

Theoretical insights into copper(I)-NHC-catalyzed C-H carboxylation of terminal alkynes with CO₂: the reaction mechanisms and the roles of NHC

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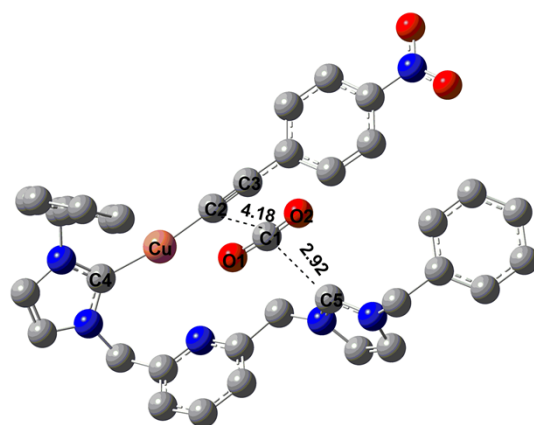
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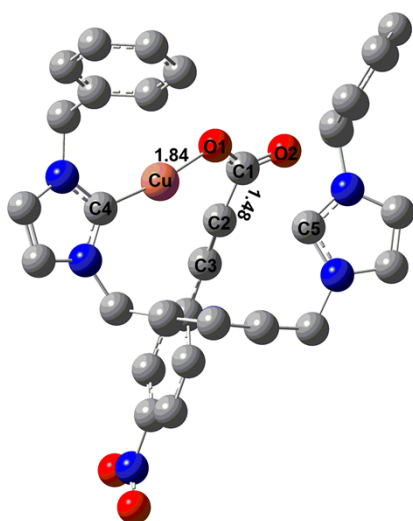
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R1



P1

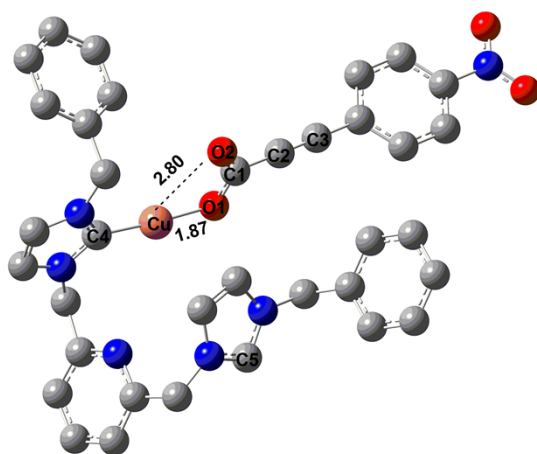


Figure S1. The structures of **R2**, **P1**, **P2** in PW-I. All the hydrogen atoms are omitted. The bond distances are measured by Å and the bond angles are measured by degree.

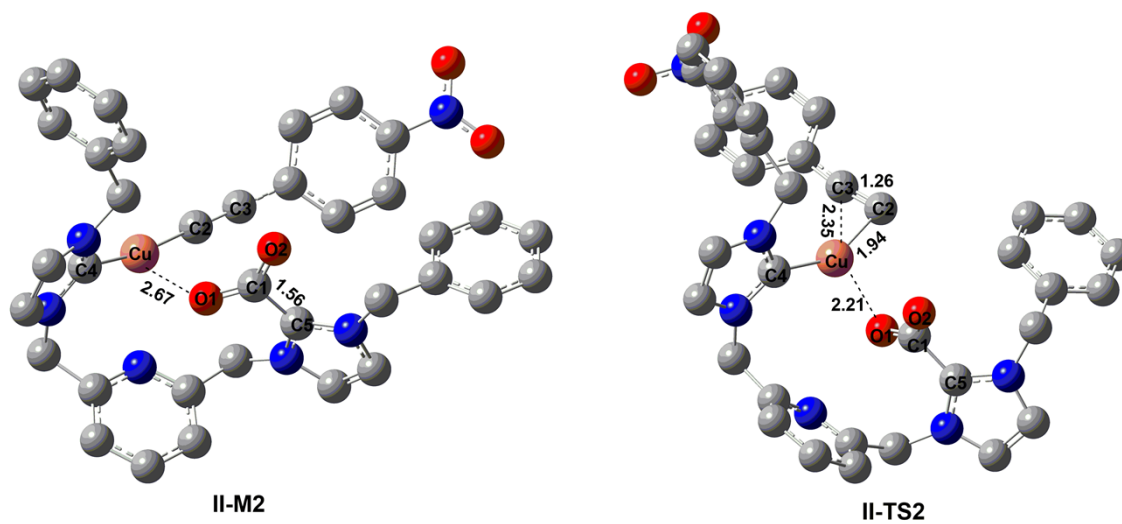


Figure S2. The structures of **II-M2**, **II-TS2** in PW-II. All the hydrogen atoms are omitted. The bond distances are measured by Å and the bond angles are measured by degree.

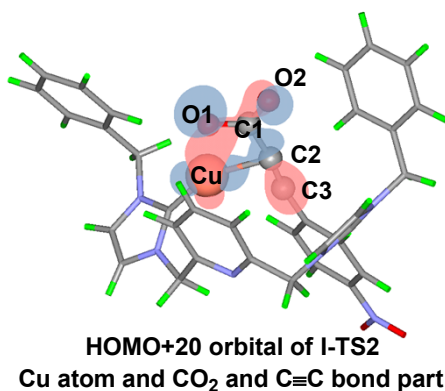


Figure S3. The part orbital diagrams of relevant complexes and transition states in PW-I.

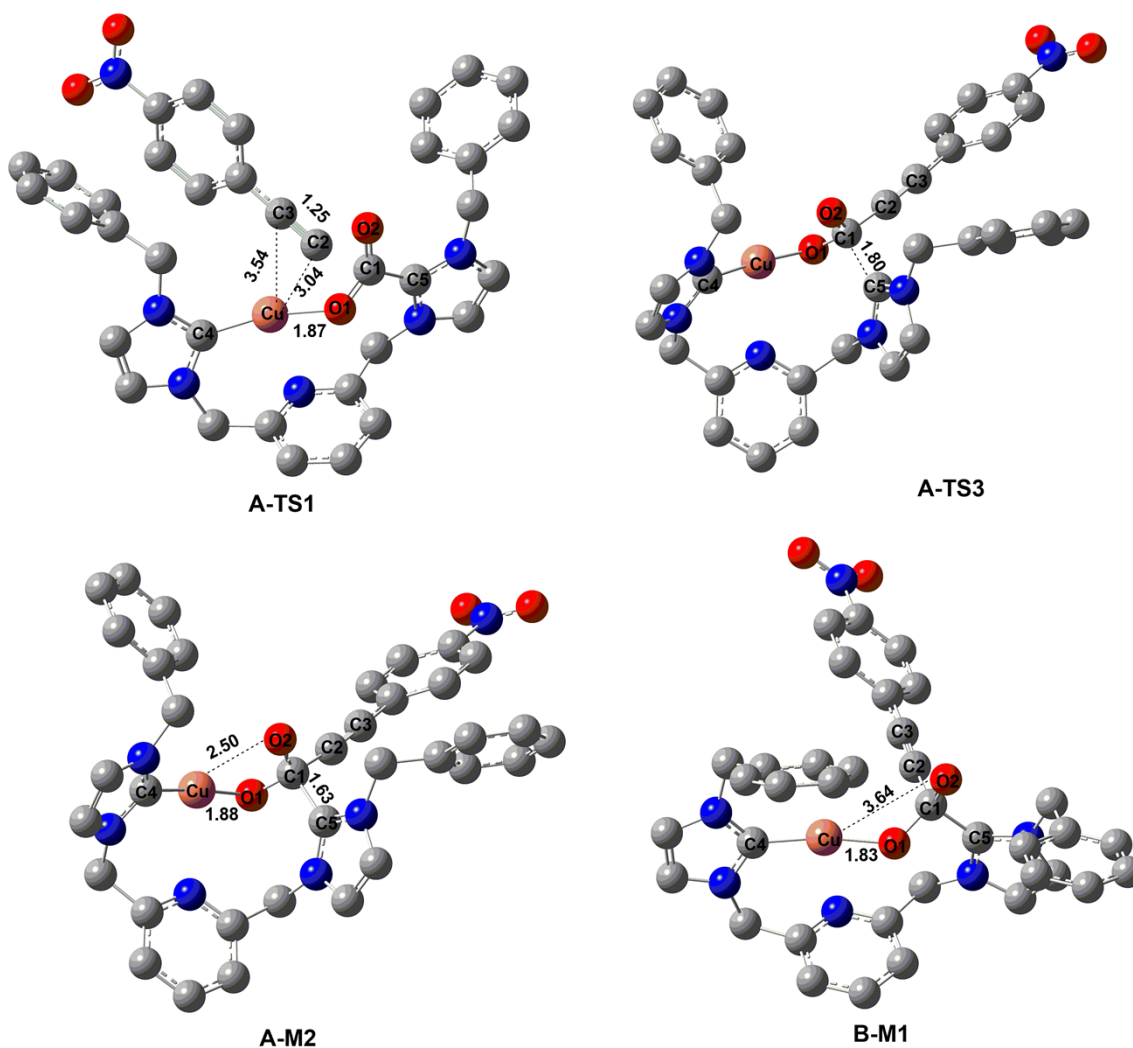


Figure S4. The structures of A-TS1, A-M2, A-TS3, B-M1 in PW-II. All the hydrogen atoms are omitted. The bond distances are measured by Å and the bond angles are measured by degree.

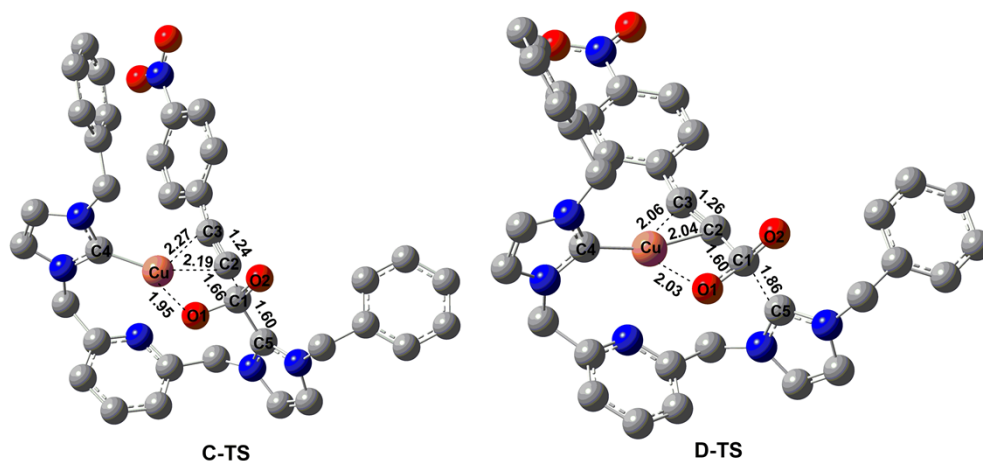
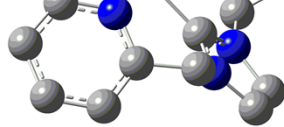
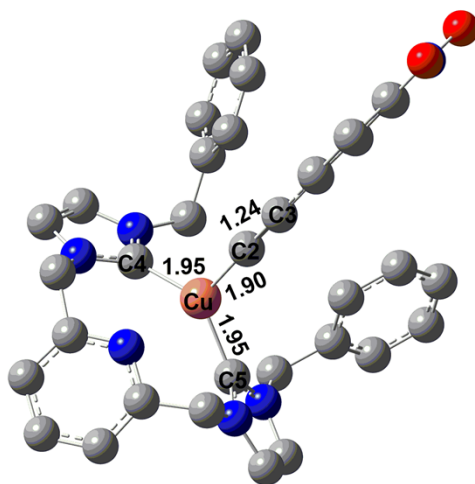


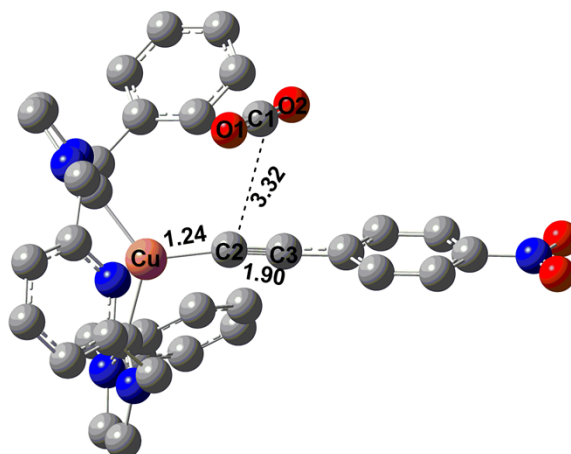
Figure S5. The structures of C-TS, D-TS in channels C and D in PW-II. All the hydrogen atoms are omitted. The bond distances are measured by Å and the bond angles are measured by degree.



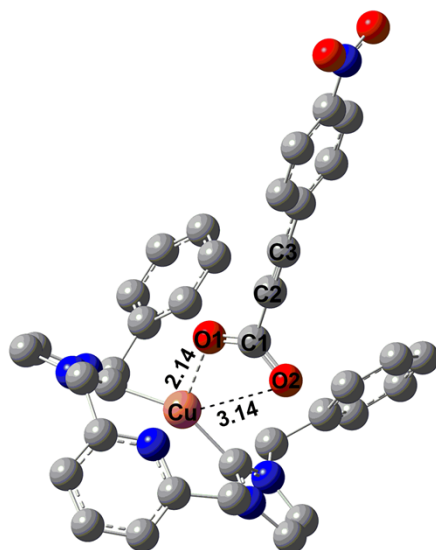
III-M3



III-M1



III-M2



III-M4

Figure S6. The structures of **III-M1**, **III-M2**, **III-M3** in PW-III. All the hydrogen atoms are omitted. The bond distances are measured by Å and the bond angles are measured by degree.

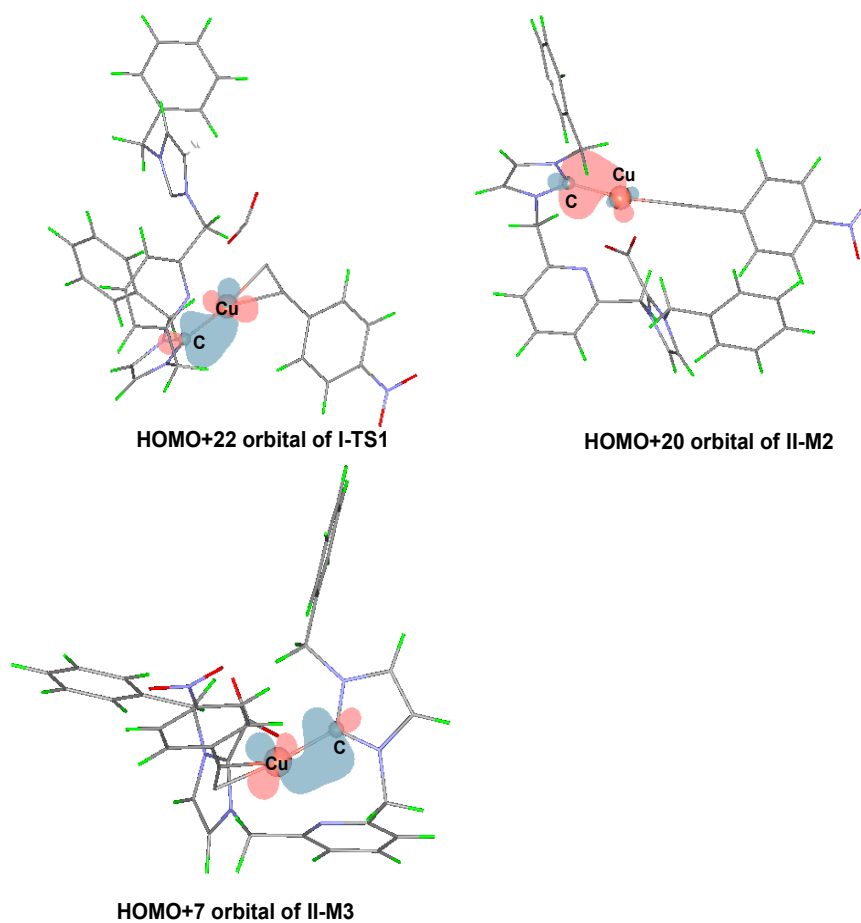


Figure S7. The $d_{\max}$ orbital diagrams of related complexes and transition states in PW-I and PW-II.

