

Insights on the Mechanism and Origin of Multifunctional Ligand Effects on Chemoselectivity in Pd-catalyzed Unnatural Prenylation and Geranylation of Oxindoles with Isoprene

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For reaction I, we have re-optimized all the species in the preferred pathway PA3 using Minnesota M06 functional with the same basis set (Figure S1, pink line). The calculating results showed that the activation energies difference of transition states **TS4a/TS5a/TS6a** and **TS4a'/TS5a'/TS6a'** is 1.3/1.1/0.4 kcal/mol.

For reaction II, we also calculated the key transition states and intermediates in pathways PB3 (Figure S3, red line). The energy difference between **TS1b/TS5b/TS6b/TS7b** and **TS1b'/TS5b'/TS6b'/TS7b'** is 1.5/1.4/0.5/0.2 kcal/mol.

Thereby, the relatively small activation energy barrier difference indicates that our results based on B3LYP-D3 functional and a mixed basis set of SDD basis set for Pd and 6-311+G(d,p) for other atoms is reasonable.

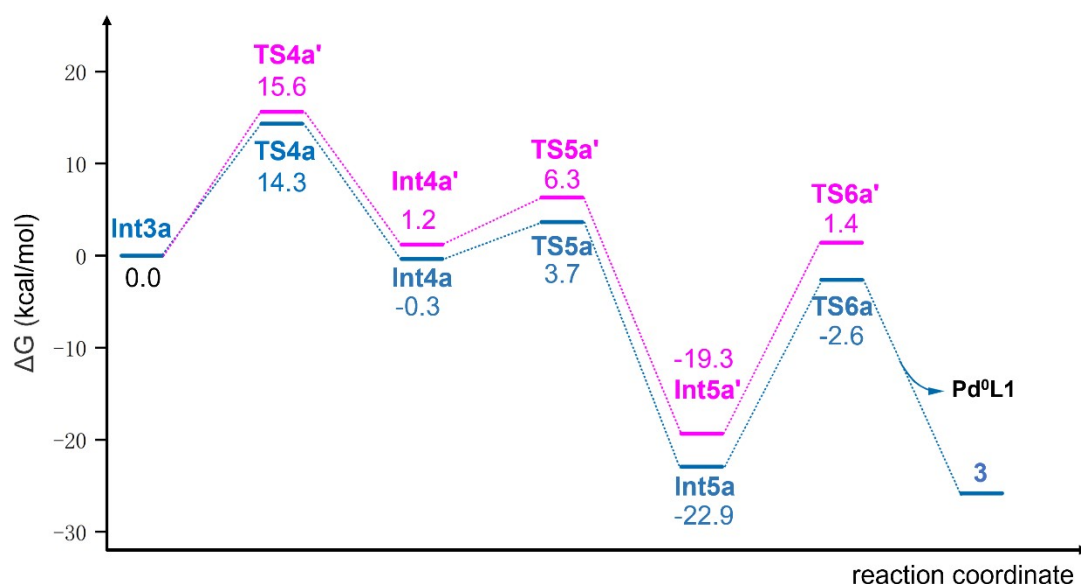


Figure S1. Energy profiles for the key structures in the most preferred pathway PA3 calculated by M06 functional (blue line) and B3LYP-D3 functional (pink line), free energies are given in kcal/mol.

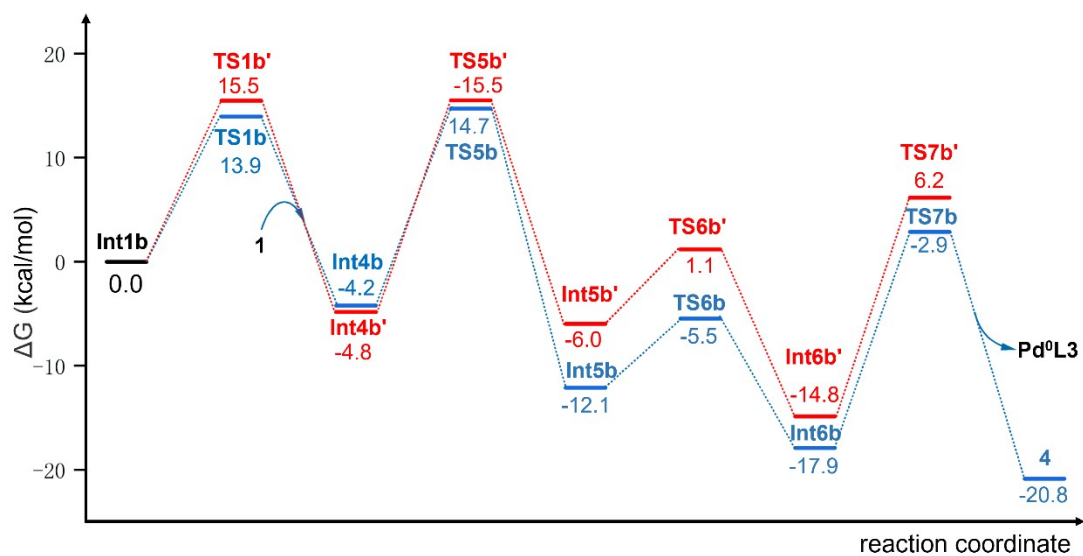


Figure S2. Energy profiles for the key structures in the most preferred pathway PB3 calculated by M06 functional (blue line) and B3LYP-D3 functional (pink line), free energies are given in kcal/mol.

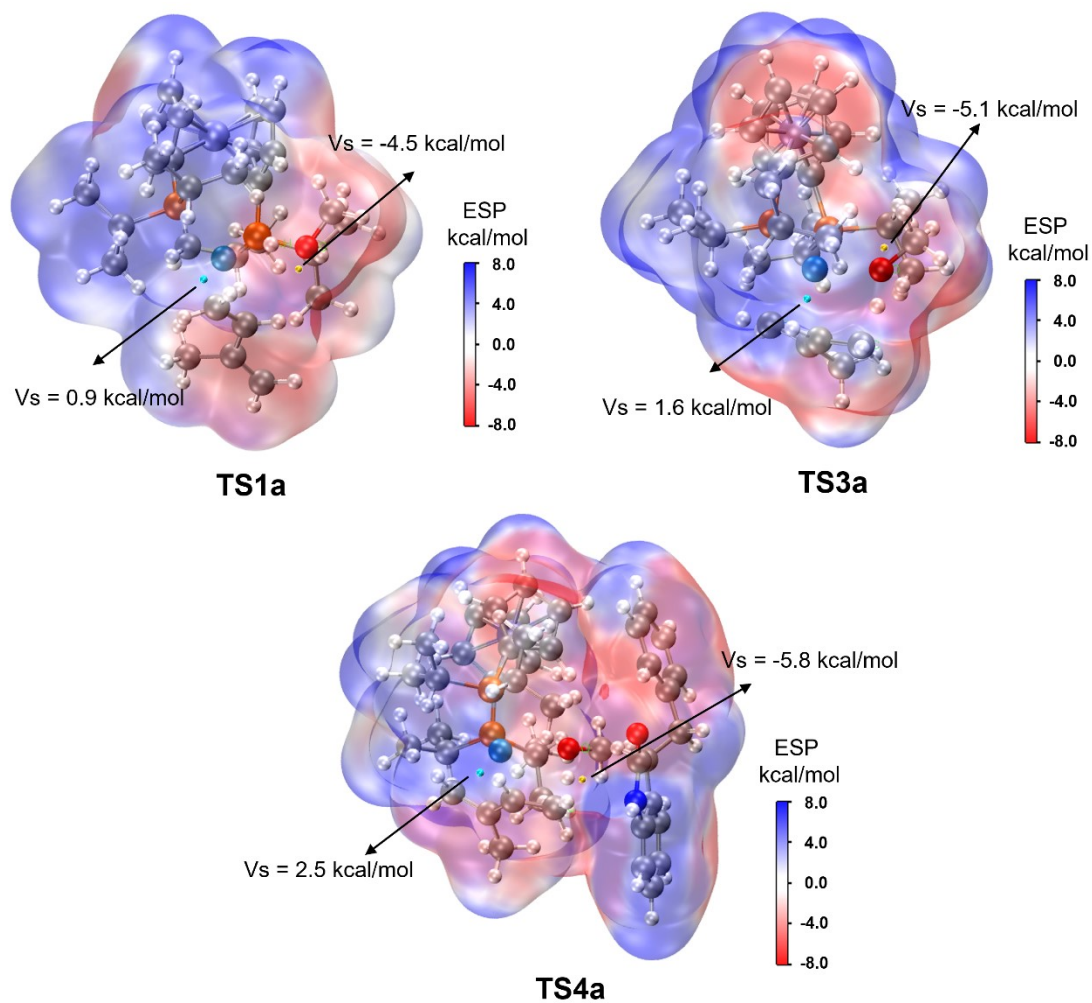


Figure S3. Electrostatic potentials on the monomers' van der Waals surface of **TS1a**, **TS3a**, and **TS4a** (red = -8 kcal/mol; blue = +8 kcal/mol).

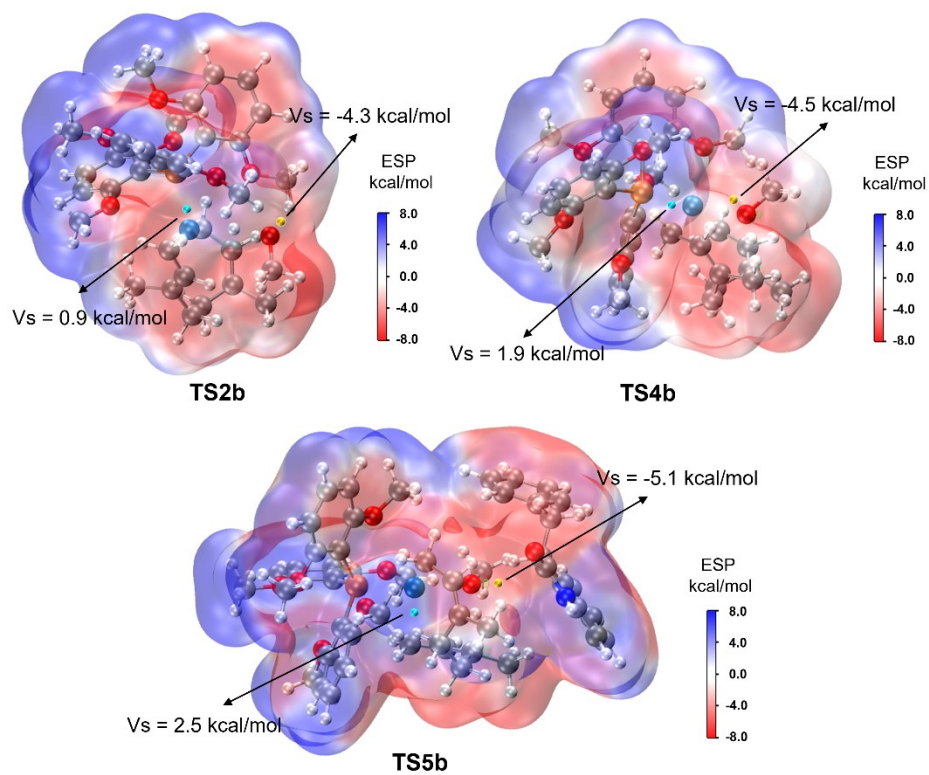


Figure S4. Electrostatic potentials on the monomers' van der Waals surface of **TS2b**, **TS4b**, and **TS5b** (red = -8 kcal/mol; blue = +8 kcal/mol).

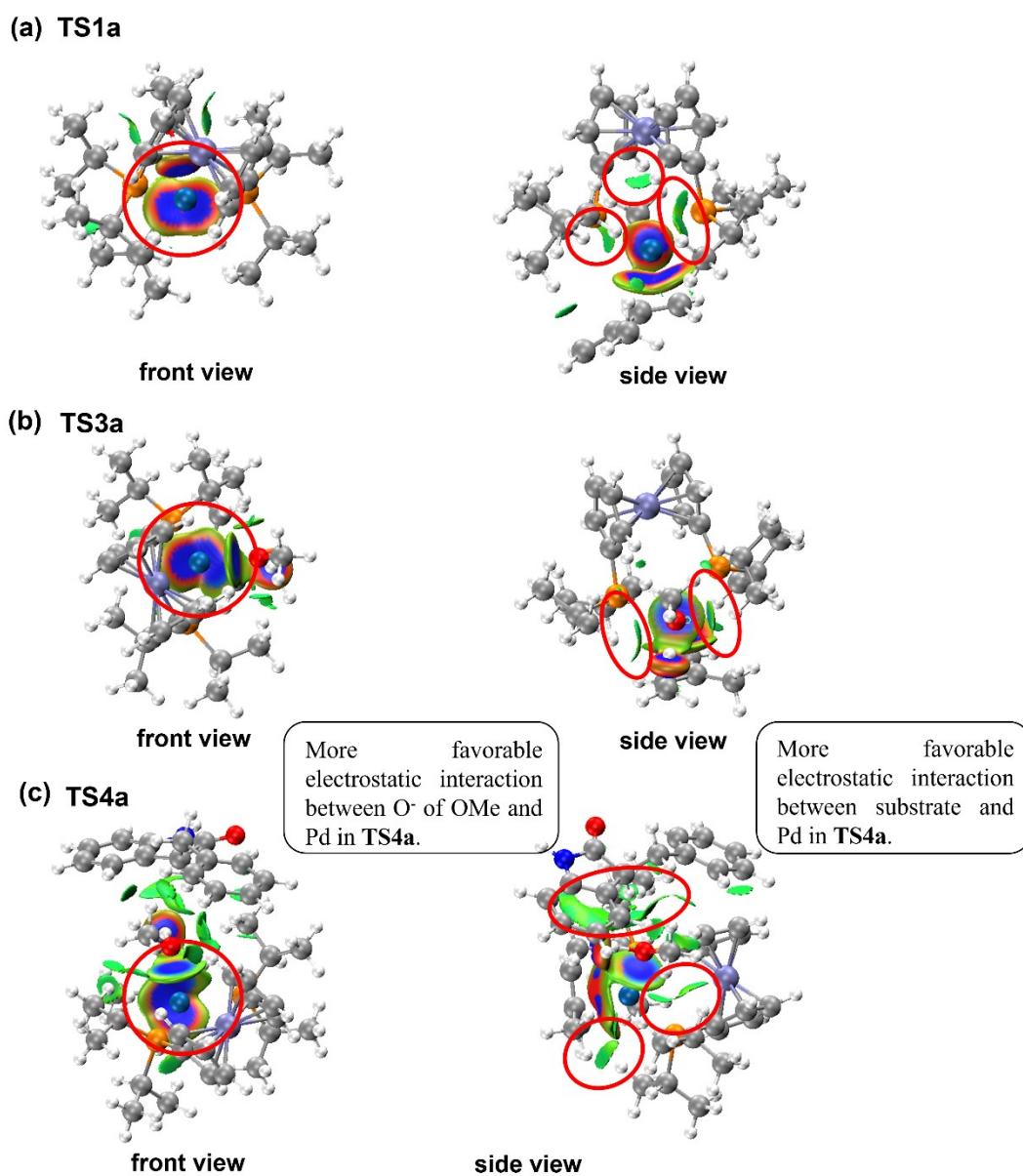
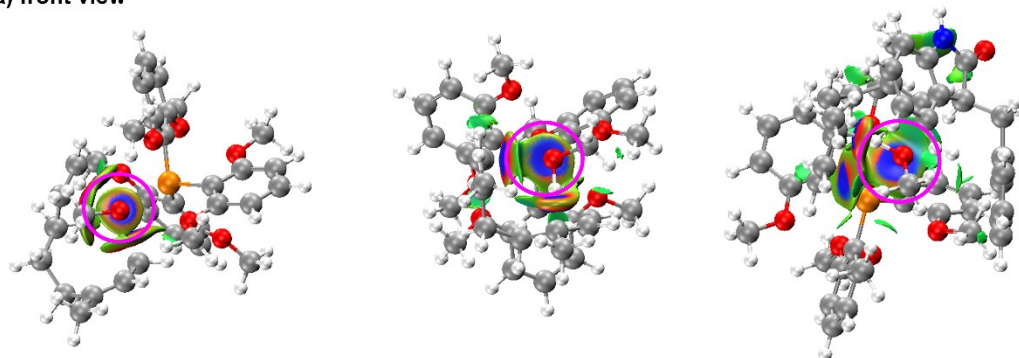


Figure S5. Noncovalent interaction analysis (blue, strong attraction; green, weak interaction) for the front view and side view of transition states **TS1a**, **TS3a**, and **TS4a**.

(a) front view

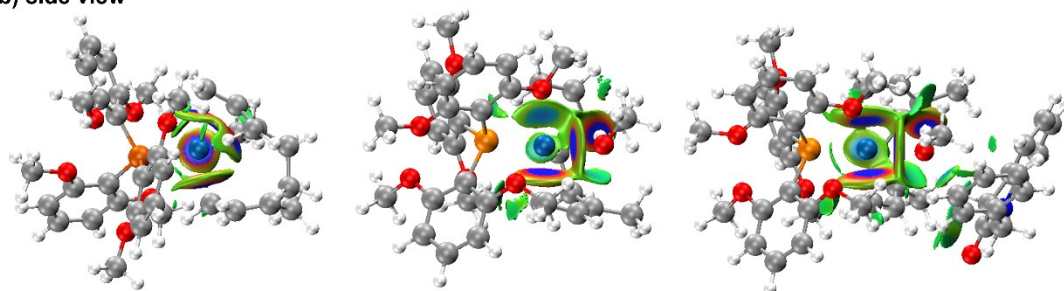


TS2b

TS4b

TS5b

(b) side view



TS2b

TS4b

TS5b

Figure S6. Noncovalent interaction analysis (blue, strong attraction; green, weak interaction) for the front view and side view of transition states **TS2b**, **TS4b**, and **TS5b**.

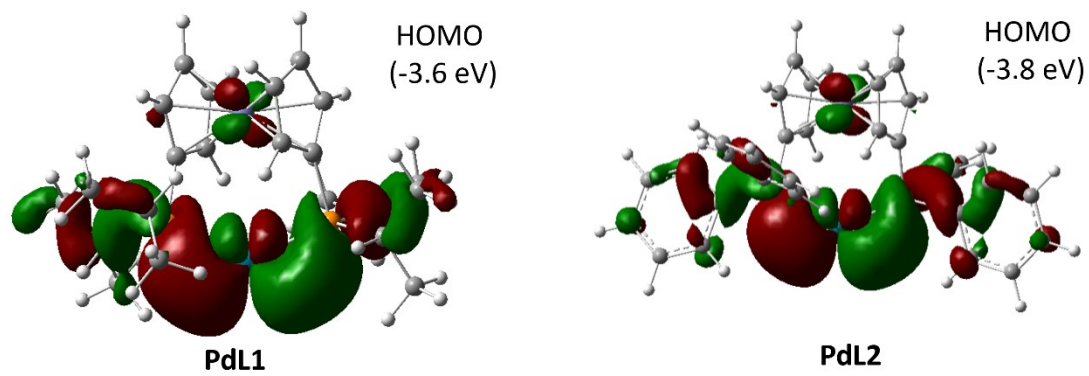


Figure S7. FMO analysis for PdL1 and PdL2.

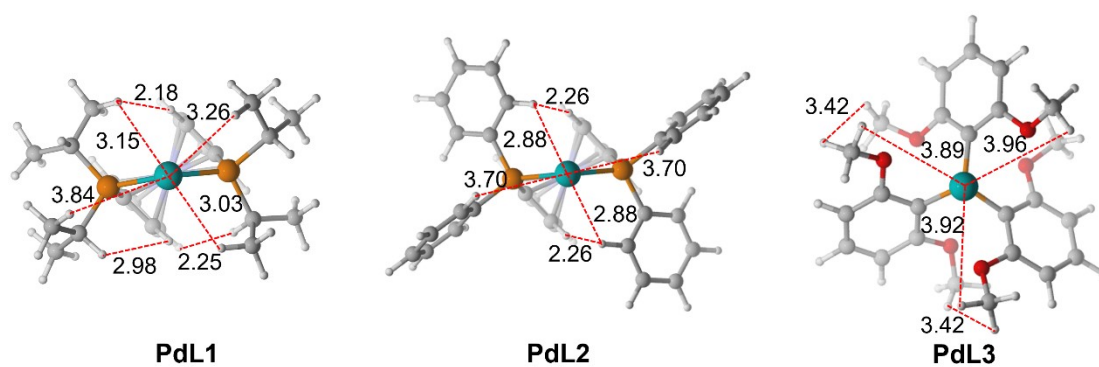


Figure S8. The structures for PdL1, PdL2, and PdL3. The distances are in Å.

Table S1. Estimation of Noncovalent Interaction Energies (E_{HB}) Using Espinosa Equation ($E_{\text{HB}} = 1/2V(r_{\text{cp}})$) in the Lower Energy Enantioccontrolling **TS1a**, **TS4a**, **TS4a**.

Noncovalent Interaction	Bond path	Distance d/Å	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho$ -2G	$E=1/2 V$ (kcal/mol)
TS1a							
N-H \cdots O	1a	2.40	0.012	-0.012	0.010	-0.02	-7.2
C-H \cdots O	1b	2.48	0.011	-0.010	0.009	-0.02	-6.4
							-13.6
TS3a							
N-H \cdots O	2a	2.25	0.015	-0.014	0.012	-0.0275	-8.6
C-H \cdots O	2b	2.49	0.011	-0.01	0.008	-0.0185	-5.8
							-14.4
TS4a							
C-H \cdots O	3a	2.44	0.013	-0.013	0.012	-0.02725	-8.5
	3b	2.54	0.008	-0.008	0.007	-0.0205	-6.4
C-H $\cdots\pi$	3c	2.72	0.008	-0.007	0.006	-0.01375	-4.3
	3d	2.74	0.008	-0.007	0.006	-0.01375	-4.3
							-23.6

Table S2. The second-order perturbation stabilization energies ($E(2)$, kcal/mol) for transition states **TS1a**, **TS2a**, **TS4a**, and **PB3-TS5b-L1** between the Pd centre and the coordination atoms (P, O, and C).

TSs	donor	acceptor	interaction	$E(2)$
TS4a				
	LP P1	LP* Pd	$n \rightarrow d^*$	102.1
	LP P2	LP* Pd	$n \rightarrow d^*$	92.3
	P1/P2...Pd			194.4
	LP Pd	LP* C4	$d \rightarrow n^*$	79.1
	BD C2-C3	LP* Pd	$\pi \rightarrow d^*$	13.7
	BD C4-C3	LP* Pd	$\pi \rightarrow d^*$	17.3
	C2/C3/C4...Pd			110.1
	BD C8-O1	LP* Pd	$\sigma \rightarrow d^*$	6.5
	LP O1	LP* Pd	$n \rightarrow d^*$	42.0
	O1...Pd			48.5
	LP O1	BD* C8'-H2	$n \rightarrow \sigma^*$	4.5
	$E(2)$ for Pd...O (MeO ⁻)/Pd...C=C (olefin)			
TS3a				
	LP P1	LP* Pd	$n \rightarrow d^*$	118.3
	LP P2	LP* Pd	$n \rightarrow d^*$	112.8
	P1/P2...Pd			231.1
	LP Pd	BD* C3-C4	$d \rightarrow \pi^*$	18.1
	BD C3-C4	LP* Pd	$\pi \rightarrow d^*$	11.6
	C3/C4...Pd			29.7
	BD C8-O1	LP* Pd	$\sigma \rightarrow d^*$	6.4
	LP O1	LP* Pd	$n \rightarrow d^*$	47.1
O1...Pd			53.5	
$E(2)$ for Pd...O (MeO ⁻)/Pd...C=C (olefin)				71.6
TS1a				
	LP P1	LP* Pd	$n \rightarrow d^*$	126.6
	LP P2	LP* Pd	$n \rightarrow d^*$	122.8
	P1/P2...Pd			249.4
	BD C1-C2	LP Pd	$\pi \rightarrow d^*$	56.8
	LP Pd	BD* C1-C2	$d \rightarrow \pi^*$	24.4
	C1/C2...Pd			81.2
$E(2)$ for Pd...C=C (olefin)				24.4

Table S3. The second-order perturbation stabilization energies ($E(2)$, kcal/mol) for transition states **TS5b**, **TS2b**, and **TS3b** between the Pd centre and the coordination atoms (P, O, and C).

TSs	donor	acceptor	interaction	$E(2)$
TS5b				
	LP P	LP* Pd	$n \rightarrow d^*$	66.6
	LP P	LP* Pd	$n \rightarrow d^*$	53.4
	P...Pd			120
	BD C1'-C2'	LP* Pd	$\pi \rightarrow d^*$	18.8
	BD C1-C2	LP* Pd	$\sigma \rightarrow d^*$	29.1
	C1-C2/C1'-C2'...Pd			47.9
	LP O1	LP*Pd	$n \rightarrow d^*$	25.1
	O1...Pd			25.1
	LP O1	BD* C11-H2	$n \rightarrow \sigma^*$	81.1
E(2) for Pd...O (MeO ⁻)/Pd...C=C (olefin)				73.0
TS4b				
	LP P	LP* Pd	$n \rightarrow d^*$	92.7
	P...Pd			92.7
	BD C1-C2	LP* Pd	$\pi \rightarrow d^*$	18.3
	BD C1'-C2'	LP* Pd	$\pi \rightarrow d^*$	5.5
	C1-C2/C1'-C2'...Pd			23.8
	LP O1	LP* Pd	$n \rightarrow d^*$	22.6
	O1...Pd			22.6
E(2) for Pd...O(MeO ⁻)/Pd...C=C(olefin)				46.4
TS2b				
	LP P	LP* Pd	$n \rightarrow d^*$	53.6
	P...Pd			53.6
	BD C1-C2	LP* Pd	$\pi \rightarrow d^*$	19.2
	BD C1'-C2'	LP* Pd	$\pi \rightarrow d^*$	5.9
	C1-C2/C1'-C2'...Pd			25.1
	Pd...C=C (olefin)			

Table S4. Estimation of Noncovalent Interaction Energies (E , in kcal/mol) Using Espinosa Equation ($E = 1/2V(r_{cp})$) in **TS4b**, and **TS5b**.

