.52512100	5.96484900	-3.00985800
H	-1.44061300	5.01969200	-2.03721500
H	-1.52054300	3.35681000	-0.19865700
N	-3.85795500	2.38443100	0.93659700
C	-2.80456100	1.75739300	1.60753300
O	-1.62403800	1.96539600	1.37503600
C	-3.22496800	0.69031300	2.64252600
C	-4.66027100	0.89736100	3.14145500
H	-4.88038100	0.16500700	3.94099200
H	-4.77029800	1.87609400	3.63617000
C	-3.06744700	-0.67606900	1.92911700
H	-3.37339000	-1.49418900	2.60052300
H	-3.68670500	-0.73073300	1.02080500
C	-2.23265400	0.75642700	3.82347400
H	-1.19577800	0.68755700	3.46330700
H	-2.33957700	1.70370600	4.37549700
H	-2.42398700	-0.07003400	4.52609900
N	-6.05315100	3.46125800	-0.10162800
Co	-5.74156900	2.04983600	1.49391600
O	-6.18730500	3.62915300	2.86835200
C	-7.37559600	3.20651500	2.94061900
O	-7.71459200	2.20382100	2.23797500
C	-8.36942500	3.85809700	3.86956700
H	-8.36278300	3.31424400	4.82863300
H	-8.09136700	4.90230300	4.06469500
H	-9.38506500	3.79301800	3.45553900
H	-2.01908300	-0.83727200	1.63557700
O	-6.38044700	-0.83753200	2.09485800
C	-6.69675400	-0.57418300	0.88614500
O	-6.38675400	0.49953100	0.31690900
C	-7.50070600	-1.60866000	0.14135900
H	-7.20422100	-2.62029700	0.44904400
H	-8.56190400	-1.47104500	0.40669300
H	-7.39016000	-1.47505400	-0.94197000
H	-5.70020300	0.03952400	2.50669300

5D

C	-7.15064900	3.74558600	-0.46500900
C	-4.82318100	3.77068800	-0.59478700
C	-4.85297900	4.66544300	-1.71255100
C	-6.12833700	5.07804000	-2.17900400
C	-7.27657100	4.62120100	-1.56415300
H	-8.03586800	3.36307400	0.05358600
C	-3.57637500	3.28552500	-0.04841400
C	-3.62954400	5.08714400	-2.29355700
H	-6.18577100	5.76109400	-3.03123700
H	-8.26771600	4.92435200	-1.90690000
C	-2.44296800	4.61919100	-1.76536100
C	-2.40160100	3.73263100	-0.66559700
H	-3.64454000	5.76946200	-3.14664000
H	-1.49430500	4.93720100	-2.20683100
H	-1.44925500	3.37906800	-0.28112800
N	-3.69528200	2.42614800	1.03821600
C	-2.60692100	1.83526700	1.61617100
O	-1.43619400	1.98072300	1.28642300
C	-2.92683500	0.81489800	2.78274400
C	-4.20389700	1.14304600	3.47569200
H	-5.05523800	0.45147700	3.46798900
H	-4.24221000	1.97354100	4.18656300
C	-2.98766100	-0.58360900	2.12765700
H	-3.12799900	-1.36284300	2.89501000
H	-3.81966100	-0.64764100	1.40943600
C	-1.75381500	0.87798400	3.78514500
H	-0.80386000	0.73340100	3.25177300
H	-1.71138500	1.85857900	4.28509900
H	-1.86524400	0.10100000	4.55781900
N	-5.97628600	3.34626100	-0.00871300
Co	-5.60818100	2.12922200	1.66452100
O	-6.30488200	3.75650700	2.99702300
C	-7.34309600	3.10878300	3.23027200
O	-7.48596700	1.95178500	2.68069800
C	-8.43052200	3.62827500	4.13578700
H	-8.59098500	2.91722800	4.96108400
H	-8.16506700	4.61417800	4.53621300
H	-9.37755400	3.69304900	3.57737700
H	-2.05113000	-0.79305000	1.58944700
O	-8.32053200	-0.02826300	1.30532200
C	-7.24971600	-0.31389800	0.60842500
O	-6.20463600	0.34054600	0.64659900
C	-7.38119800	-1.54265100	-0.24806900
H	-7.30801400	-2.43274000	0.39832700
H	-8.36839000	-1.56817300	-0.73072200
H	-6.57786500	-1.57252800	-0.99330600
H	-8.15178200	0.76389300	1.90617800