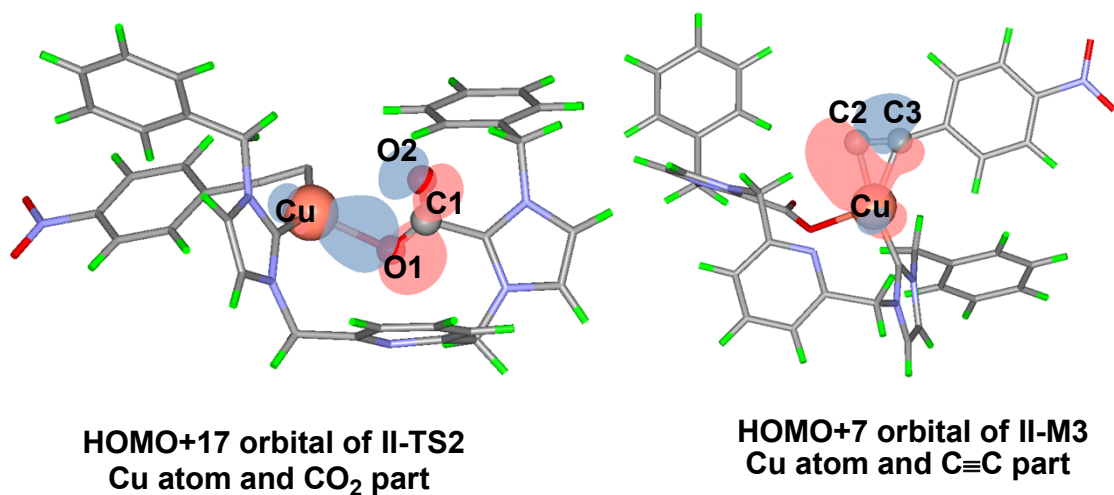


Figure S8. The part orbital diagrams of relevant complexes and transition states in PW-II.

Table S1. The second order perturbation theory analysis of Fock Matrix in NBO basis of relevant complexes and transition states in PW-I.^A

	Donor NBO (i)	Acceptor NBO (j)	E(2) /kcal mol ⁻¹	E(j)-E(i) /a.u.	F(I,j) /a.u.
R2	LP (1) C4	LP*(6)Cu	64.3	0.39	0.216
	LP (1) C2	LP*(6)Cu	77.8	0.38	0.229
I-TS1	LP (1) C4	LP*(6) Cu	59.7	0.40	0.203
	BD(3) C2 – C3	LP*(6) Cu	23.5	0.36	0.124
	LP (1) C2	LP*(1) C1	77.5	0.23	0.191
I-M1	BD(3) C2 – C3	LP*(6) Cu	21.1	0.42	0.216
I-TS3	LP (1) C4	LP*(6) Cu	54.7	0.41	0.195
	LP*(6)Cu	BD*(3) C2 – C3	25.9	0.05	0.085

A: LP-valence lone pairs; BD-valence bond; BD*-valence antibond; LP*-low occupancy lone pairs with no exact physical significance as interpreted in ref 35; E(2), E(j)-E(i), F(i,j)-reference to the formula in Scheme S1.

Table S2. The Mulliken charges of relevant complexes and transition states in PW-II.

	C4	Cu	C2	O1	C1	O2	C3	C5
R1	0.035	0.534	-0.537				-0.046	0.092
R2	0.038	0.599	-0.535	-0.339	0.655	-0.339	-0.048	0.103
II-TS1	0.047	0.623	-0.543	-0.389	0.612	-0.393	-0.041	0.190
II-M1	0.040	0.602	-0.558	-0.518	0.542	-0.537	-0.012	0.435
II-M2	0.062	0.632	-0.545	-0.550	0.557	-0.528	-0.035	0.424
II-TS2	-0.013	0.733	-0.582	-0.548	0.528	-0.513	-0.042	0.470
II-M3	0.266	0.739	-0.136	-1.046	1.308	-0.928	-0.696	0.255
A-TS1	-0.006	0.702	-0.526	-0.667	0.603	-0.475	-0.025	0.472
A-M1	-0.008	0.663	-0.497	-0.574	0.591	-0.470	-0.047	0.532
A-TS2	-0.013	0.662	-0.367	-0.713	0.570	-0.553	-0.047	0.534
A-M2	-0.010	0.689	-0.058	-0.750	0.447	-0.646	0.014	0.429
A-TS3	-0.013	0.675	-0.038	-0.732	0.442	-0.614	0.033	0.351
P2	0.016	0.645	-0.040	-0.626	0.380	-0.485	0.087	0.070

Table S3. The second order perturbation theory analysis of Fock Matrix in NBO basis of relevant complexes and transition states in the stage from A-TS1 to II-M3.^a

	Donor NBO (i)	Acceptor NBO (j)	E(2) /kcal mol ⁻¹	E(j)-E(i) /a.u.	F(I,j) /a.u.
II-M3	LP (1) C4	LP*(6) Cu	49.47	0.44	0.194
	LP (1) O1	LP*(6) Cu	3.76	0.75	0.074
	LP (2) O1	LP*(6) Cu	0.06	0.32	0.006
	LP (3) O1	LP*(6) Cu	1.53	0.32	0.028
A-TS1	LP (1) O1	LP*(6)Cu	11.40	0.63	0.116
	LP (2) O1	LP*(6)Cu	14.59	0.38	0.100
	LP (3) O1	LP*(6)Cu	15.14	0.30	0.087
	LP (1) C4	LP*(6) Cu	54.90	0.40	0.192
A-M1	LP (1) C4	LP*(6) Cu	61.28	0.39	0.200
	LP (1) O1	LP*(6) Cu	10.11	0.56	0.104
	LP (2) O1	LP*(6) Cu	28.13	0.43	0.148
	LP (3) O1	LP*(6) Cu	9.20	0.28	0.066

a: LP-valence lone pairs; LP*-low occupancy lone pairs with no exact physical significance as interpreted in ref 35; E(2), E(j)-E(i), F(i,j)-reference to the formula in Scheme S1.

Table S4. The Mulliken charges of relevant complexes and transition states in PW-III.

	C4	Cu	C2	O1	C1	O2	C3	C5
III-M1	0.051	0.841	-0.492				-0.618	0.046
III-M2	0.042	0.841	-0.515	-0.333	0.657	-0.322	-0.160	0.051
III-TS	0.041	0.833	-0.634	-0.423	0.543	-0.429	0.110	0.056
III-M3	0.029	0.785	-0.067	-0.587	0.393	-0.514	0.065	0.040

Table S5. The Mulliken charges of carbon atoms of NHCs in the complexes and transition states in three pathways.

PW-I	C4	C5	PW-II	C4	C5	PW-III	C4	C5
R1	0.035	0.092	R1	0.035	0.092	III-M1	0.051	0.046
R2	0.038	0.103	R2	0.038	0.103	III-M2	0.042	0.051
I-TS1	0.01	0.102	II-TS1	0.047	0.190	III-TS	0.041	0.056
I-M1	-0.013	0.126	II-M1	0.040	0.435	III-M3	0.029	0.040
I-TS2	-0.035	0.133	II-M2	0.062	0.424			
P1	-0.001	0.106	II-TS2	-0.013	0.470			
P2	0.016	0.07	II-M3	0.266	0.255			
I-TS3	0.014	0.116	A-TS1	-0.006	0.472			
			A-M1	-0.008	0.532			
			A-TS2	-0.013	0.534			
			A-M2	-0.010	0.429			
			A-TS3	-0.013	0.351			
			P2	0.016	0.070			

Table S6. The charge decomposition analysis of different fragments in the relevant complexes and transition states in PW-II.

	II-M2	II-TS2	II-M3 ^A	II-TS2 ^B	A-TS2 ^A
			HOMO+7	HOMO+17	HOMO+2
d×10 ⁻³			3.187	53.23	-0.147
b×10 ⁻²			1.137	0.217	4.088
(d-b)×10 ⁻³			-8.182	51.06	-41.02
r×10 ⁻¹			-0.109	-1.991	-1.905
E(int)/ kcal mol ⁻¹	-71.46	-72.50	-76.45		

5 A: This line is the charge decomposition analysis between fragment (C₆H₅NO₂)C≡C (1) and fragment L-Cu-CO₂ (2); B: This line is the charge decomposition analysis between fragment R1 (1) and fragment CO₂ (2); d—the number of electrons donated from fragment (1) to fragment (2); b—the number of electrons back donated from (2) to fragment (1); r—the number of electrons involved in repulsive polarization; E(int)—the electronic interaction energy between fragment R1 and fragment CO₂.

$$-\Delta E^{(2)} = q_i \frac{F(i,j)^2}{E(j) - E(i)}$$

F(i,j) — Fock matrix element

E(j)-E(i) — The energy difference between electron acceptor orbital (j) and electron donor orbital (i)

q_i — Occupation number of electrons on electron donor orbital

ΔE⁽²⁾ — Secondary perturbation energy

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Scheme S1. The calculation formula of the secondary perturbation energy.

List of Cartesian Coordinates for all optimized structures of complexes, transition states**Reaction I****R1**

C	1.27491900	-4.79490800	0.31579500
C	2.63231800	-4.76186700	-0.00225300
C	3.11896200	-3.68795200	-0.75531800
C	1.02294000	-2.73104900	-0.87592500
C	0.45110700	-3.75582500	-0.11592700
H	0.86520000	-5.61550400	0.89729100
H	3.30025900	-5.55293900	0.32514500
H	-0.60680200	-3.74048100	0.12624300
N	2.32102600	-2.71040400	-1.19879000
C	0.22117800	-1.55197400	-1.38630600
H	-0.85086500	-1.69940400	-1.24236400
H	0.41962000	-1.41959200	-2.45452700
C	4.58904200	-3.52724200	-1.10003800
H	5.11157000	-4.48650100	-1.03755000
H	4.67265900	-3.14100700	-2.11659900
N	0.55060200	-0.30350200	-0.68717400
C	1.81264400	0.27481900	-0.60067800
C	1.64587100	1.42448000	0.10478300
H	2.70576500	-0.19501800	-0.99104200
H	2.36116400	2.17469900	0.40236300
N	0.30054300	1.50836100	0.43341300
C	-0.39391600	0.44712600	-0.05514700
C	5.89509300	-2.92046300	0.97146100
C	5.27032900	-1.22068400	-0.45853700
C	6.34071000	-1.76025900	1.51304600
H	5.97948400	-3.93844400	1.32074900
H	6.90425700	-1.57323700	2.41425500
N	5.26277700	-2.57219200	-0.22043600
N	5.94460300	-0.75189100	0.63817100
C	6.28513700	0.65891600	0.80519200
H	6.01928200	0.97496400	1.82006600
H	5.64111800	1.19663500	0.10426300
C	-0.33785700	2.62290100	1.14887100
H	0.36324400	2.97665700	1.91006700
H	-1.20446500	2.19456400	1.65853200
C	-0.77042200	3.75931100	0.24386800
C	-0.03701100	4.94812800	0.17898400
C	-1.92639800	3.62273800	-0.53619800
C	-0.44673500	5.98685600	-0.65997800
H	0.85381500	5.06770600	0.79168000
C	-2.33576700	4.65807500	-1.37398900

H	-2.49502800	2.69701200	-0.48281300
C	-1.59582800	5.84216300	-1.43805100
H	0.12845000	6.90730300	-0.70190000
H	-3.23535000	4.54319900	-1.97135800
H	-1.91772300	6.65025200	-2.08854400
C	7.74610000	0.96747300	0.53072100
C	8.52341600	1.64602300	1.47401600
C	8.32650100	0.59365400	-0.68915600
C	9.86041000	1.95207200	1.20618100
H	8.08193200	1.93935800	2.42397100
C	9.66042800	0.89519300	-0.95652300
H	7.72306400	0.06123500	-1.41964300
C	10.43134500	1.57606100	-0.00926900
H	10.45343900	2.47898700	1.94831500
H	10.10046300	0.60133800	-1.90532500
H	11.47098400	1.81049500	-0.21915500
Cu	-2.25999500	0.16249800	0.03347800
C	-4.08617800	-0.09426400	0.10568400
C	-5.30516600	-0.24340100	0.15559000
C	-6.71063600	-0.41895600	0.21396400
C	-7.41473500	-1.02598900	-0.85427100
C	-7.45198200	0.00758000	1.34266700
C	-8.78919100	-1.20041000	-0.80067000
H	-6.85806500	-1.35620800	-1.72472400
C	-8.82660100	-0.16257400	1.40462500
H	-6.92380900	0.47391200	2.16738200
C	-9.48534100	-0.76665600	0.33056800
H	-9.33633700	-1.66343900	-1.61245200
H	-9.40186500	0.16006200	2.26355000
N	-10.93182500	-0.94900900	0.39177100
O	-11.48878600	-1.48556400	-0.57055500
O	-11.52219000	-0.55733300	1.40279100

R2

C	-2.52424800	-4.24441300	-0.07698800
C	-1.26884700	-3.67807200	-0.28363200
C	-1.15625600	-2.59844700	-1.16630800
C	-3.42420900	-2.62315400	-1.59133500
C	-3.62777900	-3.71458900	-0.74441700
H	-2.64159100	-5.08891900	0.59593900
H	-0.39152200	-4.05757000	0.22613800
H	-4.62041400	-4.13308200	-0.60802000
N	-2.21934500	-2.07712200	-1.79983400
C	-4.57418200	-1.95023200	-2.31564600

H	-5.37406400	-2.66290300	-2.53013900
H	-4.20710500	-1.54081500	-3.25899700
C	0.15563900	-1.90496000	-1.47971100
H	0.31094900	-1.91836400	-2.56360700
H	0.06669000	-0.85249500	-1.19345400
N	-5.16657000	-0.85630800	-1.53106200
C	-6.46511700	-0.84092000	-1.04225400
C	-6.60863900	0.32649500	-0.36252000
H	-7.16556600	-1.63966700	-1.22927100
H	-7.45221500	0.73288900	0.17224100
N	-5.39674600	0.98933400	-0.46407800
C	-4.48606900	0.26938400	-1.17667300
C	2.10108200	-3.50470900	-1.33859700
C	1.76544800	-2.03719600	0.40068000
C	3.07463300	-3.73796200	-0.42282300
H	1.90469600	-3.96767400	-2.29378300
H	3.90012100	-4.43279100	-0.43331400
N	1.32356500	-2.47035900	-0.82210300
N	2.84697000	-2.84383300	0.61942800
C	3.68645400	-2.74081300	1.81995200
H	3.78829400	-3.74005600	2.25775600
H	3.12314400	-2.11751800	2.51610600
C	-5.06484900	2.26634500	0.18839600
H	-5.89996000	2.95589000	0.03479000
H	-4.19552900	2.64631400	-0.35459600
C	-4.74738500	2.11255700	1.66117800
C	-5.64444500	2.54610500	2.64243200
C	-3.53690000	1.52204500	2.04776200
C	-5.34111800	2.38579000	3.99662300
H	-6.57967200	3.01868100	2.34970400
C	-3.23634100	1.35709800	3.39794000
H	-2.83461900	1.19527100	1.28520000
C	-4.13831600	1.78821400	4.37501500
H	-6.04193100	2.72921200	4.75221800
H	-2.29678200	0.89292900	3.68001600
H	-3.90130800	1.66296300	5.42771300
C	5.05501700	-2.14524500	1.55407200
C	6.18552700	-2.96240100	1.44790000
C	5.20089700	-0.75916600	1.40110700
C	7.44034800	-2.40951800	1.17978300
H	6.08720600	-4.03760800	1.58324900
C	6.45186900	-0.20377700	1.13105600
H	4.32825900	-0.11903600	1.50026000
C	7.57358500	-1.03067400	1.01628200

H	8.31037400	-3.05545300	1.10090400
H	6.55381200	0.87043800	1.00473200
H	8.54694800	-0.59748800	0.80526000
Cu	-2.66786600	0.74808000	-1.38571100
C	-0.94860000	1.43425500	-1.41212400
C	0.19011700	1.89825100	-1.34751900
C	1.51685000	2.39816700	-1.29972500
C	2.58559400	1.56847500	-0.88098300
C	1.81253200	3.73180700	-1.67284400
C	3.88632500	2.04555800	-0.84338400
H	2.37557200	0.54807400	-0.57636500
C	3.11078300	4.21777800	-1.63007200
H	1.00172600	4.37603100	-1.99571500
C	4.13966500	3.36868800	-1.21293900
H	4.70774800	1.41069400	-0.53866300
H	3.34588000	5.23720400	-1.90997300
N	5.50552300	3.87507700	-1.15447900
O	6.38936600	3.11901000	-0.73450700
O	5.71137500	5.03403700	-1.52512600
C	0.59654800	-0.04709000	2.18221700
O	1.64789800	0.34019800	2.52233500
O	-0.50469900	-0.36187200	1.93639700