Noncovalent Interaction	Bond path	Distance d/Å	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho - 2G$	$E=1/2 V$ (kcal/mol)
TS4b							
C–H···O	4a	2.14	0.018	-0.016	0.013	-0.03	-9.4
C–H···O	4b	2.23	0.015	-0.014	0.012	-0.03	-8.6
C–H···O	4c	2.45	0.010	-0.009	0.008	-0.02	-5.7
C–H···O	4d	2.46	0.010	-0.008	0.007	-0.02	-5.0
							-28.7
TS4b							
N–H···O	5a	2.30	0.015	-0.015	0.013	-0.03	-9.3
C–H···O	5b	2.50	0.012	-0.011	0.009	-0.02	-6.5
	5c	2.56	0.009	-0.008	0.008	-0.02	-5.6
							-21.5
TS5b							
C–H···O	6a	2.24	0.014	-0.012	0.011	-0.025	-7.8
	6b	2.57	0.009	-0.008	0.007	-0.016	-5.0
	6c	2.52	0.011	-0.010	0.009	-0.020	-6.4
C–H··· π	6d	2.64	0.010	-0.009	0.008	-0.018	-5.7
	6e	2.74	0.008	-0.007	0.006	-0.013	-4.3
	6f	2.70	0.008	-0.007	0.005	-0.011	-3.6
	6g	2.97	0.006	-0.005	0.004	-0.025	-7.8
							-33.0

Table S5. The electronic energy and the number of imaginary frequencies with their corresponding intensities of optimized structures for reaction I.

Stationary Points	E (SCF)	G_correction	Number of imaginary frequencies	Imaginary frequency(cm ⁻¹)
Int1a	-2106.327794	0.615485	0	\
TS1a	-2106.261346	0.612599	1	-812.41
Int2a	-2106.282451	0.613282	0	\
TS2a	-2106.253944	0.612829	1	-116.97
TS3a	-2106.264817	0.611461	1	-1080.13
Int3a	-2816.002306	0.835601	0	\
TS4a	-2815.97935	0.835502	1	-1192.53
Int4a	-2816.006199	0.838948	0	\
TS5a	-2815.997958	0.837086	1	-815.18
Int5a	-2816.046542	0.843293	0	\
TS6a	-2816.01437	0.843498	1	-169.57
3	-905.121979	0.302726	0	\

Table S6. The electronic energy and the number of imaginary frequencies with their corresponding intensities of optimized structures for reaction II.

Stationary Points	E (SCF)	G_correction	Number of imaginary frequencies	Imaginary frequency(cm^{-1})
Int1b	-2358.578593	0.653701	0	\
TS1b	-2358.557359	0.654714	1	-169.57
Int2b	-2358.586111	0.658622	0	\
TS2b	-2358.522145	0.65264	1	-1027.07
Int3b	-2358.523917	0.653265	0	\
TS3b	-2358.51208	0.654565	1	-744.10
TS4b	-2358.522353	0.651539	1	-576.17
Int4b	-3068.281517	0.878188	0	\
TS5b	-3068.248803	0.875683	1	-929.54
Int5b	-3068.294559	0.878683	0	\
TS6b	-3068.28352	0.878245	1	-835.39
Int6b	-3068.301257	0.876165	0	\
TS7b	-3068.26618	0.874166	1	-130.65
4	-1100.536064	0.41002	0	\

Table S7. The electronic energy and the number of imaginary frequencies with their corresponding intensities of optimized structures for reaction III.

Stationary Points	E (SCF)	G_correction	Number of imaginary frequencies	Imaginary frequency(cm^{-1})
PB3-TS5b-L1	-3011.378082	0.943181	1	-600.43
PA3-TS4a-L3	-2872.86015	0.764286	1	-1149.63
Int1c	-3268.61851	0.812701	0	\
TS1c	-3268.581891	0.812598	1	-1052.19
Int2c	-3268.61335	0.816197	0	\
TS2c	-3268.597451	0.81011	1	-287.71
Int3c	-3268.641592	0.807563	0	\
TS3c	-3268.610791	0.80868	1	149.7996

S1. The cartesian coordinates of key structures.

Int1a

C	2.58574700	-2.71205800	1.46141700
C	2.60342500	-3.42556100	0.21653300
C	1.39503300	-3.11055300	-0.49358700
C	0.61790100	-2.19398400	0.30586400
C	1.37214300	-1.95031300	1.51425800
H	3.38273400	-2.69679800	2.20158000
H	3.41824900	-4.04292400	-0.15647300
H	1.13904900	-3.46164100	-1.48834000
H	1.07258600	-1.26856200	2.30451200
Fe	2.46502800	-1.41566800	-0.11554100
C	2.37477500	-0.12908000	-1.67939400
C	3.56300600	-0.92748700	-1.76709900
C	2.39853700	0.60495600	-0.43356800
H	1.55898800	-0.11297700	-2.39489800
C	4.32806700	-0.70955400	-0.57314800
H	3.80525400	-1.62734100	-2.56385900
C	3.61674300	0.23143600	0.24570800
H	5.25091600	-1.21857300	-0.30223700
H	3.92078600	0.56141900	1.23389400
C	1.49323300	2.51014700	1.66749400
C	2.78993100	3.33926000	1.73705100
C	1.43764500	1.43400300	2.77156600
H	0.64274400	3.19505300	1.83333400
H	2.73910100	4.22060900	1.08133000
H	2.94326300	3.69506200	2.77076600
H	3.67077600	2.74738500	1.44763200
H	0.46194600	0.92624300	2.78562900
H	2.22342100	0.67794000	2.62867100

H	1.59423700	1.90850900	3.75536700
C	1.32535900	3.15067300	-1.25032900
C	0.46048300	2.89254500	-2.50113200
C	2.78998400	3.38530200	-1.67238600
H	0.93780900	4.04769300	-0.73408200
H	-0.58981300	2.71725400	-2.23173100
H	0.52208200	3.75345400	-3.18914000
H	0.82769700	2.00539200	-3.04299300
H	3.45953900	3.55817200	-0.82015400
H	3.16733600	2.50978400	-2.22266100
H	2.84662100	4.26041900	-2.34297800
C	-1.69310100	-2.04186700	-1.57304300
C	-1.89739600	-3.56016900	-1.73514800
C	-0.83652100	-1.45818300	-2.71711200
H	-2.67935100	-1.54774600	-1.61363700
H	-2.69085100	-3.92820300	-1.07025700
H	-2.19762100	-3.78437900	-2.77398700
H	-0.97929400	-4.12491700	-1.51586100
H	-0.71528300	-0.37074700	-2.59491300
H	0.16580400	-1.91180800	-2.73692900
H	-1.32433200	-1.65311900	-3.68714500
C	-2.00425000	-2.28555400	1.43547800
C	-1.67362000	-3.76878300	1.69229300
C	-3.50893400	-2.05296100	1.21395300
H	-1.71238800	-1.71804600	2.33323100
H	-0.59905500	-3.91646200	1.87444700
H	-2.22466800	-4.10897200	2.58631000
H	-1.97019400	-4.41050000	0.85103200
H	-3.72394700	-0.98541600	1.07811000
H	-3.87239500	-2.59108700	0.32439200

H	-4.07275500	-2.41718800	2.08888100
P	1.04390500	1.75078900	0.00388100
P	-1.02095500	-1.41935100	0.06747600
Pd	-1.13623900	0.92406600	0.01658200
C	-3.28660300	1.54869100	-0.02366200
H	-3.73701500	1.25382200	0.92943500
C	-3.94976200	1.00880700	-1.22653900
C	-5.02140000	0.18326800	-1.14095600
H	-5.44399900	-0.10336100	-0.17550300
H	-5.50152100	-0.21685700	-2.03705400
C	-3.39079200	1.40942000	-2.57852200
H	-3.92070700	0.90003900	-3.39758600
H	-3.47717100	2.49877700	-2.73512100
H	-2.31803500	1.16437300	-2.63824000
O	-1.93267600	0.60091100	3.08523600
C	-2.42130500	2.67787900	-0.02668400
H	-1.74082100	0.60625300	2.11135800
H	-2.29356700	3.24981900	0.89629100
H	-2.26816900	3.24968600	-0.94553700
C	-2.11729700	1.96055100	3.46703600
H	-1.20943600	2.56946000	3.28806000
H	-2.96481400	2.43088000	2.93268900
H	-2.33647100	1.96665000	4.54534500

TS1a

C	-2.30870500	2.73518400	1.40520100
C	-2.36960700	3.46906400	0.17306000
C	-1.22201800	3.11557600	-0.61409200
C	-0.43210200	2.16526200	0.13022700
C	-1.12515900	1.91978100	1.37405200
H	-3.05738300	2.74023500	2.19036700

H	-3.18043500	4.11819600	-0.14286500
H	-1.00453500	3.47260100	-1.61490700
H	-0.81508500	1.20339400	2.12159000
Fe	-2.33584400	1.46148800	-0.18427300
C	-2.40479500	0.09627600	-1.68625400
C	-3.52528300	0.98490000	-1.77543300
C	-2.43766600	-0.57120600	-0.40552100
H	-1.63864800	-0.04691700	-2.44071700
C	-4.25745800	0.89078500	-0.54571600
H	-3.74622400	1.65505200	-2.60318800
C	-3.59233600	-0.06356800	0.29770800
H	-5.12532500	1.48627700	-0.26939400
H	-3.87988800	-0.31496500	1.31389600
C	-1.71706400	-2.58954900	1.65055800
C	-3.09902600	-3.26752200	1.59041900
C	-1.57124400	-1.61994100	2.83917900
H	-0.95463100	-3.37855800	1.78010400
H	-3.11344400	-4.07971500	0.84889000
H	-3.33746200	-3.70314500	2.57600300
H	-3.89520800	-2.55416900	1.33155500
H	-0.51707800	-1.33715500	2.96380500
H	-2.17012300	-0.70731800	2.69644000
H	-1.91324600	-2.11135200	3.76592900
C	-1.33532100	-3.14221000	-1.21894100
C	-0.26020900	-3.00322000	-2.31406400
C	-2.73466400	-3.25854700	-1.85390700
H	-1.12354200	-4.05805800	-0.63851500
H	0.74769400	-2.96405200	-1.87809000
H	-0.31592700	-3.85464500	-3.01458500
H	-0.41619300	-2.07979000	-2.89605100

H	-3.53560400	-3.30512200	-1.10418700
H	-2.93448300	-2.39030700	-2.49973400
H	-2.78371100	-4.16763200	-2.47798300
C	1.60736100	1.88375000	-1.98100800
C	0.71200700	1.16597400	-3.01156500
H	2.62355400	1.47808300	-2.09408500
H	0.67920200	0.08101900	-2.82273100
H	-0.31397300	1.55665600	-2.96564300
H	1.09911800	1.33554800	-4.02813300
C	2.40507400	2.18964500	0.89802300
C	2.02847100	3.59365400	1.39407300
C	3.79964000	2.17396100	0.24846000
H	2.43641100	1.49742700	1.74971400
H	1.02823400	3.61255700	1.85443100
H	2.76365300	3.92245200	2.15323000
H	2.04235600	4.32899700	0.57334200
H	4.06623600	1.17538700	-0.12910000
H	3.86167300	2.89474700	-0.58352500
H	4.55348900	2.46841700	0.99808900
P	-1.13204200	-1.75787100	0.07123100
P	1.15473700	1.33634900	-0.24251300
Pd	1.09273500	-0.96756400	0.16721000
C	3.18628600	-1.79288500	0.54000900
H	3.53419800	-1.29006400	1.44572900
C	4.04008300	-1.63559500	-0.65202400
C	5.25691100	-1.04636100	-0.56442100
H	5.63873500	-0.67732600	0.39067700
H	5.89601200	-0.92479400	-1.44232400
C	3.51875800	-2.14875500	-1.97984900
H	4.25491300	-2.00035900	-2.78463100

H	3.27546500	-3.22392300	-1.92795400
H	2.58505600	-1.62523800	-2.24976800
O	1.69742400	-0.41962200	3.13589600
C	2.19757700	-2.79253100	0.69405100
H	1.22762700	-0.51424700	1.87466700
H	1.88827800	-3.07092700	1.70420900
H	2.04370200	-3.54984600	-0.08063200
C	1.05177800	0.60946200	3.85105500
H	1.12336800	1.60722800	3.37274300
H	-0.02721200	0.41277400	4.04367000
H	1.54751500	0.68493500	4.83757500
C	1.65771900	3.42554300	-2.22242500
H	2.72526600	3.78335200	-2.27632100
H	1.15134600	3.68168300	-3.19847400
H	1.13851200	4.00009200	-1.40678000

Int2a

C	3.67339100	0.43258900	1.34936800
C	4.32151200	0.19796500	0.08982700
C	3.43219500	-0.57772000	-0.72987300
C	2.22365400	-0.82029300	0.02643000
C	2.38289400	-0.18779400	1.31746900
H	4.06508800	1.04048100	2.16200600
H	5.28583400	0.59593000	-0.22023200
H	3.61634900	-0.87064600	-1.75908200
H	1.61155500	-0.19517400	2.08963000
Fe	2.54794700	1.16665500	-0.20058800
C	1.36125000	1.88233600	-1.66653400
C	2.66139700	2.47817000	-1.76440600
C	0.80777000	2.18527200	-0.36419000
H	0.88188500	1.27057900	-2.42130100

C	2.92870900	3.15400300	-0.52855200
H	3.34743800	2.37861100	-2.60268700
C	1.79105300	2.98399800	0.32977300
H	3.85713500	3.65240900	-0.25814300
H	1.71465000	3.34665500	1.34838400
C	-1.28669200	2.52413900	1.72371100
C	-1.36072400	4.05952400	1.62555500
C	-0.40131300	2.06116300	2.89929800
H	-2.30439800	2.14306400	1.91833600
H	-2.15483100	4.39337900	0.94121900
H	-1.57953400	4.47304500	2.62502100
H	-0.40535400	4.48677700	1.28408200
H	-0.29555200	0.96062200	2.91089700
H	0.60268800	2.50799200	2.84249000
H	-0.85975600	2.40246300	3.84325200
C	-1.93044000	2.41061000	-1.18671600
C	-2.16237700	1.42890300	-2.35289400
C	-1.42401100	3.75902400	-1.74158500
H	-2.88565200	2.58754900	-0.66259500
H	-2.42786900	0.42230800	-2.00320000
H	-2.96465800	1.80442200	-3.01008700
H	-1.24749600	1.34851200	-2.96095200
H	-1.20390900	4.49278800	-0.95678200
H	-0.50556800	3.60932200	-2.32762900
H	-2.19055900	4.18415700	-2.41237500
C	0.80977100	-2.46013900	-2.06293700
C	2.01346700	-3.35749600	-2.41712200
C	0.66369800	-1.30479600	-3.06978700
H	-0.10567700	-3.07431500	-2.11843200
H	2.03046700	-4.27445100	-1.81425100

H	1.94921800	-3.65009500	-3.47971200
H	2.96919100	-2.83639500	-2.26663600
H	-0.20556100	-0.67656800	-2.82505400
H	1.56644500	-0.67528700	-3.06860200
H	0.52964900	-1.71003100	-4.08687000
C	1.04026500	-3.30641100	0.83019700
C	2.51389100	-3.71599300	1.01631300
C	0.16383000	-4.50857600	0.43379200
H	0.66583500	-2.88269900	1.77785500
H	3.12124800	-2.87146900	1.37063100
H	2.56622100	-4.51709900	1.77364100
H	2.96560400	-4.10050900	0.08960400
H	-0.89281400	-4.22112500	0.31036200
H	0.50694600	-4.97772100	-0.50246000
H	0.21507600	-5.27189300	1.22786800
P	-0.84461600	1.59626100	0.14454200
P	0.73725500	-1.81918200	-0.29722600
Pd	-1.23135300	-0.78537300	0.51672700
C	-4.38191900	-0.91399000	-1.05805400
C	-3.67257700	-1.32706600	0.15484700
C	-3.34995900	-0.51994400	1.25226200
H	-3.64171100	0.53248600	1.24259800
H	-3.20089600	-0.96540700	2.23909900
O	-0.23663500	-1.00416500	2.63551300
C	-4.51145900	-1.77075700	-2.10235300
H	-1.45878800	-2.29250700	0.82766900
H	-5.07841200	-1.49869400	-2.99508400
H	-4.04534000	-2.75941800	-2.08282500
C	-1.09757900	-1.34659800	3.66481000
H	-1.79870300	-0.52003200	3.95890500

H	-1.74608500	-2.23055200	3.43237200
H	-0.53218900	-1.60825900	4.59094700
H	-3.54292800	-2.40543600	0.26480700
C	-5.06771700	0.43708900	-1.06883700
H	-5.87996500	0.45671000	-0.32164200
H	-4.37301600	1.24444000	-0.80381500
H	-5.49405700	0.65905800	-2.05809200

TS2a

C	1.06653100	-3.26169700	0.89707600
C	0.54722400	-3.91078600	-0.27429700
C	-0.56692600	-3.14245700	-0.75168700
C	-0.73537700	-2.00263700	0.12552500
C	0.28241800	-2.09040100	1.14667400
H	1.94176700	-3.57408900	1.46109400
H	0.95986500	-4.79560800	-0.75485800
H	-1.15020900	-3.36749000	-1.63860700
H	0.40238800	-1.32329700	1.90892100
Fe	1.11585500	-1.99828100	-0.71292300
C	1.31585200	-0.28606800	-1.78841500
C	1.46936900	-1.42949700	-2.64062100
C	2.31868500	-0.33047700	-0.74870000
H	0.54282100	0.47111600	-1.86089700
C	2.56301900	-2.20882700	-2.13184400
H	0.83585800	-1.68852800	-3.48532500
C	3.08138200	-1.53874400	-0.97190400
H	2.89862700	-3.16970700	-2.51726900
H	3.87893700	-1.91170100	-0.33769200
C	3.70901100	0.43217000	1.75905100
C	5.17077400	0.21893900	1.31791600
C	3.16948700	-0.81383700	2.48793600

H	3.70550900	1.26497800	2.48609800
H	5.61103300	1.13387000	0.89586800
H	5.77734400	-0.07636500	2.19264100
H	5.25973600	-0.57775100	0.56499600
H	2.16673700	-0.63515600	2.89575600
H	3.11075500	-1.67064900	1.80278200
H	3.84475700	-1.07897600	3.32022300
C	3.55427000	2.27103100	-0.53776400
C	2.67236300	3.38421700	-1.13824200
C	4.42889100	1.65009500	-1.64396400
H	4.20738100	2.72522900	0.22924200
H	2.02496800	3.84973100	-0.37827500
H	3.30226300	4.16781900	-1.59526200
H	2.02647600	2.97408700	-1.93089800
H	5.08759100	0.85803800	-1.26449800
H	3.79197800	1.20804900	-2.42616400
H	5.05441300	2.43059800	-2.11334500
C	-2.97689600	-0.83067900	-1.41293000
C	-3.88685000	-2.07002400	-1.52838600
C	-2.04746100	-0.70313900	-2.63669800
H	-3.61495700	0.06738700	-1.39903700
H	-4.68511500	-2.05677200	-0.77373000
H	-4.36109600	-2.08171200	-2.52520800
H	-3.32088100	-3.00516300	-1.40877400
H	-1.44881600	0.21266900	-2.58451800
H	-1.36466000	-1.55796100	-2.71523000
H	-2.66201000	-0.65174800	-3.55110500
C	-3.07268600	-1.21636100	1.62330000
C	-3.36945100	-2.72076800	1.75803900
C	-4.33937700	-0.34142000	1.67418600

H	-2.41805900	-0.91209400	2.45760700
H	-2.44421500	-3.31283500	1.69646200
H	-3.83286300	-2.90823200	2.74201100
H	-4.06356000	-3.08204700	0.98599900
H	-4.06759500	0.72701000	1.68217600
H	-5.00388800	-0.53025500	0.81460800
H	-4.90839500	-0.56001100	2.59326800
P	2.45497200	1.04798400	0.46096900
P	-1.99051000	-0.68866900	0.17609200
Pd	-1.26236500	1.47453300	0.95688900
C	-2.59943700	2.65661400	-0.44696800
H	-3.60537100	2.28203100	-0.23489900
C	-2.21379800	2.66769500	-1.86657500
C	-3.11952700	2.36864000	-2.82603400
H	-4.15019800	2.10642600	-2.57402200
H	-2.85033700	2.37877200	-3.88415700
C	-0.78975700	3.05256400	-2.20073800
H	-0.09193100	2.50906300	-1.54591900
H	-0.54993200	2.84043700	-3.25335400
H	-0.61199200	4.12719300	-2.02131700
O	-0.45079800	0.42861300	2.56911200
H	-0.72281400	2.78264500	1.67302300
C	0.29074200	1.13649700	3.52836900
H	1.21964300	1.58383400	3.11065000
H	-0.28799200	1.95753800	4.00779900
H	0.59509700	0.42973700	4.33166900
C	-2.00734400	3.51090300	0.51912400
H	-1.22537400	4.20413000	0.20533400
H	-2.59846400	3.83466200	1.37784100

TS3a

C	3.57716300	2.28699800	-0.60440200
C	3.59673900	1.87882100	0.77092700
C	2.23950700	1.67010000	1.18793500
C	1.35957300	1.97296000	0.08212000
C	2.20686900	2.33414700	-1.03139500
H	4.44743000	2.45961000	-1.23454900
H	4.48480500	1.69245500	1.37118600
H	1.92495100	1.30473400	2.15814400
H	1.86346300	2.56069100	-2.03607900
Fe	2.69413300	0.46554600	-0.39383900
C	3.21353500	-1.42706100	0.19345100
C	4.08786300	-0.95481400	-0.84281900
C	1.86089900	-1.41964200	-0.30643500
H	3.51686400	-1.70004000	1.19951000
C	3.28635800	-0.64910700	-1.99470800
H	5.15995400	-0.79175000	-0.74851900
C	1.91775300	-0.91954000	-1.66212200
H	3.64563700	-0.21472800	-2.92522400
H	1.04804300	-0.73750100	-2.28743600
C	0.09792700	-3.68146100	-0.42953900
C	1.42167000	-4.40747800	-0.74506100
C	-0.73495900	-3.55205900	-1.71967800
H	-0.47760200	-4.27064600	0.30884000
H	2.06808500	-4.52884100	0.13338200
H	1.20642400	-5.40801000	-1.16048700
H	1.98636400	-3.84020300	-1.50101400
H	-1.66620800	-2.99603300	-1.55934900
H	-0.15660000	-3.00959400	-2.48484000
H	-0.96348000	-4.55478000	-2.12161600
C	0.59416200	-2.40025700	2.20374800

C	1.02154200	-1.13634300	2.97201000
C	1.52082900	-3.58885700	2.51947900
H	-0.41934100	-2.67073900	2.55457800
H	0.33861000	-0.30310200	2.75266000
H	1.01447500	-1.33218200	4.05815000
H	2.03769600	-0.83216500	2.68180000
H	1.13765100	-4.52610600	2.09090900
H	2.53702700	-3.42567600	2.13078500
H	1.59341500	-3.72068500	3.61366000
C	-0.88752000	3.13921100	1.48998400
C	-0.17825600	4.50752100	1.41168700
C	-0.61385500	2.52528700	2.88112400
H	-1.97754200	3.27821700	1.37907300
H	-0.50384900	5.10976600	0.55671200
H	-0.38782000	5.08315100	2.33073800
H	0.91224900	4.36744000	1.34324100
H	-0.93471300	1.47903100	2.94716800
H	0.46180400	2.56974000	3.10967300
H	-1.13898400	3.11090900	3.65469400
C	-0.94259400	2.68722000	-1.52143300
C	-0.44756700	4.11768600	-1.83047100
C	-2.46973000	2.59933300	-1.71621400
H	-0.47172800	1.99202000	-2.23683500
H	0.56418800	4.32080800	-1.45498400
H	-0.45051800	4.27211300	-2.92359200
H	-1.13237100	4.86335300	-1.39833900
H	-2.80282600	1.55422000	-1.67432200
H	-2.99386300	3.18314900	-0.94037500
H	-2.74172000	3.02876600	-2.69635400
P	0.26739700	-1.96603100	0.39382100

P	-0.47339100	1.88019000	0.12482300
Pd	-1.45736400	-0.23497300	0.20541800
C	-3.56045700	-1.79467600	0.29170800
H	-2.96450400	-2.61870300	0.69452100
C	-3.56530600	-0.58456100	1.05098100
C	-2.61783700	-0.43169500	2.09598000
H	-2.17572600	-1.31219700	2.57183500
H	-2.68496300	0.45760500	2.72351200
C	-4.52241300	0.54172000	0.69845400
H	-4.24075400	1.46387100	1.22808400
H	-4.51179100	0.74913100	-0.38069500
H	-5.55704600	0.27573300	0.98215400
C	-1.68165400	-0.48804700	-3.26423200
H	-2.43973300	-0.86862400	-3.97852800
H	-1.46987200	0.56539300	-3.54162100
H	-0.75411700	-1.07900300	-3.42618000
O	-2.15665400	-0.58245600	-1.94843800
C	-4.14186700	-1.94453900	-1.00866000
H	-3.16659000	-1.33379700	-1.70716100
H	-4.23868700	-2.97551000	-1.37008200
H	-5.02201900	-1.32466000	-1.22290100

Int3a

C	-4.19955900	1.54861800	-2.42890700
C	-4.97222800	1.40606900	-1.22768200
C	-4.45176500	0.28452200	-0.49876700
C	-3.36568100	-0.29452000	-1.25392000
C	-3.20746000	0.51080300	-2.44200300
H	-4.29972600	2.34411600	-3.16469700
H	-5.76605600	2.07146900	-0.89448900
H	-4.79653200	-0.05987500	0.46978100

H	-2.44159000	0.37261600	-3.19960200
Fe	-3.00056300	1.68703600	-0.79152900
C	-2.76937800	2.88065100	0.85055300
C	-2.78614200	3.66288300	-0.35335900
C	-1.67649600	1.94245100	0.77163700
H	-3.48735300	2.95532500	1.66154800
C	-1.70721300	3.21247600	-1.18715500
H	-3.53109800	4.41151300	-0.61794500
C	-1.03015500	2.15220300	-0.50274400
H	-1.48167000	3.56564500	-2.18933800
H	-0.18572100	1.57151600	-0.86041900
C	0.43763200	1.82471000	2.70637600
C	0.19075700	3.34665900	2.65680200
C	1.77849000	1.50485400	2.02452900
H	0.48515500	1.49889200	3.76219500
H	-0.76972500	3.64125300	3.09980000
H	1.00164200	3.86689800	3.19677200
H	0.20261100	3.69151200	1.61216300
H	2.03401600	0.44275000	2.10575100
H	1.73096000	1.74937100	0.95535600
H	2.58835400	2.10184000	2.47413000
C	-2.18024800	0.64957900	3.40596200
C	-3.53199100	0.10231500	2.91678400
C	-2.37374900	1.89765700	4.28773900
H	-1.71464900	-0.13237700	4.03520000
H	-3.38512800	-0.78854800	2.29199800
H	-4.16971600	-0.16498000	3.77733400
H	-4.05882300	0.85862800	2.31736800
H	-1.42553800	2.24211500	4.72465600
H	-2.80737600	2.73174400	3.71635800