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C	-0.92137700	0.65973900	0.60036700
C	-0.47571300	1.97008000	0.57860600
C	-1.63605200	2.73437600	0.38464300
H	-0.39305900	-0.27674200	0.76382500

H	0.54356000	2.32519300	0.70486000	H	-1.24445900	3.41746100	-0.37863900
H	-1.74970300	3.81459400	0.32763500	C	-3.36478200	-0.35318100	0.56106300
C	-3.10413400	-0.49801100	0.43411100	C	-4.55641800	0.35088900	0.86029300
C	-4.17458800	-0.59917200	1.33016500	C	-3.29344900	-1.74500100	0.51576400
C	-2.76500900	-1.56979200	-0.40359000	C	-5.69458000	-0.43301500	1.13850900
C	-4.91252600	-1.78514300	1.37387900	H	-4.44057600	1.29076600	1.71512400
H	-4.42777300	0.23793600	1.98025800	C	-4.45019200	-2.48006800	0.79514300
C	-3.50545800	-2.75311900	-0.34191800	H	-2.36417800	-2.25715700	0.25841200
H	-1.92478900	-1.47925700	-1.09559000	C	-5.64919900	-1.82868500	1.10978800
C	-4.58080900	-2.86200900	0.54546500	H	-6.62106500	0.06196400	1.43952400
H	-5.74461300	-1.87171000	2.07654800	H	-4.41089700	-3.57149600	0.76897300
H	-3.23873900	-3.59116600	-0.98973300	H	-6.54041400	-2.41300300	1.34939100
H	-5.15586600	-3.78934800	0.59587700	Co	-4.37651200	2.21651800	-0.24146300
Co	-4.51023700	2.70512700	-0.13003800	N	-2.23565600	0.46130800	0.29955200
N	-2.26880900	0.66833800	0.41981100	N	-2.48318100	1.74858100	-0.03744500
N	-2.71528800	1.94535900	0.28561300	C	-4.16140900	3.24636300	2.40326800
C	-4.69964700	3.45007900	2.09418900	O	-4.26253700	2.07093800	2.82459500
O	-5.19005500	2.33719400	1.72302700	O	-4.19761900	3.54793900	1.16164700
O	-4.13900000	4.14021700	1.18225300	C	-4.02372600	4.37839800	3.39076600
C	-4.73992300	3.90445200	3.51834000	H	-3.47843000	4.03660700	4.28022400
H	-5.63584900	3.51491100	4.01986100	H	-3.52617900	5.24258200	2.93270100
H	-3.85489400	3.50485500	4.04100300	H	-5.03233000	4.68582400	3.71281100
H	-4.70469700	5.00034600	3.57415000	C	-5.25361300	1.43523400	-2.00934200
C	-5.68664700	1.67015800	-1.52729800	C	-4.22798800	2.36145100	-2.36452400
C	-4.49060900	2.11954500	-2.16905800	C	-4.53651700	3.62959500	-1.75686700
C	-4.40488500	3.54688000	-2.01662000	C	-5.82637300	3.50439800	-1.11558800
C	-5.61643800	3.99238600	-1.36169800	C	-5.36881100	0.02137900	-2.48825200
C	-6.21965200	0.27348100	-1.48295100	H	-5.88614400	-0.61823400	-1.76096100
H	-6.74367800	0.06916500	-0.53928700	H	-5.94478000	-0.01081700	-3.42949700
H	-6.94605000	0.12693100	-2.30167400	H	-4.38595100	-0.42545800	-2.69151200
H	-5.42874000	-0.47838100	-1.59979500	C	-6.55071000	4.62061700	-0.43842800
C	-5.94171300	5.41755100	-1.05215100	H	-6.90614400	5.34319800	-1.19272900
H	-6.21234200	5.94674700	-1.98169900	H	-7.42449900	4.26669800	0.12428500
H	-6.78715300	5.50708400	-0.35799800	H	-5.88531300	5.15764900	0.25245500
H	-5.08099100	5.93767100	-0.60792900	C	-3.75922900	4.90418400	-1.86092900
C	-3.33112700	4.43988900	-2.55587100	H	-4.25429000	5.60138800	-2.55852300
H	-3.59628400	4.78722000	-3.56977700	H	-3.69307600	5.40543500	-0.88403500
H	-3.19600800	5.33401400	-1.93059400	H	-2.73980700	4.73837900	-2.23558600
H	-2.36392700	3.92357700	-2.62973500	C	-3.04338600	2.06553900	-3.22728500
C	-3.49797300	1.26789200	-2.89178000	H	-3.30966800	2.24722600	-4.28312200
H	-3.72562900	1.29022400	-3.97177500	H	-2.18477600	2.70857200	-2.99289600
H	-2.46997600	1.63662100	-2.76961500	H	-2.72215000	1.01814300	-3.14745800
H	-3.53788200	0.22007200	-2.56842600	C	-6.25895700	2.15817400	-1.24615700
C	-6.39068200	2.84126600	-1.03732500	C	-7.58902400	1.62358700	-0.81351300
C	-7.70620300	2.80375300	-0.32763800	H	-7.88751900	1.99949800	0.17567200
H	-7.94511800	3.76269500	0.15014700	H	-8.36392000	1.94663100	-1.53019200
H	-8.51307700	2.57607400	-1.04488300	H	-7.60441900	0.52752300	-0.78715600
H	-7.71986000	2.02458300	0.44790200				