L-TS1

C	-0.41122900	1.52232600	4.64588900
C	0.00718500	0.29299900	4.15246700
C	-0.44203000	-0.11861900	2.88852900
C	-1.62876300	1.84090200	2.60791400
C	-1.24681800	2.32057100	3.85883600
H	-0.09016000	1.86240900	5.62609900
H	0.67164000	-0.34500800	4.72645400
H	-1.58312600	3.29208000	4.20828800
N	-1.24870600	0.64162200	2.14074600
C	-2.44649900	2.67005500	1.63262000
H	-2.95491800	3.49575800	2.13549900
H	-3.19606800	2.03422000	1.15680600
C	-0.05709900	-1.46257700	2.29943300
H	-0.44603300	-2.26855500	2.93131900
H	-0.51670800	-1.55160900	1.31362000
N	-1.59434000	3.23518300	0.57977000
C	-1.08341900	4.52536900	0.57548500
C	-0.19405300	4.58306700	-0.44877700
H	-1.39679500	5.27715400	1.28266100
H	0.43109900	5.38872100	-0.79832900

N	-0.18182900	3.32677000	-1.03467600
C	-1.03882000	2.47922000	-0.40992500
C	2.10774300	-2.64323900	2.83620900
C	2.15054400	-0.91612300	1.30569700
C	3.37922600	-2.54779100	2.37686900
H	1.66156400	-3.32904200	3.54067300
H	4.25681900	-3.13503100	2.59721800
N	1.38514200	-1.64884500	2.17921800
N	3.37764700	-1.50150700	1.45752400
C	4.55747500	-1.08029200	0.70129200
H	5.27289100	-0.59968200	1.38050700
H	4.19584300	-0.32249400	0.00221500
C	0.71087400	2.92740700	-2.14061800
H	0.41636200	3.47824100	-3.03987000
H	0.53439200	1.86281000	-2.30855000
C	2.16381500	3.18930100	-1.80747700
C	2.86672000	4.20406000	-2.46577400
C	2.81181100	2.43040100	-0.82029800
C	4.20014200	4.47074900	-2.14573500
H	2.37136000	4.78464000	-3.24110000
C	4.13954800	2.70806400	-0.49494400
H	2.29158700	1.61866600	-0.31646200
C	4.83637500	3.72554600	-1.15415700
H	4.73605000	5.25743400	-2.66914600
H	4.63538200	2.12323500	0.27384000
H	5.87197200	3.93101300	-0.89819700
C	5.24171300	-2.21423400	-0.03809900
C	6.60021000	-2.47404800	0.17202500
C	4.52914100	-2.99783200	-0.95834500
C	7.24786000	-3.49547500	-0.52769600
H	7.15779900	-1.87068100	0.88532900
C	5.17579800	-4.01945600	-1.65260000
H	3.47140400	-2.81255500	-1.12803200
C	6.53497600	-4.27069600	-1.44184000
H	8.30373400	-3.68488400	-0.35499500
H	4.61544400	-4.61938900	-2.36405900
H	7.03365800	-5.06707400	-1.98739400
Cu	-1.28322300	0.62301400	-0.71652600
C	-1.10790300	-1.27285400	-1.20816000
C	-2.34996700	-1.15856900	-1.09986200
C	-3.76402700	-1.35586200	-1.01604600
C	-4.30349100	-2.66154200	-1.03947300
C	-4.64622700	-0.26003400	-0.90839600
C	-5.67378700	-2.86273000	-0.95468400

H	-3.63038000	-3.50751000	-1.12420000
C	-6.01751600	-0.45227700	-0.82141000
H	-4.23365400	0.74403200	-0.90793600
C	-6.51700500	-1.75498900	-0.84296100
H	-6.10349000	-3.85657000	-0.97072300
H	-6.70746300	0.37835800	-0.74086900
N	-7.96294100	-1.96414500	-0.74541500
O	-8.37892700	-3.12378100	-0.77188400
O	-8.68141400	-0.96747800	-0.64040400
C	0.79759500	-1.42871400	-1.87457000
O	1.14924900	-2.54227500	-1.62216600
O	1.02832400	-0.35423100	-2.36055500

II

C	0.31544100	-1.64704900	2.41451300
C	-1.00432100	-1.20447800	2.46422700
C	-1.24384600	0.16630400	2.60263600
C	1.01200100	0.63668000	2.60239200
C	1.34866100	-0.71574100	2.48830300
H	0.53782500	-2.70205600	2.29189100
H	-1.82875200	-1.90218800	2.37666900
H	2.38396800	-1.03117700	2.42889200
N	-0.25328900	1.06828800	2.67044100
C	2.06124300	1.73647300	2.67177200
H	2.41324800	1.86266600	3.70131000
H	1.58838400	2.67384900	2.36765700
C	-2.64641400	0.75361200	2.67744500
H	-2.88872800	0.99139400	3.72032500
H	-2.65431200	1.69185500	2.12059300
N	3.24119400	1.47145500	1.84283500
C	4.55796300	1.60195300	2.26081100
C	5.33625200	1.25243600	1.20430200
H	4.82144700	1.92735300	3.25493900
H	6.40783700	1.18911000	1.10632500
N	4.47212400	0.92104800	0.17168400
C	3.17322400	1.05729000	0.54591900
C	-4.40647700	-1.04435600	2.88256200
C	-3.95739600	-0.17474400	0.79648200
C	-5.17179400	-1.72092700	1.98964400
H	-4.32956200	-1.13098200	3.95601600
H	-5.87991700	-2.52261700	2.13189500
N	-3.68235700	-0.11317300	2.13936500
N	-4.88617700	-1.17385200	0.74210100
C	-5.44668900	-1.66690800	-0.51926900

H	-5.20882600	-0.90044400	-1.26043600
H	-6.53684000	-1.71996300	-0.42533800
C	4.88957400	0.40768000	-1.14667200
H	5.47810900	1.18422300	-1.64612800
H	3.96443300	0.26229100	-1.70749500
C	5.67239600	-0.88542200	-1.06030300
C	7.06999400	-0.87094400	-1.14273600
C	5.00144800	-2.10648800	-0.89566400
C	7.79814600	-2.05859600	-1.04906800
H	7.59203800	0.07173000	-1.29463300
C	5.73308500	-3.29099600	-0.80410000
H	3.91394500	-2.13278300	-0.85459200
C	7.12852600	-3.27062300	-0.87681100
H	8.88195500	-2.03686300	-1.11836400
H	5.20851600	-4.23455400	-0.68483500
H	7.69110000	-4.19744800	-0.80881300
C	-4.88817800	-3.01564200	-0.93265200
C	-3.51681100	-3.16424100	-1.18212400
C	-5.73130500	-4.12216000	-1.07984300
C	-2.99779200	-4.39836300	-1.56982700
H	-2.84160100	-2.32032800	-1.07665100
C	-5.21459500	-5.36023000	-1.47115300
H	-6.79804700	-4.01568100	-0.89318300
C	-3.84761300	-5.49937200	-1.71446700
H	-1.93186100	-4.47676400	-1.75756900
H	-5.87999500	-6.21201900	-1.58353900
H	-3.44534700	-6.46193500	-2.01868900
Cu	1.64955900	0.39865700	-0.34711800
C	-0.01713300	-0.29400700	-1.22820100
C	-0.18678700	0.93553400	-1.13891000
C	-0.85835000	2.20579000	-1.22122300
C	-2.24466300	2.28407600	-0.97113700
C	-0.14069700	3.37312500	-1.54599100
C	-2.89310500	3.51135300	-1.06032200
H	-2.79839300	1.39483400	-0.66709000
C	-0.78854900	4.59685700	-1.64850000
H	0.92848600	3.30723300	-1.72002600
C	-2.16093400	4.64811500	-1.40351600
H	-3.95547500	3.59924500	-0.86887100
H	-0.25856400	5.50498100	-1.90621400
N	-2.84983400	5.94177000	-1.49932700
O	-4.06066000	5.96456200	-1.27711000
O	-2.17515000	6.92956600	-1.79531900
C	0.49246000	-1.72492300	-1.23737200

O	-0.22462800	-2.64902000	-1.59105600
O	1.70222600	-1.69750500	-0.80829000

I-TS2

C	0.28074900	-1.57799800	2.64588800
C	-1.01125500	-1.06533500	2.72425900
C	-1.18326400	0.32284300	2.68418100
C	1.08558600	0.66892000	2.44699500
C	1.35766700	-0.70046900	2.51480900
H	0.44937800	-2.64974200	2.66328300
H	-1.86861600	-1.72518500	2.79784700
H	2.37356400	-1.07318800	2.45313100
N	-0.15366800	1.16830500	2.53949900
C	2.15929400	1.73361500	2.29894300
H	2.54815600	2.00791600	3.28596700
H	1.68322700	2.62259900	1.87643600
C	-2.54341800	0.99138700	2.82005600
H	-2.76769500	1.15279200	3.88194300
H	-2.48406100	1.97040200	2.34402000
N	3.31325600	1.34750000	1.48033800
C	4.61546300	1.74398700	1.75435400
C	5.38195200	1.29790900	0.72781200
H	4.87458500	2.30943500	2.63565500
H	6.44339900	1.37371100	0.55352200
N	4.52537000	0.65135100	-0.14993800
C	3.23744300	0.67070800	0.29545500
C	-4.44592000	-0.66989600	2.89571300
C	-3.95665200	0.35541300	0.89075500
C	-5.29670500	-1.17354000	1.96686600
H	-4.35571700	-0.87000000	3.95292600
H	-6.07706700	-1.91388000	2.05106100
N	-3.64463400	0.25163300	2.22271900
N	-4.98293300	-0.53733300	0.76976800
C	-5.65804400	-0.80663800	-0.50250200
H	-5.24620200	-0.07696400	-1.20390400
H	-6.72807000	-0.59772900	-0.39000100
C	4.96161700	-0.08436200	-1.34621500
H	5.69617600	0.53228300	-1.87238200
H	4.07839900	-0.17242600	-1.98329100
C	5.53347700	-1.45190500	-1.03005400
C	6.89845700	-1.71077300	-1.18874800
C	4.68460500	-2.47313200	-0.58088000
C	7.41601100	-2.97531400	-0.89785100
H	7.55976300	-0.92556900	-1.54878300

C	5.20223600	-3.73394600	-0.29068200
H	3.62322800	-2.27605100	-0.46137900
C	6.56803700	-3.98753100	-0.44764600
H	8.47715300	-3.16820600	-1.02668500
H	4.53482600	-4.52075100	0.04789100
H	6.96771700	-4.97278000	-0.22532600
C	-5.45281800	-2.22413200	-1.00090100
C	-4.15850300	-2.71533800	-1.21864200
C	-6.54960200	-3.05295800	-1.26098600
C	-3.96596600	-4.01406600	-1.68616300
H	-3.28737100	-2.09732900	-1.02420400
C	-6.35908600	-4.35375500	-1.73480500
H	-7.55825500	-2.67923600	-1.09647600
C	-5.06672900	-4.83603500	-1.94590500
H	-2.95055600	-4.36391500	-1.84186600
H	-7.21913000	-4.98736000	-1.93429500
H	-4.91751500	-5.84832100	-2.31188200
Cu	1.78728100	-0.33549000	-0.32857900
C	-0.24557500	-0.54785700	-1.09697000
C	-0.26038000	0.68016000	-1.11340700
C	-0.55883400	2.07661100	-1.19239400
C	-1.84993500	2.53241300	-0.84715100
C	0.42019200	2.99972300	-1.61308000
C	-2.14721000	3.88790000	-0.93320200
H	-2.59729400	1.82219400	-0.48822100
C	0.12073400	4.35208500	-1.70671800
H	1.41362300	2.64256000	-1.86337600
C	-1.16308100	4.77816000	-1.36457400
H	-3.12851300	4.26537200	-0.67326100
H	0.85388100	5.07890700	-2.03280100
N	-1.48104800	6.20889200	-1.45365000
O	-2.62000600	6.56353900	-1.14855300
O	-0.58827500	6.97235600	-1.82685800
C	-0.02276600	-2.03135900	-1.00689500
O	-0.90869100	-2.82969300	-1.27260100
O	1.18906800	-2.23067100	-0.60901400

P1

C	0.47496000	0.38264400	4.06526700
C	0.22167700	-0.95041200	3.75466500
C	-0.67037000	-1.24227600	2.71836000
C	-1.03700100	0.99438500	2.30845100
C	-0.15349600	1.37882400	3.32127100
H	1.16112400	0.64300200	4.86579000

H	0.71688100	-1.75398100	4.29043500
H	0.04535100	2.42817700	3.51526700
N	-1.31047900	-0.28536600	2.03254200
C	-1.73607800	2.01309300	1.42158100
H	-2.48201500	2.58849500	1.97935700
H	-2.24396600	1.47578800	0.62029300
C	-0.93589100	-2.66852500	2.29058900
H	-0.96236700	-3.32988800	3.16406700
H	-1.91263800	-2.71140900	1.79796200
N	-0.80338300	2.96981400	0.81954000
C	-0.57788200	4.26029800	1.27686600
C	0.40403600	4.78236200	0.49669200
H	-1.14251700	4.69438300	2.08700300
H	0.87101600	5.75428800	0.50536100
N	0.74362400	3.79899100	-0.41745200
C	0.01202000	2.66485200	-0.22887000
C	0.32356300	-4.50198800	1.11561000
C	0.86884500	-2.31810100	0.60124800
C	1.27192700	-4.53818600	0.14700200
H	-0.20632300	-5.29829000	1.61633600
H	1.74007700	-5.37473600	-0.34879800
N	0.10367900	-3.15095800	1.37994200
N	1.58108500	-3.21480700	-0.14615200
C	2.58045300	-2.80653200	-1.13344000
H	2.28196600	-1.81416600	-1.48035000
H	2.50389300	-3.47134700	-1.99763700
C	1.80753600	3.91051800	-1.42960000
H	1.80027200	4.93575600	-1.80948300
H	1.51228000	3.24364000	-2.24338500
C	3.17958300	3.53438300	-0.90779100
C	4.14169200	4.51377800	-0.64205100
C	3.49535700	2.18591100	-0.69515300
C	5.40309800	4.15191400	-0.16344900
H	3.91003900	5.56204600	-0.81799700
C	4.75219900	1.82246600	-0.21610600
H	2.74554400	1.42730500	-0.90425800
C	5.70790300	2.80722200	0.05100500
H	6.14584100	4.91893500	0.03641000
H	4.98474600	0.77355800	-0.05767800
H	6.68992200	2.52463100	0.41933300
C	3.99722600	-2.79349300	-0.58722000
C	4.28542500	-2.16803500	0.63485100
C	5.04603700	-3.36795200	-1.31294700
C	5.59398700	-2.12263100	1.11648700

H	3.46920100	-1.72863500	1.20252200
C	6.35822900	-3.31920800	-0.83496600
H	4.83497900	-3.85644700	-2.26138200
C	6.63613200	-2.69727200	0.38217800
H	5.80207400	-1.64155800	2.06886200
H	7.15993900	-3.77275800	-1.41138000
H	7.65454800	-2.66327900	0.75918400
Cu	0.22813900	1.09982300	-1.20493100
C	-1.60994900	-0.96927200	-2.09466600
C	-2.77144200	-0.83976800	-1.75170400
C	-4.10882400	-0.65793400	-1.30587700
C	-5.16654500	-0.51166300	-2.23020200
C	-4.39533300	-0.62186200	0.07828800
C	-6.47010400	-0.32947500	-1.78920500
H	-4.94973200	-0.54526100	-3.29228400
C	-5.69849200	-0.44230400	0.52205300
H	-3.57786400	-0.72674000	0.78554100
C	-6.72136300	-0.29610300	-0.41653200
H	-7.29401800	-0.21526300	-2.48246300
H	-5.94051100	-0.41143800	1.57717100
N	-8.09516300	-0.09810100	0.05240200
O	-8.98004100	0.02570300	-0.79620000
O	-8.28688400	-0.06380600	1.26985900
C	-0.23065700	-1.26330300	-2.54418700
O	-0.00692700	-2.33123000	-3.09966600
O	0.63134400	-0.32376900	-2.29868500

P2

C	-5.85098700	-3.57400100	-2.60170800
C	-5.19372100	-4.14878400	-1.51789500
C	-4.35938700	-3.34204600	-0.73198500
C	-4.79389800	-1.49879500	-2.04477900
C	-5.65053800	-2.21999300	-2.87826900
H	-6.50384700	-4.17247900	-3.23043500
H	-5.31308600	-5.20320400	-1.28794500
H	-6.13841300	-1.74231000	-3.72265900
N	-4.17677500	-2.04579500	-0.99268400
C	-4.45434900	-0.04157800	-2.31676400
H	-5.11602600	0.37876500	-3.07996700
H	-3.42468600	0.02740300	-2.68178800
C	-3.62278600	-3.91215900	0.47452400
H	-4.25312000	-3.80700100	1.36738500
H	-3.43571500	-4.97703300	0.32068000
N	-4.50975900	0.79018400	-1.12084700

