

Supporting Information for:

**Mechanism of Palladium-Catalyzed Allylic Substitution of Tertiary
Allylic Carbonates with Sodium Sulfinates: Unusual Bifunctional
Nucleophile-Enabled Inner-Sphere Pathway and Origin of Regio- and
Enantioselectivities**

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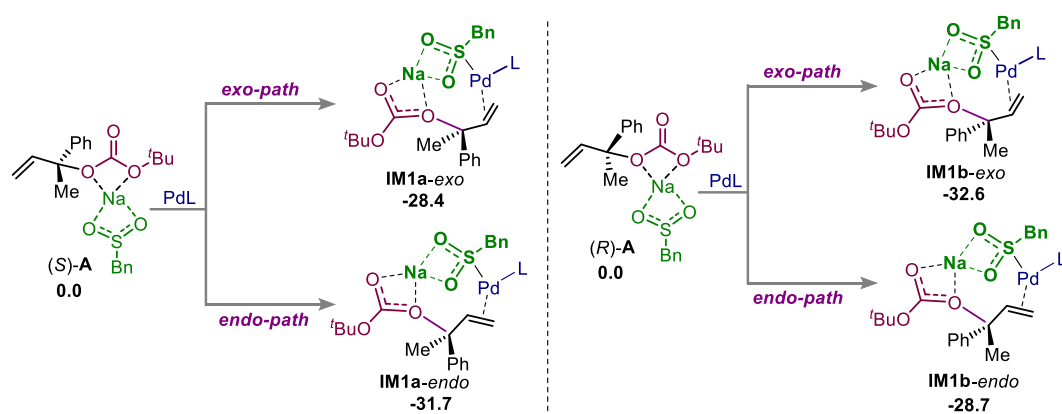
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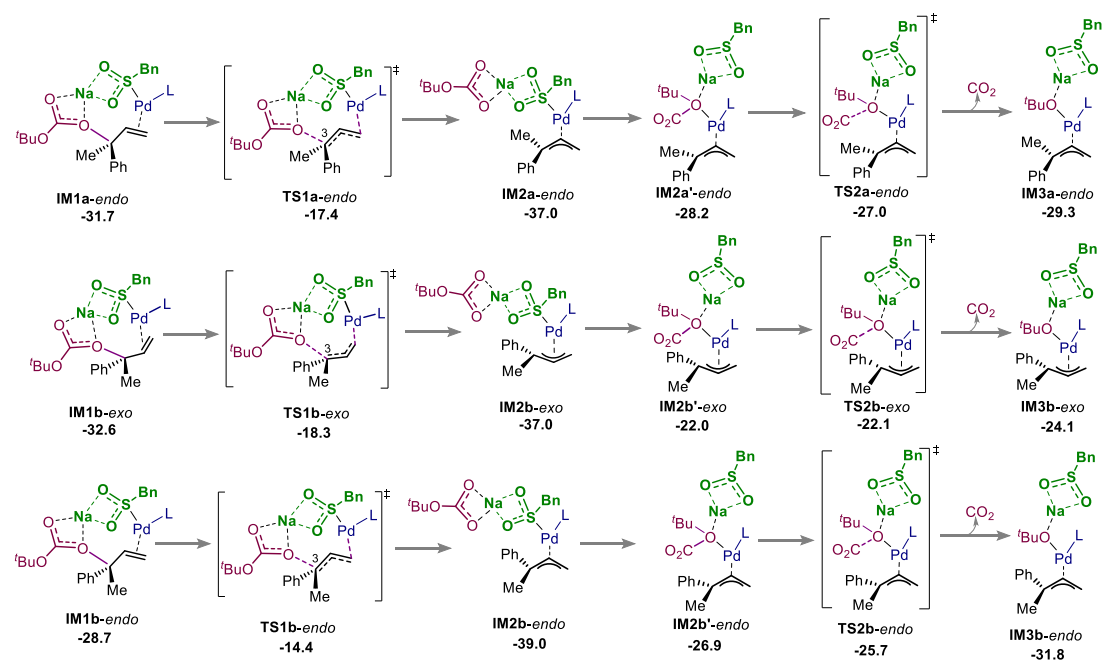
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The formation of species IM1a and IM1b from (*rac*)-A and PdL



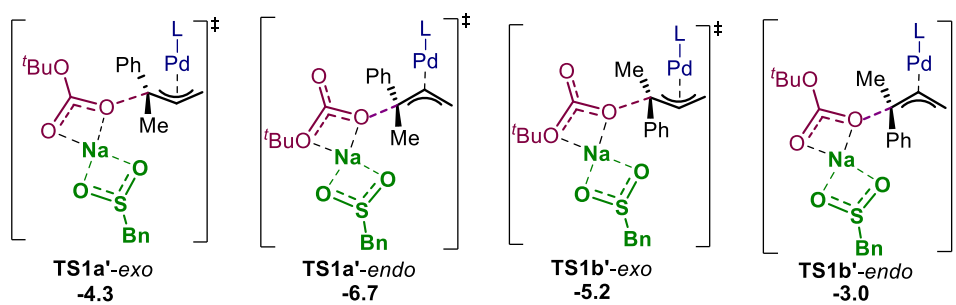
Scheme S1. The formation of species IM1a-*endo/exo* and IM1b-*endo/exo*. Gibbs free energies are given in kcal/mol.