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C	-0.89887200	0.24699600	0.42086800
C	-0.26348100	1.44754800	0.14599600
C	-1.30158000	2.35980100	-0.12969000
H	-0.50248800	-0.72101600	0.71753700
H	0.80558300	1.64337500	0.15871500

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C	-1.22103000	-0.45402700	0.18085800
C	-0.41035400	0.49993400	-0.41689800
C	-1.27473800	1.56171500	-0.74355500
H	-0.98318200	-1.42745600	0.60191500
H	0.66082000	0.43817200	-0.59007600
H	-1.04484200	2.51233400	-1.21820300

C	-3.69839500	-0.41126500	0.77106800	C	-3.89064300	-0.63934500	0.97318500
C	-4.76553500	0.50859600	0.66616500	C	-2.03138900	-1.33728400	-0.44025200
C	-3.79895000	-1.63785300	1.43142200	C	-4.50393300	-1.87735300	0.75675200
C	-5.95379200	0.14858300	1.32234200	H	-4.35429500	0.09727300	1.63256300
H	-4.39769900	1.48346300	2.40545200	C	-2.64636900	-2.57666300	-0.63016600
C	-5.00929200	-1.96686700	2.04812400	H	-1.07542200	-1.11550300	-0.91940700
H	-2.95411900	-2.32786000	1.48087300	C	-3.88507700	-2.84702100	-0.03842700
C	-6.07940200	-1.07001100	2.00779500	H	-5.46109000	-2.09158400	1.23773900
H	-6.80954400	0.82776900	1.31387600	H	-2.15755800	-3.33095300	-1.25080900
H	-5.10729600	-2.92003800	2.57186900	H	-4.36277800	-3.81750800	-0.19010400
H	-7.01854700	-1.31655100	2.50862400	Co	-4.59289500	2.43670400	0.05514100
Co	-4.31051900	2.08478200	-0.41865400	N	-2.00452500	0.87615200	0.58896800
N	-2.48491500	0.03836000	0.18928800	N	-2.66683100	2.06109000	0.57132900
N	-2.52522100	1.26669200	-0.37701400	C	-5.26068700	3.26344600	2.25308400
C	-3.72629300	3.24844700	2.32198900	O	-5.61345100	2.13711000	1.74435600
O	-4.04977000	2.18196200	3.01118500	O	-4.55939400	4.02905200	1.54392700
O	-3.82677500	3.32380200	1.09254100	C	-5.66840100	3.61069500	3.65546700
C	-3.22913200	4.39105500	3.15282400	H	-4.99906500	3.08572800	4.35688300
H	-2.40875900	4.04633800	3.80042200	H	-5.57896300	4.69049600	3.82792600
H	-2.89319300	5.21549700	2.51452800	H	-6.69178000	3.26491300	3.85606000
H	-4.03868100	4.73345100	3.81715500	C	-6.03840300	1.75726700	-1.46427600
C	-4.86007800	1.64223600	-2.36621500	C	-4.77279400	1.79071100	-2.07041900
C	-4.14356100	2.90832300	-2.42837700	C	-4.30520400	3.20221000	-2.08273500