C	-5.67715600	1.21871600	-0.50537000
C	-5.30016800	1.86895500	0.62488600
H	-6.65540300	1.02348500	-0.91536900
H	-5.88838300	2.36450700	1.38037700
N	-3.91592200	1.80528000	0.67737000
C	-3.41005800	1.13773900	-0.39576900
C	-2.17340000	-2.08643100	1.42229400
C	-1.19613000	-3.70791000	0.09739700
C	-0.86954000	-1.74608500	1.27229700
H	-2.97716600	-1.59007400	1.94323000
H	-0.30779900	-0.91000300	1.66087500
N	-2.34552100	-3.27427700	0.71587700
N	-0.30743000	-2.73753100	0.46899800
C	1.10026100	-2.76861400	0.07308200
H	1.37613500	-1.78215800	-0.30933300
H	1.15112800	-3.47911800	-0.75526800
C	-3.07233400	2.42316800	1.71876800
H	-2.11639800	1.89647300	1.68838200
H	-3.54899200	2.22376800	2.68381800
C	-2.85321200	3.90892100	1.51686300
C	-1.66846100	4.35836400	0.92023500
C	-3.81659900	4.84351200	1.91745000
C	-1.46171600	5.72364600	0.71442500
H	-0.90385400	3.63586000	0.64645500
C	-3.61122300	6.20710800	1.70706600
H	-4.72819000	4.50813900	2.40767300
C	-2.43286100	6.64883800	1.10100400
H	-0.53655400	6.06387200	0.25824400
H	-4.36380900	6.92356900	2.02389000
H	-2.26878700	7.71081100	0.94179400
C	2.02834700	-3.19453800	1.19570100
C	2.98130500	-2.31341700	1.71749700
C	1.93782600	-4.48970500	1.72424200
C	3.83930100	-2.72076900	2.74371500
H	3.04513200	-1.30113900	1.32613800
C	2.79167900	-4.89711000	2.74765300
H	1.18452100	-5.16699900	1.32969700
C	3.74774100	-4.01368700	3.25863600
H	4.57278400	-2.02519200	3.14226000
H	2.71439500	-5.90456300	3.14750900
H	4.41397300	-4.33239300	4.05545600
Cu	-1.61350100	0.79695000	-0.70670000
C	0.91870500	1.13274600	-0.13090200
O	0.21033200	0.56214700	-1.04307500

O	0.50211900	1.69040700	0.89764000
C	2.36458400	1.08155100	-0.36560500
C	3.56938400	1.05300200	-0.52448400
C	4.97877200	1.02197700	-0.72254800
C	5.70913700	-0.16442200	-0.49553100
C	5.66341900	2.17941500	-1.15114100
C	7.08379500	-0.19330700	-0.68908000
H	5.18772400	-1.05598500	-0.16435500
C	7.03711200	2.15405100	-1.34978600
H	5.10430300	3.09221300	-1.32478300
C	7.73088700	0.96671100	-1.11532800
H	7.66211100	-1.09278300	-0.51925200
H	7.58037700	3.03078500	-1.67912800
N	9.18323800	0.93793100	-1.32218100
O	9.72839500	1.97556300	-1.70125300
O	9.77189800	-0.12183700	-1.10453400

I-TS3

C	2.77848700	-3.25002200	-1.44843600
C	1.73023800	-4.12197500	-1.18089100
C	1.34814600	-4.32863800	0.15052000
C	2.97673400	-2.89280700	0.91215900
C	3.41791800	-2.61577100	-0.38233600
H	3.07446000	-3.03469500	-2.46916500
H	1.18525700	-4.60215500	-1.98673300
H	4.22326400	-1.91122100	-0.55848700
N	1.96799000	-3.73616200	1.17717700
C	3.62399700	-2.29131000	2.14309400
H	4.59304700	-2.76710500	2.33255800
H	2.97394800	-2.50348500	2.99604200
C	0.16756200	-5.21501800	0.50061500
H	0.34569200	-6.24533100	0.17261100
H	0.05277700	-5.21580400	1.58761800
N	3.87721300	-0.84625700	2.05642500
C	4.91163400	-0.22005200	2.73819500
C	4.77082200	1.11247000	2.52301900
H	5.64075200	-0.77028800	3.31193800
H	5.36802200	1.94847000	2.85052700
N	3.64737800	1.26273000	1.72799100
C	3.07899200	0.06079000	1.42676700
C	-1.94745600	-5.53290400	-0.86510100
C	-1.38549400	-3.41091400	-0.15393300
C	-2.89100700	-4.68322700	-1.34411900
H	-1.83798700	-6.60136500	-0.97454000

H	-3.76192600	-4.86996000	-1.95363400
N	-1.05302800	-4.74043600	-0.14733000
N	-2.52564200	-3.41263600	-0.90709900
C	-3.23433200	-2.17872500	-1.24361800
H	-3.71338300	-2.31368200	-2.21814200
H	-2.46310600	-1.41363700	-1.36935100
C	3.16180800	2.54288600	1.18635300
H	3.17969500	3.27881200	1.99561800
H	2.11975000	2.36431700	0.90918200
C	3.96043400	3.03035300	-0.00486700
C	4.85163600	4.10112600	0.12330500
C	3.80704400	2.40572900	-1.25067200
C	5.58946600	4.54319800	-0.97713300
H	4.96388800	4.59919800	1.08410900
C	4.54552600	2.84744100	-2.34749300
H	3.11346300	1.57648600	-1.36638100
C	5.43803200	3.91477400	-2.21372300
H	6.27617000	5.37779500	-0.86828000
H	4.41506200	2.35888400	-3.30850700
H	6.00852800	4.25865300	-3.07183000
C	-4.26510300	-1.74942100	-0.21333100
C	-5.51518000	-1.27126000	-0.62157800
C	-3.96163700	-1.76943100	1.15587800
C	-6.44660300	-0.81482200	0.31443300
H	-5.76220700	-1.25156400	-1.68069900
C	-4.89341500	-1.31949800	2.09221400
H	-2.99028400	-2.14164000	1.46993200
C	-6.13822700	-0.83812000	1.67525700
H	-7.41292200	-0.44741200	-0.01972000
H	-4.64777800	-1.34401400	3.15059100
H	-6.86290400	-0.48957700	2.40577300
Cu	1.65128000	-0.11163600	0.19881000
C	0.01332300	0.43883900	-0.71124200
C	-0.86173200	1.29806900	-0.54866600
C	-1.88037900	2.25708400	-0.31527100
C	-3.04551000	1.90470100	0.40403700
C	-1.74827400	3.57870100	-0.80132900
C	-4.04304800	2.84218700	0.63457200
H	-3.15815900	0.89082400	0.77089000
C	-2.74550800	4.51753700	-0.57943800
H	-0.85687900	3.84992700	-1.35665700
C	-3.87989300	4.13682600	0.13994600
H	-4.94266700	2.58519000	1.17906800
H	-2.66475500	5.53319400	-0.94568200

N	-4.93322800	5.13015200	0.38155800
O	-5.92259200	4.77223700	1.02202900
O	-4.76534500	6.26461300	-0.06909100
C	0.63112600	-0.46003900	-2.07540800
O	-0.25138600	-1.07916300	-2.62403600
O	1.84788700	-0.26714200	-2.19213700

Reaction II

II-TS1

C	-1.77416500	-5.04934200	-0.66892700
C	-0.64017800	-4.26262600	-0.84706600
C	-0.79903300	-2.94971700	-1.30429000
C	-3.09204500	-3.18301800	-1.38632400
C	-3.02904700	-4.50459900	-0.94319200
H	-1.68366700	-6.07373400	-0.31948400
H	0.34956000	-4.65162300	-0.63673800
H	-3.93474500	-5.08883900	-0.81198100
N	-2.00347800	-2.42246900	-1.56511800
C	-4.41375600	-2.49139600	-1.65864800
H	-5.20124300	-3.21917700	-1.86673700
H	-4.30470600	-1.83850600	-2.52773500
C	0.35839700	-2.00936600	-1.57462200
H	0.51949000	-1.93742200	-2.65613200
H	0.07710600	-1.01051700	-1.23216500
N	-4.85969600	-1.67878200	-0.51769200
C	-6.01241300	-1.90951100	0.22013500
C	-6.03698000	-0.96842900	1.19924800
H	-6.70020400	-2.70785900	-0.01001100
H	-6.75440200	-0.78356400	1.98279300
N	-4.89354700	-0.20357700	1.03641000
C	-4.15240400	-0.62330800	-0.02572500
C	2.65869800	-3.05841400	-1.59779200
C	1.95127700	-2.05914800	0.32849400
C	3.67005100	-3.15535100	-0.69825800
H	2.59364600	-3.38290000	-2.62509400
H	4.66069900	-3.57244300	-0.78816000
N	1.62231200	-2.38807800	-0.95292400
N	3.21515900	-2.54136300	0.46463300
C	4.00975500	-2.40192300	1.69315400
H	4.21255600	-3.40003300	2.09708300
H	3.36700000	-1.87201100	2.39903200
C	-4.52574100	0.96262400	1.85689900
H	-3.43520800	1.01567800	1.82212800
H	-4.82601700	0.75376300	2.88723400

C	-5.13437200	2.25970700	1.36456500
C	-4.59958800	2.88223300	0.22886800
C	-6.21523600	2.85051100	2.02632300
C	-5.14572000	4.07483300	-0.24071500
H	-3.75749600	2.41519000	-0.27664500
C	-6.76280500	4.04660800	1.55626000
H	-6.62613200	2.38122800	2.91769900
C	-6.22931200	4.65888200	0.42159500
H	-4.72068900	4.55268100	-1.11850000
H	-7.60020600	4.50032000	2.07863100
H	-6.65157100	5.59114400	0.05751900
C	5.31078400	-1.65462900	1.47582300
C	6.53666800	-2.25055200	1.78813400
C	5.29759200	-0.34307700	0.98027200
C	7.73222100	-1.54758300	1.61461500
H	6.55766100	-3.26711300	2.17512100
C	6.48789600	0.36073200	0.80401300
H	4.34912200	0.12433300	0.73151200
C	7.70883000	-0.24279900	1.12282500
H	8.67794700	-2.02116300	1.86304600
H	6.46346700	1.38063100	0.42990400
H	8.63641000	0.30621400	0.98867000
Cu	-2.51953100	0.14837400	-0.60501400
C	-0.97732300	1.13123400	-0.91045200
C	0.09032700	1.74581600	-0.90700300
C	1.34608400	2.40285500	-0.90775600
C	1.77629300	3.16977700	-2.01779300
C	2.21624200	2.29027800	0.20594800
C	3.02413800	3.77456000	-2.03135700
H	1.11428300	3.26985700	-2.87128500
C	3.46568400	2.89110000	0.19787800
H	1.89799800	1.71008200	1.06559000
C	3.86628400	3.61924000	-0.92664000
H	3.36615900	4.35390800	-2.88007100
H	4.13730600	2.80604800	1.04315700
N	5.19531700	4.21452900	-0.95473200
O	5.49030900	4.93510000	-1.91175700
O	5.96557800	3.96234300	-0.01912100
C	0.59701900	-1.04575500	1.87360100
O	1.38331200	-0.43725000	2.52494200
O	-0.46856500	-1.45538400	1.55348900

III

C	3.10828600	4.30236800	-0.32365000
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C	1.82924000	3.81119000	-0.56354200
C	1.69648900	2.59487600	-1.24151000
C	3.98092900	2.36381700	-1.42584400
C	4.21171600	3.56593600	-0.75695600
H	3.24625900	5.24344500	0.20054400
H	0.95409500	4.35517700	-0.22574700
H	5.22376300	3.91467700	-0.57612000
N	2.75054200	1.89597300	-1.67435300
C	5.11479800	1.46341700	-1.88133100
H	6.05610000	2.01474500	-1.94090300
H	4.88110700	1.06311200	-2.87022300
C	0.36541300	1.96530700	-1.60086300
H	0.13431200	2.15681000	-2.65402700
H	0.44583600	0.88376000	-1.47419300
N	5.31656700	0.33266300	-0.96889600
C	6.35760300	0.21796000	-0.05716400
C	6.13227300	-0.92465300	0.64191300
H	7.16005900	0.93634700	0.00295700
H	6.69166900	-1.38604700	1.44002800
N	4.96476600	-1.47141700	0.13629000
C	4.43643900	-0.70232900	-0.85459200
C	-1.68691700	3.40544800	-1.27850100
C	-1.15142400	2.03812400	0.40365100
C	-2.62196400	3.56234000	-0.30341800
H	-1.59811000	3.86028900	-2.25212400
H	-3.50457400	4.17947000	-0.25932000
N	-0.77896300	2.46403200	-0.82553500
N	-2.27533300	2.70973300	0.72841400
C	-3.04355400	2.56965100	1.99297100
H	-3.03044500	3.54541200	2.48728700
H	-2.48581500	1.84248700	2.58489400
C	4.30697500	-2.69060500	0.63724900
H	5.06368300	-3.47741800	0.71440200
H	3.59875300	-2.96928300	-0.14788900
C	3.59063300	-2.49740600	1.95734300
C	4.03765400	-3.14647000	3.11348200
C	2.45001000	-1.68607600	2.01945400
C	3.35019500	-2.98966800	4.31935800
H	4.91762300	-3.78542100	3.07017800
C	1.76035400	-1.53080900	3.22087700
H	2.09060800	-1.16509200	1.13701900
C	2.21067200	-2.18483400	4.37167500
H	3.70137800	-3.50027500	5.21199000
H	0.86931100	-0.90958400	3.23248400

H	1.67148200	-2.06999400	5.30821100
C	-4.45929100	2.10670900	1.73738400
C	-5.54339700	2.97344100	1.91217500
C	-4.69033400	0.78870200	1.31867700
C	-6.84600600	2.53018600	1.66901800
H	-5.37191400	3.99318600	2.25095400
C	-5.98874400	0.34709300	1.06821000
H	-3.84393700	0.11863800	1.19808600
C	-7.06761600	1.21994200	1.24398300
H	-7.68322600	3.20734000	1.81271800
H	-6.16027300	-0.67446900	0.74030400
H	-8.07936400	0.87423000	1.05267300
Cu	2.70201400	-0.93892500	-1.57431000
C	0.95479100	-1.41649500	-1.95914900
C	-0.22482800	-1.76540800	-1.88355400
C	-1.58503600	-2.13765500	-1.74771400
C	-2.36003300	-2.53794000	-2.86352300
C	-2.20666100	-2.11088500	-0.47274700
C	-3.69618700	-2.88040600	-2.72265500
H	-1.89089100	-2.56919200	-3.84116400
C	-3.54121800	-2.45548400	-0.32629300
H	-1.62924500	-1.79945600	0.39182500
C	-4.28068200	-2.82816100	-1.45363800
H	-4.29878600	-3.18095500	-3.57087500
H	-4.02121700	-2.44535300	0.64439900
N	-5.69092600	-3.15603900	-1.30595800
O	-6.30385800	-3.55704500	-2.29885500
O	-6.20976900	-3.01131400	-0.19037000
C	-0.39488500	0.97699700	1.25099400
O	-1.12404700	0.32006400	2.02461900
O	0.82425000	0.95308500	1.01288900

II2

C	-3.00083100	-4.85853100	0.03806700
C	-1.68435600	-4.43381400	-0.12226100
C	-1.44067400	-3.29778800	-0.90128000
C	-3.68749100	-3.00273100	-1.31313300
C	-4.02915000	-4.12531700	-0.55648600
H	-3.22594400	-5.73985000	0.63159500
H	-0.86594100	-4.96685300	0.35195100
H	-5.06827500	-4.41097400	-0.42427200
N	-2.42042500	-2.62295800	-1.50712300
C	-4.72171300	-2.03495300	-1.86612000
H	-5.71705000	-2.48431600	-1.90458800