H	-3.06489100	1.66055100	5.11602900
C	-3.71107800	-3.07252400	-0.45127400
C	-4.94696300	-3.03917400	-1.37567200
C	-4.19441700	-3.01933600	1.01295800
H	-3.16433800	-4.02120200	-0.60108200
H	-4.70303100	-3.19101800	-2.43235100
H	-5.65190600	-3.83219800	-1.06925800
H	-5.46438100	-2.07234800	-1.28186100
H	-3.36169900	-2.93145100	1.72039400
H	-4.86044200	-2.15562500	1.16446000
H	-4.77510700	-3.92807700	1.24701100
C	-1.59423300	-2.23416000	-2.42667100
C	-2.52374000	-2.55222500	-3.61346600
C	-0.59143600	-3.37892300	-2.20388300
H	-1.01641300	-1.33078500	-2.67440500
H	-3.34610700	-1.82961800	-3.71179500
H	-1.93687800	-2.53967200	-4.54871900
H	-2.95257100	-3.56131000	-3.51202200
H	0.13580700	-3.10598900	-1.42974300
H	-1.10881600	-4.29940300	-1.88391800
H	-0.05789100	-3.60264700	-3.14390800
P	-0.96416000	0.75314100	1.95984100
P	-2.37270200	-1.75400200	-0.76786200
Pd	-0.65106800	-1.44435200	0.77407400
C	1.49121700	-2.19317100	2.02862100
H	1.27638500	-1.50623200	2.85210300
C	0.49457900	-3.18196400	1.76291700
C	-0.79794600	-3.01286400	2.32479000
H	-0.93276500	-2.42480100	3.23870200
H	-1.53277400	-3.80380300	2.16334900

C	0.79708400	-4.37049800	0.86935900
H	-0.13339300	-4.82395600	0.49836100
H	1.41141900	-4.08803000	0.00347800
H	1.35732800	-5.13691800	1.43558000
C	1.37392500	-0.51053700	-1.80463700
H	2.30735300	0.02986800	-2.05153000
H	1.42972600	-1.52159300	-2.25819300
H	0.55459800	0.04450600	-2.29871000
O	1.15026300	-0.53635600	-0.41451600
C	2.64263900	-1.93843300	1.22172700
H	1.85280805	-1.04285959	0.13254883
H	3.41810800	-1.32002800	1.68429000
H	3.05121200	-2.77491300	0.64333600
C	5.76164200	-1.14494600	0.31293700
C	4.92093500	-0.72757800	-0.74059300
C	4.68268100	-1.58829400	-1.80980900
C	5.27998400	-2.86615400	-1.81239000
C	6.10581800	-3.26670200	-0.74891600
C	6.36249300	-2.40559700	0.33568200
C	5.13365900	1.02280400	0.87795800
H	4.03240300	-1.28109900	-2.62969500
H	5.09831000	-3.54771000	-2.64530600
H	6.56035600	-4.25934700	-0.75944800
H	7.00240700	-2.71613900	1.16368300
N	5.83890300	-0.11522800	1.26263700
H	6.44465900	-0.11454800	2.07626700
O	5.14880300	2.08697400	1.48639700
C	4.37993300	0.65111300	-0.42428600
H	3.31443400	0.56022800	-0.15084000
C	4.52036900	1.70924700	-1.56346400

H	4.58243000	1.16720200	-2.52000200
H	5.47944200	2.23899300	-1.43732900
C	3.38019300	2.71137400	-1.63791300
C	3.10006700	3.57795100	-0.56245300
C	2.58215600	2.79000800	-2.79501300
C	2.04883300	4.50222100	-0.64912300
H	3.70620300	3.51093200	0.34079800
C	1.53219000	3.71801100	-2.88592600
H	2.79028400	2.11949100	-3.63312400
C	1.26444500	4.57988900	-1.81143100
H	1.84032500	5.16244200	0.19526200
H	0.92729700	3.76666000	-3.79477200
H	0.44646300	5.29977900	-1.87348500

TS4a

C	-4.19955900	1.54861800	-2.42890700
C	-4.97222800	1.40606900	-1.22768200
C	-4.45176500	0.28452200	-0.49876700
C	-3.36568100	-0.29452000	-1.25392000
C	-3.20746000	0.51080300	-2.44200300
H	-4.29972600	2.34411600	-3.16469700
H	-5.76605600	2.07146900	-0.89448900
H	-4.79653200	-0.05987500	0.46978100
H	-2.44159000	0.37261600	-3.19960200
Fe	-3.00056300	1.68703600	-0.79152900
C	-2.76937800	2.88065100	0.85055300
C	-2.78614200	3.66288300	-0.35335900
C	-1.67649600	1.94245100	0.77163700
H	-3.48735300	2.95532500	1.66154800
C	-1.70721300	3.21247600	-1.18715500
H	-3.53109800	4.41151300	-0.61794500

C	-1.03015500	2.15220300	-0.50274400
H	-1.48167000	3.56564500	-2.18933800
H	-0.18572100	1.57151600	-0.86041900
C	0.43763200	1.82471000	2.70637600
C	0.19075700	3.34665900	2.65680200
C	1.77849000	1.50485400	2.02452900
H	0.48515500	1.49889200	3.76219500
H	-0.76972500	3.64125300	3.09980000
H	1.00164200	3.86689800	3.19677200
H	0.20261100	3.69151200	1.61216300
H	2.03401600	0.44275000	2.10575100
H	1.73096000	1.74937100	0.95535600
H	2.58835400	2.10184000	2.47413000
C	-2.18024800	0.64957900	3.40596200
C	-3.53199100	0.10231500	2.91678400
C	-2.37374900	1.89765700	4.28773900
H	-1.71464900	-0.13237700	4.03520000
H	-3.38512800	-0.78854800	2.29199800
H	-4.16971600	-0.16498000	3.77733400
H	-4.05882300	0.85862800	2.31736800
H	-1.42553800	2.24211500	4.72465600
H	-2.80737600	2.73174400	3.71635800
H	-3.06489100	1.66055100	5.11602900
C	-3.71107800	-3.07252400	-0.45127400
C	-4.94696300	-3.03917400	-1.37567200
C	-4.19441700	-3.01933600	1.01295800
H	-3.16433800	-4.02120200	-0.60108200
H	-4.70303100	-3.19101800	-2.43235100
H	-5.65190600	-3.83219800	-1.06925800
H	-5.46438100	-2.07234800	-1.28186100

H	-3.36169900	-2.93145100	1.72039400
H	-4.86044200	-2.15562500	1.16446000
H	-4.77510700	-3.92807700	1.24701100
C	-1.59423300	-2.23416000	-2.42667100
C	-2.52374000	-2.55222500	-3.61346600
C	-0.59143600	-3.37892300	-2.20388300
H	-1.01641300	-1.33078500	-2.67440500
H	-3.34610700	-1.82961800	-3.71179500
H	-1.93687800	-2.53967200	-4.54871900
H	-2.95257100	-3.56131000	-3.51202200
H	0.13580700	-3.10598900	-1.42974300
H	-1.10881600	-4.29940300	-1.88391800
H	-0.05789100	-3.60264700	-3.14390800
P	-0.96416000	0.75314100	1.95984100
P	-2.37270200	-1.75400200	-0.76786200
Pd	-0.65106800	-1.44435200	0.77407400
C	1.49121700	-2.19317100	2.02862100
H	1.27638500	-1.50623200	2.85210300
C	0.49457900	-3.18196400	1.76291700
C	-0.79794600	-3.01286400	2.32479000
H	-0.93276500	-2.42480100	3.23870200
H	-1.53277400	-3.80380300	2.16334900
C	0.79708400	-4.37049800	0.86935900
H	-0.13339300	-4.82395600	0.49836100
H	1.41141900	-4.08803000	0.00347800
H	1.35732800	-5.13691800	1.43558000
C	1.37392500	-0.51053700	-1.80463700
H	2.30735300	0.02986800	-2.05153000
H	1.42972600	-1.52159300	-2.25819300
H	0.55459800	0.04450600	-2.29871000

O	1.15026300	-0.53635600	-0.41451600
C	2.64263900	-1.93843300	1.22172700
H	2.02720500	-1.16859200	0.26835000
H	3.41810800	-1.32002800	1.68429000
H	3.05121200	-2.77491300	0.64333600
C	5.76164200	-1.14494600	0.31293700
C	4.92093500	-0.72757800	-0.74059300
C	4.68268100	-1.58829400	-1.80980900
C	5.27998400	-2.86615400	-1.81239000
C	6.10581800	-3.26670200	-0.74891600
C	6.36249300	-2.40559700	0.33568200
C	5.13365900	1.02280400	0.87795800
H	4.03240300	-1.28109900	-2.62969500
H	5.09831000	-3.54771000	-2.64530600
H	6.56035600	-4.25934700	-0.75944800
H	7.00240700	-2.71613900	1.16368300
N	5.83890300	-0.11522800	1.26263700
H	6.44465900	-0.11454800	2.07626700
O	5.14880300	2.08697400	1.48639700
C	4.37993300	0.65111300	-0.42428600
H	3.31443400	0.56022800	-0.15084000
C	4.52036900	1.70924700	-1.56346400
H	4.58243000	1.16720200	-2.52000200
H	5.47944200	2.23899300	-1.43732900
C	3.38019300	2.71137400	-1.63791300
C	3.10006700	3.57795100	-0.56245300
C	2.58215600	2.79000800	-2.79501300
C	2.04883300	4.50222100	-0.64912300
H	3.70620300	3.51093200	0.34079800
C	1.53219000	3.71801100	-2.88592600

H	2.79028400	2.11949100	-3.63312400
C	1.26444500	4.57988900	-1.81143100
H	1.84032500	5.16244200	0.19526200
H	0.92729700	3.76666000	-3.79477200
H	0.44646300	5.29977900	-1.87348500

Int4a

C	-3.22617300	-2.83194400	-2.30711700
C	-4.26706500	-2.74822500	-1.32203700
C	-3.67901100	-2.27266700	-0.10077400
C	-2.25634100	-2.10723000	-0.30336800
C	-1.99796200	-2.42142800	-1.68822100
H	-3.35465600	-3.09806300	-3.35419700
H	-5.32543200	-2.93697600	-1.48968700
H	-4.21407900	-2.06917000	0.82139300
H	-1.02827200	-2.35824900	-2.17238400
Fe	-3.40417400	-0.93295000	-1.59926500
C	-4.61266000	0.66921000	-1.21874900
C	-4.89676700	0.11106000	-2.50958700
C	-3.23050200	1.08884500	-1.18781100
H	-5.31916500	0.73549300	-0.39899100
C	-3.69550500	0.17192300	-3.29173600
H	-5.84091500	-0.33475200	-2.81666100
C	-2.67039300	0.75744400	-2.47975700
H	-3.56650500	-0.21830400	-4.29894700
H	-1.63602800	0.90601700	-2.76722600
C	-1.82793900	3.56182300	-0.50356900
C	-2.82877900	4.14268400	-1.52200700
C	-0.40028400	3.60683600	-1.08763100
H	-1.84831800	4.17593400	0.41598100
H	-3.86133800	4.15887500	-1.14964300

H	-2.53515800	5.17404200	-1.78624200
H	-2.81506400	3.54013900	-2.44341300
H	0.31269100	2.99896600	-0.51630600
H	-0.40677000	3.22465600	-2.12118300
H	-0.04186500	4.64921800	-1.12477800
C	-3.47406100	2.21345000	1.52665800
C	-3.95562600	0.90752700	2.18415700
C	-4.63660200	3.17019000	1.20283300
H	-2.82687800	2.72238700	2.26495200
H	-3.09254700	0.28366800	2.44276400
H	-4.52594200	1.13170100	3.10218200
H	-4.60389700	0.32583600	1.51349000
H	-4.26870200	4.17312000	0.94298600
H	-5.24888800	2.80397000	0.36584500
H	-5.29115800	3.27008400	2.08679200
C	-1.54841700	-2.83418900	2.42750900
C	-2.06319500	-4.23747600	2.03779600
C	-2.58594100	-2.17263600	3.35543000
H	-0.61142900	-2.94672200	2.99914400
H	-1.36651400	-4.79297200	1.40253900
H	-2.23355400	-4.82272900	2.95841000
H	-3.02119200	-4.16394200	1.50332500
H	-2.26110800	-1.19120100	3.71444300
H	-3.55234900	-2.04440200	2.84580700
H	-2.75726300	-2.82549000	4.22850800
C	0.57255800	-2.55515500	0.33727500
C	0.51556700	-4.02246800	-0.12891300
C	1.68621400	-2.35815800	1.38265100
H	0.83577900	-1.91736700	-0.51591800
H	-0.39284200	-4.25421300	-0.70402900

H	1.39406100	-4.21627200	-0.76589200
H	0.57463700	-4.71229600	0.72757300
H	1.87028100	-1.28983700	1.54758200
H	1.43107900	-2.83175400	2.34600900
H	2.60688900	-2.83198000	1.01530300
P	-2.23369400	1.82019700	0.15672100
P	-1.00071600	-1.72413900	0.97705700
Pd	-0.31971100	0.52229800	1.28750800
C	0.84097900	2.36376100	2.14632100
H	0.00190900	3.06541500	2.10166000
C	0.73842300	1.29241200	3.06866900
C	-0.59985800	0.89211100	3.40829400
H	-1.39050000	1.64533300	3.48821600
H	-0.70858300	0.03593800	4.07639700
C	1.94346800	0.52172000	3.56937500
H	1.64957400	-0.49419300	3.87267300
H	2.73559300	0.45263400	2.81307000
H	2.37034200	1.03290900	4.45193200
C	0.69371000	0.31306100	-1.71772600
H	1.57047300	-0.04073100	-2.31349900
H	-0.11249700	-0.43880100	-1.86030100
H	0.34622700	1.24808900	-2.21760800
O	1.05281800	0.49842100	-0.39519200
C	2.11125300	2.75957000	1.44838100
H	2.18906900	2.20285300	0.49726000
H	2.12049500	3.83201300	1.20938200
H	3.00707400	2.51293200	2.03490100
C	4.79203500	-2.54756000	-0.23055100
C	3.97054600	-1.80584800	-1.10987600
C	3.37773300	-2.44466400	-2.19707900

C	3.60609600	-3.82326700	-2.39769600
C	4.42301600	-4.54391500	-1.51046600
C	5.03112000	-3.91362500	-0.40646400
C	4.71413600	-0.40139000	0.66768100
H	2.73484300	-1.88277300	-2.87796700
H	3.14327000	-4.33287800	-3.24484000
H	4.59084900	-5.61053900	-1.67293600
H	5.66110500	-4.47535500	0.28607800
N	5.23564000	-1.69417500	0.78698200
H	5.78240100	-1.97669100	1.59313700
O	4.90790700	0.49451600	1.48433100
C	3.90146000	-0.37368600	-0.63857600
H	2.85644000	-0.05785600	-0.40939300
C	4.50339800	0.60875600	-1.70052000
H	4.05416400	0.33263600	-2.66723800
H	5.58590700	0.41330000	-1.78222700
C	4.25248500	2.08115200	-1.44459800
C	5.09249400	2.83242300	-0.60100000
C	3.17243500	2.72901300	-2.07313200
C	4.85745800	4.19942900	-0.39222100
H	5.92102200	2.33741700	-0.09442900
C	2.93841900	4.09706300	-1.87378000
H	2.50961200	2.15140600	-2.71938600
C	3.78185600	4.83801900	-1.03126200
H	5.51692900	4.76703000	0.26834100
H	2.09646300	4.58025500	-2.37274000
H	3.60364400	5.90441200	-0.87402300

TS5a

C	-2.72091900	-2.89420700	-2.48269100
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C	-3.86772300	-3.00764500	-1.62496500
C	-3.48500900	-2.56217300	-0.31407900
C	-2.08789500	-2.19495700	-0.34726500
C	-1.63013200	-2.38225300	-1.70371700
H	-2.70036200	-3.09548100	-3.55135400
H	-4.86729400	-3.31089400	-1.92868200
H	-4.13891700	-2.49368300	0.54977000
H	-0.63119700	-2.14565500	-2.05933400
Fe	-3.20242500	-1.08958500	-1.67559300
C	-4.42470000	0.45436100	-1.17219400
C	-4.78343500	-0.07182500	-2.45867200
C	-3.04923400	0.89634900	-1.22593600
H	-5.07284900	0.48772100	-0.30306000
C	-3.63822300	0.03382700	-3.31719800
H	-5.73644600	-0.52931300	-2.71523700
C	-2.56916800	0.61850000	-2.56123500
H	-3.56882800	-0.33073900	-4.33947800
H	-1.56022000	0.80092900	-2.91723400
C	-1.38230800	3.26274100	-0.82278800
C	-2.23393100	3.78959900	-1.99883000
C	0.07768200	3.08707100	-1.27451800
H	-1.41280900	4.01038900	-0.01303600
H	-3.30773600	3.84417900	-1.77975600
H	-1.87754300	4.79894400	-2.26576200
H	-2.10675100	3.14726100	-2.88137300
H	0.68832000	2.51138100	-0.56675700
H	0.11712600	2.55393500	-2.23501800
H	0.54026700	4.07261200	-1.42482800
C	-3.31807200	2.51578000	1.24427900
C	-3.90080500	1.47458100	2.21641200

C	-4.41409600	3.38839200	0.60235400
H	-2.66340500	3.17694800	1.83840400
H	-3.08893700	0.97012900	2.75502500
H	-4.56266200	1.97395200	2.94442200
H	-4.48769400	0.70135600	1.69921900
H	-3.98968800	4.28991700	0.14011300
H	-4.98055100	2.83963200	-0.16401700
H	-5.12231300	3.71406900	1.38340200
C	-1.70181300	-2.63118500	2.54165200
C	-2.16803000	-4.08406000	2.31277700
C	-2.81194400	-1.81242000	3.22593200
H	-0.83548200	-2.65002200	3.22359100
H	-1.39441200	-4.70845800	1.85352900
H	-2.43524000	-4.52656900	3.28782400
H	-3.05892200	-4.12411900	1.67130200
H	-2.43842500	-0.82658800	3.52759100
H	-3.67296800	-1.65793600	2.55737000
H	-3.17001000	-2.34699600	4.12227800
C	0.61338400	-2.59509700	0.62104900
C	0.52394400	-4.07634000	0.19722100
C	1.63628900	-2.40726600	1.75239800
H	0.98657000	-1.99909000	-0.21819400
H	-0.35038300	-4.29391700	-0.43319900
H	1.43507100	-4.31691200	-0.37283100
H	0.49927700	-4.74034100	1.07562800
H	1.91114800	-1.35069800	1.83497000
H	1.26119200	-2.77987600	2.72124900
H	2.53817100	-2.97927000	1.49991500
P	-2.06033300	1.73056000	0.06605700
P	-1.00025900	-1.71654400	1.04277500

Pd	-0.59775800	0.54665300	1.48718100
C	0.01186600	2.42143000	2.67168000
H	-0.91510100	2.49521500	3.25372200
C	0.88962300	1.34493600	2.98901800
C	0.29379600	0.16815400	3.51089500
H	-0.61960900	0.23461800	4.10968400
H	0.90981800	-0.71385100	3.67232600
C	2.33818300	1.37794500	2.56111600
H	2.85738400	0.44402200	2.80397400
H	2.41553500	1.53880800	1.47804400
H	2.85827900	2.20670100	3.06965400
C	1.10674700	0.10306400	-1.59480600
H	1.24564200	-0.93248200	-1.99404600
H	0.02334000	0.32332600	-1.66151300
H	1.62500500	0.78187000	-2.31169100
O	1.55247500	0.25158400	-0.28363800
C	0.52939700	3.71234000	2.08521500
H	-0.29198700	4.34575900	1.72185000
H	1.06575300	4.28852000	2.86407600
H	1.23446600	3.53924400	1.26236100
C	4.49509800	-2.61253300	-0.07666400
C	4.04232100	-1.73371700	-1.10031600
C	3.57465200	-2.28733300	-2.29843500
C	3.55201600	-3.68823100	-2.46083200
C	3.99166900	-4.53722800	-1.42909000
C	4.47117300	-4.00377500	-0.21470400
C	4.81806000	-0.45060400	0.71141400
H	3.23156400	-1.63409200	-3.10370400
H	3.19259700	-4.11780800	-3.39882200
H	3.96892700	-5.62055400	-1.56679500

H	4.82320600	-4.65747500	0.58712400
N	4.90267200	-1.83074900	1.00066300
H	5.37483500	-2.16916700	1.83120300
O	5.24917500	0.41526100	1.48631600
C	4.10865800	-0.33653500	-0.59941600
H	2.85847800	-0.03959800	-0.33669700
C	4.59114800	0.75069000	-1.58688300
H	4.36112500	0.40086200	-2.60627900
H	5.69344400	0.82146900	-1.52866300
C	4.02641000	2.15554400	-1.42976800
C	4.08925700	2.84019200	-0.19886400
C	3.51463700	2.83852500	-2.54982100
C	3.65292700	4.16998800	-0.09832300
H	4.50374000	2.31778300	0.66401200
C	3.09011400	4.17418800	-2.45639800
H	3.46539500	2.31962500	-3.51137300
C	3.15799400	4.84693800	-1.22680700
H	3.71685900	4.68683000	0.86303200
H	2.70386800	4.68538000	-3.34190900
H	2.83158900	5.88711700	-1.14866200

Int5a

C	2.51447900	-1.97100800	1.82462200
C	1.83067400	-2.59968300	2.91794800
C	0.57535300	-1.93061600	3.10053900
C	0.47426800	-0.88502100	2.10376400
C	1.68873500	-0.91852000	1.31488400
H	3.45972600	-2.28369700	1.38921400
H	2.16720100	-3.47634200	3.46761300
H	-0.18381300	-2.20515100	3.82513600
H	1.89717900	-0.33626300	0.41988500

Fe	0.69074200	-2.67726600	1.21807000
C	-1.02474700	-3.60985100	0.68723600
C	-0.01751600	-4.58019900	1.01200900
C	-0.53048600	-2.79415000	-0.40269900
H	-1.98111700	-3.49018700	1.18664400
C	1.10247600	-4.36167200	0.14107500
H	-0.07021600	-5.30746100	1.81949900
C	0.79838900	-3.25982300	-0.72498300
H	2.05568600	-4.88385800	0.18161100
H	1.46610600	-2.81095100	-1.45969600
C	-0.52401800	-1.26767800	-2.88740400
C	-1.25750100	-0.26798300	-3.80078100
C	-0.20484400	-2.54351200	-3.70152800
H	0.41782500	-0.80731200	-2.54455300
H	-1.56952700	0.63436300	-3.26151400
H	-0.59078300	0.02041100	-4.63121000
H	-2.15304800	-0.72933900	-4.24808300
H	0.04039000	-3.41053800	-3.07794700
H	-1.05304800	-2.81176900	-4.35261500
H	0.67191400	-2.34071300	-4.33453000
C	-3.08066200	-2.31633300	-1.73123500
C	-4.12456400	-2.17481400	-0.60881800
C	-2.95800900	-3.79356200	-2.15475600
H	-3.42346600	-1.72241500	-2.59390100
H	-4.18238000	-1.14032400	-0.24395500
H	-5.11806100	-2.48432000	-0.97642900
H	-3.86945300	-2.82206800	0.24423900
H	-2.28249900	-3.93057100	-3.00674900
H	-2.58283300	-4.40471600	-1.32060300
H	-3.95500800	-4.17382600	-2.43732900

C	-2.14212500	0.07611900	3.15607200
C	-1.75985400	0.14218200	4.64836500
C	-2.85421600	-1.24351700	2.80122600
H	-2.85043800	0.89720500	2.95456800
H	-1.44986200	1.15438800	4.93962200
H	-2.63863100	-0.13274800	5.25686600
H	-0.94290700	-0.54709600	4.89970900
H	-3.18084900	-1.23442900	1.75248400
H	-2.18724300	-2.10548700	2.94192700
H	-3.73783200	-1.37653000	3.44838300
C	0.16765100	1.93383600	2.55544300
C	1.16459700	1.60755800	3.69079400
C	-0.73705500	3.12735600	2.93285000
H	0.74342300	2.23363600	1.67267400
H	1.84675600	0.79092500	3.42195600
H	1.77042700	2.50973500	3.87729300
H	0.65751600	1.34039000	4.62869900
H	-1.08661000	3.65628600	2.04041500
H	-1.60086500	2.83544000	3.55139700
H	-0.14065700	3.84640300	3.51770500
P	-1.44984700	-1.47594100	-1.26410000
P	-0.77404200	0.42025700	1.90834300
Pd	-1.90583500	0.57764900	-0.15071200
C	-3.42670700	1.54314500	-1.66322600
H	-2.64693700	2.15215700	-2.13206100
C	-3.74973400	1.87752400	-0.32688400
C	-2.74398400	2.52586600	0.44372600
H	-2.95223000	2.70164900	1.49858400
H	-2.02255600	3.19932900	-0.03034700
C	-5.03469500	1.43727500	0.34651700

H	-5.48033400	0.55105100	-0.12317600
H	-4.86016700	1.22428500	1.41181600
H	-5.77315700	2.25524300	0.28159400
C	4.02719000	-2.24753600	-1.92530900
H	3.66608300	-2.58096700	-0.92888600
H	4.60541200	-3.07267500	-2.37382500
H	4.69296900	-1.38222300	-1.77288500
O	2.94927000	-1.94148900	-2.80657700
C	0.17747100	3.27146400	-1.56871100
C	1.09368000	3.51352400	-0.48504700
C	0.96308400	4.72286000	0.23369800
C	-0.01776500	5.65650700	-0.14686000
C	-0.87554800	5.41465800	-1.23993100
C	-0.77766200	4.20729500	-1.96820000
C	1.54224400	1.42111100	-1.33210200
H	1.62547700	4.93367400	1.07749300
H	-0.10971700	6.59320200	0.40888300
H	-1.61448100	6.16324700	-1.53286300
H	-1.43430400	4.01343300	-2.82172900
N	0.42440500	1.98381500	-2.02735900
H	0.18994800	1.65990600	-2.95662000
O	1.96200900	0.24782500	-1.58954000
C	1.95079400	2.37114900	-0.36674400
H	2.61307700	-1.06236400	-2.50515300
C	3.09840600	2.20493700	0.59803200
H	2.80224000	1.67023900	1.52001200
H	3.40181600	3.21506600	0.93498600
C	4.33114700	1.49697100	0.04597200
C	5.03345800	0.57569200	0.84444500
C	4.81981500	1.77644300	-1.24418000