C	-4.82507000	3.83137300	-1.611188200	C	-5.29602700	4.00860900	-1.50068400
C	-5.99539900	3.16599900	-1.05080100	C	-6.95826900	0.58661400	-1.29784800
C	-4.52360500	0.40789000	-3.14544600	H	-7.39600100	0.55643800	-0.28868100
H	-4.92363100	-0.49620400	-2.66556600	H	-7.79364000	0.64791100	-2.01622900
H	-4.95478000	0.46142600	-4.16046500	H	-6.44024300	-0.36613700	-1.47046700
H	-3.43784000	0.27828700	-3.25862800	C	-5.28557800	5.49323000	-1.30239200
C	-7.02409400	3.83862700	-0.19412900	H	-6.15076100	5.95959500	-1.80112300
H	-7.72145900	4.42580700	-0.81659800	H	-5.33233300	5.74891600	-0.23243400
H	-7.62448700	3.11638200	0.37626400	H	-4.37824300	5.95197700	-1.71697000
H	-6.56104100	4.53563900	0.51913100	C	-3.02715400	3.64534000	-2.71496600
C	-4.45613700	5.25577800	-1.34535100	H	-3.11454300	3.59109700	-3.81477900
H	-5.19235600	5.93318900	-1.81013200	H	-2.77301400	4.68050600	-2.45263400
H	-4.44656800	5.47001200	-0.26654700	H	-2.18260000	2.99976900	-2.43140300
H	-3.46781300	5.50974000	-1.75093800	C	-4.06357900	0.67259600	-2.76434600
C	-2.93644000	3.17222000	-3.27419300	H	-4.26708400	0.72090100	-3.84912000
H	-3.25487000	3.47205000	-4.28778300	H	-2.97338800	0.73427500	-2.64040200
H	-2.31540000	3.98785500	-2.87746600	H	-4.39333700	-0.31198500	-2.40779700
H	-2.30764300	2.27911800	-3.38941200	C	-6.34753700	3.12280800	-1.04646600
C	-6.06202400	1.85383500	-1.60722200	C	-7.61721400	3.55183300	-0.39679600
C	-7.20971000	0.89882300	-1.52577200	H	-7.50351200	4.50753100	0.13265200
H	-7.87963100	1.11551800	-0.68445700	H	-8.39381300	3.69333100	-1.17109000
H	-7.80729700	0.99164800	-2.44967000	H	-7.98909500	2.79600800	0.30847600
H	-6.88359900	-0.14657000	-1.44777400				

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³ E				C	-0.59264100	1.44275600	0.80074900
C	-0.70659000	1.06747900	0.94253700	C	-0.41900000	2.81372000	0.89684500
C	-0.51907200	2.42389600	1.15450300	C	-1.69516300	3.35856900	0.64856900
C	-1.77646200	3.00112000	0.91827200	H	0.10619000	0.62276400	0.94663100
H	-0.03013900	0.22295700	1.05327000	H	0.50041500	3.34573500	1.12759200
H	0.39645300	2.92387900	1.45937500	H	-2.00375800	4.40269200	0.63065300
H	-2.09323900	4.03902300	0.99640000	C	-2.64379300	0.01994200	0.36773500
C	-2.65829900	-0.37465000	0.36135100	C	-4.03763400	0.12294400	0.59151200