H	-4.43359900	-1.72335000	-2.87221200
C	-0.05494900	-2.74749200	-1.17264400
H	0.46331700	-3.36536700	-1.91388200
H	-0.15930600	-1.74001000	-1.57862100
N	-4.78624800	-0.84167200	-1.01704900
C	-5.70932500	-0.64235500	0.00401900
C	-5.28175300	0.44015700	0.70342600
H	-6.58665100	-1.25857400	0.12395200
H	-5.71195800	0.95044600	1.54964200
N	-4.11224600	0.86703000	0.09324800
C	-3.77864300	0.07715900	-0.96247700
C	1.94036300	-3.52570500	0.14954600
C	0.84856400	-1.76258100	0.98328700
C	2.62078200	-3.10143400	1.24733300
H	2.14808500	-4.32575500	-0.54290100
H	3.53289000	-3.45496500	1.69942600
N	0.84505500	-2.69472200	-0.00332000
N	1.93745700	-2.00965800	1.74581300
C	2.37883400	-1.23085000	2.93416600
H	2.17415000	-1.83935200	3.82032300
H	1.72824200	-0.35233400	2.94589900
C	-3.17307500	1.87084300	0.62731400
H	-2.56982000	2.18404000	-0.23073600
H	-2.48884000	1.36534800	1.31615900
C	-3.86126900	3.04359500	1.28455600
C	-4.74048500	3.86433400	0.56225200
C	-3.60782500	3.34319800	2.62788700
C	-5.35362000	4.95739600	1.17214000
H	-4.94201800	3.64263400	-0.48276900
C	-4.21647600	4.44195500	3.23970800
H	-2.92202100	2.71616500	3.19154600
C	-5.09218400	5.24943700	2.51404900
H	-6.03050400	5.58599500	0.60030300
H	-4.00606400	4.66422400	4.28200600
H	-5.56721900	6.10361200	2.98819000
C	3.84780200	-0.88353300	2.85047400
C	4.75101200	-1.38664100	3.79365100
C	4.32304800	-0.04924600	1.82698100
C	6.10821100	-1.06238500	3.71957200
H	4.39092600	-2.02891500	4.59433900
C	5.67934000	0.26315600	1.74250600
H	3.62948300	0.35140100	1.09246200
C	6.57356800	-0.24287600	2.69149400
H	6.79832800	-1.45486100	4.46099000

H	6.04275200	0.89387000	0.93610800
H	7.62911500	0.00398900	2.62593200
Cu	-2.05379000	0.10496800	-1.76228600
C	-0.33565300	0.48502100	-2.35666900
C	0.84968300	0.82526300	-2.40520000
C	2.20627900	1.22110500	-2.39698700
C	2.58995900	2.55290900	-2.69792300
C	3.22828200	0.30847800	-2.02834000
C	3.91046200	2.96115400	-2.59886900
H	1.82242000	3.26094900	-2.99065700
C	4.54918600	0.70996300	-1.91662400
H	2.95715400	-0.72082200	-1.81770900
C	4.88092100	2.04094700	-2.18892200
H	4.20640400	3.98101500	-2.81201200
H	5.32886000	0.02072900	-1.61701400
N	6.25653800	2.47873900	-2.01856800
O	6.55758200	3.61557500	-2.39117400
O	7.05695600	1.68870600	-1.49786100
C	-0.23726100	-0.66703900	1.20991000
O	0.08709800	0.25700900	1.97638800
O	-1.29104900	-0.90432300	0.58782600

II-TS2

C	3.50426600	-4.36240200	-0.87392300
C	4.27843900	-3.28987200	-1.32062800
C	3.64405000	-2.27200100	-2.03529900
C	1.59077500	-3.29428700	-1.85399100
C	2.13386900	-4.35549600	-1.11803300
H	3.96049900	-5.17448400	-0.31589200
H	5.34024500	-3.23828200	-1.09815400
H	1.49572300	-5.14170700	-0.72724100
N	2.34246000	-2.30529900	-2.33973500
C	0.09648900	-3.12744900	-2.08006800
H	-0.31956100	-3.95714900	-2.66092800
H	-0.04973500	-2.20215100	-2.63805300
C	4.34875400	-0.99190100	-2.44646900
H	5.18797300	-1.18224000	-3.12169800
H	3.61330300	-0.35387100	-2.93742700
N	-0.65396400	-3.04917500	-0.82649600
C	-1.34659400	-4.12387200	-0.27836900
C	-1.87211700	-3.68896700	0.89380100
H	-1.42768400	-5.07724100	-0.77717700
H	-2.49934800	-4.18541300	1.61645700
N	-1.48859100	-2.36458600	1.02530000

C	-0.72279200	-1.93741000	-0.02540400
C	6.20922500	0.23536000	-1.22971400
C	4.24635200	0.11408900	-0.17824600
C	6.32135200	0.91359200	-0.05531100
H	6.92749700	0.05705800	-2.01379300
H	7.15252300	1.45023300	0.37253500
N	4.91450000	-0.25257300	-1.29577400
N	5.10179100	0.81605200	0.58758400
C	4.75073100	1.45812700	1.88589800
H	5.67508000	1.47960100	2.46867400
H	4.03606800	0.78064400	2.35483500
C	-1.80676300	-1.50103600	2.17575600
H	-1.56851500	-0.48748100	1.83842500
H	-1.12560800	-1.74718000	2.99725200
C	-3.24398800	-1.62044700	2.62860600
C	-4.28221500	-1.08391900	1.85302900
C	-3.55917900	-2.26279800	3.83178900
C	-5.60663300	-1.19451500	2.27296300
H	-4.05017700	-0.56961900	0.92438800
C	-4.88600800	-2.37284800	4.25517700
H	-2.75964200	-2.67087100	4.44601800
C	-5.91204100	-1.84049800	3.47455400
H	-6.40055800	-0.76887000	1.66617800
H	-5.11492500	-2.87030000	5.19342300
H	-6.94462900	-1.92179400	3.80180000
C	4.17779600	2.84771200	1.70830400
C	5.00628100	3.97299200	1.81241300
C	2.81616600	3.01822700	1.42026100
C	4.48552400	5.25391600	1.62477100
H	6.06098500	3.84959800	2.05190400
C	2.30064700	4.29932800	1.22303700
H	2.13401400	2.17569800	1.34225100
C	3.13076700	5.41736200	1.32488200
H	5.13455400	6.12056100	1.71459300
H	1.24508700	4.39708600	0.98834700
H	2.72519500	6.41426300	1.17563900
Cu	-0.06138300	-0.15002000	-0.08189700
C	-0.29761700	1.74109900	0.29616900
C	-1.42719900	1.75996800	-0.25462200
C	-2.71024200	1.97682400	-0.81419000
C	-3.35146500	3.23914000	-0.72058000
C	-3.39960400	0.93196600	-1.48197600
C	-4.61070900	3.44404200	-1.25936900
H	-2.83693200	4.04845100	-0.21404700

C	-4.66090900	1.12902100	-2.01998000
H	-2.91002800	-0.03278900	-1.56857300
C	-5.26191800	2.38677100	-1.90550300
H	-5.10706400	4.40429100	-1.19095800
H	-5.19196600	0.33562900	-2.53147000
N	-6.58542100	2.59802700	-2.46790900
O	-7.09231000	3.71982800	-2.35736200
O	-7.13857400	1.64352800	-3.02695300
C	2.77710400	-0.18621300	0.16222000
O	2.56954100	-0.53293700	1.33513300
O	2.01368600	-0.01540300	-0.81516800

II3

C	-2.67970700	4.95027000	-1.10157300
C	-3.12185700	3.69491500	-1.50827800
C	-2.17582600	2.69504300	-1.76354700
C	-0.43718500	4.11154000	-1.21780800
C	-1.31032100	5.16586300	-0.94495800
H	-3.38973200	5.74750200	-0.90178900
H	-4.18205100	3.49140000	-1.62529400
H	-0.92975200	6.12604300	-0.61056400
N	-0.86138200	2.91231400	-1.63769300
C	1.05878300	4.21499400	-0.96249400
H	1.36439200	5.25427800	-0.82120900
H	1.60701300	3.80210800	-1.81281600
C	-2.56363200	1.31101100	-2.24829300
H	-2.95279300	1.36655600	-3.27034100
H	-1.67992900	0.65527800	-2.25766500
N	1.43100100	3.45825700	0.23496200
C	1.67932900	3.99521600	1.49345100
C	1.77939500	2.94132400	2.34484800
H	1.79034500	5.05445600	1.66571900
H	1.99540100	2.90443900	3.40021600
N	1.58306100	1.79770600	1.58441600
C	1.35155400	2.09774000	0.27961600
C	-4.92299900	0.48630600	-1.93194900
C	-3.52839300	0.09444300	-0.23581900
C	-5.61172300	-0.20307500	-0.98271500
H	-5.22587700	0.84199500	-2.90363200
H	-6.62993700	-0.55622100	-0.96303400
N	-3.63899000	0.67212400	-1.45727700
N	-4.73812000	-0.43358400	0.05951000
C	-5.10877200	-1.17931500	1.29138000
H	-6.05564400	-0.75526100	1.63682900

H	-4.31498200	-0.97195500	2.00780300
C	1.41378100	0.42663300	2.10664700
H	1.60689500	-0.23214200	1.25630200
H	0.36117400	0.29109100	2.37440700
C	2.33171900	0.11980400	3.26612100
C	3.68862100	-0.15946900	3.04875500
C	1.84063700	0.10883100	4.57731000
C	4.53647000	-0.43647100	4.12006300
H	4.07545500	-0.17093900	2.03292300
C	2.68806700	-0.16753500	5.65290700
H	0.78606300	0.30656500	4.75279800
C	4.03771400	-0.43834200	5.42578600
H	5.58377200	-0.65866200	3.93674500
H	2.29228700	-0.17713100	6.66454000
H	4.69776200	-0.65802000	6.26009900
C	-5.23981500	-2.66503400	1.03705400
C	-6.49969300	-3.26942600	0.96350000
C	-4.08713700	-3.44759200	0.87525000
C	-6.61324700	-4.64070400	0.72376100
H	-7.39667500	-2.67007200	1.10624400
C	-4.20336500	-4.81527400	0.63151800
H	-3.11400500	-2.97085400	0.95380800
C	-5.46433600	-5.41376000	0.55360800
H	-7.59525400	-5.10219700	0.67273200
H	-3.30758700	-5.41684200	0.50799300
H	-5.54984400	-6.48038200	0.36663900
Cu	0.63641800	0.92264800	-1.04344700
C	0.14893600	-0.46640300	-2.35810700
C	1.36350800	-0.71349000	-2.11027900
C	2.67111500	-1.28364700	-2.09969500
C	2.93192100	-2.51112600	-2.75712600
C	3.74430500	-0.64402100	-1.43526900
C	4.19922800	-3.07180500	-2.74792800
H	2.11735000	-3.01048900	-3.27033900
C	5.01528000	-1.19644600	-1.42277000
H	3.55113700	0.30111400	-0.93799800
C	5.23471500	-2.41115200	-2.07852200
H	4.40780000	-4.01067600	-3.24592900
H	5.84353600	-0.71048100	-0.92180200
N	6.56721200	-2.99799800	-2.06495000
O	6.73607200	-4.06913300	-2.65637800
O	7.46082300	-2.39402600	-1.46149400
C	-2.26190800	0.07645400	0.65959600
O	-2.27210100	-0.75809900	1.58425400

0	-1.41515200	0.92790500	0.32231200
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A-TS1

C	2.98986400	-5.08909100	-0.11250800
C	3.53856200	-3.87425500	-0.51246600
C	2.70996400	-2.94634500	-1.15214500
C	0.89703200	-4.38037900	-1.03990700
C	1.64070600	-5.35166200	-0.36989300
H	3.60270800	-5.82675700	0.39719300
H	4.57944600	-3.63954900	-0.31324900
H	1.18351700	-6.28512700	-0.05661700
N	1.42814000	-3.21227600	-1.43081000
C	-0.56008000	-4.57448500	-1.40755400
H	-0.81305400	-5.63809700	-1.39435800
H	-0.70621900	-4.19694200	-2.42465800
C	3.13737600	-1.57767700	-1.63159800
H	3.60642600	-1.65453700	-2.61786200
H	2.24229500	-0.91938900	-1.69460100
N	-1.52686000	-3.89795700	-0.51849800
C	-2.84108500	-4.33385600	-0.39913500
C	-3.48122200	-3.43592800	0.39119800
H	-3.20228200	-5.22419300	-0.88967300
H	-4.50355900	-3.39059900	0.72933100
N	-2.54480100	-2.47076300	0.72421900
C	-1.32997200	-2.73193200	0.16743500
C	5.28808900	-0.33881800	-1.28127900
C	3.76791600	-0.12155500	0.33121700
C	5.71874600	0.63544400	-0.43729100
H	5.71949300	-0.71962000	-2.19291800
H	6.59882000	1.25730300	-0.46121800
N	4.08470400	-0.81504800	-0.79427300
N	4.77110800	0.75318200	0.55909300
C	4.82392800	1.79179500	1.61564500
H	5.82574700	1.75536900	2.05215200
H	4.08221300	1.49942700	2.35876000
C	-2.77092200	-1.34790700	1.65538800
H	-1.99148300	-0.61757100	1.42399100
H	-2.59905800	-1.70634000	2.67646400
C	-4.15503900	-0.75145900	1.54005400
C	-4.48945900	0.06726900	0.45250900
C	-5.12101000	-1.00987000	2.52020000
C	-5.76691300	0.61678800	0.34691300
H	-3.74428000	0.28571100	-0.30686800
C	-6.40155200	-0.46145000	2.41648000

H	-4.86680200	-1.63406000	3.37408400
C	-6.72505400	0.35149800	1.32961100
H	-6.00927500	1.26336000	-0.49169700
H	-7.14042900	-0.66436200	3.18651400
H	-7.71733200	0.78598300	1.25052800
C	4.52389500	3.16684600	1.05480000
C	5.42838900	4.21599800	1.24972800
C	3.32587400	3.40365700	0.36328500
C	5.14332300	5.49530000	0.76659200
H	6.35685100	4.03599200	1.78767200
C	3.05129200	4.67967900	-0.12696200
H	2.61347500	2.59848300	0.19657700
C	3.95435200	5.72749000	0.07523500
H	5.85098900	6.30385900	0.92648400
H	2.12490000	4.85315000	-0.66648100
H	3.73157800	6.71991600	-0.30635700
Cu	0.28914500	-1.87950100	0.47199600
C	1.05917200	0.62820100	-1.06748400
C	-0.00985000	1.26597500	-1.11366200
C	-1.22233200	1.98928700	-1.16602200
C	-1.53541100	2.98052800	-0.19640400
C	-2.18449100	1.74118900	-2.18351000
C	-2.73793000	3.66628500	-0.22642800
H	-0.81089500	3.18538400	0.58475600
C	-3.39610700	2.41188600	-2.21135300
H	-1.95256100	1.00298500	-2.94412600
C	-3.67223900	3.36720200	-1.22532000
H	-2.98336800	4.41586000	0.51610700
H	-4.13665000	2.21488200	-2.97720300
N	-4.95912000	4.03446800	-1.22067300
O	-5.12484400	4.98419400	-0.44816100
O	-5.83788100	3.60934300	-1.98617600
C	2.56038700	-0.35876200	1.23684200
O	2.29731200	0.48210200	2.09227100
O	2.03443400	-1.50033000	1.02240500

A-M1

C	-5.00639600	2.95327200	0.46046100
C	-3.74138800	3.13929100	1.01391800
C	-3.15425700	2.08497300	1.72179900
C	-4.98502600	0.72586300	1.34748700
C	-5.64408500	1.72455400	0.62658100
H	-5.48785800	3.75390500	-0.09285100
H	-3.21573100	4.08133800	0.89316200

H	-6.62524300	1.54176800	0.19920700
N	-3.77073800	0.90554700	1.88982200
C	-5.59984100	-0.65018000	1.54521000
H	-6.67260200	-0.56506400	1.73787700
H	-5.12628100	-1.11713400	2.41231500
C	-1.77089700	2.20617500	2.34911400
H	-1.81862600	2.82311300	3.25270500
H	-1.41982600	1.21040500	2.60965600
N	-5.44451900	-1.53531900	0.37615600
C	-6.44194300	-2.34541500	-0.14940200
C	-5.86641000	-3.05896100	-1.15285600
H	-7.44968400	-2.35512000	0.23553500
H	-6.28422200	-3.79427000	-1.82246700
N	-4.53520900	-2.67370600	-1.20434200
C	-4.25769200	-1.73338300	-0.26521100
C	-0.19147900	4.08332600	1.72616800
C	-0.26156800	2.35592200	0.32060500
C	0.66024500	4.34098500	0.69673900
H	-0.42255100	4.65465600	2.61057900
H	1.32446400	5.17002300	0.52092200
N	-0.77526200	2.85117900	1.47459600
N	0.57831100	3.27968600	-0.18029200
C	1.43093200	3.03853200	-1.37287600
H	0.80542300	3.16347300	-2.25828900
H	1.71799100	1.98333000	-1.27345200
C	-3.56073400	-3.14170500	-2.22488200
H	-3.55101100	-2.40859000	-3.03792400
H	-3.96254300	-4.07744900	-2.62304600
C	-2.16755400	-3.34369200	-1.67579400
C	-1.22942800	-2.30067500	-1.72168500
C	-1.81656700	-4.55393100	-1.06518000
C	0.03624200	-2.46027200	-1.14959200
H	-1.46239700	-1.36013100	-2.21441500
C	-0.54956200	-4.71831800	-0.50412900
H	-2.53715500	-5.36806900	-1.02551200
C	0.37329400	-3.66886100	-0.53887900
H	0.73746600	-1.63058100	-1.14545900
H	-0.28441600	-5.66257200	-0.03706000
H	1.35532100	-3.78846500	-0.09121500
C	2.64778600	3.92808800	-1.38938400
C	2.69099100	5.08955600	-2.17055900
C	3.76693200	3.57445700	-0.61919900
C	3.83341700	5.89318100	-2.18168500
H	1.83156900	5.35960200	-2.78018100