C	6.20360200	-0.04444300	0.37659000
H	4.65292400	0.34280000	1.84275900
C	5.98768300	1.16273900	-1.71717300
H	4.26106400	2.47004900	-1.87532400
C	6.68805900	0.25073500	-0.90732100
H	6.73397900	-0.75755800	1.01305900
H	6.34993000	1.38888300	-2.72295400
H	7.59492100	-0.23182900	-1.27903000
C	-4.38174800	0.84537000	-2.59965400
H	-3.85489000	0.46322400	-3.48295400
H	-4.90248600	0.00662600	-2.11726200
H	-5.15409400	1.55306000	-2.95632300

TS6a

C	2.18019200	2.63317800	-2.65505000
C	3.27769800	3.18068900	-1.90970400
C	3.04273400	2.91396100	-0.51861800
C	1.79113500	2.20435800	-0.38748700
C	1.27404100	2.02482000	-1.72465500
H	2.08797700	2.62100100	-3.73894900
H	4.16600700	3.65072100	-2.32747000
H	3.72775700	3.15716800	0.28602600
H	0.35699600	1.49893200	-1.96194600
Fe	3.12271100	1.18126000	-1.57449900
C	4.42714800	-0.07353100	-0.64725800
C	5.01335000	0.47493700	-1.83805500
C	3.23400700	-0.80014900	-1.01300700
H	4.80211700	0.04989900	0.36476100
C	4.17561400	0.11462800	-2.94753800
H	5.89559300	1.11045900	-1.88143300
C	3.07827900	-0.66120400	-2.44307100

H	4.31107000	0.43093500	-3.98003500
H	2.23864300	-1.03347700	-3.02277900
C	1.35745400	-2.93230400	-1.12293100
C	0.20922300	-3.72646700	-0.48042500
C	2.32506600	-3.88011400	-1.85373100
H	0.91058200	-2.26247400	-1.87032600
H	-0.55445200	-3.04326200	-0.08463600
H	-0.25645100	-4.38219100	-1.23562000
H	0.56894300	-4.36264100	0.34595300
H	3.14223700	-3.33369300	-2.34859900
H	2.76778400	-4.61170800	-1.15874700
H	1.76977300	-4.43788100	-2.62686600
C	3.39022400	-2.84527700	1.05227600
C	3.80056500	-2.16796200	2.37644500
C	4.65094500	-3.31507300	0.26662900
H	2.76805300	-3.72128300	1.30309500
H	2.92483700	-1.82679900	2.94044600
H	4.38217800	-2.87185900	2.99714800
H	4.43966400	-1.29142700	2.17648500
H	4.63183700	-3.01373000	-0.79667300
H	5.56727200	-2.87342800	0.71249800
H	4.75180600	-4.41846400	0.30738700
C	1.86443300	2.28680700	2.56068300
C	2.17197400	3.79543800	2.66024100
C	3.14361200	1.43117400	2.67509900
H	1.21981100	2.01997800	3.41592600
H	1.25991300	4.38984400	2.80192300
H	2.82879300	3.97375500	3.52972600
H	2.68054900	4.18018100	1.76680300
H	2.88324700	0.36473300	2.70282900

H	3.81175400	1.59245600	1.81574700
H	3.69408100	1.69309800	3.59564200
C	-0.63282600	2.85745700	0.99780700
C	-0.40142800	4.23679300	0.35098900
C	-1.26966700	3.00395100	2.39318800
H	-1.32956100	2.30568400	0.34929500
H	0.00574500	4.14108500	-0.66538700
H	-1.36809300	4.76639500	0.28631700
H	0.29062100	4.85657700	0.93952900
H	-1.37056900	2.03597600	2.90449700
H	-0.66993800	3.66377800	3.03770800
H	-2.27052700	3.45211100	2.29411900
P	2.14805800	-1.74009900	0.12553100
P	0.84824400	1.66702500	1.09053600
Pd	0.48968100	-0.68177800	1.41461000
C	-0.28307500	-2.29680300	2.63042600
H	-0.37015700	-3.21476300	2.04728600
C	-1.37956100	-1.37964600	2.54774400
C	-2.51244200	-1.82353100	1.69224400
H	-3.45674900	-1.92129400	2.24812800
H	-2.31400400	-2.73064300	1.11350900
C	-1.76581400	-0.53345800	3.75965900
H	-0.88057600	-0.10512900	4.25342900
H	-2.43152800	0.29166000	3.47939000
H	-2.30554600	-1.15059100	4.50654400
C	-0.24482800	0.07978400	-4.31745400
H	0.69391800	0.65942000	-4.24437000
H	-0.29931000	-0.38362900	-5.31400500
H	-1.09893200	0.77405900	-4.19998700
O	-0.28095500	-0.97272900	-3.35274500

C	-3.90268300	-2.15893100	-1.40559700
C	-4.35054300	-1.51730200	-0.22671700
C	-5.62274100	-1.80151900	0.27262200
C	-6.44032900	-2.71706300	-0.41797700
C	-5.97745300	-3.34820700	-1.58722000
C	-4.69313400	-3.07826800	-2.10101500
C	-2.22451000	-0.70444100	-0.80435900
H	-5.98480500	-1.30781700	1.17938500
H	-7.44211200	-2.93845300	-0.04539200
H	-6.62187700	-4.05651900	-2.11164100
H	-4.33434400	-3.56294600	-3.01092600
N	-2.61327300	-1.69053000	-1.69958300
H	-2.08562700	-1.84401900	-2.56068000
O	-1.21266300	0.00403900	-0.94655800
C	-3.24185900	-0.67982700	0.30210900
H	-0.38348000	-0.54405100	-2.46395800
C	-3.51498400	0.64369100	0.98340800
H	-2.56152400	0.98412400	1.40990000
H	-4.18276600	0.46104600	1.84262800
C	-4.10468200	1.76228100	0.13172800
C	-4.50166500	2.95319500	0.77523600
C	-4.25045100	1.68208100	-1.26503000
C	-4.99790400	4.04299400	0.04701000
H	-4.42023200	3.01975300	1.86301000
C	-4.75040400	2.76980900	-2.00019800
H	-3.98560300	0.76527600	-1.79052500
C	-5.11890100	3.95667400	-1.35027100
H	-5.29469900	4.95554900	0.56902200
H	-4.85398100	2.68386500	-3.08423900
H	-5.50498400	4.80237400	-1.92321500

C	0.51806800	-2.47441800	3.91331700
H	1.38180900	-3.13451300	3.74219300
H	0.89404000	-1.51305500	4.29929100
H	-0.10473200	-2.93098800	4.70729700

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C	-0.28307500	-2.29680300	2.63042600
H	-0.37015700	-3.21476300	2.04728600
C	-1.37956100	-1.37964600	2.54774400
C	-2.51244200	-1.82353100	1.69224400
H	-3.45674900	-1.92129400	2.24812800
H	-2.31400400	-2.73064300	1.11350900
C	-1.76581400	-0.53345800	3.75965900
H	-0.88057600	-0.10512900	4.25342900
H	-2.43152800	0.29166000	3.47939000
H	-2.30554600	-1.15059100	4.50654400
C	-3.90268300	-2.15893100	-1.40559700
C	-4.35054300	-1.51730200	-0.22671700
C	-5.62274100	-1.80151900	0.27262200
C	-6.44032900	-2.71706300	-0.41797700
C	-5.97745300	-3.34820700	-1.58722000
C	-4.69313400	-3.07826800	-2.10101500
C	-2.22451000	-0.70444100	-0.80435900
H	-5.98480500	-1.30781700	1.17938500
H	-7.44211200	-2.93845300	-0.04539200
H	-6.62187700	-4.05651900	-2.11164100
H	-4.33434400	-3.56294600	-3.01092600
N	-2.61327300	-1.69053000	-1.69958300
H	-2.08562700	-1.84401900	-2.56068000
O	-1.21266300	0.00403900	-0.94655800
C	-3.24185900	-0.67982700	0.30210900

C	-3.51498400	0.64369100	0.98340800
H	-2.56152400	0.98412400	1.40990000
H	-4.18276600	0.46104600	1.84262800
C	-4.10468200	1.76228100	0.13172800
C	-4.50166500	2.95319500	0.77523600
C	-4.25045100	1.68208100	-1.26503000
C	-4.99790400	4.04299400	0.04701000
H	-4.42023200	3.01975300	1.86301000
C	-4.75040400	2.76980900	-2.00019800
H	-3.98560300	0.76527600	-1.79052500
C	-5.11890100	3.95667400	-1.35027100
H	-5.29469900	4.95554900	0.56902200
H	-4.85398100	2.68386500	-3.08423900
H	-5.50498400	4.80237400	-1.92321500
C	0.51806800	-2.47441800	3.91331700
H	1.38180900	-3.13451300	3.74219300
H	0.89404000	-1.51305500	4.29929100
H	-0.10473200	-2.93098800	4.70729700

Int1b

C	-3.16558600	0.33869200	1.70048800
H	-3.73053100	1.26041400	1.55214400
C	-3.96735700	-0.90727700	1.65229400
C	-5.46132900	-0.70643100	1.51305900
H	-5.67180000	-0.13923900	0.59053300
H	-5.99934800	-1.66642900	1.47362200
H	-5.86152600	-0.11274600	2.35459500
C	-1.86031000	0.42118800	2.21110600
H	-1.39323800	-0.44599300	2.67971400
H	-1.43788800	1.39330600	2.47623100

Pd	-1.62486200	0.27503200	0.03194000
C	1.32771600	-1.67172200	-0.88182700
C	2.70815100	-1.83744100	-1.16431900
C	0.45280200	-2.73461800	-1.21937000
C	3.20212300	-2.99428300	-1.79722900
C	0.93921100	-3.89905200	-1.85610900
C	2.30338500	-4.01187200	-2.14010400
H	4.26281800	-3.10212100	-2.01781500
H	0.26169300	-4.70608900	-2.12785700
H	2.67478300	-4.91251400	-2.63400300
O	-0.86484000	-2.58243300	-0.89113000
O	3.50229200	-0.79740500	-0.78572300
C	4.90681500	-0.88846000	-0.98153800
H	5.31394200	0.03989200	-0.56332800
H	5.32994200	-1.76027000	-0.45079900
H	5.15758100	-0.96352000	-2.05540300
C	-1.74757100	-3.68821400	-1.05263900
H	-1.36135200	-4.58359400	-0.53253600
H	-2.69255600	-3.36893900	-0.59818600
H	-1.90006900	-3.92991500	-2.11978500
P	0.71169400	-0.16640300	0.01645800
C	1.66780900	-0.37917400	1.60799500
C	2.76686300	0.38687600	2.07925300
C	1.20550000	-1.42362300	2.45447500
C	3.27826400	0.20484000	3.38260900
C	1.71987000	-1.62338100	3.74939700
C	2.74461600	-0.78803300	4.20843000
H	4.11198000	0.81231700	3.73193400
H	1.33041200	-2.41373700	4.38822700
H	3.14612300	-0.92883000	5.21408100

C	1.34980000	1.35304400	-0.83058200
C	1.73573200	1.42199600	-2.19174700
C	1.24299000	2.57831200	-0.12101900
C	2.11090000	2.64641700	-2.78351000
C	1.60767200	3.80529800	-0.70291900
C	2.05192300	3.82340700	-2.03009000
H	2.42222800	2.68447800	-3.82574500
H	1.51460600	4.73380900	-0.14401200
H	2.32996800	4.77272100	-2.49229300
O	0.23078500	-2.22472100	1.91572300
O	3.34194100	1.27075400	1.21008200
O	1.68537100	0.24958400	-2.89870200
O	0.77473300	2.46895900	1.16098600
C	-0.12477900	-3.41993200	2.60594900
H	0.76885600	-4.03271400	2.81724300
H	-0.65128800	-3.19659700	3.55059800
H	-0.79924000	-3.95734900	1.92883100
C	4.08725400	2.36283700	1.73830900
H	3.54804400	2.84754900	2.57043500
H	5.08359900	2.04143400	2.09446000
H	4.19800400	3.06881200	0.90446900
C	2.19244800	0.22336100	-4.22699100
H	3.24409600	0.56149900	-4.26075200
H	2.12734200	-0.82613800	-4.54170400
H	1.58875200	0.85712200	-4.90150800
C	0.60202600	3.65852800	1.93259800
H	1.56581900	4.17920900	2.07530000
H	-0.12687300	4.32308500	1.44525500
H	0.21986100	3.31750800	2.90350400
C	-2.90317200	0.98087600	-1.76435000

H	-2.90204000	2.06992500	-1.67270700
C	-1.70705900	0.37550600	-2.17921100
H	-0.87586800	1.00682800	-2.49555100
H	-1.68853500	-0.65624400	-2.53639300
C	-4.32611200	-1.14866500	-1.85135000
H	-5.37080800	-1.48251600	-1.94506900
H	-3.75446900	-1.53803500	-2.71069400
H	-3.89184600	-1.58674500	-0.93976200
C	-3.07488900	3.68887400	0.63600800
H	-3.40740700	4.73531500	0.55646300
H	-3.85410800	3.03440500	0.20214000
H	-2.96711900	3.43460000	1.70959800
O	-1.84184800	3.58894800	-0.06849100
H	-1.56127500	2.64382100	-0.00649900
C	-4.23609000	0.35909000	-1.77468500
C	-5.35100300	1.12949000	-1.72222800
C	-3.41911100	-2.14454700	1.71073400
H	-6.34955500	0.68706700	-1.75101900
H	-5.28450400	2.21878600	-1.65776000
H	-4.04534400	-3.04023600	1.70865900
H	-2.33810700	-2.26973600	1.72972700

TS1b

C	3.21516600	-0.57242100	1.74528900
H	3.06314800	-1.64015400	1.93399900
C	4.54742600	-0.20018500	1.38856800
C	4.91436700	1.06978400	0.92664500
H	5.95833900	1.37803800	1.03256000
H	4.18458100	1.88205100	0.97409700
C	5.61315600	-1.28197200	1.36379300
H	5.85415900	-1.59425000	0.32841100

H	6.55547300	-0.91897500	1.80871800
H	5.29823200	-2.18200400	1.91475100
C	2.10505300	0.26069200	2.01722600
H	2.26631200	1.33711500	2.13460300
H	1.29319200	-0.15097700	2.62123300
Pd	1.56568800	-0.00303500	-0.07025400
C	-1.55623000	1.74106100	-0.42037100
C	-2.95964000	1.80775000	-0.62126800
C	-0.82593200	2.95245500	-0.48026400
C	-3.60942100	3.02223300	-0.91323200
C	-1.46871900	4.17704500	-0.76751200
C	-2.84924200	4.19602300	-0.98583400
H	-4.68539800	3.05505300	-1.07606800
H	-0.89833700	5.10237300	-0.82227600
H	-3.34358500	5.14335900	-1.21178200
O	0.51864900	2.88070000	-0.23684300
O	-3.61554400	0.61943700	-0.50848800
C	-5.03395800	0.59744100	-0.59619700
H	-5.31509200	-0.44604800	-0.41054300
H	-5.49186400	1.25440200	0.16489800
H	-5.37879800	0.91126400	-1.59835300
C	1.22974700	4.08436600	0.03348500
H	0.73709600	4.65982300	0.83716500
H	2.23009500	3.76335000	0.34875600
H	1.31692200	4.71819700	-0.86668600
P	-0.74356200	0.14540000	0.07898300
C	-1.63264700	-0.11360300	1.70468000
C	-2.60448300	-1.10063700	2.02013800
C	-1.23191500	0.74999400	2.76174800
C	-3.02191300	-1.31406800	3.35157000

C	-1.64553000	0.54709200	4.09271700
C	-2.52645600	-0.50228800	4.37612300
H	-3.75350400	-2.08852000	3.57763200
H	-1.30170100	1.20367000	4.88965800
H	-2.85276500	-0.67040600	5.40458500
C	-1.27783800	-1.19504500	-1.08127900
C	-1.71339900	-0.98553500	-2.41199600
C	-1.01462900	-2.53106700	-0.68440600
C	-2.00519800	-2.07240900	-3.26244400
C	-1.29501800	-3.62239600	-1.52490800
C	-1.80477400	-3.37936000	-2.80574100
H	-2.35959800	-1.90125000	-4.27718600
H	-1.08641800	-4.64013900	-1.20277100
H	-2.01938700	-4.21997500	-3.46862100
O	-0.43608400	1.79759100	2.38664200
O	-3.14651800	-1.80884200	0.98470300
O	-1.79302900	0.31634400	-2.82869500
O	-0.46981500	-2.66869900	0.56620400
C	0.17706500	2.58807100	3.39836400
H	-0.57803800	3.14273900	3.98379700
H	0.78431600	1.96232200	4.07465500
H	0.82579700	3.29325400	2.86507800
C	-3.72981700	-3.07920900	1.25632000
H	-3.08119200	-3.68234600	1.91470700
H	-4.72480700	-2.97702600	1.72779500
H	-3.82689500	-3.56942500	0.27853200
C	-2.35618900	0.59699000	-4.10398400
H	-3.37587900	0.17989200	-4.19179900
H	-2.39388100	1.69196500	-4.17069700
H	-1.72958000	0.19135400	-4.91867700

C	-0.12673600	-3.97800900	1.02168800
H	-1.02558800	-4.61499500	1.10464300
H	0.60361900	-4.43663900	0.33855400
H	0.31531800	-3.83010600	2.01531400
C	5.06907800	0.93193900	-1.20003900
H	5.74107400	1.78842300	-1.30618200
H	5.56781800	-0.04074500	-1.18117400
C	3.79611600	1.02054500	-1.77583700
C	2.97663800	-0.14634500	-1.92047900
H	3.46882500	-1.11248700	-1.78289900
C	1.61230600	-0.16159300	-2.29291800
H	1.15790700	-1.10824000	-2.58820700
H	1.13151000	0.73389400	-2.69179200
C	3.24411300	2.37231200	-2.18227200
H	3.25445800	2.48312500	-3.28286800
H	2.20286700	2.49291900	-1.85564300
H	3.84675500	3.19135900	-1.75754300
C	3.26081000	-3.49052500	-0.26583800
H	3.74816000	-4.37802000	-0.69832500
H	3.97839400	-2.65331900	-0.26253300
H	2.99330700	-3.71625200	0.78714500
O	2.11866900	-3.21102200	-1.06694000
H	1.73767400	-2.36783400	-0.73360000

Int2b

C	3.23240800	0.31936800	-1.83694800
H	3.13620800	1.38234500	-2.08629200
C	4.49289200	-0.14519900	-1.59056700
C	4.74505400	-1.55056500	-1.12664000
H	5.77203700	-1.85349700	-1.39328900
H	4.06149200	-2.26565600	-1.61179900

C	5.69804700	0.76603900	-1.64037300
H	5.41552100	1.79668700	-1.91237600
H	6.21719400	0.80625400	-0.66136900
H	6.45027700	0.41320400	-2.37204400
C	1.97956700	-0.43048700	-1.74967600
H	2.06599400	-1.50227800	-1.99067500
H	1.16463400	0.03129200	-2.31713600
Pd	1.45418800	-0.48804800	0.34743100
C	-1.83869200	0.02484400	1.46897500
C	-2.99490500	-0.78005000	1.64125300
C	-1.43356000	0.82630400	2.57284500
C	-3.64292400	-0.86657600	2.89218600
C	-2.08222000	0.75119000	3.82157700
C	-3.17491600	-0.10893900	3.96999500
H	-4.52266700	-1.49645600	3.01399700
H	-1.74711500	1.35737500	4.66041200
H	-3.68177200	-0.17440500	4.93507500
O	-0.38628200	1.66950900	2.33322500
O	-3.47359900	-1.43885800	0.54199100
C	-4.38399300	-2.51513100	0.72905800
H	-4.01797100	-3.22249200	1.49405300
H	-5.38567600	-2.15446400	1.02839000
H	-4.44450400	-3.01664500	-0.24597400
C	0.07053900	2.51593500	3.39243000
H	-0.73777000	3.19052600	3.72530400
H	0.42431500	1.91528000	4.24805000
H	0.90771800	3.08009000	2.97164700
P	-0.72917500	0.13937600	-0.02329000
C	-1.26340400	-1.13351800	-1.26294500
C	-1.48342300	-0.86452500	-2.63625000

C	-1.25745500	-2.49452100	-0.85958000
C	-1.78978000	-1.90080800	-3.54454800
C	-1.55888300	-3.53502100	-1.75653800
C	-1.83392200	-3.22274500	-3.09421100
H	-1.97444500	-1.67912900	-4.59386500
H	-1.56538400	-4.57221500	-1.42681900
H	-2.06550200	-4.02467000	-3.79814300
C	-1.20890500	1.82256700	-0.63319400
C	-2.57261500	2.12730700	-0.87805000
C	-0.26162700	2.86899100	-0.76653300
C	-2.99705200	3.43143000	-1.19404700
C	-0.68130500	4.18278200	-1.07902400
C	-2.03847500	4.44757400	-1.28292700
H	-4.04813000	3.64903400	-1.37592500
H	0.04131900	4.99188400	-1.15701800
H	-2.35462000	5.46543900	-1.52164300
O	-0.94505800	-2.71883200	0.45671500
O	-1.35883300	0.43968300	-3.02826100
O	-3.42371500	1.06439400	-0.81016300
O	1.05041100	2.54678500	-0.58321800
C	-1.04161600	-4.04517900	0.96377900
H	-2.06106300	-4.44808100	0.83119000
H	-0.31814900	-4.71689100	0.46968400
H	-0.80599800	-3.96807500	2.03273200
C	-1.65838400	0.79075300	-4.37409500
H	-0.95966500	0.30679700	-5.07970400
H	-2.69388800	0.51086400	-4.63938900
H	-1.54259400	1.88110500	-4.42068600
C	-4.82593300	1.29824400	-0.84386800
H	-5.28338700	0.31764600	-0.66618100

H	-5.13094400	2.00790900	-0.05449600
H	-5.14378000	1.69143300	-1.82675100
C	2.02891100	3.57555500	-0.73618600
H	2.99445900	3.07643700	-0.62688200
H	1.95600600	4.03896900	-1.73600900
H	1.91731200	4.34740100	0.04310400
C	4.59740100	-1.71324800	0.43756100
H	5.20891100	-2.59077200	0.72218800
H	5.04620600	-0.83382200	0.92695300
C	3.19535200	-1.93692800	0.93945500
C	2.71593500	-1.15853200	2.03449100
H	3.36741500	-0.35162200	2.37876800
C	1.39214300	-1.15813000	2.52784400
H	1.11568000	-0.42049400	3.27994700
H	0.73403800	-2.02334000	2.43757300
C	2.60248200	-3.29216900	0.58973200
H	3.21035900	-4.10500500	1.03558800
H	1.57052200	-3.38687700	0.94604400
H	2.59497800	-3.44793900	-0.50146600
C	4.13430900	1.95801400	1.41710700
H	4.75717100	1.37295300	2.12303600
H	4.10196000	1.41583200	0.45990400
H	4.62438600	2.93611600	1.26483300
O	2.82445800	2.17846300	1.94080000
H	2.20855400	1.57462100	1.47374000

TS2

C	3.29231600	0.96959800	-1.57321000
H	3.27268100	2.04246000	-1.36380300
C	4.51260000	0.35676700	-1.55088000
C	4.66500300	-1.12845300	-1.66820300

H	5.65032400	-1.37530100	-2.09828900
H	3.89983100	-1.57639700	-2.32122600
C	5.77153800	1.13088900	-1.24570700
H	5.55560600	2.19447000	-1.06039000
H	6.28262700	0.72990500	-0.34711000
H	6.50448100	1.06414300	-2.07286000
C	1.99131200	0.33368500	-1.75616900
H	1.99309700	-0.58010800	-2.37024000
H	1.20208400	1.02571200	-2.07002700
Pd	1.47436600	-0.44094600	0.19617700
C	-1.72764500	-0.35304100	1.53582500
C	-2.82437200	-1.24860300	1.61649900
C	-1.21343500	0.17256300	2.75289300
C	-3.31948200	-1.66646100	2.87082100
C	-1.70379100	-0.23981300	4.00683400
C	-2.75091600	-1.16551200	4.04858300
H	-4.15634000	-2.36020100	2.93052500
H	-1.28619800	0.17306000	4.92349900
H	-3.14605200	-1.49043500	5.01347600
O	-0.22754900	1.09544800	2.60339300
O	-3.37823100	-1.67716800	0.44018600
C	-4.28674100	-2.77037500	0.47130000
H	-3.86003100	-3.63425100	1.01151300
H	-5.24383900	-2.49075100	0.94934500
H	-4.45927500	-3.03493600	-0.58041200
C	0.62993400	1.40873200	3.71182500
H	0.10944800	2.07457600	4.42292000
H	0.93400400	0.48541300	4.23407200
H	1.50515900	1.89219900	3.25403600
P	-0.76346500	0.19978000	0.05083400

C	-1.27110500	-0.79554000	-1.43431200
C	-1.52641900	-0.22423400	-2.70865600
C	-1.22350300	-2.21177200	-1.36020500
C	-1.84344600	-1.03207400	-3.82180700
C	-1.53191400	-3.02650100	-2.46468100
C	-1.85290600	-2.42268700	-3.68612000
H	-2.05965800	-0.57934400	-4.78746000
H	-1.50522200	-4.11132600	-2.38237300
H	-2.09136900	-3.04701100	-4.54952200
C	-1.41165200	1.91899100	-0.17802500
C	-2.80872100	2.12773400	-0.31271100
C	-0.56389700	3.05671600	-0.20160200
C	-3.36031200	3.41861500	-0.41089900
C	-1.11341600	4.35625400	-0.31301800
C	-2.49735100	4.52084700	-0.40689500
H	-4.43519500	3.56160100	-0.50559500
H	-0.46429600	5.22851600	-0.32766900
H	-2.91234400	5.52804400	-0.48747100
O	-0.84294900	-2.72630800	-0.14907600
O	-1.42464500	1.13369600	-2.79840300
O	-3.56284100	0.99299300	-0.37694100
O	0.76974400	2.83178600	-0.12556900
C	-0.92125500	-4.13298700	0.05364800
H	-1.94283600	-4.50415600	-0.14127500
H	-0.20734600	-4.67121400	-0.59063100
H	-0.66219100	-4.29292200	1.10955000
C	-1.79964800	1.78536100	-4.00780000
H	-1.12830100	1.50406700	-4.83852600
H	-2.84168100	1.54407700	-4.28337300
H	-1.70676600	2.85784800	-3.79601900