C	-2.01737400	-1.18135800	0.02841500	C	-4.72881100	-1.04629900	0.11207200
C	-4.78579900	-1.06639400	0.45881500	H	-4.59826900	0.46742200	2.13993400
H	-4.34405500	0.79007100	1.72008300	C	-2.77333300	-2.36065400	0.68690900
C	-2.80009800	-2.33371600	-0.08723800	H	-0.93298600	-1.26125900	0.95296500
H	-0.94269900	-1.22748800	-0.15831500	C	-4.13836400	-2.28620200	0.39877300
C	-4.18343300	-2.28220500	0.12950400	H	-5.79724300	-1.01962500	-0.11316700
H	-5.85986600	-1.04629800	0.66567100	H	-2.30756300	-3.32493100	0.90118700
H	-2.32292900	-3.28087200	-0.34969000	H	-4.74689000	-3.19349600	0.39220600
H	-4.78202900	-3.19281800	0.05407400	Co	-4.53961200	2.01544000	-0.26554800
Co	-4.65333400	2.12059500	-0.02620700	N	-1.89242000	1.24990900	0.49588800
N	-1.90278200	1.22181500	0.50872500	N	-2.60162100	2.37894000	0.26028500
N	-2.58057300	2.38937100	0.41433900	C	-5.15358300	2.15584200	2.79928400
C	-5.08305100	2.42026100	2.76273500	O	-4.83029500	0.89451300	2.99613700
O	-4.55484200	1.28404600	2.88841400	O	-5.15315700	2.68230100	1.68551300
O	-5.29916300	2.96074500	1.62615000	C	-5.53247400	2.88713500	4.05012700
C	-5.51809300	3.16547700	3.99562500	H	-4.71859600	2.80432700	4.78670800
H	-5.03070200	2.75492800	4.88807200	H	-5.74367200	3.93909700	3.82944900
H	-5.30448900	4.23759900	3.88671400	H	-6.41803100	2.40853100	4.49743000
H	-6.60941400	3.05299400	4.10462300	C	-6.09618200	1.74129300	-1.72720100
C	-6.13622700	1.66616600	-1.65163000	C	-4.84224900	1.76792600	-2.50654900
C	-4.79208800	1.66903000	-2.24682700	C	-4.27466300	3.04363600	-2.36220000
C	-4.25754800	2.99714500	-2.17288300	C	-5.12222500	3.80473100	-1.45741100
C	-5.18704600	3.78032400	-1.44650300	C	-7.12639800	0.65762200	-1.80897800
C	-7.10146900	0.52239200	-1.72395200	H	-7.72063700	0.57402800	-0.88718400
H	-7.86137100	0.57285200	-0.93142400	H	-7.83308000	0.88335400	-2.62734000
H	-7.63519300	0.53690200	-2.69038200	H	-6.68474700	-0.32249800	-2.03065800
H	-6.59523900	-0.44941800	-1.64989200	C	-4.90761300	5.23059300	-1.05218600
C	-5.08597500	5.22786700	-1.09431100	H	-5.50548500	5.90229400	-1.69329600
H	-5.78733300	5.81796000	-1.71049100	H	-5.22292000	5.41109200	-0.01387900
H	-5.36111800	5.40212600	-0.04247100	H	-3.85835000	5.53994900	-1.15765000
H	-4.07839800	5.62902100	-1.26607800	C	-3.02796100	3.55404900	-3.01636400
C	-2.95426700	3.44754800	-2.75910900	H	-3.28023100	4.19959500	-3.87549500
H	-3.06396700	3.64250400	-3.83984700	H	-2.41314300	4.15861600	-2.33334600
H	-2.59462500	4.37636500	-2.29643600	H	-2.39985400	2.73623100	-3.39515600
H	-2.16465100	2.69073000	-2.64482300	C	-4.36294800	0.65378500	-3.38326100
C	-4.19284900	0.52541400	-2.99426900	H	-4.91021200	0.66050500	-4.34248500
H	-4.61960500	0.49294900	-4.01381500	H	-3.29327200	0.74611100	-3.61613700
H	-3.10427600	0.62432200	-3.10131100	H	-4.52347000	-0.33085200	-2.92199000
H	-4.41315700	-0.44149800	-2.52091700	C	-6.28390800	3.02852400	-1.14670400
C	-6.37868100	2.95634500	-1.16303800	C	-7.47818000	3.49935300	-0.37178600
C	-7.61926900	3.48126800	-0.51627900	H	-7.19434000	4.18827200	0.43613500
H	-7.38901600	3.97882900	0.43788900	H	-8.18118900	4.03547200	-1.03264900
H	-8.10739200	4.22490700	-1.16938500	H	-8.03012400	2.66272500	0.07976700
H	-8.34719200	2.68317300	-0.31881400				