C	4.90639500	4.37838500	-0.63131900
H	3.72832900	2.66073000	-0.02972800
C	4.94138900	5.53874100	-1.41013400
H	3.85978000	6.78904000	-2.79572200
H	5.77189500	4.09423300	-0.03963300
H	5.83241900	6.16029300	-1.42138600
Cu	-2.67512600	-0.82680300	0.03813600
C	1.97631100	0.54004300	0.45652000
C	2.94259300	-0.24682400	0.49808100
C	4.04091300	-1.13512700	0.58200700
C	4.75477200	-1.31373700	1.79776600
C	4.47323900	-1.88662000	-0.54410100
C	5.82768100	-2.18437200	1.88671000
H	4.43873400	-0.74948700	2.66894100
C	5.54448700	-2.76072600	-0.46389900
H	3.94471600	-1.76090900	-1.48344400
C	6.21927500	-2.90724100	0.75357800
H	6.37232300	-2.32287100	2.81274800
H	5.87543100	-3.33451400	-1.32095600
N	7.34106500	-3.82378200	0.84263300
O	7.92232400	-3.93142200	1.92966400
O	7.66190500	-4.45439300	-0.17249100
C	-0.77677400	1.11981000	-0.37296400
O	-0.78477600	1.09638100	-1.60432900
O	-1.26499600	0.28576900	0.46828700

A-TS2

C	4.77841000	3.03074300	-0.45706500
C	3.50899000	3.35228800	-0.93061400
C	2.87305300	2.46933000	-1.81060200
C	4.66745800	1.01759300	-1.75363200
C	5.37278600	1.83975100	-0.87329500
H	5.29644900	3.69621000	0.22686600
H	3.01518300	4.26631000	-0.61620000
H	6.35679700	1.55172600	-0.51619300
N	3.44589700	1.32749800	-2.21569400
C	5.22048600	-0.31794100	-2.21680300
H	6.30722700	-0.27027500	-2.32131200
H	4.78673500	-0.55524200	-3.19121200
C	1.48493000	2.74573100	-2.37304900
H	1.52220100	3.55804500	-3.10685400
H	1.11404900	1.83300300	-2.83345300
N	4.92645800	-1.41580700	-1.28191400
C	5.86992600	-2.29150800	-0.76108600

C	5.18825000	-3.18054600	0.00719500
H	6.92198000	-2.21491200	-0.98707400
H	5.53543200	-4.01359500	0.59721900
N	3.85048300	-2.82955600	-0.07520100
C	3.66615800	-1.73830100	-0.86509900
C	0.13938400	4.47814900	-1.10707100
C	-0.06839900	2.35620600	-0.42579500
C	-0.68532800	4.46590300	-0.02818800
H	0.46593200	5.28792100	-1.73963400
H	-1.22234900	5.26016900	0.46346600
N	0.52118700	3.16167300	-1.34132700
N	-0.79136200	3.15056700	0.38692500
C	-1.52421600	2.68691800	1.58940500
H	-0.87945700	2.86963900	2.45363700
H	-1.63565400	1.60851200	1.46608500
C	2.74568500	-3.49071000	0.64319400
H	2.87723700	-4.57166800	0.53561800
H	1.84105600	-3.19579800	0.10687800
C	2.65098500	-3.09478600	2.10140500
C	3.18365300	-3.91771300	3.10070300
C	2.02206700	-1.89265400	2.45397100
C	3.10159300	-3.54283200	4.44303100
H	3.65258300	-4.86236500	2.83174500
C	1.94147200	-1.52273500	3.79661300
H	1.58608900	-1.24247500	1.69600100
C	2.48099900	-2.34176200	4.79163700
H	3.51294300	-4.18991800	5.21272100
H	1.44450300	-0.59311100	4.05744200
H	2.41027200	-2.05086400	5.83621000
C	-2.85858200	3.37874300	1.73343800
C	-3.05564600	4.36823900	2.70383300
C	-3.92338500	3.02097600	0.89250300
C	-4.29575900	4.99893700	2.83326200
H	-2.23857500	4.63851000	3.36930300
C	-5.15956200	3.65213000	1.02119500
H	-3.77038200	2.23635000	0.15578200
C	-5.34821100	4.64295400	1.98960600
H	-4.43863100	5.76183000	3.59337300
H	-5.98107000	3.36444700	0.37135000
H	-6.31434600	5.12947800	2.08979900
Cu	2.12053900	-0.75458600	-1.10072400
C	-1.76129400	0.32410100	-0.42447100
C	-2.71387400	-0.44777400	-0.57763900
C	-3.80186300	-1.33905900	-0.75718700

C	-4.70707200	-1.18528200	-1.83700300
C	-4.01815700	-2.41488500	0.14016600
C	-5.77075800	-2.05607100	-2.01377400
H	-4.55115800	-0.36848400	-2.53380400
C	-5.07836600	-3.29114000	-0.02986700
H	-3.33300200	-2.54361200	0.97124200
C	-5.94988300	-3.10540300	-1.10740400
H	-6.46532500	-1.94559300	-2.83737700
H	-5.24997300	-4.11572900	0.65097200
N	-7.06551600	-4.02367100	-1.29006600
O	-7.82311500	-3.83397600	-2.24760800
O	-7.19781600	-4.94562300	-0.47826800
C	0.17789600	0.85487000	-0.24006100
O	0.58129500	0.57785700	0.92245300
O	0.64021600	0.31234000	-1.35524900

A-M2

C	-4.83764500	-3.76860600	-2.26618600
C	-3.44468300	-3.79426500	-2.28536600
C	-2.74178000	-2.59050400	-2.13959500
C	-4.71354300	-1.38859300	-1.99266300
C	-5.48907100	-2.54521200	-2.10651200
H	-5.40785200	-4.68612100	-2.37790200
H	-2.91085600	-4.72986300	-2.42534200
H	-6.57332800	-2.48925600	-2.08747500
N	-3.37471800	-1.41628600	-2.01614800
C	-5.33670500	-0.00537700	-1.85438800
H	-6.40944400	-0.04628500	-2.05748600
H	-4.87289100	0.66061300	-2.58648600
C	-1.22214500	-2.54122900	-2.11982300
H	-0.80394900	-3.34924700	-2.72774800
H	-0.87829500	-1.55502100	-2.44953700
N	-5.15332300	0.58571200	-0.52672600
C	-6.15112800	0.76099700	0.42533200
C	-5.54244200	1.28173300	1.52341800
H	-7.18544700	0.51673000	0.24030900
H	-5.94847800	1.57410500	2.47903800
N	-4.19639400	1.39788500	1.21519500
C	-3.93328600	0.98146500	-0.05312100
C	-0.72975300	-3.88746000	-0.03484400
C	-0.05545000	-1.74367200	-0.01704500
C	-0.12246600	-3.65814800	1.15589000
H	-1.18786100	-4.77847400	-0.43198500
H	0.06297500	-4.30921400	1.99509900

N	-0.67989900	-2.69772800	-0.75168400
N	0.28368600	-2.33450900	1.15206500
C	0.90781200	-1.66005200	2.30668700
H	0.20648400	-1.73953300	3.14372500
H	0.94549400	-0.59889800	2.03050100
C	-3.12900900	1.88533600	2.11450400
H	-2.28509100	1.19963400	1.99753800
H	-3.51774800	1.80961400	3.13458300
C	-2.68482000	3.29954800	1.80201000
C	-1.53502900	3.50054200	1.02581600
C	-3.40721200	4.40447000	2.26891100
C	-1.12342400	4.80018700	0.72195100
H	-0.96896700	2.63398700	0.68482900
C	-2.99483700	5.70075400	1.95943800
H	-4.29451300	4.25284100	2.88081700
C	-1.85069300	5.89939300	1.18266200
H	-0.22809200	4.95181900	0.12555000
H	-3.55954000	6.55269600	2.32833300
H	-1.52464700	6.90830300	0.94458700
C	2.24034700	-2.26628400	2.68670100
C	2.51660000	-2.55627700	4.02797600
C	3.22836500	-2.51978400	1.72362900
C	3.75548100	-3.07861600	4.40642800
H	1.75782400	-2.36754100	4.78392400
C	4.46174000	-3.05207000	2.09905700
H	3.02984000	-2.29041200	0.68082000
C	4.73085600	-3.33102900	3.44203300
H	3.95310800	-3.29424100	5.45263000
H	5.21587100	-3.24671100	1.34153100
H	5.69304300	-3.74304600	3.73198000
Cu	-2.27143200	0.64039400	-0.76752400
C	0.09323800	-0.14826600	-0.32719100
O	-0.61445000	0.11361300	-1.47084200
O	-0.31180500	0.47345300	0.78051200
C	1.56218000	0.08363100	-0.59594900
C	2.73375600	0.36803300	-0.77495500
C	4.08070800	0.73975100	-1.03343000
C	4.39067700	1.57593800	-2.13144100
C	5.13663100	0.28986400	-0.20810000
C	5.70106900	1.94379200	-2.39917300
H	3.58431000	1.92693800	-2.76608700
C	6.44989100	0.65169900	-0.47205300
H	4.90862100	-0.34150300	0.64365700
C	6.72012900	1.47469800	-1.56709900

H	5.95258100	2.58229400	-3.23679300
H	7.26845700	0.31534600	0.15199100
N	8.10360800	1.85415200	-1.84908900
O	8.98413700	1.42214600	-1.10049000
O	8.31499700	2.58404900	-2.82077500

A-TS3

C	-4.51381600	-3.99715700	-2.49051500
C	-3.12440600	-3.93967200	-2.40072900
C	-2.51390200	-2.70812600	-2.12799700
C	-4.56337200	-1.63615200	-2.06914800
C	-5.25269700	-2.82722800	-2.31343500
H	-5.01437400	-4.93818300	-2.69895900
H	-2.52134000	-4.83064000	-2.54977300
H	-6.33651600	-2.83685200	-2.37887100
N	-3.22894700	-1.58505100	-1.98358500
C	-5.28438900	-0.30037000	-1.93247700
H	-6.34848100	-0.41845400	-2.15005000
H	-4.86314100	0.39629500	-2.66252100
C	-1.00716600	-2.56750800	-1.98727600
H	-0.49651100	-3.35604800	-2.54897600
H	-0.69600000	-1.57221200	-2.32077900
N	-5.16196700	0.31095400	-0.60813300
C	-6.18386900	0.41965700	0.32842000
C	-5.63684900	1.01116600	1.42301900
H	-7.19078900	0.08365400	0.13642300
H	-6.07904600	1.28525200	2.36791000
N	-4.30156200	1.23571400	1.12849600
C	-3.98735100	0.81933200	-0.12779200
C	-0.71443800	-3.78881000	0.21476400
C	0.04278400	-1.66316900	0.11135800
C	-0.17448700	-3.48690700	1.42188000
H	-1.18531100	-4.69123300	-0.14074800
H	-0.06757800	-4.07756200	2.31797100
N	-0.57162400	-2.65620800	-0.58055500
N	0.28086800	-2.17917000	1.33984700
C	0.89621800	-1.44575400	2.45957200
H	0.19992600	-1.49072200	3.30343200
H	0.93191700	-0.39976900	2.13110100
C	-3.29359200	1.84065400	2.02514100
H	-2.38628600	1.23801000	1.92767500
H	-3.68038600	1.74726100	3.04437100
C	-2.98310900	3.28407200	1.68586800
C	-1.85310900	3.57607300	0.90979600

C	-3.80811600	4.32577000	2.12689300
C	-1.56155500	4.90166500	0.58097200
H	-1.20685300	2.76067300	0.58804300
C	-3.51593200	5.64833700	1.79254800
H	-4.68064100	4.10443600	2.73870700
C	-2.39059700	5.93718400	1.01659400
H	-0.68055000	5.12380100	-0.01456000
H	-4.15938300	6.45127000	2.14179400
H	-2.15825700	6.96713500	0.75969200
C	2.23865500	-2.01513200	2.86625100
C	2.51403000	-2.26496500	4.21541100
C	3.23510600	-2.27575600	1.91408500
C	3.76001300	-2.75643000	4.61225300
H	1.74886500	-2.06945200	4.96324500
C	4.47600800	-2.77618300	2.30778800
H	3.03592400	-2.07834800	0.86475100
C	4.74380500	-3.01635400	3.65863500
H	3.95680500	-2.94170900	5.66445800
H	5.23687600	-2.97690900	1.55857000
H	5.71173400	-3.40399000	3.96290800
Cu	-2.29011400	0.60329000	-0.80841700
C	0.15606600	0.08357400	-0.29213900
O	-0.56729900	0.21888700	-1.42465300
O	-0.24125900	0.69156600	0.79287700
C	1.61707400	0.26553300	-0.58062200
C	2.79617400	0.50002800	-0.77564800
C	4.15675400	0.80651000	-1.05013400
C	4.50387600	1.52490000	-2.21773900
C	5.18844600	0.40851700	-0.16970800
C	5.82757500	1.82999300	-2.49929000
H	3.71594200	1.83613300	-2.89486500
C	6.51491300	0.70763800	-0.44695500
H	4.93145800	-0.13300800	0.73409800
C	6.82188900	1.41489400	-1.61084800
H	6.10775600	2.37889700	-3.38964200
H	7.31565600	0.41008000	0.21853200
N	8.21946100	1.72883200	-1.90658500
O	9.07788200	1.34527400	-1.10798100
O	8.46298600	2.35831700	-2.93887200

B-TS1

C	-3.67213000	-2.78721200	-2.77988000
C	-2.28654900	-2.89962300	-2.72890600
C	-1.52048200	-1.72978100	-2.73649200

C	-3.41023900	-0.40639800	-2.86629700
C	-4.25308500	-1.51768500	-2.84206800
H	-4.29657300	-3.67558100	-2.76567500
H	-1.80780400	-3.87082800	-2.65841000
H	-5.33168800	-1.39699500	-2.86428900
N	-2.07233800	-0.51430800	-2.83366900
C	-3.94557900	1.01061200	-2.93777000
H	-4.93057900	1.01955900	-3.41215200
H	-3.25964200	1.60536500	-3.54851000
C	-0.00350900	-1.71183900	-2.68504800
H	0.40895600	-1.86276100	-3.68892800
H	0.31109600	-0.72931200	-2.32274300
N	-4.09947400	1.67592300	-1.62655400
C	-5.01910200	2.69233800	-1.39835100
C	-4.78863100	3.15042900	-0.14060500
H	-5.73831700	3.00190500	-2.14039000
H	-5.27964600	3.92367500	0.42880900
N	-3.72846400	2.41155100	0.35863500
C	-3.28678300	1.49533500	-0.54438000
C	1.37133100	-3.79727200	-2.28212400
C	0.76983900	-2.62059300	-0.47645200
C	1.94265900	-4.38067400	-1.19733900
H	1.42879200	-4.04573500	-3.32992900
H	2.58553400	-5.24155800	-1.11226800
N	0.63344900	-2.71657000	-1.82332100
N	1.55107600	-3.64503300	-0.08891400
C	1.97988200	-3.93807200	1.30407900
H	1.89357200	-5.02062100	1.43326500
H	1.26225600	-3.41360300	1.93691000
C	-3.14875800	2.53386000	1.70906300
H	-3.28877800	3.57034700	2.02829600
H	-2.07770700	2.35439200	1.59480900
C	-3.73458900	1.57251100	2.72386600
C	-4.79986700	1.96225100	3.54406200
C	-3.20533700	0.28092600	2.85253300
C	-5.33789500	1.07386200	4.47639200
H	-5.20505100	2.96875800	3.46238700
C	-3.74115200	-0.60466200	3.78729800
H	-2.37861000	-0.03786000	2.22241700
C	-4.80821300	-0.21212100	4.59840200
H	-6.16183600	1.38809000	5.11085500
H	-3.31537800	-1.59888300	3.88289300
H	-5.22047700	-0.90256600	5.32887800
C	3.39089800	-3.46397600	1.57549900