C	-4.98007100	1.10210600	-0.34768100
H	-5.34582500	0.06892300	-0.31830800
H	-5.31964200	1.65082000	0.54861700
H	-5.36153100	1.61296100	-1.25049500
C	1.65392200	3.95827100	-0.07143000
H	2.63743600	3.52547800	0.12888200
H	1.62586500	4.51708400	-1.02434100
H	1.37726600	4.62946600	0.75919500
C	4.58087600	-1.83853600	-0.25210200
H	5.12748800	-2.79617900	-0.35074200
H	5.12243000	-1.22257500	0.48085500
C	3.19521600	-2.14552300	0.22882000
C	2.77721000	-1.69787000	1.51287400
H	3.47925000	-1.05856800	2.05047400
C	1.47844700	-1.83367100	2.04409200
H	1.24442900	-1.38412400	3.00873900
H	0.79102800	-2.60017600	1.68816500
C	2.47273000	-3.28749400	-0.48637000
H	2.30017000	-4.12288600	0.21414300
H	1.48110300	-2.99595400	-0.89063600
H	3.08683800	-3.65630900	-1.32614400
C	4.17644200	1.39629800	2.20456100
H	4.00419500	0.72504800	3.08199900
H	4.68070300	0.79637200	1.41848000
H	4.89807800	2.17265300	2.53750400
O	3.01932900	2.03860900	1.75167000
H	2.18529700	1.00089400	1.01969100

Int3b

C	3.29249300	0.97321000	-1.57113700
H	3.27232500	2.04584500	-1.36062000

C	4.51304900	0.36090700	-1.54915500
C	4.66615000	-1.12412200	-1.66798600
H	5.65168400	-1.37007800	-2.09809400
H	3.90133500	-1.57173100	-2.32165600
C	5.77156500	1.13527900	-1.24287800
H	5.55510900	2.19856900	-1.05650700
H	6.28262200	0.73359100	-0.34457700
H	6.50473400	1.06972300	-2.06992600
C	1.99182000	0.33690100	-1.75506600
H	1.99416300	-0.57625200	-2.37008700
H	1.20235400	1.02889800	-2.06839200
Pd	1.47476100	-0.43999200	0.19635000
C	-1.72760700	-0.35492400	1.53532900
C	-2.82394900	-1.25106400	1.61481100
C	-1.21392300	0.16964600	2.75306400
C	-3.31916700	-1.67045000	2.86858000
C	-1.70439000	-0.24425500	4.00646000
C	-2.75110700	-1.17046900	4.04699700
H	-4.15572600	-2.36462900	2.92736400
H	-1.28720000	0.16785300	4.92365200
H	-3.14632500	-1.49657300	5.01145800
O	-0.22841800	1.09313000	2.60475800
O	-3.37733600	-1.67865600	0.43792200
C	-4.28536000	-2.77230400	0.46768300
H	-3.85838800	-3.63654900	1.00709900
H	-5.24269700	-2.49360900	0.94579100
H	-4.45752500	-3.03584900	-0.58434400
C	0.62866100	1.40564800	3.71371900
H	0.10770600	2.07051800	4.42538200
H	0.93302400	0.48192400	4.23507800

H	1.50377600	1.88998600	3.25664100
P	-0.76332500	0.19987500	0.05114200
C	-1.27016300	-0.79412900	-1.43515800
C	-1.52543300	-0.22161400	-2.70896800
C	-1.22194000	-2.21041600	-1.36251200
C	-1.84183200	-1.02843900	-3.82303400
C	-1.52972100	-3.02413500	-2.46790800
C	-1.85069600	-2.41919600	-3.68879500
H	-2.05801900	-0.57480200	-4.78826700
H	-1.50255900	-4.10903300	-2.38672200
H	-2.08867300	-3.04273000	-4.55290200
C	-1.41223300	1.91903100	-0.17608300
C	-2.80936400	2.12728300	-0.31088400
C	-0.56498600	3.05716200	-0.19827600
C	-3.36151400	3.41801700	-0.40786100
C	-1.11506500	4.35656700	-0.30847200
C	-2.49905200	4.52063300	-0.40250600
H	-4.43643900	3.56061700	-0.50266300
H	-0.46633500	5.22913600	-0.32206200
H	-2.91448000	5.52772600	-0.48213300
O	-0.84144100	-2.72603900	-0.15182900
O	-1.42425100	1.13645500	-2.79727900
O	-3.56295700	0.99227000	-0.37647300
O	0.76873800	2.83275400	-0.12216000
C	-0.91916000	-4.13296300	0.04941400
H	-1.94052700	-4.50439000	-0.14613700
H	-0.20485600	-4.67019800	-0.59525500
H	-0.66027400	-4.29387900	1.10521100
C	-1.79926100	1.78920800	-4.00608700
H	-1.12759000	1.50908000	-4.83694600

H	-2.84112000	1.54774000	-4.28215800
H	-1.70691300	2.86151600	-3.79316900
C	-4.98024300	1.10071300	-0.34743600
H	-5.34553700	0.06733500	-0.31922400
H	-5.32027400	1.64834200	0.54935100
H	-5.36171900	1.61233500	-1.24980900
C	1.65239500	3.95958100	-0.06664000
H	2.63605700	3.52702400	0.13345500
H	1.62431200	4.51937200	-1.01897600
H	1.37523900	4.62978700	0.76461600
C	4.58200700	-1.83571400	-0.25264400
H	5.12907500	-2.79300800	-0.35214900
H	5.12311000	-1.22027200	0.48108200
C	3.19637200	-2.14382600	0.22763000
C	2.77786000	-1.69769700	1.51204900
H	3.47948400	-1.05863800	2.05048000
C	1.47903200	-1.83463600	2.04281700
H	1.24458300	-1.38619800	3.00787600
H	0.79204400	-2.60108000	1.68593000
C	2.47457100	-3.28537900	-0.48891900
H	2.30222200	-4.12157600	0.21068500
H	1.48290800	-2.99386600	-0.89311700
H	3.08904400	-3.65304300	-1.32893000
C	4.17553100	1.39638100	2.20728500
H	4.00337900	0.72414100	3.08398400
H	4.68024900	0.79750000	1.42070100
H	4.89673800	2.17271500	2.54120600
O	3.01823600	2.03864000	1.75478700
H	2.09413600	0.81719100	0.91611800

TS3b

C	3.34421600	1.04012400	1.98176700
H	3.12464600	0.10122500	2.49867200
C	3.66138000	0.88573500	0.53460700
C	3.92596700	2.19806500	-0.20993300
H	4.86178900	2.64835400	0.17521400
H	3.11542500	2.90799300	0.02765900
C	4.70523500	-0.22833100	0.29583800
H	5.44029400	-0.26534700	1.14653700
H	4.21393500	-1.22145700	0.17153900
H	5.28876100	-0.03496300	-0.63954400
C	3.33531600	2.18002100	2.70479400
H	3.56128000	3.15141800	2.26066400
H	3.09555400	2.16637200	3.76831700
Pd	1.25475800	-1.11708900	-0.67670900
C	-2.22126900	-1.17185700	-0.34989800
C	-3.51909700	-0.68204200	-0.66343400
C	-2.02668300	-2.57869200	-0.41544400
C	-4.52187800	-1.54879700	-1.14521000
C	-3.02223500	-3.44748700	-0.90077400
C	-4.26044300	-2.91859900	-1.27549300
H	-5.50759200	-1.15979900	-1.39619200
H	-2.82945500	-4.51862800	-0.95041800
H	-5.04463400	-3.58247900	-1.64547000
O	-0.83055100	-3.04663200	0.04761300
O	-3.75342900	0.65161700	-0.47487900
C	-4.83724200	1.25797200	-1.17124200
H	-4.67253600	2.33991000	-1.08174600
H	-4.84029200	0.96562200	-2.23582500
H	-5.81080800	0.98697100	-0.72305300
C	-0.22443200	-4.18098900	-0.60125800

H	-0.47837500	-4.19247600	-1.67324500
H	0.85863700	-4.03636100	-0.48681600
H	-0.56425000	-5.11885600	-0.12860200
P	-0.69354900	-0.18326600	0.05371400
C	-1.01168700	1.58654900	-0.35436600
C	-0.63841200	2.65656400	0.49916200
C	-1.50166500	1.91857700	-1.64196300
C	-0.84971400	3.99893700	0.11740100
C	-1.72401700	3.25238000	-2.02854000
C	-1.40059900	4.28134900	-1.13601800
H	-0.57097400	4.81158000	0.78519800
H	-2.11324300	3.48949100	-3.01664200
H	-1.55866500	5.32009900	-1.43280200
C	-0.63115000	-0.40698800	1.89741800
C	-1.65061500	0.08351300	2.75080800
C	0.40817200	-1.16610200	2.48171100
C	-1.62533800	-0.15373400	4.13815900
C	0.44586800	-1.41405800	3.86884300
C	-0.57085200	-0.90096200	4.67969800
H	-2.40978400	0.23506500	4.78521200
H	1.25792400	-1.99222400	4.30448200
H	-0.54318500	-1.08772700	5.75519100
O	-1.73437500	0.85502700	-2.47631900
O	-0.04556600	2.31146100	1.67387300
O	-2.62856800	0.79685100	2.12642300
O	1.37843300	-1.64418700	1.63954700
C	-2.14465200	1.11048100	-3.81649200
H	-3.12041000	1.62695000	-3.84323500
H	-1.39557600	1.72061600	-4.35092300
H	-2.23200600	0.12381100	-4.28770400

C	0.18906700	3.31783900	2.65444600
H	0.93900100	4.04716500	2.30484500
H	-0.74917600	3.84323800	2.90945700
H	0.58130300	2.78321700	3.52621800
C	-3.75451900	1.23012400	2.87978800
H	-4.26495600	0.37682300	3.36073600
H	-3.46032300	1.95942900	3.65622700
H	-4.42212900	1.70500600	2.15097400
C	2.31200900	-2.63727500	2.09426000
H	3.01769300	-2.19309900	2.81322600
H	1.76922200	-3.47429200	2.56817600
H	2.82133700	-2.95718700	1.17766700
C	4.04651600	2.09355200	-1.76363800
H	4.29095600	3.09874800	-2.14826200
H	4.88478300	1.43040600	-2.02468100
C	2.76031100	1.57544500	-2.36163100
C	2.61034000	0.23639500	-2.56526400
H	3.49794000	-0.38712600	-2.42858500
C	1.34785600	-0.49856600	-2.67969600
H	1.39386100	-1.44635300	-3.23415700
H	0.46148400	0.09080200	-2.92547200
C	1.64763000	2.58185700	-2.49378400
H	2.00795300	3.48326400	-3.02040200
H	0.78448000	2.18565600	-3.03873800
H	1.28714000	2.91935600	-1.50736400
C	3.05628500	-3.16896000	-2.15047200
H	3.87512500	-3.90323600	-2.00107600
H	2.20175000	-3.71890400	-2.61993100
H	3.42297000	-2.44062000	-2.90998400
O	2.72477600	-2.58019400	-0.93299900

H	2.37373300	0.30382400	-0.02343400
TS4b			
C	3.12194500	1.85924700	-1.60274300
H	3.59669100	2.85020000	-1.53685100
C	4.01227800	0.76950800	-1.32907200
C	3.50293000	-0.64877200	-1.53701300
H	3.65609000	-0.95177200	-2.59513400
H	2.41822600	-0.67926900	-1.36076400
C	5.49280400	0.97724100	-1.62207100
H	5.74261700	0.77882000	-2.68725700
H	5.80002500	2.01532900	-1.40378500
H	6.12911000	0.30606600	-1.02109800
C	1.74293300	1.84219200	-1.76034800
H	1.21547200	0.94097400	-2.06218600
H	1.18651000	2.77738000	-1.84618900
Pd	1.25942000	0.41312500	0.66445700
C	-1.63795300	-1.44681500	0.99620300
C	-2.32316300	-2.54496300	0.41880200
C	-1.40499000	-1.48504400	2.39631400
C	-2.62152900	-3.69276400	1.18141000
C	-1.70283000	-2.62452300	3.16732100
C	-2.29555900	-3.72754600	2.54281000
H	-3.13187500	-4.53798000	0.72133200
H	-1.49097200	-2.63888900	4.23533300
H	-2.53189800	-4.61738300	3.12999600
O	-0.88278100	-0.34174600	2.93509100
O	-2.70981200	-2.42488500	-0.88692300
C	-2.88933400	-3.61551700	-1.64982400
H	-2.91113500	-3.29058200	-2.69858500
H	-2.05189500	-4.31584200	-1.49039300

H	-3.83864100	-4.12194400	-1.39610400
C	-0.13614200	-0.43244800	4.15017100
H	0.60348800	-1.24813500	4.09544600
H	0.37999300	0.53056400	4.24699900
H	-0.80375400	-0.59294000	5.01521100
P	-0.87151300	-0.00596900	0.11953000
C	-1.04451600	-0.21395900	-1.71548800
C	-1.52005700	0.80551200	-2.58549800
C	-0.44043800	-1.34611500	-2.32611000
C	-1.46042200	0.66073000	-3.98745000
C	-0.37065600	-1.49393700	-3.72326700
C	-0.89288600	-0.48786500	-4.54314400
H	-1.83971800	1.44566800	-4.63837800
H	0.09076700	-2.37340100	-4.16737800
H	-0.83964100	-0.59331600	-5.62837600
C	-1.98140500	1.38552500	0.64179700
C	-3.39392600	1.25241000	0.60185300
C	-1.45080200	2.62596200	1.06075100
C	-4.24285700	2.28958100	1.03453000
C	-2.29157100	3.67991300	1.47442400
C	-3.67777000	3.49561000	1.46815200
H	-5.32468700	2.17034100	1.00942000
H	-1.86037700	4.62209000	1.80995100
H	-4.33043300	4.30552600	1.80104300
O	0.06121800	-2.28715800	-1.46647500
O	-2.00690500	1.93706400	-1.99675700
O	-3.85350300	0.08838900	0.06337100
O	-0.08766700	2.76979000	1.04413600
C	0.88555700	-3.32402200	-1.99796700
H	0.30595700	-3.99614400	-2.65529900

H	1.73606200	-2.89918200	-2.55696400
H	1.25093400	-3.88036900	-1.12622300
C	-2.39581400	3.03767500	-2.81060400
H	-2.69805700	3.82175700	-2.10447900
H	-1.55438400	3.38898100	-3.43378100
H	-3.24703100	2.77483000	-3.46435700
C	-5.25195600	-0.17191000	0.05877000
H	-5.79310000	0.56418000	-0.56301400
H	-5.35370500	-1.17515800	-0.37235700
H	-5.66510400	-0.15468600	1.08295300
C	0.44978200	4.07061700	0.78508500
H	-0.14345400	4.58912500	0.01335000
H	0.47324600	4.68290500	1.70369400
H	1.46685100	3.89221300	0.41994800
C	4.15254100	-1.81005800	-0.69183900
H	3.56560100	-2.71312900	-0.93680900
H	5.17126500	-1.98670600	-1.07591500
C	4.22575100	-1.65982300	0.81509800
C	3.13433800	-1.62211200	1.63679400
H	3.32853900	-1.42813900	2.69743200
C	1.73898400	-1.62942800	1.23471400
H	1.03276000	-1.90954000	2.02193400
H	1.52208900	-2.14719300	0.29803500
C	5.60067500	-1.41632600	1.38845200
H	5.98245300	-0.43758600	1.04399700
H	5.58870700	-1.40271400	2.48987400
H	6.32867000	-2.17707500	1.04949200
C	3.50241100	2.44948600	1.61855300
H	2.65516000	2.75150500	2.25511400
H	4.44251400	2.57678500	2.18904100

H	3.53492000	3.10950200	0.73111900
O	3.32550800	1.08910400	1.23954400
H	3.75794900	0.97210300	0.20966200
Int4b			
C	0.51562900	-1.90084400	-2.45286600
H	1.27006500	-1.29281800	-2.96274100
C	0.99338900	-2.77324500	-1.41784800
C	0.20862400	-3.97805300	-0.92699300
H	0.78773100	-4.88617700	-1.18187600
H	-0.75693700	-4.04360400	-1.45317100
C	2.49379700	-2.90726800	-1.25319300
H	2.85002700	-3.83603400	-1.74200700
H	3.03389000	-2.06559800	-1.70493500
H	2.77450500	-2.97732000	-0.19478100
C	-0.82669800	-1.59568600	-2.71050400
H	-1.63656400	-2.26848400	-2.42840500
H	-1.07249700	-0.82583500	-3.44047300
Pd	-0.16248200	-0.98680900	-0.53548100
C	-2.77263200	0.23872800	1.69992000
C	-4.00596600	-0.29125500	2.16786600
C	-1.88880400	0.76683900	2.68210000
C	-4.25340500	-0.46075000	3.54603600
C	-2.12869600	0.59985500	4.06224500
C	-3.30138000	-0.03547900	4.47795000
H	-5.19352800	-0.88933300	3.88912800
H	-1.41674100	0.96360300	4.79922800
H	-3.49040400	-0.17436700	5.54443900
O	-0.82250900	1.46674700	2.19757300
O	-4.96194600	-0.57768600	1.23285300
C	-6.07205700	-1.38418100	1.60616000

H	-6.57146600	-1.64474400	0.66372400
H	-5.74596100	-2.30245900	2.12524300
H	-6.77073400	-0.83353100	2.26304500
C	0.11835200	1.99715400	3.13537100
H	0.61409400	1.18216600	3.69019800
H	0.85351600	2.54289000	2.53829700
H	-0.38264000	2.67941900	3.84427300
P	-2.12777000	0.27043600	-0.05359000
C	-3.39646400	-0.56321600	-1.12870800
C	-3.93660400	0.00091900	-2.30914700
C	-3.71857500	-1.91862100	-0.85535200
C	-4.84260900	-0.71556600	-3.12031600
C	-4.60861200	-2.64855900	-1.66415700
C	-5.17660800	-2.02992500	-2.78588900
H	-5.26127900	-0.25701100	-4.01446000
H	-4.85157000	-3.68367400	-1.43229500
H	-5.86927500	-2.58956600	-3.41759400
C	-2.23097900	2.09156500	-0.39868200
C	-3.37208100	2.85976100	-0.03622000
C	-1.13339400	2.77968400	-0.94651500
C	-3.36891900	4.26328900	-0.13326300
C	-1.12594800	4.18345200	-1.06539200
C	-2.23621700	4.91770900	-0.64223500
H	-4.24350800	4.84013600	0.16470200
H	-0.24592000	4.67040700	-1.48699500
H	-2.23326900	6.00726800	-0.71675300
O	-3.10919800	-2.45530100	0.24631400
O	-3.50013600	1.25472400	-2.64625200
O	-4.46278500	2.14113900	0.35501500
O	-0.02116900	2.08418800	-1.37628700

C	-3.47721200	-3.77027500	0.65653500
H	-4.56591000	-3.84052900	0.82271000
H	-3.17110400	-4.52000900	-0.09335700
H	-2.93785900	-3.94665600	1.59368400
C	-4.23554600	2.01207200	-3.60221000
H	-3.80435100	3.02089200	-3.56522100
H	-4.12653900	1.59547300	-4.61992700
H	-5.30697600	2.04865200	-3.33809500
C	-5.54815300	2.81832500	0.97865300
H	-6.07023800	3.48325700	0.26642600
H	-6.22637000	2.02472200	1.31493700
H	-5.20182400	3.41262800	1.84233500
C	0.01992900	1.94405900	-2.80920900
H	0.02709400	2.93738800	-3.29510200
H	0.95360900	1.41456700	-3.02350800
H	-0.85527100	1.37252200	-3.15653100
C	-0.09632800	-4.03021400	0.62234300
H	-0.89889200	-3.30807000	0.80542800
H	-0.47898600	-5.04326300	0.84254900
C	1.09699100	-3.69817000	1.47383800
C	1.36673600	-2.40162800	1.79030400
H	2.34670200	-2.20624400	2.24002300
C	0.49100200	-1.24157400	1.51609900
H	0.93915100	-0.29815600	1.85051000
H	-0.50228300	-1.35391500	1.97984300
C	2.05961100	-4.82346700	1.76470100
H	2.35066300	-5.33844000	0.82671600
H	2.97656100	-4.45614400	2.24668900
H	1.59956900	-5.59660700	2.41017900
C	3.76625600	0.01927100	-2.96666100

H	4.34398000	0.82972800	-3.43191500
H	4.48134200	-0.66805900	-2.47967300
H	3.21663800	-0.53191200	-3.75438800
O	2.88938100	0.64233600	-2.02880900
H	2.27959200	-0.02402200	-1.65205500
C	6.75564700	-0.67798100	-0.32983400
C	5.69306700	0.23907100	-0.17026500
C	5.76852600	1.49266600	-0.77980400
C	6.91737500	1.81786600	-1.53083200
C	7.96592200	0.89437400	-1.67502900
C	7.89911600	-0.37850600	-1.07585200
C	5.21476200	-1.79673700	1.00636800
H	4.94476800	2.19704700	-0.68790100
H	6.98906300	2.79736000	-2.00754100
H	8.84752400	1.16015500	-2.26237600
H	8.70902000	-1.10162000	-1.19130100
N	6.44058300	-1.86512000	0.35137200
H	7.05958500	-2.66141400	0.45789600
O	4.76025300	-2.66859600	1.73804200
C	4.60664800	-0.41760800	0.65626100
H	3.70773300	-0.57892200	0.04169700
C	4.16309900	0.32866500	1.94806100
H	4.99478200	0.32148700	2.67047300
H	3.33770900	-0.25288600	2.38643200
C	3.74480400	1.75530600	1.66203600
C	2.64552500	2.03412500	0.82623900
C	4.50686300	2.82796600	2.16149600
C	2.32975300	3.35838000	0.48718100
H	2.03215000	1.22382200	0.43049000
C	4.18478000	4.15521900	1.83761500

H	5.36986100	2.61469600	2.79744400
C	3.09624200	4.42240200	0.99230500
H	1.48291700	3.54270900	-0.17097600
H	4.78851400	4.97443900	2.23525900
H	2.84672200	5.45259700	0.72690000
TS5b			
C	0.84067300	-0.81083200	-2.91723700
H	1.24522600	-0.01738300	-3.56145900
C	1.82347200	-1.65843200	-2.32462100
C	1.36882400	-2.95288000	-1.63045100
H	2.24711300	-3.60999400	-1.51412400
H	0.67638600	-3.48713700	-2.31011400
C	3.17587400	-1.77643400	-3.03052500
H	3.17865500	-2.58153500	-3.79419100
H	3.44251800	-0.83528600	-3.54044000
H	3.98387100	-2.00349500	-2.31658700
C	-0.51812100	-0.71009300	-2.58675900
H	-1.04056200	-1.58766300	-2.20269900
H	-1.14277800	0.00590400	-3.12169200
Pd	-0.14833800	0.13719700	-0.28382200
C	-2.90308900	0.64637800	1.76023500
C	-3.80564900	-0.05502100	2.59940600
C	-2.21792200	1.75534200	2.32264800
C	-3.91006300	0.26343200	3.96983800
C	-2.31322800	2.07940600	3.68797900
C	-3.15431900	1.31432500	4.50329000
H	-4.59614900	-0.29078100	4.60889800
H	-1.75752800	2.92277400	4.09549000
H	-3.24240400	1.55465800	5.56485600
O	-1.47713000	2.48488900	1.43737200

O	-4.57449700	-1.03107500	2.02841600
C	-5.06181500	-2.07932600	2.86210300
H	-5.38042800	-2.87505100	2.17543100
H	-4.26791500	-2.45545100	3.52930000
H	-5.92049400	-1.74658400	3.47374100
C	-0.37091100	3.24468000	1.91875700
H	0.23728400	2.65112700	2.62049000
H	0.21948100	3.48520500	1.02717300
H	-0.71014100	4.17222500	2.41420100
P	-2.36183000	0.22010000	0.03559800
C	-3.06506400	-1.43120400	-0.43203300
C	-3.68530300	-1.70741300	-1.67853000
C	-2.75435300	-2.54392700	0.39599300
C	-4.04630000	-3.02239600	-2.04159100
C	-3.11658900	-3.85750800	0.04409800
C	-3.76754000	-4.08203500	-1.17358800
H	-4.53040400	-3.21756900	-2.99630300
H	-2.87883200	-4.69120400	0.70182500
H	-4.04532800	-5.09891400	-1.45815700
C	-3.22187800	1.54332700	-0.94049800
C	-4.63809100	1.63935400	-0.89297500
C	-2.52661400	2.47424300	-1.75020700
C	-5.34279200	2.59813600	-1.64367200
C	-3.22755300	3.43099500	-2.51827400
C	-4.62254100	3.48172600	-2.45717700
H	-6.42938100	2.65024000	-1.60385800
H	-2.68399900	4.14227700	-3.13749900
H	-5.15908900	4.22876200	-3.04621100
O	-2.07947100	-2.25155200	1.54538200
O	-3.89100500	-0.64133000	-2.50833800