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3F				C	-0.55372200	1.19066400	0.71317400
C	-0.60733400	1.54759500	0.81423500	C	-0.43395100	2.55682600	0.92601200
C	-0.48258000	2.92901100	0.78440500	C	-1.73760600	3.05631200	0.78996500
C	-1.76081400	3.40201100	0.43457000	H	0.18279100	0.39098600	0.75348100
H	0.12146600	0.77404000	1.04154300	H	0.47107800	3.10958700	1.16404500
H	0.41061800	3.51304900	0.99056800	H	-2.10935300	4.07386000	0.89752100
H	-2.10509100	4.42701000	0.31245800	C	-2.46749700	-0.34943600	0.23204600
C	-2.60954700	0.02599500	0.43933600	C	-3.64049300	-0.69022300	0.92062200
C	-3.98095300	0.14113900	0.11769600	C	-1.87069800	-1.24659500	-0.66197300
C	-1.99632600	-1.19954900	0.71363500	C	-4.22710900	-1.93843100	0.68661700

H	-4.06992500	-0.01188300	1.66171700	C	-3.22990800	-2.72058500	0.38633100
C	-2.45651100	-2.49777000	-0.86834900	H	-1.28284200	-1.87120800	-0.02649900
H	-0.96360000	-0.96412800	-1.20046300	C	-4.56202700	-2.46624100	0.73327900
C	-3.63781900	-2.84284900	-0.20252900	H	-6.00887300	-0.97502700	1.28961300
H	-5.13565500	-2.21275500	1.22769000	H	-2.90049700	-3.74341100	0.18924400
H	-1.99150600	-3.20197500	-1.56186400	H	-5.27078500	-3.29288300	0.81982100
H	-4.09259500	-3.82179500	-0.36929900	Co	-4.44000400	1.88038200	0.01315600
Co	-4.62304600	2.26704000	0.22097200	N	-1.84897600	0.73066100	0.41936000
N	-1.85971200	0.92322500	0.46132500	N	-2.36539600	1.94404200	0.10688500
N	-2.59302600	2.06374600	0.50285700	C	-4.95056500	2.65711000	2.69011600
C	-5.22355600	3.14996500	2.40499300	O	-4.52873200	1.49875000	2.97770500
O	-5.45908200	1.94639300	2.01292200	O	-5.06625100	3.07650100	1.49257600
O	-4.70183200	3.94788500	1.58013700	C	-5.36029200	3.56976700	3.81314100
C	-5.56115000	3.55493800	3.80854700	H	-4.92811100	3.23253700	4.76310200
H	-4.95152500	2.96375700	4.51018500	H	-5.06496300	4.60427800	3.59094400
H	-5.37399100	4.62399700	3.96454300	H	-6.45936200	3.54735900	3.90005600
H	-6.61406500	3.31424500	4.01922600	C	-5.83885800	1.69462600	-1.72531700
C	-6.25209000	1.83497400	-1.28867000	C	-4.62061600	2.08480700	-2.37950300
C	-5.00133400	1.76734300	-2.04431700	C	-4.39647500	3.50887300	-2.14115500
C	-4.43794900	3.07905700	-2.09825500	C	-5.47153600	3.99541200	-1.39695400
C	-5.33681400	3.96676700	-1.43896400	C	-6.56309600	0.38986800	-1.92594000
C	-7.19626400	0.68987000	-1.07721100	H	-7.26994500	0.18333400	-1.10976500
H	-7.84499500	0.85387700	-0.20575500	H	-7.14445000	0.40742200	-2.86398100
H	-7.84967600	0.56074900	-1.95801400	H	-5.87064300	-0.46173500	-1.98232100
H	-6.66387700	-0.26072800	-0.92721600	C	-5.69390700	5.37875300	-0.88080000
C	-5.19321100	5.43898300	-1.26349500	H	-6.66146800	5.78153700	-1.22417000
H	-6.07404100	5.96599000	-1.66815000	H	-5.71722100	5.37529700	0.22194100
H	-5.13092500	5.69359200	-0.19168800	H	-4.90897900	6.07471900	-1.20517600
H	-4.30164400	5.83387100	-1.76783800	C	-3.24003400	4.27955600	-2.69643500
C	-3.17337700	3.46966500	-2.80266100	H	-3.36482400	4.43928700	-3.78220500
H	-3.38600800	3.79448500	-3.83606800	H	-3.14417700	5.27046500	-2.23199900
H	-2.66372600	4.30398800	-2.29962500	H	-2.28582300	3.74575300	-2.56763400
H	-2.46321500	2.63328300	-2.86601200	C	-3.77454300	1.22451500	-3.25527000
C	-4.49056200	0.54768600	-2.73843700	H	-4.03428500	1.40287200	-4.31581600
H	-5.02208400	0.41658900	-3.69913900	H	-2.70366700	1.45623000	-3.15262200
H	-3.41911900	0.61870200	-2.96899000	H	-3.92537200	0.15331400	-3.06242100
H	-4.66016900	-0.36839800	-2.15417400	C	-6.39791500	2.89116100	-1.16449500
C	-6.46126400	3.18658000	-0.93250400	C	-7.71204400	3.03522700	-0.48132900
C	-7.63641200	3.76961500	-0.21711500	H	-7.60711400	3.59817800	0.45930500
H	-7.32410100	4.52355500	0.52124900	H	-8.40971300	3.61000500	-1.11772400
H	-8.30574600	4.27880200	-0.93330800	H	-8.18411600	2.06760400	-0.26481400
H	-8.22880100	3.00194300	0.29841300				