C	4.46476000	-4.36104500	1.58451100
C	3.62424700	-2.10239000	1.82062400
C	5.76368800	-3.90820200	1.82724200
H	4.28570500	-5.42087300	1.41307400
C	4.92294000	-1.65288700	2.05917000
H	2.77779900	-1.42021500	1.82576300
C	5.99383900	-2.55186500	2.06103100
H	6.59063900	-4.61277900	1.83693800
H	5.09800600	-0.59792600	2.25052300
H	7.00297400	-2.19680400	2.25094900
Cu	-2.08932100	0.11998500	-0.25923700
C	1.11365200	-0.08140900	-0.28791000
C	1.91982500	0.85248000	-0.33132400
C	2.84714500	1.92299000	-0.39373200
C	4.24048600	1.67027100	-0.45420200
C	2.41513100	3.27195700	-0.40357700
C	5.15566500	2.70912000	-0.52337400
H	4.58402200	0.64129500	-0.44000400
C	3.32396800	4.31634800	-0.47238200
H	1.35125800	3.47876200	-0.35717400
C	4.69005600	4.02706800	-0.53342100
H	6.22206200	2.52594300	-0.56951000
H	3.00279600	5.35060700	-0.48130900
N	5.64895400	5.12237200	-0.60952700
O	6.84979300	4.83861300	-0.66075300
O	5.21050300	6.27698400	-0.61961300
C	0.08536200	-1.55380100	0.42609800
O	0.36862500	-1.57956700	1.65287500
O	-1.15096200	-1.43177900	-0.05245600

B-M1

C	2.80130200	2.07403400	3.28899900
C	2.42090200	0.73981000	3.19591000
C	1.06821900	0.44300000	2.99956400
C	0.49934600	2.68025900	3.01447800
C	1.82652900	3.07065100	3.18965500
H	3.84481900	2.33908500	3.43041000
H	3.15876300	-0.05405900	3.24451000
H	2.09358300	4.12164700	3.23939800
N	0.12664900	1.39182600	2.94338400
C	-0.62619600	3.68744200	2.89773500
H	-0.36880100	4.60614700	3.43197100
H	-1.52021000	3.25664500	3.35866800
C	0.52625400	-0.97183700	2.88643800

H	0.35227800	-1.39201100	3.88433800
H	-0.43113700	-0.91816000	2.36975000
N	-0.95955200	4.08270700	1.51294400
C	-1.53616200	5.30857100	1.20709600
C	-1.82787500	5.27770400	-0.11815100
H	-1.68298700	6.08203300	1.94453400
H	-2.27282200	6.02217100	-0.75950300
N	-1.42600400	4.03612500	-0.58352700
C	-0.89119800	3.27512100	0.41213800
C	2.20353100	-2.86517900	2.79909600
C	1.48364700	-2.05578500	0.83414500
C	2.80853300	-3.57337100	1.81044300
H	2.27374100	-2.94654700	3.87237400
H	3.52472400	-4.37801400	1.85064800
N	1.38997500	-1.92594300	2.18166100
N	2.34208200	-3.06601700	0.60707700
C	2.75311800	-3.56600900	-0.73041400
H	2.04767300	-3.09236200	-1.42264900
H	2.63516200	-4.65347400	-0.71054700
C	-1.60591800	3.56414400	-1.97537200
H	-2.11114100	4.37296200	-2.50983700
H	-2.28841300	2.70997400	-1.94590800
C	-0.31671900	3.18334100	-2.66676400
C	0.43071200	4.13500900	-3.37143400
C	0.16242300	1.87117200	-2.57571300
C	1.63606700	3.77461000	-3.97532300
H	0.06841900	5.15794300	-3.45147600
C	1.37211000	1.50666200	-3.16786900
H	-0.40451500	1.10983800	-2.05003400
C	2.10818500	2.46225600	-3.86977500
H	2.20602200	4.51709500	-4.52728500
H	1.71074100	0.48399200	-3.02978500
H	3.04966600	2.18794700	-4.33813800
C	4.17510700	-3.17301500	-1.06136200
C	4.45483600	-1.84079300	-1.40259300
C	5.21198500	-4.11207800	-1.03892100
C	5.76203100	-1.46239600	-1.70535100
H	3.62539500	-1.13583400	-1.43443000
C	6.52007300	-3.73031600	-1.34798600
H	4.99605500	-5.14957600	-0.79074900
C	6.79656200	-2.40316900	-1.67784500
H	5.97515200	-0.43073900	-1.97213600
H	7.31798700	-4.46767500	-1.33284100
H	7.81288700	-2.10355200	-1.91900300

Cu	-0.02863600	1.63891000	0.29602100
C	-0.68789900	-1.42108300	-0.19948700
C	-1.87300100	-1.71457000	-0.25748500
C	-3.25230300	-2.03763100	-0.32588700
C	-3.78013800	-3.12634100	0.40795000
C	-4.13553200	-1.27643100	-1.12759700
C	-5.12964200	-3.43942000	0.34904100
H	-3.11148400	-3.71968800	1.02234600
C	-5.48623300	-1.58335700	-1.19037700
H	-3.73889500	-0.44574200	-1.70112100
C	-5.97285200	-2.66263000	-0.44892700
H	-5.54573600	-4.26956200	0.90612300
H	-6.17215500	-1.00895600	-1.80045900
N	-7.39584000	-2.98591100	-0.50879900
O	-7.79770000	-3.94597000	0.15417900
O	-8.11847800	-2.28020400	-1.21762900
C	0.80209600	-1.07247200	-0.25558200
O	1.27444700	-1.27562800	-1.45940900
O	1.02086700	0.14495000	0.35688600

B-TS2

C	2.72549900	2.26087200	3.16169900
C	2.42281700	0.90482600	3.09540000
C	1.08268200	0.52435600	2.97398900
C	0.38159800	2.72406500	2.99029600
C	1.68900600	3.19564600	3.10494800
H	3.75684000	2.58946500	3.24859200
H	3.20868500	0.15764600	3.10862000
H	1.89351900	4.26132500	3.13609500
N	0.08479700	1.41519900	2.94540700
C	-0.80605700	3.65945400	2.90599700
H	-0.59250500	4.59334700	3.43318900
H	-1.66008700	3.17478000	3.38844200
C	0.61985300	-0.92082800	2.89150900
H	0.43628200	-1.31287900	3.89916600
H	-0.32579700	-0.93130800	2.35095700
N	-1.19349600	4.02902900	1.52879500
C	-1.84803800	5.21687600	1.23137700
C	-2.15443400	5.16757600	-0.08998100
H	-2.03307200	5.97961300	1.97134800
H	-2.65324000	5.88260200	-0.72515000
N	-1.68287600	3.95306900	-0.56087800
C	-1.08921400	3.22687000	0.42773900
C	2.50179100	-2.61605000	2.87291700

C	1.57794200	-2.05310600	0.88771700
C	3.14338400	-3.31981800	1.90493200
H	2.63111000	-2.60779700	3.94427400
H	3.95570100	-4.02658800	1.96399400
N	1.54373100	-1.83909100	2.22912100
N	2.55427700	-2.96354000	0.69798700
C	2.94404200	-3.50700300	-0.62331900
H	2.21054600	-3.09631300	-1.32286400
H	2.85896100	-4.59690000	-0.56820700
C	-1.84230700	3.47665100	-1.95362400
H	-2.40118600	4.25449800	-2.48057300
H	-2.46839800	2.58038800	-1.92524900
C	-0.53393200	3.18377300	-2.65206300
C	0.16781200	4.19426300	-3.32075700
C	0.01137000	1.89574800	-2.59762500
C	1.39508700	3.91588700	-3.92361100
H	-0.24621500	5.19916000	-3.37196200
C	1.24353100	1.61298100	-3.18903000
H	-0.52409400	1.09446900	-2.09907900
C	1.93448000	2.62744900	-3.85297100
H	1.93007700	4.70353800	-4.44712100
H	1.64118500	0.60805600	-3.08096000
H	2.89354000	2.41715300	-4.31852200
C	4.34532600	-3.09109800	-1.01425200
C	4.57807500	-1.77341700	-1.43716900
C	5.41124000	-3.99585100	-0.96197100
C	5.86670400	-1.37462600	-1.78965200
H	3.72973600	-1.09365400	-1.49386700
C	6.70094300	-3.59430200	-1.31964900
H	5.23186000	-5.02331000	-0.65106200
C	6.93020800	-2.28092600	-1.73045900
H	6.04249400	-0.35438100	-2.12004100
H	7.52110300	-4.30592900	-1.27983300
H	7.93181400	-1.96578700	-2.01033600
Cu	-0.13017100	1.64422400	0.28362300
C	-0.62867900	-1.39904100	-0.33025700
C	-1.79616000	-1.75550000	-0.34826900
C	-3.15768700	-2.15585500	-0.37216000
C	-3.66563100	-3.06225100	0.58756000
C	-4.04047100	-1.65271500	-1.35639200
C	-4.99817000	-3.44651500	0.57056000
H	-2.99607000	-3.45740200	1.34393400
C	-5.37449900	-2.03143400	-1.37837500
H	-3.65736300	-0.96536100	-2.10289000

C	-5.84233500	-2.92449100	-0.41188900
H	-5.39999500	-4.13855100	1.30009900
H	-6.06059900	-1.65393700	-2.12628600
N	-7.24889100	-3.32134100	-0.42809600
O	-7.63389200	-4.11475800	0.43455800
O	-7.97364800	-2.83928700	-1.30224200
C	0.81824900	-0.96667100	-0.40337500
O	1.37322400	-1.22892600	-1.52555200
O	1.01346000	0.21341400	0.22137800

C-TS

C	-1.84379000	5.00105800	-0.19316900
C	-2.58408000	3.95272800	-0.72798600
C	-1.90160800	2.91193500	-1.36413500
C	0.14080100	3.90878800	-0.97707700
C	-0.45239500	4.98013700	-0.30991400
H	-2.34019600	5.82221000	0.31517000
H	-3.66471500	3.92681900	-0.63372200
H	0.15611600	5.77339200	0.11308700
N	-0.57264600	2.90473900	-1.50983400
C	1.64253500	3.78554800	-1.13038100
H	2.10303400	4.77473000	-1.19885800
H	1.85178200	3.24181700	-2.05649700
C	-2.60279300	1.72614600	-2.00502500
H	-3.03425800	2.01639900	-2.96901000
H	-1.85450500	0.95395300	-2.18445200
N	2.29005300	3.09155100	-0.00581600
C	3.53330200	3.45467400	0.49974500
C	3.84816100	2.54074900	1.45049400
H	4.07819000	4.31260200	0.13782700
H	4.71811800	2.44395500	2.07983200
N	2.79325100	1.64113200	1.49362000
C	1.81395300	1.95730900	0.59541500
C	-5.04233900	1.32961300	-1.49843900
C	-3.55494100	0.38029800	-0.10663400
C	-5.73502000	0.66405000	-0.53998200
H	-5.37897800	1.89399600	-2.35369300
H	-6.79513100	0.53934200	-0.39030300
N	-3.69548200	1.15182900	-1.21608300
N	-4.80368800	0.09090000	0.31086400
C	-5.17004300	-0.73321500	1.49447400
H	-6.00433700	-0.21739400	1.97847500
H	-4.27691000	-0.72570200	2.12457400
C	2.68788700	0.51705700	2.43221400

H	1.81120500	-0.04864000	2.10296500
H	2.46638900	0.90725500	3.43167700
C	3.92887300	-0.34955600	2.47092200
C	4.37602000	-1.00402800	1.31437500
C	4.63052000	-0.53091600	3.66733100
C	5.49632000	-1.83205100	1.35639100
H	3.83802500	-0.86914500	0.38137200
C	5.75603000	-1.35795000	3.71216000
H	4.29002800	-0.03055000	4.57088100
C	6.18921700	-2.01015700	2.55782300
H	5.81820800	-2.34946200	0.45690200
H	6.28999900	-1.49245200	4.64851700
H	7.06070100	-2.65751000	2.59173000
C	-5.55018200	-2.14569100	1.10874200
C	-6.89057200	-2.54171100	1.03775700
C	-4.53876200	-3.07454100	0.82062000
C	-7.22510500	-3.84831400	0.67436500
H	-7.67848000	-1.83023900	1.27827000
C	-4.87627700	-4.37712200	0.45493200
H	-3.50498400	-2.74400100	0.90440200
C	-6.21690700	-4.76668500	0.37860900
H	-8.26854800	-4.14748900	0.62601200
H	-4.09033200	-5.09467900	0.23550500
H	-6.47413700	-5.78402200	0.09647700
Cu	0.13595700	1.14428200	0.41450800
C	-1.08653000	-0.46580800	-0.42120000
C	0.05396200	-0.77522100	-0.80239100
C	1.22522900	-1.37279600	-1.34718100
C	1.73810200	-2.57624400	-0.80575700
C	1.91914500	-0.76797500	-2.42319400
C	2.91177400	-3.13193200	-1.29276900
H	1.20513500	-3.05275400	0.00983500
C	3.08276500	-1.32746600	-2.92620900
H	1.52919300	0.15336500	-2.84313400
C	3.58097000	-2.49755300	-2.34364900
H	3.32512100	-4.04040300	-0.87270400
H	3.62650300	-0.87284600	-3.74508200
N	4.84152700	-3.04896900	-2.82321900
O	5.34462000	-3.98022100	-2.18398300
O	5.34572800	-2.54970300	-3.83318100
C	-2.21008100	0.04945800	0.68537500
O	-2.36866400	-0.86319000	1.57239600
O	-1.71680200	1.28803000	0.99684200

D-TS

C	1.64853400	-4.98581500	-1.41373800
C	2.42150100	-3.84857000	-1.62236200
C	1.77684000	-2.65492100	-1.96038800
C	-0.29311100	-3.66684500	-1.89312800
C	0.26205700	-4.89907600	-1.54812300
H	2.11704400	-5.92810700	-1.14567300
H	3.49988000	-3.87761200	-1.50760300
H	-0.37153500	-5.76489800	-1.38183100
N	0.44989700	-2.57116700	-2.10477500
C	-1.78928100	-3.46333000	-2.01507300
H	-2.28008900	-4.38051700	-2.34968000
H	-1.97675900	-2.67876600	-2.75324700
C	2.52612700	-1.36604500	-2.25274400
H	2.95273400	-1.40132200	-3.26165100
H	1.80992700	-0.54489700	-2.22262100
N	-2.41533000	-3.08297100	-0.73997100
C	-3.54157700	-3.69842400	-0.20760600
C	-3.83529000	-3.04181400	0.94279300
H	-4.03197800	-4.52877900	-0.69117300
H	-4.63012800	-3.18499300	1.65680100
N	-2.88402700	-2.04163900	1.07642900
C	-1.99327800	-2.04550900	0.04244100
C	4.96032400	-1.34964800	-1.56742500
C	3.44434200	-0.53308600	-0.09313100
C	5.63180000	-0.97187100	-0.44984600
H	5.31225500	-1.76433000	-2.49946000
H	6.68380800	-1.00238100	-0.21403200
N	3.61781800	-1.07550900	-1.32788500
N	4.68454100	-0.48362500	0.44062200
C	5.00777800	0.04908600	1.78584300
H	5.82412900	-0.56568000	2.17618800
H	4.10145700	-0.09557300	2.37820000
C	-2.76869000	-1.13184800	2.22794700
H	-2.01883800	-0.39192900	1.93659500
H	-2.36262800	-1.69075600	3.07741700
C	-4.08051300	-0.47839900	2.60229300
C	-4.62823800	0.53028100	1.79684000
C	-4.76598300	-0.87060300	3.75773400
C	-5.84008900	1.12763700	2.13860100
H	-4.09711300	0.85424600	0.90560500
C	-5.98046500	-0.27237500	4.10276100
H	-4.34171100	-1.64152200	4.39685200
C	-6.52016700	0.72598100	3.29200000

H	-6.25101400	1.91243800	1.51019000
H	-6.49934300	-0.58378300	5.00473300
H	-7.46251900	1.19525100	3.55925200
C	5.39868400	1.51152800	1.75488200
C	6.74207500	1.90348300	1.73341500
C	4.39511400	2.49152800	1.74872200
C	7.08601900	3.25648600	1.69501500
H	7.52594400	1.14879800	1.75775400
C	4.74116200	3.84233300	1.70932200
H	3.35817200	2.16304300	1.78633300
C	6.08424400	4.22817400	1.67972100
H	8.13212600	3.55020000	1.68211500
H	3.96037400	4.59823000	1.71009500
H	6.34913400	5.28171300	1.65266600
Cu	-0.41425100	-1.01854900	-0.03822500
C	0.91801000	0.52063700	-0.07494100
C	-0.16809300	0.96704000	-0.51784100
C	-1.05473400	1.95373000	-1.06101400
C	-2.35042500	1.60091800	-1.49291100
C	-0.64740300	3.30201100	-1.17796100
C	-3.21423300	2.55198100	-2.01889100
H	-2.65635600	0.56320000	-1.41099200
C	-1.50238400	4.25989700	-1.70399400
H	0.34670500	3.57992300	-0.84531800
C	-2.77976000	3.87450300	-2.11802500
H	-4.21025200	2.29448900	-2.35697300
H	-1.20527100	5.29700300	-1.79799000
N	-3.68600300	4.88233400	-2.67069800
O	-4.81215100	4.51570200	-3.01537200
O	-3.27330500	6.04036600	-2.76020500
C	1.86158500	-0.36663700	0.86937200
O	2.11939100	0.21815000	1.95919200
O	1.36005900	-1.59687700	0.75345600