O	-5.24760700	0.71395000	-0.10248500
O	-1.16054500	2.42534900	-1.74827900
C	-1.57702000	-3.31424500	2.35318500
H	-2.40541100	-3.87962400	2.81717700
H	-0.94775000	-3.99464700	1.75967000
H	-0.96512000	-2.82776500	3.12045600
C	-4.35790000	-0.87233200	-3.83280800
H	-4.38396000	0.11806300	-4.30472400
H	-3.67157100	-1.53907600	-4.38369100
H	-5.37203000	-1.31168000	-3.83268200
C	-6.66722600	0.67781400	-0.03931600
H	-7.10386300	0.48274600	-1.03542300
H	-6.90042500	-0.14585300	0.64557700
H	-7.07521500	1.62545300	0.35583100
C	-0.45638000	2.97911800	-2.85958800
H	-0.89512700	2.63885900	-3.81327400
H	-0.46054900	4.08350400	-2.82942600
H	0.56959600	2.60706100	-2.76379400
C	0.63100600	-2.89933200	-0.24423100
H	-0.22657100	-2.21916200	-0.30740300
H	0.22249900	-3.91844500	-0.10051300
C	1.47791800	-2.56089500	0.96370900
C	1.35927200	-1.45349100	1.74330800
H	2.12590900	-1.35041800	2.52441000
C	0.37039700	-0.32465000	1.71396300
H	0.81222500	0.57661200	2.16979400
H	-0.56701600	-0.55858500	2.23361000
C	2.53157200	-3.60443100	1.28392000
H	3.26561400	-3.69675300	0.46320700
H	3.07381400	-3.36895300	2.21023800

H	2.06325700	-4.60206500	1.39232400
C	2.48145600	1.42527500	-1.18980800
H	1.83346800	2.26669700	-0.90226700
H	3.51480900	1.67570500	-0.90758200
H	2.42558100	1.28599200	-2.28609500
O	2.04697200	0.24563600	-0.51215100
H	2.09162700	-0.63601500	-1.27388900
C	5.99196800	-1.84180100	-0.05673300
C	5.57162100	-0.49347900	-0.14435400
C	5.85629700	0.22963600	-1.30327400
C	6.54688300	-0.39889000	-2.36062700
C	6.93865900	-1.74241100	-2.25847300
C	6.66582300	-2.48873500	-1.09594000
C	4.98033200	-1.41493700	1.98820100
H	5.54974200	1.27056300	-1.39286600
H	6.76751200	0.16295600	-3.26999400
H	7.46093200	-2.22140800	-3.08905000
H	6.97278300	-3.53290200	-1.00980400
N	5.63343000	-2.35241200	1.19886300
H	5.80513400	-3.29936400	1.51717600
O	4.60613200	-1.59319600	3.14266600
C	4.83528000	-0.13791600	1.13141100
H	3.75642200	-0.02126600	0.91705300
C	5.33486000	1.09560300	1.93370300
H	6.43372800	1.05394900	2.00447900
H	4.92872000	0.98909600	2.95235500
C	4.89582600	2.41519900	1.33790000
C	3.60752500	2.91884700	1.60492700
C	5.74518400	3.14989700	0.48911100
C	3.17918200	4.12616800	1.03532900

H	2.93650300	2.34790400	2.25092200
C	5.31427800	4.35082600	-0.09713600
H	6.74773500	2.76836300	0.28286400
C	4.02815600	4.84346000	0.17599200
H	2.18348300	4.51174200	1.26199900
H	5.98514700	4.90509000	-0.75746700
H	3.69299600	5.78260400	-0.26958900

Int5b

C	-0.11809700	-2.96151400	-2.11729900
H	0.03482900	-1.97786200	-2.57171400
C	1.15807700	-3.61478000	-1.62937000
C	0.93591500	-4.77028900	-0.63542800
H	1.87689600	-5.33432200	-0.52807600
H	0.19404200	-5.48380500	-1.03485300
C	1.98380800	-4.08852200	-2.84993000
H	1.46670700	-4.91133100	-3.37343400
H	2.13675100	-3.26719400	-3.56924500
H	2.97533500	-4.44748600	-2.52576300
C	-1.36276000	-3.46611400	-2.10058400
H	-1.58857000	-4.43887700	-1.65639300
H	-2.20942000	-2.91138500	-2.50679900
Pd	0.05422600	-0.30583400	-0.20195800
C	-2.69856300	0.70055800	1.77416800
C	-3.92880400	0.30121000	2.35891400
C	-1.76508300	1.37237300	2.61058200
C	-4.14500800	0.41326200	3.74671600
C	-1.97441200	1.48670500	4.00021800
C	-3.15694500	0.98768500	4.55474900
H	-5.08523500	0.08256400	4.18548500
H	-1.23526400	1.97203700	4.63389500

H	-3.32422100	1.07363400	5.63039700
O	-0.68205600	1.90847200	1.97844600
O	-4.89834600	-0.15683800	1.51233100
C	-5.92867600	-0.98648100	2.04294900
H	-6.41795100	-1.43912200	1.17084900
H	-5.50736600	-1.77578500	2.68905900
H	-6.66284400	-0.39869800	2.62361300
C	0.43764900	2.32397400	2.77091900
H	0.79610000	1.49113800	3.39942100
H	1.20882000	2.61845300	2.05324600
H	0.16731900	3.18216400	3.41010300
P	-2.12245900	0.30892200	0.06129700
C	-3.33169100	-0.87263100	-0.71087500
C	-3.97281800	-0.68062700	-1.96239600
C	-3.54373400	-2.12032000	-0.06521300
C	-4.80823500	-1.67234800	-2.52016900
C	-4.38646500	-3.10811500	-0.60494100
C	-5.01237700	-2.87233100	-1.83305500
H	-5.29334500	-1.50948600	-3.48038100
H	-4.53896800	-4.05225100	-0.08642400
H	-5.65776100	-3.63851500	-2.26670300
C	-2.24636600	1.92164200	-0.84440400
C	-3.26908700	2.88251800	-0.61972000
C	-1.25246700	2.24076100	-1.78461300
C	-3.23396800	4.13693300	-1.26013600
C	-1.21672600	3.47591100	-2.45083800
C	-2.20538700	4.42453100	-2.16956900
H	-4.00838500	4.87759600	-1.06641700
H	-0.41452300	3.67760300	-3.16095600
H	-2.18186700	5.39836100	-2.66245500

O	-2.90459300	-2.27401400	1.13158300
O	-3.72809600	0.50380300	-2.60449600
O	-4.27926700	2.48761700	0.20257300
O	-0.24673800	1.31375500	-2.07171700
C	-2.98531700	-3.52985500	1.80548000
H	-4.02268400	-3.74252600	2.11843100
H	-2.61576800	-4.34525800	1.16257800
H	-2.33843300	-3.42816000	2.68492900
C	-4.39786600	0.78719400	-3.82916600
H	-4.06853200	1.79591100	-4.10894300
H	-4.11685300	0.06617200	-4.61762500
H	-5.49409500	0.77039100	-3.69735100
C	-5.25134100	3.44481200	0.61279400
H	-5.85349200	3.79610200	-0.24458100
H	-5.89234100	2.91562300	1.32850200
H	-4.77351800	4.31200100	1.10131400
C	-0.41690600	0.66284000	-3.35377500
H	-0.49533800	1.41836100	-4.15319700
H	0.48123700	0.05304400	-3.49404400
H	-1.31959300	0.03497700	-3.33698400
C	0.47928100	-4.26672700	0.75807100
H	-0.43994100	-3.68231400	0.62318300
H	0.23746100	-5.14835900	1.38449900
C	1.54612900	-3.44043900	1.44789600
C	1.38580400	-2.13373300	1.79578400
H	2.25317000	-1.62287200	2.21936200
C	0.16800900	-1.33781700	1.64492800
H	0.12304700	-0.49266300	2.34473000
H	-0.76132600	-1.90914600	1.66623300
C	2.86728900	-4.13308400	1.69493400

H	3.39702400	-4.32081900	0.74213400
H	3.52356700	-3.52510100	2.33337500
H	2.71558100	-5.12239300	2.16662700
C	2.53341800	-0.39515400	-1.86628800
H	2.28289600	0.64261400	-2.18524100
H	3.63865500	-0.48306900	-1.90903300
H	2.12615300	-1.09062200	-2.63975200
O	2.08727600	-0.70443700	-0.57619800
H	1.73092700	-2.82539100	-1.11373900
C	6.59688100	-0.71576600	0.16660400
C	5.65176000	0.31014100	-0.06726800
C	5.83493300	1.17777400	-1.14567000
C	6.96266200	1.01115200	-1.97687400
C	7.88691000	-0.01782200	-1.73128400
C	7.71600100	-0.90365700	-0.64933500
C	5.05330500	-0.92112800	1.89132900
H	5.11145900	1.96945000	-1.33883000
H	7.11565100	1.68659600	-2.82094800
H	8.75295600	-0.13799000	-2.38588200
H	8.43360500	-1.70379900	-0.45579700
N	6.20485700	-1.43967800	1.30379000
H	6.73266700	-2.19408200	1.72888200
O	4.56207000	-1.31551000	2.94699800
C	4.55881900	0.20478100	0.97066100
H	3.61294800	-0.15832900	0.49839100
C	4.24290800	1.48838200	1.77822100
H	5.14448100	1.80977600	2.32566400
H	3.48995700	1.20728100	2.53428400
C	3.73563600	2.63184600	0.91958500
C	2.64936700	2.44192700	0.03965500

C	4.34203900	3.90026700	0.98142200
C	2.17619500	3.50166400	-0.74742800
H	2.18802400	1.45489500	-0.03174500
C	3.87148800	4.96315100	0.19223300
H	5.19398300	4.05173400	1.64968900
C	2.78438800	4.76675000	-0.67428600
H	1.33150600	3.32913700	-1.41430700
H	4.35691000	5.94032000	0.25248900
H	2.41601000	5.59161100	-1.28923300

TS6b

C	-0.04361600	3.45353300	1.17704600
H	-0.67823700	2.85990000	0.51518100
C	1.19118200	4.02696600	0.52135500
C	0.78385500	4.80038500	-0.76477900
H	1.63114300	5.42619200	-1.08844700
H	-0.04910700	5.48762700	-0.53308600
C	2.03299400	4.90901800	1.45631300
H	1.46011600	5.79096100	1.79051400
H	2.34984000	4.34885400	2.35070300
H	2.93650500	5.26131500	0.93390600
C	-0.44355900	3.61201300	2.45103700
H	0.13252700	4.19752300	3.17288900
H	-1.37750800	3.16431900	2.79769600
Pd	0.20544000	0.42185400	-0.10902700
C	-2.82944100	-0.88997300	-1.44541600
C	-4.13867100	-0.51208400	-1.84139000
C	-2.09095200	-1.72643700	-2.32614500
C	-4.62096700	-0.81521500	-3.13141100
C	-2.56774100	-2.03542100	-3.61541100
C	-3.82308100	-1.55748300	-4.00867500

H	-5.61925600	-0.50382900	-3.43373100
H	-1.97863300	-2.64829400	-4.29393800
H	-4.19737700	-1.79158000	-5.00732600
O	-0.93138600	-2.22407100	-1.81746600
O	-4.90688500	0.11844100	-0.90625700
C	-6.07687000	0.81360700	-1.32913900
H	-6.40323400	1.39198800	-0.45549800
H	-5.85276900	1.49406500	-2.16934500
H	-6.87291100	0.11169100	-1.63549600
C	-0.07650500	-2.98637200	-2.67971300
H	0.24375200	-2.37719600	-3.54254000
H	0.78241100	-3.26469900	-2.06788300
H	-0.59864900	-3.88918300	-3.04031200
P	-1.95200500	-0.28341800	0.05055100
C	-2.98313700	1.05507200	0.82067600
C	-3.55607200	1.02692700	2.11967300
C	-3.16384100	2.24232100	0.06219500
C	-4.17946100	2.17057300	2.66612400
C	-3.80316900	3.37704300	0.58904200
C	-4.29013600	3.33390900	1.90014600
H	-4.60014100	2.14004600	3.66932700
H	-3.90857900	4.28278300	-0.00410200
H	-4.77282800	4.21583000	2.32516200
C	-1.78640900	-1.66108200	1.27709700
C	-2.32990500	-2.95936600	1.14582000
C	-0.97811900	-1.39587700	2.41317000
C	-2.04724500	-3.96043500	2.10293400
C	-0.72827900	-2.36848100	3.39262000
C	-1.26359400	-3.65449500	3.21720500
H	-2.46536300	-4.95878100	1.98489700

H	-0.10285600	-2.14646800	4.25462900
H	-1.05559000	-4.42740100	3.95930400
O	-2.68972300	2.19228100	-1.22207600
O	-3.51557400	-0.16003000	2.78882100
O	-3.16151200	-3.18399500	0.08948900
O	-0.47478800	-0.11880100	2.48077600
C	-3.04169200	3.24508200	-2.12183100
H	-4.13822100	3.35608100	-2.17741200
H	-2.58723400	4.20165000	-1.81535200
H	-2.63845100	2.94207100	-3.09531700
C	-3.83672100	-0.18961300	4.17680400
H	-3.57603200	-1.20185800	4.51038900
H	-3.24683200	0.55708400	4.73739900
H	-4.91214000	-0.00154300	4.34488800
C	-3.27619900	-4.51725800	-0.41049300
H	-3.90495600	-5.14371000	0.24724100
H	-3.75448000	-4.41800300	-1.39368100
H	-2.28033200	-4.97950600	-0.51850200
C	0.18705700	0.30078600	3.67975700
H	1.12538400	-0.25732800	3.82692300
H	0.39584500	1.36484900	3.52801100
H	-0.47804700	0.15383000	4.54752500
C	0.37019800	3.86645000	-1.93146400
H	-0.48438000	3.25784900	-1.61648100
H	0.03609400	4.50502400	-2.77285400
C	1.49817300	2.97385600	-2.40371400
C	1.39621900	1.61330200	-2.48974900
H	2.30492700	1.07029600	-2.76092700
C	0.21456900	0.81175800	-2.18904900
H	0.24834400	-0.20215000	-2.60315100

H	-0.75810700	1.28602400	-2.35177000
C	2.80026700	3.65953100	-2.73566900
H	3.25475100	4.07582600	-1.81717400
H	3.52434300	2.96047500	-3.17385000
H	2.63336100	4.51670600	-3.41499900
C	2.71220500	0.98801500	1.54851600
H	2.61931600	0.02135400	2.07876700
H	3.76228700	1.31178300	1.61574000
H	2.06347200	1.73506800	2.03340300
O	2.32615800	0.88012300	0.17598100
H	1.80922700	3.17250600	0.19360300
C	5.95680300	0.54391900	0.32431400
C	5.13911500	-0.62899600	0.27179800
C	5.20935100	-1.54362500	1.33470100
C	6.06004200	-1.27555800	2.42601400
C	6.83413400	-0.10188600	2.46938100
C	6.79018200	0.82762900	1.40930900
C	4.85629900	0.58400600	-1.71439900
H	4.60748600	-2.45313500	1.31283000
H	6.11942700	-1.99163600	3.24960500
H	7.48484200	0.09196200	3.32531900
H	7.40054200	1.73422200	1.43021100
N	5.72738500	1.27566900	-0.83937200
H	6.27469900	2.06971100	-1.15019300
O	4.63461200	0.93453200	-2.88706800
C	4.30020700	-0.53410300	-0.93186200
H	3.13626600	0.22043000	-0.36905000
C	3.84099900	-1.74013400	-1.73832100
H	4.71016400	-2.22475900	-2.22398400
H	3.22285900	-1.35793600	-2.57211300

C	3.05546500	-2.81596800	-1.00828400
C	2.16009400	-2.52145000	0.03902000
C	3.15883600	-4.15726300	-1.43408800
C	1.36437200	-3.52478500	0.61198100
H	2.08279800	-1.49628300	0.39452300
C	2.36968700	-5.16750300	-0.86141900
H	3.86256800	-4.40319900	-2.23404100
C	1.45951800	-4.85082100	0.16077300
H	0.66492500	-3.26903200	1.40466700
H	2.46725200	-6.19787100	-1.21290400
H	0.83706300	-5.62814500	0.61079900

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C	1.54645000	6.66363900	-1.14215900
H	1.88483600	6.79834400	-2.17723600
C	2.39259700	4.32210100	-1.06276500
H	3.20389300	4.61906900	-0.37529700
H	2.76001400	4.50803800	-2.08733800
Pd	0.07201200	0.35633900	-1.17782300
C	3.01068900	-1.70386500	-0.91188700
C	4.03503400	-2.40876200	-0.22818000
C	2.96976700	-1.80303900	-2.32468800
C	4.99935800	-3.16611600	-0.91941600
C	3.93445100	-2.55907700	-3.02661600
C	4.93577500	-3.22826600	-2.31672700
H	5.78312600	-3.69729200	-0.38227900
H	3.90271400	-2.62858700	-4.11199800
H	5.67900000	-3.81312900	-2.86254400
O	1.95726200	-1.14435400	-2.96297500
O	4.01599300	-2.28454400	1.12896200
C	4.89961300	-3.08240000	1.90840500

H	4.63830000	-2.86537100	2.95095000
H	4.75661900	-4.15662400	1.69714800
H	5.95491500	-2.81327700	1.72100700
C	1.77598900	-1.34321400	-4.36127000
H	1.65791400	-2.41492800	-4.59742900
H	0.85681200	-0.80047700	-4.61307900
H	2.62236400	-0.93238300	-4.93972900
P	1.67677300	-0.84273500	0.04485300
C	0.95382000	-2.29349900	0.93983500
C	1.07541000	-2.65320600	2.30645900
C	0.19067900	-3.14638700	0.09546200
C	0.39998600	-3.78166600	2.81531000
C	-0.48304800	-4.27486100	0.59753300
C	-0.37916200	-4.56966200	1.95858200
H	0.48358300	-4.05199000	3.86609500
H	-1.10492300	-4.88055800	-0.05566300
H	-0.90888500	-5.43486900	2.36201500
C	2.45111500	0.31291300	1.25980800
C	3.75630300	0.85483800	1.15533600
C	1.61882100	0.82419600	2.28669100
C	4.23704800	1.78359600	2.10121800
C	2.08451200	1.75063200	3.23530500
C	3.40176800	2.21380800	3.13791800
H	5.24627400	2.18236700	2.01860700
H	1.42552000	2.11331400	4.02235900
H	3.77514100	2.93840500	3.86404400
O	0.20453600	-2.80821300	-1.22267900
O	1.88706000	-1.87493600	3.09107400
O	4.49324900	0.46723700	0.07011800
O	0.32705000	0.36642200	2.27623500

C	-0.45071300	-3.66044900	-2.17250100
H	-0.30335700	-3.16533800	-3.14019500
H	0.02659400	-4.65677500	-2.18065400
H	-1.52186900	-3.74260100	-1.93582600
C	1.99939000	-2.18273500	4.47476100
H	1.01649400	-2.15334900	4.97878100
H	2.44786900	-3.18087900	4.63144500
H	2.65411200	-1.40631000	4.89208100
C	5.87651800	0.80580200	0.01834800
H	6.40225000	0.46607000	0.92793400
H	6.27035700	0.28062700	-0.86096700
H	6.01863500	1.89511100	-0.09783000
C	-0.43103000	0.40446400	3.49324300
H	-0.72494800	1.43715300	3.74739700
H	-1.32810700	-0.19018800	3.28896200
H	0.15396700	-0.03222900	4.31708900
C	2.13717400	2.80447400	-0.87230100
H	3.10269500	2.28500600	-0.94304000
H	1.76143500	2.62726600	0.14328500
C	1.19498500	2.19026400	-1.88990800
C	-0.21810000	2.41700800	-1.72676800
H	-0.56627000	2.96992200	-0.85143700
C	-1.17079000	1.69913900	-2.47071400
H	-2.21971400	1.73350600	-2.17233300
H	-0.94958700	1.31093600	-3.46856200
C	1.81531600	1.95834400	-3.25502000
H	1.10915700	1.52319500	-3.97357700
H	2.17064500	2.92290300	-3.66557700
H	2.67998600	1.28627500	-3.17000300
C	-3.76272200	-3.15589700	0.46948700

H	-4.57679200	-3.89029200	0.36803300
H	-3.01070900	-3.54427700	1.18563700
H	-4.19582800	-2.22635900	0.87737100
O	-3.20534200	-2.94610400	-0.82530600
C	-3.05400700	2.27774700	1.05869200
C	-4.20152000	1.89691400	0.27998000
C	-5.32089300	2.75843400	0.27481900
C	-5.27428400	3.95248700	1.01059200
C	-4.13182700	4.30639000	1.76365200
C	-3.00489900	3.46473700	1.79790200
C	-2.58560500	0.30812700	-0.00564800
H	-6.21250000	2.49327000	-0.29827500
H	-6.13792900	4.62196400	1.00265200
H	-4.12186600	5.24194800	2.32740000
H	-2.11684300	3.73265400	2.37757400
N	-2.11412900	1.27780500	0.89765600
H	-1.14616800	1.27816900	1.20143200
O	-1.78781300	-0.65327700	-0.40463300
C	-3.89092100	0.66045700	-0.38539500
H	-2.64258100	-2.13197000	-0.74553300
C	-4.74555600	-0.09308500	-1.36480300
H	-4.10192000	-0.77144100	-1.94640800
H	-5.18886800	0.62422000	-2.08463100
C	-5.88562800	-0.92689700	-0.77533900
C	-6.33034400	-2.07270800	-1.46261900
C	-6.51583000	-0.58428900	0.43598700
C	-7.37960700	-2.85575100	-0.95963300
H	-5.82279200	-2.36585200	-2.38400600
C	-7.56835000	-1.36430900	0.94282900
H	-6.16828900	0.28879500	0.98896200

C	-8.00551100	-2.50309200	0.24798200
H	-7.70108700	-3.74788900	-1.50340000
H	-8.04316600	-1.08298900	1.88634500
H	-8.82043500	-3.11326100	0.64516800
C	1.53288300	7.72895700	-0.32610700
H	1.20788100	7.65670700	0.71426600
H	1.84048400	8.71607700	-0.67919000
C	1.16914500	5.23910400	-0.78979900
H	0.36902300	4.93722300	-1.49099000
C	0.63831900	5.08183500	0.64592300
H	0.30488000	4.05237100	0.83885100
H	1.42831000	5.32272200	1.37670700
H	-0.21697100	5.75175500	0.82178700

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C	0.35639900	6.96250000	-1.99530400
H	0.69295600	6.72867800	-3.01341100
C	1.47420600	4.93822500	-1.05178400
H	2.21807000	5.51894800	-0.47894200
H	1.87761000	4.82601100	-2.07239200
Pd	0.07783100	0.78778900	-0.12878100
C	3.62241600	-0.19878200	0.11665400
C	4.52252800	-0.31826900	1.20525700
C	4.11589500	0.39244000	-1.07592700
C	5.81222200	0.25117800	1.14338800
C	5.41108500	0.93601500	-1.15752900
C	6.24128100	0.87699700	-0.03109800
H	6.48697900	0.16804200	1.99420300
H	5.76406100	1.39727000	-2.07832300
H	7.24418100	1.30623500	-0.07807900
O	3.23900000	0.39033100	-2.12934500

O	4.11223600	-1.05064700	2.28317500
C	4.68880200	-0.76283800	3.55516500
H	4.04795000	-1.27094200	4.28803900
H	5.72038100	-1.15225300	3.63172100
H	4.69028900	0.32299100	3.74824400
C	3.74450700	0.65165100	-3.43639000
H	4.59855600	-0.00881100	-3.66541500
H	2.90935000	0.44414300	-4.11631200
H	4.05855400	1.70546700	-3.54504700
P	1.84005900	-0.70627000	0.07779300
C	1.87875500	-2.11885000	-1.11215700
C	2.71498000	-3.23412600	-0.85129400
C	1.07557100	-2.14231500	-2.28201300
C	2.72417200	-4.36351000	-1.68977600
C	1.07527300	-3.27828000	-3.12470500
C	1.89227100	-4.37045700	-2.81631300
H	3.36044800	-5.21881300	-1.46882400
H	0.44141700	-3.31087700	-4.00766300
H	1.88422900	-5.24379900	-3.47223400
C	1.34079400	-1.34935400	1.75205500
C	1.33037100	-0.37501900	2.78518400
C	0.63289300	-2.56040500	1.99163900
C	0.64592100	-0.57388500	3.99549000
C	-0.08232800	-2.75178200	3.19626000
C	-0.06988200	-1.76289700	4.18714700
H	0.66399200	0.19360200	4.76804400
H	-0.63835900	-3.67438300	3.35365000
H	-0.62296600	-1.92088700	5.11472600
O	0.32906000	-1.03624600	-2.55429200
O	3.47228300	-3.13529000	0.27778900

O	2.02246600	0.78387200	2.52524900
O	0.65154900	-3.50692700	1.01397800
C	-0.56917000	-1.07453800	-3.67070600
H	-1.07363700	-0.10069100	-3.66438000
H	-0.01080300	-1.19323200	-4.61705800
H	-1.31671900	-1.87494200	-3.55793100
C	4.07930200	-4.31005400	0.80342200
H	3.32434700	-5.09893900	0.96470800
H	4.87183400	-4.69076400	0.13411000
H	4.51792800	-4.00139700	1.76030400
C	1.41740600	2.02005300	2.93098100
H	1.38315300	2.11685200	4.03017700
H	2.06084800	2.80536700	2.51638000
H	0.40291700	2.10224500	2.50975400
C	-0.46846700	-4.39337600	0.88529900
H	-1.40627800	-3.81919100	0.85342700
H	-0.31220300	-4.90317100	-0.07335400
H	-0.49005000	-5.13687600	1.70223700
C	1.33217700	3.53186500	-0.41280100
H	2.32623300	3.05465700	-0.39536100
H	1.00112100	3.62942200	0.63067500
C	0.37791500	2.60747300	-1.16020700
C	-1.02351900	2.62908300	-0.75642100
H	-1.28967200	3.22157000	0.12280400
C	-2.08758600	2.05536700	-1.47610000
H	-3.09673200	2.42980100	-1.33107400
H	-1.89732500	1.50175200	-2.39540200
C	0.73264600	2.41246400	-2.62692600
H	0.24007600	1.53181200	-3.05366300
H	0.43751700	3.30362200	-3.21225300