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C	-0.51086000	0.81560900	0.62181900	C	-0.18521900	2.14923800	0.30922500
C	-0.14426800	2.14134000	0.43232400	C	-1.39483300	2.77253000	-0.04085300
C	-1.34170800	2.80600900	0.11696500	H	0.07960000	-0.00910500	0.89231500
H	0.07618600	-0.05289900	0.91121300	H	0.80361900	2.59582600	0.37319100
H	0.85120500	2.56810000	0.52385000	H	-1.58086700	3.80934000	-0.31377800
H	-1.50769500	3.85932400	-0.10129400	C	-2.74166200	-0.41425600	0.55440800
C	-2.74946800	-0.37086900	0.53874400	C	-4.12908300	-0.14327000	0.54280300
C	-4.08346200	-0.06304500	0.90045300	C	-2.21519700	-1.69688200	0.73310700
C	-2.31263200	-1.67117100	0.27689300	C	-4.97705000	-1.25237400	0.72989500
C	-4.97415900	-1.15479400	0.98132700	H	-4.56979200	0.75775000	2.28970500
H	-4.31109400	0.82891300	1.93665100	C	-3.09746800	-2.76311900	0.92778000

H	-1.13966800	-1.88279500	0.71395400	H	-7.35394800	0.28929900	-1.24913200
C	-4.47823800	-2.54506800	0.93010700	H	-7.31733100	0.62302400	-2.98912200
H	-6.06286300	-1.11049600	0.72998000	H	-6.03406300	-0.35225200	-2.24156900
H	-2.69906400	-3.76982900	1.07268700	C	-5.54908700	5.39825400	-0.78689900
H	-5.16373300	-3.38210000	1.08208900	H	-6.48581400	5.87846400	-1.11711200
Co	-4.48571100	1.75617200	-0.11285900	H	-5.58338000	5.34693400	0.31387700
N	-1.86629800	0.70677700	0.36922800	H	-4.72126700	6.06224200	-1.06978000
N	-2.40220900	1.89325900	-0.00634600	C	-3.24057900	4.31113100	-2.79225900
C	-5.00673300	2.55821500	2.72464000	H	-3.41895000	4.53705600	-3.85886000
O	-4.75917000	1.32465700	3.08688100	H	-3.07494600	5.27020800	-2.28218300
O	-5.00050100	2.93059400	1.54240500	H	-2.30494400	3.73210600	-2.75064000
C	-5.30483400	3.48793800	3.85904900	C	-3.90783800	1.31302500	-3.47756500
H	-4.47599600	3.45949400	4.58300400	H	-4.16992500	1.57907300	-4.51892600
H	-5.45675700	4.50897700	3.49254800	H	-2.82379300	1.47566600	-3.37695500
H	-6.20369000	3.13668800	4.39007800	H	-4.11487600	0.24108700	-3.35458500
C	-5.89325200	1.77825000	-1.85074100	C	-6.35974200	2.95215300	-1.16683600
C	-4.68945500	2.15335900	-2.52601400	C	-7.64766000	3.10126100	-0.43155400
C	-4.39576400	3.55640100	-2.21483100	H	-7.52967300	3.72237400	0.46876700
C	-5.40261400	4.03299500	-1.37968300	H	-8.39157900	3.61018400	-1.07262700
C	-6.68478800	0.52043000	-2.09044300	H	-8.08136400	2.13398400	-0.14159200