Reaction III

III1

C	5.30882900	-3.39870700	-1.11102300
C	4.74270600	-2.67001100	-2.15798200
C	3.45621400	-2.15110200	-1.99076800
C	3.31119700	-2.99653400	0.15527800
C	4.58491200	-3.56572800	0.06883000
H	6.30019800	-3.82969700	-1.21452000
H	5.28351000	-2.51798900	-3.08702300
H	4.99821700	-4.12352400	0.90360200

N	2.76057200	-2.32043100	-0.86014800
C	2.46509900	-3.02811600	1.41053500
H	2.76262500	-3.84326200	2.07391700
H	1.41531400	-3.15203600	1.12722400
C	2.72579700	-1.39674500	-3.07994900
H	3.25829100	-1.49307800	-4.02891200
H	1.73188900	-1.84286100	-3.19631000
N	2.59550500	-1.77096800	2.15167900
C	3.05474200	-1.65226700	3.45766300
C	2.99552800	-0.33269500	3.76263500
H	3.37382800	-2.50005700	4.04379500
H	3.24434400	0.19453100	4.67010900
N	2.51827900	0.31215400	2.62736700
C	2.24959500	-0.56128800	1.61023400
C	2.75958500	1.00551600	-3.80085500
C	1.96179400	0.56179300	-1.69985800
C	2.28579200	2.16990300	-3.29825600
H	3.21400500	0.78081800	-4.75331100
H	2.23747600	3.15773400	-3.72822300
N	2.56126700	0.03808900	-2.81789000
N	1.81139900	1.88174800	-2.02447200
C	1.08852100	2.84042500	-1.18214400
H	1.72690300	3.71368000	-1.00785600
H	0.93320300	2.33162500	-0.22853000
C	2.27993400	1.75231900	2.54239700
H	2.36259500	2.00289000	1.48103400
H	3.09389600	2.26451100	3.06550500
C	0.93983900	2.19077800	3.10417400
C	-0.25127300	1.64277500	2.60572500
C	0.87931000	3.16264500	4.10833800
C	-1.47970600	2.06510500	3.11237400
H	-0.21766500	0.88399900	1.82712100
C	-0.35254200	3.58787300	4.61120000
H	1.79959000	3.59184800	4.49962200
C	-1.53448400	3.03779700	4.11450800
H	-2.39501600	1.62993700	2.72163800
H	-0.38659200	4.34292000	5.39161600
H	-2.49390600	3.36409000	4.50584600
C	-0.24094400	3.26562100	-1.77355000
C	-0.42580900	4.56572400	-2.25479000
C	-1.30118000	2.34915500	-1.84166400
C	-1.65184400	4.95232200	-2.80268300
H	0.38918100	5.28409900	-2.19402200
C	-2.52330100	2.73624200	-2.38996700

H	-1.17069300	1.33953800	-1.45700000
C	-2.70152300	4.03654800	-2.87237500
H	-1.78476800	5.96576900	-3.17068600
H	-3.33986800	2.02101500	-2.43439100
H	-3.65658200	4.33410100	-3.29613400
Cu	1.34532100	-0.37219800	-0.10866500
C	-0.46435300	-0.94832800	-0.13840700
C	-1.67431200	-1.20548600	-0.12331900
C	-3.05075300	-1.51891700	-0.11555300
C	-3.50414100	-2.85053100	-0.30646100
C	-4.03370700	-0.51349900	0.08590700
C	-4.85348600	-3.16225700	-0.29412600
H	-2.76753300	-3.63152400	-0.46336700
C	-5.38501900	-0.81714400	0.09954500
H	-3.70680200	0.51169100	0.22842500
C	-5.78991600	-2.14289300	-0.08984200
H	-5.20377600	-4.17705600	-0.43823400
H	-6.13804200	-0.05390200	0.25352000
N	-7.20674700	-2.46673400	-0.07501400
O	-8.01164000	-1.54575500	0.10870000
O	-7.53669500	-3.64609900	-0.24725200

III2

C	4.33624300	-4.44523200	-0.84671600
C	4.16638800	-3.49159600	-1.85112500
C	3.08291400	-2.61319200	-1.76223600
C	2.39294700	-3.54834800	0.23633700
C	3.43712300	-4.47741600	0.21866400
H	5.15849700	-5.15307500	-0.89442900
H	4.85284600	-3.43862300	-2.69057300
H	3.54321200	-5.20442900	1.01807000
N	2.21828100	-2.65231000	-0.74192100
C	1.40396800	-3.42257900	1.37638800
H	1.36165700	-4.33703100	1.97230000
H	0.41316700	-3.20648700	0.96492200
C	2.76705000	-1.58781100	-2.82929100
H	3.40086900	-1.74929800	-3.70428400
H	1.72291900	-1.71381800	-3.13228300
N	1.77834800	-2.31985500	2.26670200
C	2.07167900	-2.44332400	3.61877900
C	2.34514800	-1.19244900	4.06434900
H	2.05796400	-3.39063300	4.13486900
H	2.60774400	-0.83418300	5.04723500
N	2.22529900	-0.34934400	2.96548200

C	1.86240600	-1.02397800	1.83326200
C	3.60055300	0.74754400	-3.21144300
C	2.34707800	0.39115100	-1.32859500
C	3.40052300	1.95399000	-2.63015300
H	4.13435700	0.47668400	-4.10908700
H	3.71731800	2.94175700	-2.92501700
N	2.95936600	-0.19278600	-2.40898100
N	2.64578700	1.71687400	-1.48815400
C	2.09021600	2.77539800	-0.63840500
H	2.90472700	3.43204200	-0.31391000
H	1.68731000	2.26765600	0.24012500
C	2.41997100	1.09852100	3.01934700
H	2.73203800	1.39278500	2.01331900
H	3.25549800	1.30523000	3.69565800
C	1.18974400	1.87255800	3.45667800
C	-0.02327600	1.72335300	2.76872100
C	1.26108600	2.76090600	4.53479200
C	-1.14373100	2.45387000	3.16223100
H	-0.09106000	1.03252600	1.93150800
C	0.13868100	3.49547300	4.92449400
H	2.19874400	2.88121500	5.07337900
C	-1.06663300	3.34124900	4.23915400
H	-2.07886300	2.32632700	2.62499200
H	0.20621700	4.18146400	5.76420100
H	-1.94218900	3.90822500	4.54232700
C	1.00331400	3.57581200	-1.32767600
C	1.23068900	4.89596900	-1.72959600
C	-0.24347100	2.98488300	-1.57953200
C	0.22966900	5.62074300	-2.38137500
H	2.19213900	5.36331000	-1.52675700
C	-1.23953900	3.70634400	-2.23592400
H	-0.43283900	1.96435100	-1.25397200
C	-1.00511200	5.02468200	-2.63830000
H	0.41556000	6.64676000	-2.68642800
H	-2.19717700	3.23462800	-2.43326100
H	-1.78445200	5.58528900	-3.14684100
Cu	1.27685000	-0.46394400	0.05214500
C	-1.41385400	-0.34830000	-3.36856900
O	-0.63409600	-1.18673200	-3.61247200
O	-2.20200100	0.49516600	-3.18791100
C	-0.60581500	-0.64969800	-0.16426300
C	-1.83212000	-0.81076900	-0.11593000
C	-3.23343700	-0.99634500	-0.09291600
C	-3.80689800	-2.28305400	-0.26347600

C	-4.11696100	0.09597100	0.10557100
C	-5.17890700	-2.47122000	-0.23546900
H	-3.14629600	-3.12983400	-0.41789400
C	-5.48999700	-0.08343000	0.13647800
H	-3.69635400	1.08831000	0.22965300
C	-6.01514000	-1.36850700	-0.03386900
H	-5.62122200	-3.45140900	-0.36425900
H	-6.16859700	0.74702000	0.28765600
N	-7.45635200	-1.56198600	-0.00019200
O	-8.17174100	-0.57055900	0.18149800
O	-7.89247100	-2.70831800	-0.15440400

III-TS

C	-0.21052600	5.80497600	0.95576300
C	-1.05135900	5.33113700	-0.05125100
C	-0.89547300	4.01209700	-0.48723100
C	0.84008500	3.64850700	1.00251700
C	0.75334000	4.95275500	1.49562800
H	-0.30103300	6.82702900	1.31150400
H	-1.80673500	5.97265900	-0.49451200
H	1.42668600	5.29471400	2.27557400
N	0.03211600	3.19982400	0.03371100
C	1.85699100	2.63957500	1.49666400
H	2.64726000	3.13522300	2.06454700
H	2.29964900	2.14173100	0.62859900
C	-1.73504700	3.39363200	-1.58568500
H	-2.27596600	4.16713300	-2.13515700
H	-1.08288400	2.85372900	-2.27941200
N	1.27052400	1.61027800	2.36415100
C	1.77558900	1.25764800	3.60918900
C	1.03049400	0.21028200	4.04113500
H	2.60270300	1.77474800	4.06990100
H	1.08335000	-0.36614100	4.95112600
N	0.08962700	-0.03790900	3.05035500
C	0.22562200	0.81115900	1.99091900
C	-4.08615900	2.50475800	-1.37621000
C	-2.40767900	1.27958900	-0.43066700
C	-4.63977500	1.36182100	-0.90251600
H	-4.52593100	3.33524400	-1.90588200
H	-5.65298900	0.99648800	-0.94014600
N	-2.73111100	2.43952200	-1.07908800
N	-3.60380000	0.63124100	-0.33548900
C	-3.77005500	-0.69263300	0.28262500
H	-4.18433600	-0.56450700	1.29011000

H	-2.76387200	-1.10479900	0.37446600
C	-0.90513300	-1.11499000	3.11110800
H	-1.77825800	-0.74689800	2.56673800
H	-1.19437500	-1.24026600	4.15879400
C	-0.43053900	-2.43384100	2.53166700
C	-0.21180900	-2.55201400	1.15267000
C	-0.22941100	-3.54719200	3.35431400
C	0.19967100	-3.76618800	0.60565200
H	-0.34523300	-1.69192700	0.50500300
C	0.18734200	-4.76361100	2.80791800
H	-0.40412700	-3.46763000	4.42531600
C	0.40173100	-4.87461200	1.43305200
H	0.34809700	-3.83421000	-0.46759800
H	0.34054200	-5.62238600	3.45542700
H	0.71995700	-5.82215400	1.00749700
C	-4.65392500	-1.61766600	-0.52701100
C	-5.94461300	-1.93015300	-0.08483300
C	-4.18535700	-2.16905600	-1.72929500
C	-6.76550500	-2.77915400	-0.83122900
H	-6.30764500	-1.51295800	0.85215400
C	-5.00775100	-3.01448900	-2.47309400
H	-3.17718000	-1.94266300	-2.06918500
C	-6.29734100	-3.32060700	-2.02846500
H	-7.76430900	-3.01708300	-0.47631000
H	-4.63754300	-3.44134500	-3.40081500
H	-6.93180400	-3.98257800	-2.61119500
Cu	-0.61211100	0.85683900	0.23505200
C	-0.53399700	-0.32207700	-2.35154000
O	-0.60405300	0.58217300	-3.14398000
O	-0.93009600	-1.42998200	-2.06535600
C	0.78327500	0.15064100	-1.02085900
C	1.98708900	-0.11848400	-1.14325500
C	3.36607600	-0.42229200	-1.24310700
C	4.25713200	0.43702400	-1.93248600
C	3.89218400	-1.59524600	-0.64659000
C	5.61049000	0.14676900	-2.01502900
H	3.86095100	1.33044000	-2.40334300
C	5.24454300	-1.89090000	-0.72367400
H	3.21541400	-2.26105400	-0.12166000
C	6.09306900	-1.01419100	-1.40516000
H	6.30162200	0.79491500	-2.53935000
H	5.65941200	-2.78186000	-0.26898700
N	7.52022800	-1.31758000	-1.48000400
O	7.92076200	-2.34815300	-0.93201400

0	8.24802500	-0.52496600	-2.08427000
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III3

C	-3.13976200	-5.28649200	-1.05478900
C	-2.52814500	-5.02966500	0.17276200
C	-1.78353300	-3.85625400	0.31234700
C	-2.21477000	-3.22635800	-1.87584200
C	-2.98389400	-4.37222400	-2.09710400
H	-3.72314900	-6.19091800	-1.19980900
H	-2.62293200	-5.72595500	1.00047700
H	-3.44064100	-4.54953000	-3.06593100
N	-1.63515400	-2.98111800	-0.69189100
C	-1.92761700	-2.20170000	-2.95220400
H	-2.19154500	-2.60272100	-3.93359600
H	-0.85954100	-1.95685900	-2.92699600
C	-1.08680600	-3.45815500	1.59829500
H	-0.93284900	-4.32524600	2.24448200
H	-0.12029500	-3.01276200	1.34659000
N	-2.65564500	-0.93441700	-2.78903500
C	-3.19312600	-0.22923200	-3.85956200
C	-3.48434800	1.01196100	-3.40158700
H	-3.31831100	-0.66720900	-4.83752300
H	-3.90659200	1.87013100	-3.89944300
N	-3.11145700	1.03078000	-2.06274500
C	-2.58168200	-0.16099200	-1.66341400
C	-2.16121600	-2.55814200	3.71384200
C	-2.26934600	-1.28023000	1.82613300
C	-2.78474200	-1.39903800	4.04543500
H	-1.91497100	-3.42306900	4.30976900
H	-3.18235500	-1.05569000	4.98737200
N	-1.85741700	-2.46610500	2.36243300
N	-2.84960300	-0.64282300	2.88231700
C	-3.39252700	0.71354300	2.79573300
H	-4.24871300	0.78273600	3.47344300
H	-3.76759000	0.81525300	1.77281100
C	-3.12252300	2.22541600	-1.22298300
H	-2.82912900	1.87902300	-0.22734900
H	-4.14466300	2.61536000	-1.15613200
C	-2.17745400	3.30834700	-1.71085000
C	-0.86477400	2.99376400	-2.09375400
C	-2.60354700	4.64021300	-1.74955300
C	-0.00005300	4.00803400	-2.50523600
H	-0.51879700	1.96205800	-2.08158200
C	-1.73295300	5.65371200	-2.15634200

H	-3.62187400	4.88799300	-1.45753500
C	-0.42842900	5.33809600	-2.53629100
H	1.01366400	3.75499700	-2.80242600
H	-2.07673300	6.68402000	-2.18215100
H	0.25047800	6.12282400	-2.85827300
C	-2.38171400	1.80186500	3.10928600
C	-2.63913700	2.73562200	4.11828400
C	-1.19326600	1.89784700	2.37065800
C	-1.72504200	3.75648900	4.38972300
H	-3.55953600	2.66749500	4.69450700
C	-0.28087700	2.91550800	2.64506400
H	-0.97848700	1.17185000	1.59063100
C	-0.54343700	3.84670200	3.65358400
H	-1.93555800	4.47552400	5.17644900
H	0.63635500	2.97773600	2.06739000
H	0.17029200	4.63809800	3.86408000
Cu	-1.88229500	-0.72769400	0.02067000
C	0.89558800	-0.41691900	-0.82560300
O	0.48000600	-0.28733700	-1.99441600
O	0.23716500	-0.56526000	0.25109300
C	2.36289600	-0.39340100	-0.64310900
C	3.57148500	-0.37475300	-0.49774500
C	4.98013800	-0.35162500	-0.32446600
C	5.73115100	-1.54846800	-0.36379600
C	5.65942600	0.86854700	-0.10596600
C	7.10734500	-1.52936700	-0.18976900
H	5.21665200	-2.48813300	-0.53250900
C	7.03546500	0.89381200	0.06843100
H	5.08954700	1.79072200	-0.07542100
C	7.74652500	-0.30694400	0.02542000
H	7.69634900	-2.43757100	-0.21658300
H	7.57003900	1.82023400	0.23705100
N	9.19722500	-0.28364200	0.21139300
O	9.73628600	0.80964700	0.39831500
O	9.80029700	-1.35868700	0.17141800