H	1.81493300	2.27600200	-2.72312000
C	-2.60026100	-4.32197100	-2.44500000
H	-2.89064500	-4.97475200	-3.28388800
H	-1.50044600	-4.37619300	-2.32128000
H	-3.07495000	-4.70822800	-1.52130300
O	-3.03742900	-3.00288600	-2.75544500
C	-2.45596000	0.82737300	1.84056400
C	-3.48677700	1.21540600	0.93330900
C	-4.24153700	2.37087000	1.22383900
C	-3.98437600	3.08232300	2.40591300
C	-2.98238300	2.65716100	3.30504800
C	-2.20069700	1.52079400	3.02633800
C	-2.49095700	-0.71811900	0.12080300
H	-5.02536700	2.70219100	0.53870900
H	-4.57599500	3.97002100	2.64033000
H	-2.81308300	3.21204600	4.23028000
H	-1.42660000	1.17716700	3.71251000
N	-1.79339400	-0.28103400	1.29468900
H	-1.28467600	-0.95475300	1.86120400
O	-2.23756300	-1.81198300	-0.42904400
C	-3.44422600	0.33019000	-0.20007400
H	-2.82123900	-2.46095700	-1.95237200
C	-4.53237300	0.12552700	-1.22334900
H	-4.11255300	-0.37522800	-2.10996900
H	-4.91916600	1.10758700	-1.54938700
C	-5.67413100	-0.71711000	-0.65988400
C	-5.78802100	-2.08103500	-0.99070000
C	-6.59888000	-0.15528700	0.24296900
C	-6.80915900	-2.86525400	-0.42960300
H	-5.07537900	-2.52252000	-1.69016300

C	-7.61792600	-0.93846600	0.80410500
H	-6.50898500	0.89740900	0.51731900
C	-7.72687400	-2.29894300	0.46929200
H	-6.88756900	-3.92158600	-0.69899300
H	-8.32758700	-0.48691000	1.50168900
H	-8.52130200	-2.90989500	0.90452600
C	0.19607800	8.24998900	-1.65145800
H	-0.13260900	8.54487900	-0.65226300
H	0.38478900	9.05481900	-2.36588300
C	0.15222700	5.74899700	-1.11280200
H	-0.59680900	5.10309500	-1.60909300
C	-0.37084200	6.09066900	0.29258300
H	-0.56431100	5.17843600	0.87478500
H	0.36828300	6.69899800	0.84039100
H	-1.30971000	6.66289200	0.23331300

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C	-5.16392100	-1.13266600	-0.01459500
H	-4.11435500	-1.31466800	0.23037500
C	-5.05899000	1.40332900	-0.20628000
H	-5.62803400	2.30420300	0.08180000
H	-5.17999600	1.28942000	-1.29657500
C	-3.57419600	1.67108600	0.14304400
H	-3.31360200	2.65021300	-0.30348100
H	-3.47818300	1.78548500	1.23598400
C	-2.56713700	0.64883600	-0.35411400
C	-1.70150400	0.07584000	0.50943100
H	-1.74286900	0.38684900	1.55600200
C	-0.62289000	-0.92622500	0.18830900
H	-0.67545200	-1.77176800	0.89604500
H	-0.75089100	-1.35234900	-0.81791600

C	-2.62587300	0.36633000	-1.83929200
H	-1.76334200	-0.20740700	-2.20397100
H	-3.54289700	-0.19583700	-2.08608600
H	-2.66816200	1.31367500	-2.40515700
C	2.70702400	-1.57168400	1.08705100
C	1.85713900	-1.43136500	-0.02885400
C	2.05595000	-2.22559900	-1.15498400
C	3.11649600	-3.15501200	-1.16211800
C	3.95896500	-3.27508700	-0.04487300
C	3.76531600	-2.48357900	1.10370500
C	1.19629500	0.08467900	1.70119100
H	1.40191800	-2.12401000	-2.02427800
H	3.28454300	-3.78218600	-2.03923000
H	4.77937100	-3.99519600	-0.06108600
H	4.42050900	-2.57958200	1.97137200
N	2.29041800	-0.68147800	2.08681600
H	2.74787800	-0.54977900	2.98234300
O	0.65279400	0.93977800	2.38956600
C	0.83417500	-0.35209900	0.25333900
C	0.98033500	0.86993500	-0.70590900
H	0.21779300	1.60462300	-0.40939200
H	0.73190400	0.51771400	-1.72062800
C	2.36001400	1.49543300	-0.68417500
C	3.37751900	1.03405100	-1.54055900
C	2.66015700	2.51951400	0.23520000
C	4.66713400	1.58219800	-1.48222900
H	3.15599500	0.23303800	-2.24827500
C	3.94909900	3.06978100	0.29660400
H	1.87850300	2.86898900	0.91184900
C	4.95685700	2.60269400	-0.56235000

H	5.44481400	1.21269400	-2.15441900
H	4.16522500	3.86518500	1.01348300
H	5.96001900	3.03244200	-0.51727800
C	-5.82557500	-2.04574500	-0.74362500
H	-6.87492300	-1.92168100	-1.02175500
H	-5.33313100	-2.96046000	-1.08268900
C	-5.71948400	0.18228900	0.49816000
H	-5.45314000	0.25440500	1.57077000
C	-7.25142000	0.28416900	0.37470000
H	-7.61083500	1.21564300	0.83939000
H	-7.55549200	0.29490900	-0.68513000
H	-7.74736000	-0.56904400	0.86302900

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C	-0.37623000	-2.57491700	1.75115000
H	0.24295200	-1.86848700	2.30996900
C	-1.69846700	-2.08546900	1.42996700
C	-2.66351800	-3.07764100	0.76715700
H	-3.68972700	-2.83861900	1.08775500
H	-2.46654100	-4.11375100	1.09995000
C	-2.31989400	-1.22345400	2.54545500
H	-3.16988800	-0.64339600	2.16170200
H	-2.68771200	-1.83282100	3.39138200
H	-1.57347700	-0.51062700	2.93420400
C	0.26486100	-3.74802000	1.34267800
H	-0.32431300	-4.61447800	1.02905700
H	1.23719800	-3.97228200	1.78159500
C	-2.66751000	-3.03750800	-0.79303000
H	-3.54944400	-3.61034900	-1.13959000
H	-2.81710500	-1.99834500	-1.10995900

C	-1.44408500	-3.60537900	-1.47945200
C	-0.74913900	-2.77533700	-2.39682200
H	-1.11549100	-1.75434900	-2.51291200
C	0.54773100	-3.06403400	-2.89870800
H	1.04703000	-2.30845800	-3.50604300
H	0.88555300	-4.09294600	-3.05362500
C	-1.33332800	-5.11841700	-1.48796800
H	-1.49467900	-5.53030200	-0.47941000
H	-2.12354600	-5.54118200	-2.13766500
H	-0.35812800	-5.47011300	-1.85252300
C	-1.33347600	0.45207100	-1.21093200
H	-2.23271900	-0.04078400	-1.65318300
H	-1.68766600	1.43153400	-0.81121600
H	-0.66893200	0.70488300	-2.06815500
O	-0.67394800	-0.32738600	-0.26687600
H	-1.35630300	-1.20580800	0.57299500
C	5.16251700	2.01473400	0.84974500
C	4.67024400	2.49471100	2.10998500
C	3.31792400	2.94337100	1.91595700
C	2.95448600	2.75522400	0.53060500
C	4.11096200	2.17256800	-0.11104500
H	6.13957100	1.57259900	0.66779600
H	5.20041100	2.46161400	3.06000000
H	2.65902300	3.30636200	2.69855300
H	4.15672700	1.88667500	-1.15664900
Fe	3.49698600	0.97711600	1.44779800
C	1.85996800	-0.24834400	1.48329500
C	2.21591000	0.17874200	2.80533500
C	2.97470400	-0.98650700	0.94071100
H	0.92237400	-0.08337600	0.94652200

C	3.56300000	-0.24504800	3.07292200
H	1.60001500	0.77981800	3.46926800
C	4.04285200	-0.94120300	1.91389900
H	4.14248600	-0.01381700	3.96444600
H	5.03296300	-1.37312900	1.79108000
C	3.35623100	-1.14292400	-2.01191800
C	4.81983300	-0.67459100	-1.91350100
C	2.35556200	0.00268500	-2.23928200
H	3.26129300	-1.86744900	-2.83790300
H	5.51684300	-1.52546300	-1.97096800
H	5.05484300	0.01521400	-2.74240600
H	4.99179900	-0.14738700	-0.96433700
H	1.33322900	-0.38007800	-2.36282900
H	2.32843700	0.68058700	-1.37935300
H	2.64055500	0.58246300	-3.13402300
C	4.18080000	-3.35952300	-0.25160200
C	4.31645900	-4.22102000	-1.52211800
C	3.89122400	-4.24695700	0.97243600
H	5.11940200	-2.80350000	-0.08756300
H	4.61826800	-3.62486500	-2.39635400
H	5.07409200	-5.00651100	-1.36296400
H	3.35504600	-4.71059400	-1.75065600
H	3.73352200	-3.65106100	1.88399000
H	2.98804300	-4.84952100	0.79109500
H	4.73787100	-4.93301100	1.14481900
C	0.14167400	3.73990100	0.76183300
C	0.37908600	4.98674200	1.63719900
C	-0.25891700	2.53008200	1.63451700
H	-0.70971900	3.95390500	0.09234500
H	0.46515400	5.90236800	1.03575900

H	-0.47335700	5.11778900	2.32845400
H	1.29202300	4.89531300	2.24373900
H	-1.16810400	2.78057100	2.20986400
H	-0.45695400	1.62537900	1.04026700
H	0.54243300	2.29876200	2.35106100
C	2.16121500	4.84095900	-1.22062100
C	3.05467400	5.73079000	-0.33393600
C	1.01573400	5.64348300	-1.86797200
H	2.79839000	4.45975100	-2.03959700
H	3.89105300	5.15705000	0.09156300
H	3.47371700	6.55325200	-0.94164300
H	2.49331000	6.18028300	0.49670800
H	0.41188400	5.01135900	-2.53636100
H	0.34383400	6.06560400	-1.10441100
H	1.42450200	6.48382800	-2.45540000
P	2.81623200	-2.09709000	-0.49618100
P	1.47908800	3.21019800	-0.47522700
Pd	0.66501700	-2.85526000	-0.70545400
C	-5.85601400	-0.89072100	1.26181200
C	-5.31652000	0.41312200	1.27025300
C	-5.31231800	1.15197400	2.45122300
C	-5.84784500	0.57682300	3.62231900
C	-6.37262700	-0.72590900	3.59704900
C	-6.38532300	-1.48456000	2.41014600
C	-5.15916100	-0.52185700	-0.92788400
H	-4.88706600	2.15803500	2.47011700
H	-5.84798600	1.14380300	4.55470200
H	-6.77794100	-1.16364300	4.51135400
H	-6.79131100	-2.49761700	2.39220300
N	-5.73593700	-1.41821100	-0.03241900

H	-6.08264300	-2.32245300	-0.33292800
O	-5.02119800	-0.72863100	-2.12806900
C	-4.75531000	0.72449400	-0.09926500
H	-3.65340600	0.71855300	-0.05029200
C	-5.21512900	2.07976700	-0.72664500
H	-5.49007700	2.75430000	0.09934300
H	-6.13079600	1.90448400	-1.31468900
C	-4.15631200	2.75066600	-1.58381300
C	-3.75960900	2.19366800	-2.81571400
C	-3.53357700	3.93198100	-1.14033100
C	-2.76188300	2.80935600	-3.58418500
H	-4.21983600	1.26339300	-3.14798600
C	-2.53788800	4.55390700	-1.91136100
H	-3.83296100	4.36790000	-0.18297700
C	-2.15045800	3.99237700	-3.13754300
H	-2.45956300	2.36334100	-4.53425500
H	-2.06583600	5.47190700	-1.55616300
H	-1.38079800	4.47471500	-3.74291900

PA3-TS4a-L3

C	1.98457900	-3.14087600	-0.46742700
H	2.26805300	-3.01476500	0.58274700
C	0.62647400	-3.51502700	-0.70031000
C	-0.31561800	-3.39568600	0.36749900
H	0.03611600	-3.44349900	1.40381100
H	-1.34644600	-3.71910500	0.20344200
C	0.16730400	-3.91162200	-2.09460000
H	0.51671700	-3.18832500	-2.84701700
H	0.56858800	-4.90341400	-2.37063400
H	-0.93125200	-3.95191400	-2.13638500

C	1.57733100	0.34082000	-2.62206600
H	0.94941300	1.21971900	-2.40908000
H	2.55303500	0.69456500	-3.01073800
H	1.07503200	-0.24623300	-3.42123100
O	1.75623900	-0.40803000	-1.43880600
C	2.92430700	-2.74160600	-1.46761900
H	2.47562200	-1.44430200	-1.58845100
H	3.97284800	-2.69051600	-1.15764400
H	2.78259700	-3.15772800	-2.47382700
Pd	0.12904500	-1.38259100	-0.25857500
C	-1.92697700	0.91727100	1.70210300
C	-3.08627600	1.71315000	1.89030900
C	-1.05654000	0.73829700	2.80309000
C	-3.38483600	2.29967700	3.13372200
C	-1.35287200	1.31787200	4.05765900
C	-2.50870100	2.08879400	4.20706600
H	-4.27709000	2.91000600	3.26434900
H	-0.68288700	1.17507900	4.90306000
P	-1.67993900	-0.02621300	0.12733400
C	-3.29080100	-0.97009500	0.09561300
C	-4.36617200	-0.82747200	-0.81735700
C	-3.39991200	-2.00822300	1.06373000
C	-5.41815100	-1.76791000	-0.85982600
C	-4.45021100	-2.94590900	1.03479100
C	-5.44275100	-2.82483900	0.05474000
H	-6.22653800	-1.65194900	-1.58061200
H	-4.50274500	-3.74635600	1.77046800
C	-1.67648400	1.17505200	-1.28500900
C	-1.43389800	2.56746000	-1.16825200
C	-1.74013900	0.63718100	-2.59734600

C	-1.36548000	3.39670300	-2.30949900
C	-1.66477400	1.45296100	-3.74127500
C	-1.49059600	2.83304000	-3.58311100
H	-1.19714000	4.46660000	-2.20031600
H	-1.72788900	1.02149200	-4.73838700
O	-1.89470000	-0.72186200	-2.66624800
O	-1.22579500	3.04617600	0.09171900
O	0.06462000	-0.01461400	2.59744700
O	-3.86900200	1.86821100	0.78351800
O	-2.42270200	-2.01987800	2.01936300
O	-4.36587800	0.27654300	-1.62573300
C	-1.78819700	-1.35706500	-3.93643600
H	-2.61604200	-1.05676600	-4.60389400
H	-0.82495200	-1.11565500	-4.41814100
H	-1.84328400	-2.43213100	-3.73073200
C	-1.20378400	4.45287700	0.31279200
H	-0.30135300	4.91069900	-0.12660700
H	-2.10760800	4.93247400	-0.10349600
H	-1.18308800	4.57077200	1.40355900
C	0.69931200	-0.59975600	3.74017600
H	1.18403900	0.16933800	4.36772600
H	-0.03867300	-1.14841600	4.35193300
H	1.46571300	-1.27281800	3.34162800
C	-5.15368000	2.46195100	0.92414900
H	-5.75554900	1.93421200	1.68516100
H	-5.07502200	3.52899600	1.20210000
H	-5.62311100	2.36375700	-0.06213900
C	-5.06935700	0.21259900	-2.86244100
H	-4.85560500	-0.73210400	-3.39176400
H	-6.16146400	0.30383000	-2.71563700

H	-4.70055300	1.06295400	-3.45151100
C	-2.37818300	-3.09630800	2.94872700
H	-3.27802700	-3.10710500	3.58930800
H	-2.28413500	-4.06564200	2.42924200
H	-1.48586100	-2.91610700	3.56049600
H	-2.73085400	2.53901200	5.17713200
H	-1.43000500	3.47398500	-4.46497800
H	-6.25997100	-3.54847600	0.02271200
C	5.80026000	-1.16946800	0.23333300
C	4.84799300	-0.15721900	-0.01166600
C	5.03448100	0.71853900	-1.08151000
C	6.18809000	0.58149200	-1.88157900
C	7.13014600	-0.42592500	-1.61565900
C	6.94751800	-1.32699400	-0.54806200
C	4.13115300	-1.53102300	1.81001400
H	4.29626900	1.49005800	-1.29225300
H	6.34674100	1.26294500	-2.71963000
H	8.01673100	-0.52116100	-2.24625600
H	7.67103300	-2.11953700	-0.34636500
N	5.36394400	-1.94487900	1.32265300
H	5.83254200	-2.77027200	1.68006100
O	3.52392100	-2.08024200	2.72890300
C	3.72377300	-0.29298400	0.98869600
H	2.77689300	-0.50132900	0.46848800
C	3.48914500	0.94504100	1.90723700
H	4.36992800	1.09430100	2.55273300
H	2.63009200	0.71220200	2.55026300
C	3.23045200	2.19312000	1.08889600
C	2.10664500	2.27265300	0.24232100
C	4.16410000	3.24555000	1.08330000

C	1.94725300	3.37086500	-0.61503000
H	1.39122300	1.45109700	0.21518600
C	3.99339900	4.35762500	0.24357100
H	5.04411500	3.17812700	1.72810000
C	2.88699800	4.41649500	-0.61795400
H	1.09597100	3.39908500	-1.29492800
H	4.73145800	5.16322100	0.24938500
H	2.76021400	5.26672400	-1.29287700

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C	-3.15704800	-4.11195400	-1.32399600
C	-3.79668700	-3.54550000	-0.17044000
C	-2.84087100	-2.71163300	0.49804000
C	-1.59518200	-2.75740000	-0.23200800
C	-1.80378100	-3.63313600	-1.36366600
H	-3.63228700	-4.73963200	-2.07533000
H	-4.84006800	-3.66838600	0.11159000
H	-3.03352400	-2.09336500	1.36624400
H	-1.07632500	-3.83145300	-2.14498800
Fe	-3.10448300	-2.06888900	-1.40591100
C	-4.59424800	-0.70153000	-1.64951200
C	-4.42177500	-1.46716200	-2.85236400
C	-3.33806600	-0.05866800	-1.33922800
H	-5.48646600	-0.66290200	-1.03070500
C	-3.06671500	-1.29817400	-3.30039700
H	-5.16738600	-2.11718100	-3.30638100
C	-2.39838900	-0.43441900	-2.37163500
H	-2.60650100	-1.79488400	-4.15165600
H	-1.34553900	-0.16776000	-2.37592800
P	-2.84187400	0.96902700	0.09315800

P	-0.12621300	-1.73501100	0.20031700
Pd	-0.65202900	0.46599500	0.71305300
C	0.43170600	2.73841000	2.47858300
H	-0.58270300	3.14514200	2.55253400
C	0.55512100	1.30809800	2.73946000
C	-0.57534900	0.56616100	3.05729300
H	-1.51628800	1.07221600	3.28152400
H	-0.47685100	-0.47074000	3.38452900
C	1.93467600	0.68189100	2.72500400
H	2.57629900	1.14191900	3.49858100
H	1.87461600	-0.39881400	2.90385200
H	2.43727900	0.84813900	1.76064900
C	-0.01807200	2.83123900	-1.38411000
H	-0.69897600	3.50813800	-0.84777200
H	0.71177100	3.40438500	-1.97887400
H	-0.60793900	2.19724500	-2.05573800
O	0.65716900	1.94600100	-0.46719300
C	1.44706500	3.55778600	2.08334500
H	1.02199700	2.51570800	0.25513200
H	1.27077000	4.61882100	1.89671500
H	2.47656500	3.20562300	2.01136100
C	0.67803200	-2.76508100	1.51293800
C	-0.07464300	-3.49951100	2.45379600
C	2.07827100	-2.68761300	1.68016600
C	0.56014800	-4.14089100	3.53046800
H	-1.15627600	-3.58268200	2.33640700
C	2.71164100	-3.33465400	2.74916800
H	2.67680200	-2.11336500	0.97331500
C	1.95390300	-4.06312500	3.68329900
H	-0.03760800	-4.71038100	4.24631000

H	3.79704900	-3.26227700	2.84952100
H	2.44445900	-4.56404000	4.52064700
C	0.95468500	-2.08962100	-1.26595700
C	1.44605800	-3.38256400	-1.55004600
C	1.25992600	-1.03296700	-2.14400200
C	2.20529900	-3.61543900	-2.70628100
H	1.23063000	-4.20087800	-0.86085900
C	2.01947500	-1.26357500	-3.30452300
H	0.92101600	-0.02396500	-1.90605800
C	2.48682800	-2.55623100	-3.58904800
H	2.58303400	-4.61876100	-2.91649100
H	2.25695300	-0.42082600	-3.95373600
H	3.08337000	-2.73825300	-4.48571700
C	-3.24690800	2.67654900	-0.50916100
C	-3.15927300	3.73783600	0.42025000
C	-3.49982600	2.97953700	-1.86235000
C	-3.31778200	5.06658300	0.00745300
H	-2.95780200	3.51553900	1.47141600
C	-3.64247600	4.31396400	-2.27905800
H	-3.57589400	2.17176600	-2.59190700
C	-3.55098100	5.36095600	-1.34918600
H	-3.25320700	5.87451600	0.74021100
H	-3.83123100	4.53297000	-3.33279500
H	-3.66232800	6.39745000	-1.67474800
C	-4.25076300	0.68847000	1.26910000
C	-4.01646400	-0.03198400	2.45614100
C	-5.54967000	1.17514000	1.01036700
C	-5.06224600	-0.28636100	3.35807900
H	-3.00623900	-0.38808000	2.66130500
C	-6.59562400	0.92420000	1.91120900

H	-5.73525800	1.75501500	0.10439800
C	-6.35479500	0.18945600	3.08546700
H	-4.86570600	-0.84817100	4.27413300
H	-7.59804500	1.30348100	1.69924000
H	-7.16936000	-0.00275800	3.78723200
C	4.02956600	3.47103200	-0.44501300
C	4.25760800	2.12681100	-0.07286400
C	4.86287600	1.84629100	1.15249800
C	5.24352400	2.91607100	1.99032100
C	5.02079400	4.24562200	1.59593700
C	4.40535300	4.54550200	0.36524700
C	3.16293300	2.21917800	-2.20187300
H	5.03540500	0.81471300	1.45658900
H	5.71188700	2.70714200	2.95349800
H	5.31824400	5.06351000	2.25499400
H	4.22118100	5.57807100	0.06294100
N	3.39622200	3.49506200	-1.69614800
H	3.11272500	4.33187500	-2.19369900
O	2.61980300	1.97786100	-3.27396600
C	3.76542900	1.22599200	-1.18270200
H	2.96732600	0.54528100	-0.85302500
C	4.88372600	0.38931500	-1.87613600
H	5.67948600	1.07414700	-2.21056500
H	4.43093400	-0.07048200	-2.76730800
C	5.45167300	-0.67382500	-0.96262300
C	4.71234000	-1.84424400	-0.70477900
C	6.69384500	-0.50044400	-0.32414900
C	5.20390400	-2.82097300	0.17373900
H	3.75124400	-1.98892800	-1.19733200
C	7.18754900	-1.47376000	0.55974900

H	7.26847600	0.40884400	-0.51510100
C	6.44215500	-2.63705300	0.81268000
H	4.61286200	-3.71875600	0.36316100
H	8.15269500	-1.32369000	1.04886000
H	6.82574500	-3.39703500	1.49709700
TS1c			
C	3.12169900	-4.03572300	1.52716300
C	3.77799800	-3.52143900	0.35881600
C	2.82672100	-2.73616600	-0.37143800
C	1.56787700	-2.75892000	0.33706300
C	1.76258500	-3.57317200	1.51684100
H	3.58870800	-4.61812400	2.31879500
H	4.82793300	-3.64592500	0.10351600
H	3.02982500	-2.16541900	-1.26873500
H	1.02174100	-3.73962800	2.29274600
Fe	3.03891300	-1.99158000	1.50164500
C	4.51047000	-0.60278500	1.73051800
C	4.29415400	-1.30379000	2.96475500
C	3.26372800	0.01414600	1.33821300
H	5.42639000	-0.58921300	1.14631800
C	2.92138900	-1.12065500	3.34905100
H	5.02455600	-1.92232200	3.48265500
C	2.28512000	-0.31313400	2.35068900
H	2.42981600	-1.57380600	4.20692400
H	1.23325000	-0.04920700	2.30344700
P	2.83003900	0.96481500	-0.16198900
P	0.10151300	-1.76790100	-0.15302500
Pd	0.56075500	0.42238300	-0.80501600
C	-0.24695700	2.41361300	-2.31726800
H	0.78449700	2.75261700	-2.45119800

C	-0.54028100	1.07754800	-2.72999500
C	0.54583500	0.21646700	-3.02903500
H	1.50098100	0.65126000	-3.33434100
H	0.34458700	-0.80185300	-3.36999000
C	-1.97654200	0.58678100	-2.75739500
H	-2.55321000	1.13379500	-3.52423900
H	-2.01600400	-0.48687400	-2.98156100
H	-2.47379300	0.76579800	-1.79451200
C	0.09161000	2.68113100	1.49021200
H	0.64233300	3.48178100	0.95979500
H	-0.60227400	3.14160100	2.21938900
H	0.83003600	2.09738400	2.06350800
O	-0.60635300	1.84056100	0.58207700
C	-1.15442600	3.23553200	-1.57712800
H	-0.99529300	2.64836900	-0.41147600
H	-0.86932200	4.28987800	-1.47464400
H	-2.22113500	3.09202200	-1.78140800
C	-0.68152000	-2.82168400	-1.45463200
C	0.08464600	-3.59605900	-2.34987600
C	-2.07677300	-2.73810700	-1.64833300
C	-0.53490000	-4.27245700	-3.41407200
H	1.16307900	-3.68175700	-2.20775800
C	-2.69461900	-3.41958100	-2.70525200
H	-2.68363300	-2.13510500	-0.97345200
C	-1.92471000	-4.18785000	-3.59614900
H	0.07096800	-4.87313800	-4.09655200
H	-3.77707300	-3.34266800	-2.82899200
H	-2.40346300	-4.71594400	-4.42349800
C	-1.00508700	-2.05342100	1.30105000
C	-1.48778500	-3.34243900	1.61772400

C	-1.32810700	-0.96786700	2.13619400
C	-2.25730700	-3.54468900	2.77235200
H	-1.25720400	-4.18101400	0.95836300
C	-2.09676800	-1.17255000	3.29622700
H	-1.00767500	0.03902100	1.85822400
C	-2.55418000	-2.45975200	3.61816600
H	-2.62961900	-4.54387000	3.00981700
H	-2.35039300	-0.31126300	3.91383300
H	-3.15741800	-2.61829300	4.51487500
C	3.22464700	2.70205300	0.34589600
C	3.09084100	3.71463900	-0.62921800
C	3.55693300	3.06660300	1.66554600
C	3.28112900	5.06079400	-0.29250800
H	2.83318700	3.44434000	-1.65621700
C	3.73536400	4.41759400	2.00562600
H	3.66403100	2.29528800	2.42950300
C	3.59677000	5.41777200	1.03090000
H	3.17628200	5.83237400	-1.05869300
H	3.98539900	4.68670100	3.03450600
H	3.73404100	6.46782000	1.29771300
C	4.27513600	0.60974000	-1.27239700
C	4.08637900	-0.18308400	-2.42108400
C	5.56290200	1.11841200	-0.99900200
C	5.16487600	-0.48741900	-3.26748500
H	3.08836700	-0.56029700	-2.64464200
C	6.64151300	0.81603600	-1.84339500
H	5.71377300	1.75658500	-0.12648400
C	6.44552500	0.00919300	-2.97792900
H	5.00243500	-1.10470600	-4.15392300
H	7.63440500	1.21250200	-1.61894000

H	7.28535600	-0.22229600	-3.63658600
C	-3.90826600	3.57467300	0.38924600
C	-4.21208700	2.24399400	0.02268200
C	-4.79344600	1.98948000	-1.21893700
C	-5.07095100	3.07086100	-2.08252100
C	-4.76986500	4.38691700	-1.69571200
C	-4.18200600	4.66049900	-0.44566100
C	-3.17926600	2.29453300	2.18318400
H	-5.02337900	0.96766400	-1.51879300
H	-5.52054900	2.88114600	-3.05880200
H	-4.98648400	5.21450700	-2.37420700
H	-3.93570900	5.68172700	-0.14914400
N	-3.31886200	3.57440500	1.65974200
H	-2.95744800	4.39202800	2.13779000
O	-2.70661200	2.03388200	3.28420300
C	-3.78596200	1.32389900	1.14383300
H	-2.98427800	0.64088300	0.82796300
C	-4.93269200	0.49852800	1.79582600
H	-5.74039200	1.18782700	2.09014900
H	-4.52027600	0.04762100	2.71102000
C	-5.46797800	-0.57686900	0.87579900
C	-4.73982700	-1.76786100	0.68718400
C	-6.67310000	-0.40077000	0.17006800
C	-5.20730100	-2.76125900	-0.18615500
H	-3.80767300	-1.91642100	1.23166200
C	-7.14044400	-1.38921400	-0.71135600
H	-7.23976600	0.52296100	0.30775100
C	-6.40757700	-2.57363500	-0.89268700
H	-4.62771700	-3.67694600	-0.31714800
H	-8.07687100	-1.23548800	-1.25250000

H	-6.77260200	-3.34707200	-1.57230700
Int2c			
C	-3.02912700	-3.92980200	-1.76427100
C	-3.73361800	-3.45677100	-0.60632600
C	-2.80888700	-2.71981700	0.20384100
C	-1.51901600	-2.73186700	-0.44650900
C	-1.66614600	-3.49083500	-1.66994600
H	-3.46559700	-4.47049600	-2.60142200
H	-4.79581100	-3.57698100	-0.40559900
H	-3.04797100	-2.19418800	1.11922200
H	-0.88623300	-3.63732900	-2.41085800
Fe	-2.91666600	-1.88930100	-1.64035200
C	-4.37101900	-0.49590600	-1.90685600
C	-4.05195400	-1.12396800	-3.15833800
C	-3.16175400	0.10422200	-1.38768500
H	-5.33053200	-0.52103700	-1.39782000
C	-2.65417200	-0.91358700	-3.42150400
H	-4.73477700	-1.71364100	-3.76689400
C	-2.10264600	-0.16039300	-2.33594800
H	-2.09340700	-1.31663700	-4.26169200
H	-1.06333300	0.11780100	-2.18020600
P	-2.82884000	0.95032500	0.19432500
P	-0.05072400	-1.79547900	0.11799500
Pd	-0.40302800	0.42645500	0.81769800
C	0.10737800	2.25352900	2.20141800
H	-0.92067600	2.54763100	2.42557200
C	0.56681000	1.01891600	2.71920900
C	-0.45233500	0.03607400	2.96995400
H	-1.42702900	0.37969700	3.32635400
H	-0.15485400	-0.96619400	3.28587800

C	2.04309600	0.70461300	2.83933700
H	2.46095400	1.20122700	3.73447500
H	2.20421300	-0.37666100	2.93696400
H	2.59757400	1.07803900	1.96965000
C	-0.18549300	2.51892200	-1.42445400
H	-0.41231200	3.29147400	-0.65741900
H	0.45317100	2.98918000	-2.20220900
H	-1.15146000	2.27670500	-1.91872000
O	0.46730700	1.39737000	-0.90514300
C	1.02830800	3.29154200	1.62295200
H	1.46701900	2.90296100	0.69018300
H	0.48405600	4.21760500	1.39107900
H	1.86278300	3.52954000	2.30437400
C	0.63149500	-2.84268700	1.47975200
C	-0.17239200	-3.69547000	2.26037400
C	1.99536600	-2.69539700	1.80810500
C	0.37999600	-4.38409600	3.35415600
H	-1.22549200	-3.82998000	2.00948500
C	2.54658100	-3.38842100	2.89390700
H	2.62991600	-2.03918000	1.21213700
C	1.73827400	-4.23313000	3.67502400
H	-0.25309500	-5.04537800	3.95019600
H	3.60650700	-3.26340800	3.12557200
H	2.16451100	-4.77065000	4.52466000
C	1.12503600	-2.15256400	-1.26002500
C	1.63651400	-3.45747800	-1.44207800
C	1.45933300	-1.13421400	-2.17255100
C	2.46500400	-3.74117600	-2.53643000
H	1.38597100	-4.24341400	-0.72761600
C	2.28722400	-1.42768300	-3.27163500

H	1.09847900	-0.11428200	-1.99596800
C	2.78593300	-2.72606300	-3.45696600
H	2.86260300	-4.74990200	-2.66944500
H	2.55039700	-0.61894500	-3.95337900
H	3.43533200	-2.94871500	-4.30680900
C	-3.28776000	2.70874400	-0.16235900
C	-3.22353400	3.63332000	0.90252900
C	-3.63953000	3.17025500	-1.44616400
C	-3.50210700	4.99026500	0.68840600
H	-2.96459700	3.28726100	1.90615700
C	-3.91178200	4.53057500	-1.66148900
H	-3.69006000	2.46572100	-2.27757700
C	-3.84246600	5.44419300	-0.59746600
H	-3.45075500	5.69314300	1.52305100
H	-4.18064400	4.87530500	-2.66263200
H	-4.05339000	6.50214400	-0.76750000
C	-4.28738100	0.46009900	1.23541900
C	-4.09021800	-0.34654200	2.37324800
C	-5.59449200	0.89477700	0.92740500
C	-5.17728500	-0.74056700	3.17075300
H	-3.08056100	-0.67133800	2.62573700
C	-6.68185300	0.50012900	1.72041700
H	-5.75337300	1.55121600	0.07008300
C	-6.47594600	-0.32180400	2.84243800
H	-5.00751400	-1.36786900	4.04867200
H	-7.68934000	0.83821300	1.46741600
H	-7.32282800	-0.62445200	3.46200500
C	3.68281000	3.65950500	-0.62121900
C	4.08767000	2.39046800	-0.14602800
C	4.69147200	2.28978100	1.10720100

C	4.88108500	3.45737700	1.87735900
C	4.46970100	4.70757600	1.38802900
C	3.86251800	4.82830700	0.12312600
C	3.09543100	2.18734700	-2.31876700
H	5.00778000	1.31908300	1.48757100
H	5.35020500	3.38595900	2.86040400
H	4.61936400	5.60366000	1.99400600
H	3.53806400	5.79879500	-0.25701400
N	3.11343800	3.51108100	-1.89077000
H	2.69894600	4.25683000	-2.43806100
O	2.68742500	1.80871100	-3.40995400
C	3.72971800	1.34901800	-1.18346300
H	2.93974600	0.67584300	-0.81690900
C	4.91663100	0.50698900	-1.72913600
H	5.71682700	1.19161500	-2.05356800
H	4.54590600	-0.02713900	-2.61676900
C	5.44900900	-0.47872300	-0.71110300
C	4.74455000	-1.67075500	-0.45052200
C	6.62957700	-0.21937100	0.01046100
C	5.20903300	-2.58081200	0.51087100
H	3.83592900	-1.88730100	-1.01107400
C	7.09303100	-1.12340200	0.98039400
H	7.18028100	0.70362600	-0.18539800
C	6.38233000	-2.30781200	1.23475900
H	4.65011200	-3.50071100	0.69285000
H	8.00996600	-0.90468600	1.53255900
H	6.74513900	-3.01634200	1.98298000

TS2c

C	-2.30012900	-1.64887400	-3.81131100
C	-3.22165100	-2.58219900	-3.22839700

C	-2.73836300	-2.92833800	-1.92436000
C	-1.50449000	-2.21698300	-1.69789300
C	-1.25519100	-1.40646000	-2.86482500
H	-2.41204600	-1.15585600	-4.77445700
H	-4.15771500	-2.91854600	-3.66958000
H	-3.22476500	-3.58555400	-1.21046300
H	-0.41655200	-0.73626200	-2.98115000
Fe	-3.09157800	-0.91114200	-2.06974600
C	-4.24481100	-0.29370300	-0.50397100
C	-5.04614200	-0.53312300	-1.66989500
C	-3.30966600	0.76739300	-0.80487500
H	-4.34382000	-0.79597000	0.45303200
C	-4.57000500	0.32721100	-2.71672900
H	-5.82307800	-1.28855000	-1.76530900
C	-3.48958500	1.11168400	-2.19165800
H	-4.92139700	0.33646000	-3.74627600
H	-2.90719100	1.85032100	-2.73345200
P	-2.14303900	1.52788300	0.38195500
P	-0.50284100	-2.27645100	-0.16627300
Pd	-0.47011000	-0.02991200	0.58100300
C	1.40773200	-1.37130300	3.20916000
H	0.96063600	-2.33285800	2.93552300
C	0.59236900	-0.28185900	3.10246300
C	-0.79242700	-0.47115000	2.62280800
H	-1.52188900	0.23766700	3.03042900
H	-1.14387900	-1.50252700	2.72354400
C	1.01462000	1.13919300	3.42883000
H	0.83234200	1.79692900	2.56420000
H	0.41822600	1.53165400	4.27156900
H	2.07695800	1.22118400	3.69453800

C	0.38868400	1.44423600	-2.30576800
H	0.80418400	1.11627600	-3.27687300
H	-0.69521900	1.58807600	-2.40536700
H	0.86209000	2.39771300	-2.03010700
O	0.63228500	0.43986700	-1.31606100
C	3.61170800	2.84998800	-1.72741100
C	3.27610500	2.14982700	-0.52301000
C	3.06155300	2.89117100	0.65070400
C	3.18052000	4.29569900	0.61914100
C	3.50258800	4.96410200	-0.57728200
C	3.71519200	4.24234700	-1.77257500
C	3.69255000	0.57311900	-2.20787300
H	2.83214500	2.37759300	1.58594400
H	3.03160700	4.87110700	1.53632100
H	3.60027700	6.05231700	-0.58418100
H	3.97912300	4.75852800	-2.69906500
N	3.79525800	1.89930800	-2.72314500
H	4.16407700	2.08088900	-3.64917100
O	3.92601700	-0.43623000	-2.89296700
C	3.19963300	0.73005400	-0.83227700
H	1.73666000	0.53035600	-1.10076500
C	3.41342800	-0.35409600	0.21432300
H	3.10525300	-1.31883600	-0.20699500
H	2.75781000	-0.15438200	1.07746000
C	4.86111500	-0.43484400	0.66175200
C	5.31008500	0.22681400	1.82022400
C	5.80135200	-1.13273600	-0.12441100
C	6.66140000	0.18218200	2.19947100
H	4.59187500	0.78648300	2.42303100
C	7.15137000	-1.18050100	0.25119900

H	5.45851500	-1.60653400	-1.04474800
C	7.58676400	-0.52754000	1.41811300
H	6.99091100	0.70244500	3.10250700
H	7.86822100	-1.72572100	-0.36839100
H	8.63862600	-0.56663200	1.71132300
C	2.84624500	-1.43645000	3.62679100
H	3.23129500	-0.47957300	4.00336600
H	2.98758300	-2.19838800	4.41436600
H	3.48465500	-1.73293600	2.77536100
C	1.08710000	-3.08091300	-0.58996900
C	1.69618200	-2.87052800	-1.84271400
C	1.82106400	-3.72382500	0.43463400
C	3.01057200	-3.30405800	-2.07186000
H	1.16766500	-2.33569700	-2.62853200
C	3.12756400	-4.16792100	0.19606000
H	1.37025200	-3.87755000	1.41551500
C	3.72553000	-3.95800500	-1.05791900
H	3.48283400	-3.08242100	-3.02695500
H	3.68430200	-4.66167600	0.99514000
H	4.75406200	-4.27807700	-1.23217700
C	-1.46772500	-3.51235500	0.79980900
C	-1.17872700	-4.89177000	0.80079900
C	-2.61887000	-3.05131400	1.47337600
C	-2.01734300	-5.78887900	1.48078300
H	-0.30460900	-5.26234000	0.26511400
C	-3.46286400	-3.95002500	2.14135000
H	-2.84546100	-1.98530100	1.46240400
C	-3.15979200	-5.32182700	2.15143700
H	-1.78195100	-6.85520300	1.47769100
H	-4.34961400	-3.57886100	2.65969300

H	-3.81021100	-6.02280700	2.67850600
C	-3.19255400	2.00154100	1.82696100
C	-4.59853600	1.91762700	1.85504800
C	-2.51245100	2.52414400	2.94927100
C	-5.30842800	2.33491900	2.99293600
H	-5.14189500	1.54136200	0.98877100
C	-3.22434500	2.94639900	4.08009000
H	-1.42357200	2.60005700	2.93343700
C	-4.62553400	2.84675500	4.10717500
H	-6.39848400	2.26682200	3.00234100
H	-2.68494300	3.34834600	4.94018700
H	-5.18101000	3.16932700	4.99004600
C	-1.75400900	3.18030900	-0.32469900
C	-2.75628600	4.00391900	-0.88001400
C	-0.43544100	3.65824600	-0.21313100
C	-2.42985100	5.28548800	-1.34337700
H	-3.78378900	3.64168500	-0.94550900
C	-0.11185800	4.94461000	-0.67375200
H	0.34919400	3.01775300	0.19430400
C	-1.10721000	5.75437200	-1.24174800
H	-3.20568400	5.91924300	-1.77888300
H	0.92125600	5.28553800	-0.59951900
H	-0.85525300	6.75225800	-1.60749500

Int3c

C	4.57463200	-0.18537800	-2.92251400
C	5.67947500	-0.04346200	-2.01642000
C	5.19209600	0.53963900	-0.79945400
C	3.77143700	0.76471800	-0.94590600
C	3.40066700	0.31247000	-2.26972300
H	4.61036900	-0.64941000	-3.90534600

H	6.69664700	-0.38710600	-2.19228500
H	5.77522200	0.71355800	0.09920900
H	2.37991800	0.29812300	-2.64548000
Fe	4.20481300	-1.19625200	-1.17667300
C	3.76650900	-2.19511600	0.54172400
C	4.99610100	-2.68278100	-0.01039400
C	2.72626300	-2.38678700	-0.44417000
H	3.63806200	-1.72948500	1.51301100
C	4.73248300	-3.16973000	-1.33490700
H	5.97087700	-2.62969400	0.46932200
C	3.33481400	-2.99394300	-1.60419800
H	5.47235400	-3.55025500	-2.03566200
H	2.81750400	-3.22516200	-2.53105200
P	0.98429200	-1.84450500	-0.28687800
P	2.50637400	1.37324700	0.21547900
Pd	0.46702200	0.42732100	-0.37552500
C	-0.83785700	2.31715600	-0.51023000
H	-1.04297200	2.28000000	0.56275600
C	-1.42181400	1.30806400	-1.31706200
C	-1.74141500	0.07132800	-0.70257800
H	-2.06020600	-0.76860400	-1.31760700
H	-1.96873100	0.01281700	0.35566300
C	-1.55215100	1.47418200	-2.81434900
H	-2.42634200	2.11626600	-3.01458900
H	-0.66478100	1.95638300	-3.25356900
H	-1.71753000	0.50359500	-3.30406300
C	-0.80400700	1.01497300	4.08353900
H	-0.67052800	-0.05326000	4.35280900
H	0.13675600	1.54087200	4.31037900
H	-1.60680100	1.43082500	4.72412600

O	-1.08286800	1.18438700	2.70175300
C	-4.01873500	2.75232200	-0.12586000
C	-4.63139900	1.66899100	-0.84898000
C	-5.11815200	1.92347200	-2.15004500
C	-4.96956800	3.20430800	-2.70590800
C	-4.35740400	4.25062200	-1.97906400
C	-3.88572100	4.03264200	-0.66871500
C	-3.88766800	0.86084500	1.17901600
H	-5.59928700	1.12479400	-2.72023400
H	-5.34317100	3.39987900	-3.71433800
H	-4.26184700	5.24207800	-2.42724100
H	-3.42251100	4.84033900	-0.09597600
N	-3.62992600	2.24918600	1.10717700
H	-3.02430700	2.70936800	1.77668800
O	-3.47107400	0.14238200	2.15558000
C	-4.52760500	0.49649400	-0.04011500
H	-1.98655700	0.75885000	2.54160700
C	-4.99738900	-0.89786400	-0.34750500
H	-4.30658700	-1.60957900	0.13966700
H	-4.95096100	-1.08160500	-1.43537200
C	-6.41271400	-1.17305000	0.14962900
C	-7.47632200	-1.39380500	-0.74221600
C	-6.67386200	-1.17988400	1.53562300
C	-8.77951200	-1.61981200	-0.26661400
H	-7.28004000	-1.38508000	-1.81833800
C	-7.97136300	-1.40941700	2.01337800
H	-5.84690900	-0.99139900	2.22406600
C	-9.03040000	-1.63045600	1.11386000
H	-9.59618300	-1.78602600	-0.97390400
H	-8.16057000	-1.41396100	3.08998700

H	-10.04208900	-1.80628900	1.48747600
C	-0.38842900	3.64095300	-1.06815100
H	-1.28119000	4.23600500	-1.33862600
H	0.19935500	4.20304100	-0.33124300
H	0.22056400	3.52363900	-1.97763800
C	0.20281200	-2.73924300	-1.69700500
C	-0.02895300	-2.01235500	-2.88198000
C	-0.14250000	-4.10277300	-1.63889200
C	-0.58710000	-2.64441100	-4.00288100
H	0.20632600	-0.94598000	-2.90588900
C	-0.71388900	-4.73043600	-2.75687300
H	0.01909500	-4.66508100	-0.71796800
C	-0.93247300	-4.00498400	-3.94002400
H	-0.76699400	-2.07310600	-4.91601500
H	-0.99324800	-5.78456600	-2.70202700
H	-1.38072000	-4.49558300	-4.80629600
C	0.42000800	-2.70542000	1.23804200
C	1.00405600	-3.91488900	1.67205400
C	-0.62230000	-2.12863100	1.99199000
C	0.53859700	-4.54217000	2.83765100
H	1.82688900	-4.35492300	1.10601900
C	-1.09307500	-2.76474900	3.15023800
H	-1.05114400	-1.17200300	1.70617300
C	-0.51384100	-3.97171400	3.57470400
H	0.99719700	-5.47628500	3.16925600
H	-1.91310800	-2.30755400	3.70591300
H	-0.87677000	-4.46607800	4.47831700
C	2.72965300	3.19452300	0.23042500
C	2.30351500	3.93184400	1.35582100
C	3.18954000	3.87711500	-0.91353200

C	2.34238800	5.33298100	1.33481200
H	1.93750000	3.40816200	2.24110000
C	3.22391800	5.27974800	-0.93029600
H	3.52006200	3.31157100	-1.78691200
C	2.79983200	6.01075400	0.19122300
H	2.01280700	5.89601900	2.21046700
H	3.58364600	5.80105600	-1.81990700
H	2.82505700	7.10206000	0.17526400
C	3.03888000	0.85552100	1.89543400
C	2.14054100	0.09467900	2.66851900
C	4.31538300	1.16180500	2.41094300
C	2.53675900	-0.40984300	3.91745500
H	1.13259000	-0.08849700	2.29897900
C	4.70981900	0.65557900	3.65752200
H	4.99166200	1.80268000	1.84351400
C	3.82564100	-0.14392100	4.40533000
H	1.83431800	-1.00852200	4.49942000
H	5.70275900	0.88701900	4.04892200
H	4.13821900	-0.54196400	5.37297800

TS3c

C	4.59887200	-0.04493800	-2.86050800
C	5.68957900	0.06865600	-1.93277000
C	5.18176500	0.61557800	-0.70657800
C	3.76546300	0.85078800	-0.87160100
C	3.41497400	0.43327100	-2.21057100
H	4.65163900	-0.47657200	-3.85738800
H	6.70933600	-0.27055000	-2.10273300
H	5.74361000	0.76010900	0.21132800
H	2.40068700	0.44373600	-2.60370000
Fe	4.21159000	-1.11633500	-1.15356000

C	3.77830900	-2.17662400	0.53115300
C	5.02864600	-2.60991600	-0.01896900
C	2.75255700	-2.37708800	-0.46731200
H	3.62709800	-1.73750700	1.51161900
C	4.79241800	-3.06964200	-1.35776700
H	5.99642700	-2.53768700	0.47220500
C	3.39201100	-2.93098000	-1.63631600
H	5.54978900	-3.40809200	-2.06159300
H	2.89551700	-3.16254300	-2.57369900
P	1.00425600	-1.87283800	-0.25513400
P	2.47897600	1.39003800	0.29791700
Pd	0.48755800	0.38265900	-0.27903000
C	-0.80371300	2.16258600	-0.79574900
H	-1.04801900	2.44617100	0.23103200
C	-1.42787200	0.99159900	-1.31084600
C	-1.89413800	0.01684900	-0.39237300
H	-2.20595900	-0.95936400	-0.75774400
H	-1.91218000	0.18928600	0.67968100
C	-1.52841100	0.72974300	-2.79993800
H	-2.36093900	1.31356900	-3.22405300
H	-0.60343700	1.02526100	-3.31990300
H	-1.71260400	-0.33478200	-2.99549900
O	-0.84711700	1.39770000	2.57084700
C	-4.21348800	2.43676900	-1.31842700
C	-4.60711900	1.05702900	-1.32411900
C	-5.06899800	0.49127200	-2.52792300
C	-5.10325000	1.27926200	-3.69005600
C	-4.68829300	2.62813100	-3.66706000
C	-4.24599400	3.22652200	-2.46914200
C	-3.87717500	1.61463800	0.81117300

H	-5.38730100	-0.55354600	-2.55611100
H	-5.45534200	0.84244300	-4.62760300
H	-4.72055000	3.22226700	-4.58281600
H	-3.93676900	4.27457200	-2.44425000
N	-3.81841200	2.74707700	-0.02256500
H	-3.43510700	3.63125000	0.28686500
O	-3.48962300	1.62247000	2.01867900
C	-4.33710100	0.52945500	-0.01698100
H	-1.79527000	1.57688100	2.30711900
C	-4.69401800	-0.82584900	0.52816000
H	-3.98853600	-1.06449300	1.34389900
H	-4.56530600	-1.59312000	-0.25535200
C	-6.11756100	-0.88626900	1.06806100
C	-7.11851600	-1.62393900	0.41255000
C	-6.45411700	-0.16254100	2.23074000
C	-8.43433800	-1.64589900	0.90530700
H	-6.86304100	-2.18329000	-0.49200900
C	-7.76506100	-0.18550800	2.72640200
H	-5.67711600	0.42447200	2.72524200
C	-8.76081200	-0.92786600	2.06589100
H	-9.20182500	-2.22249700	0.38281300
H	-8.01348500	0.37808400	3.62928200
H	-9.78266100	-0.94330400	2.45235000
C	-0.30869900	3.27513400	-1.68876200
H	-1.16579000	3.84195900	-2.10018000
H	0.33186700	3.97069500	-1.13076400
H	0.26366200	2.88649300	-2.54508800
C	0.15156600	-2.68928000	-1.66675900
C	0.44374300	-2.23162000	-2.97080700
C	-0.87493400	-3.63656800	-1.48368600

C	-0.26164100	-2.73174600	-4.07283300
H	1.21218500	-1.47052100	-3.11525800
C	-1.59396300	-4.12013100	-2.58950100
H	-1.11574900	-3.98954900	-0.48025600
C	-1.28801000	-3.67437300	-3.88459500
H	-0.02537500	-2.37125300	-5.07622200
H	-2.39341900	-4.84785400	-2.43528500
H	-1.84985300	-4.05071500	-4.74154100
C	0.47209700	-2.79811000	1.24036600
C	0.90605800	-4.11456600	1.50023900
C	-0.38875900	-2.15192000	2.15128700
C	0.47730200	-4.77949900	2.65817600
H	1.57942900	-4.61038000	0.79830300
C	-0.81718900	-2.82236600	3.30807900
H	-0.69625200	-1.12050300	1.96741500
C	-0.38629200	-4.13464700	3.56147600
H	0.81630000	-5.79841100	2.85707700
H	-1.48160500	-2.31456800	4.00957300
H	-0.71830300	-4.65436100	4.46268700
C	3.11231500	0.93891000	1.96561900
C	2.33619500	0.07655500	2.76112100
C	4.33897100	1.42617900	2.46046000
C	2.80306500	-0.34103700	4.01728100
H	1.37001200	-0.25741400	2.38885200
C	4.80630000	1.00789300	3.71529000
H	4.91754500	2.13959500	1.87060000
C	4.04387500	0.11539500	4.49048100
H	2.19505100	-1.01974700	4.61885000
H	5.76034200	1.38239500	4.09262200
H	4.41142000	-0.20922300	5.46619000

C	2.54926700	3.22323600	0.32672700
C	1.66451900	3.88153300	1.21099400
C	3.36434300	3.97509700	-0.53943400
C	1.61325200	5.28112200	1.23028600
H	1.00413700	3.29588600	1.85633000
C	3.29758800	5.37871900	-0.52300400
H	4.04317100	3.46536900	-1.22592000
C	2.42620500	6.03288800	0.36136200
H	0.92978600	5.78749400	1.91532500
H	3.92845300	5.95869700	-1.20025900
H	2.37538700	7.12362900	0.37201500
C	-0.91034300	1.00760000	3.93817900
H	0.10699900	0.73132400	4.25377800
H	-1.27036700	1.82846700	4.58881700
H	-1.58106800	0.13835400	4.08646300