C-O oxidative addition/CO₂ extrusion of IM1a-endo, IM1b-exo and IM1b-endo.



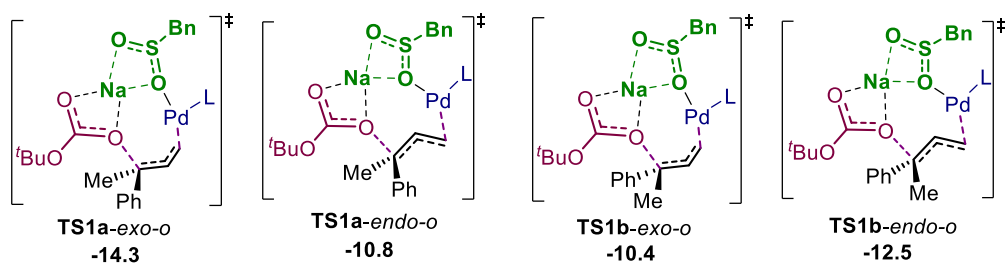
Scheme S2. C-O oxidative addition/CO₂ extrusion of IM1a-endo, IM1b-exo and IM1b-endo. Gibbs free energies are given in kcal/mol.

C–O oxidative addition via the S_N2 back-side attack transition states without the Pd-S interaction



Scheme S3. S_N2 back-side attack transition states without the Pd-S interaction. Gibbs free energies are given in kcal/mol.

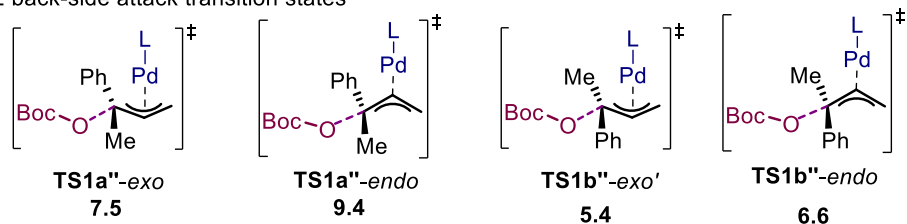
C–O oxidative addition via S_N2 front-side attack transition states with the Pd-O interaction



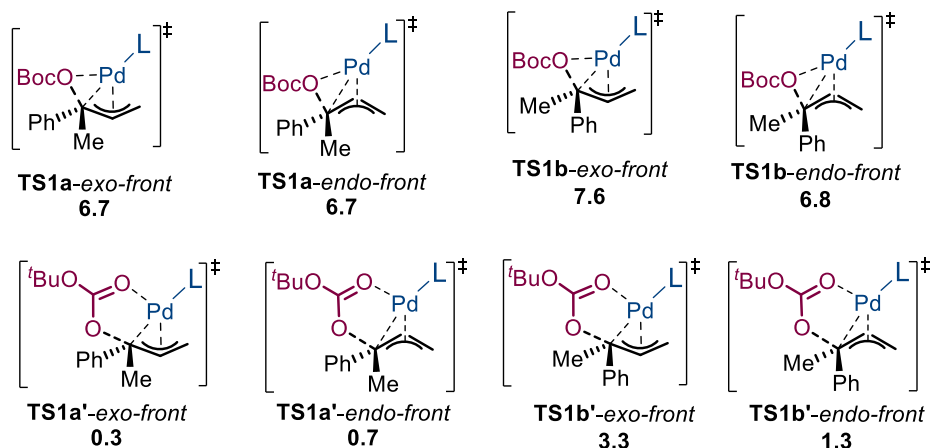
Scheme S4. S_N2 front-side attack transition states with the Pd-O interaction. Gibbs free energies are given in kcal/mol.

C–O oxidative addition in the absence of sodium benzenesulfonate

S_N2 back-side attack transition states

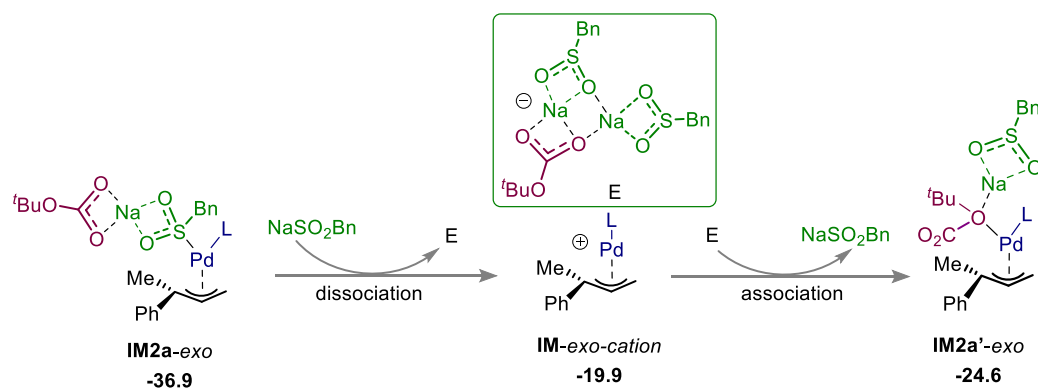


Front-side attack transition states



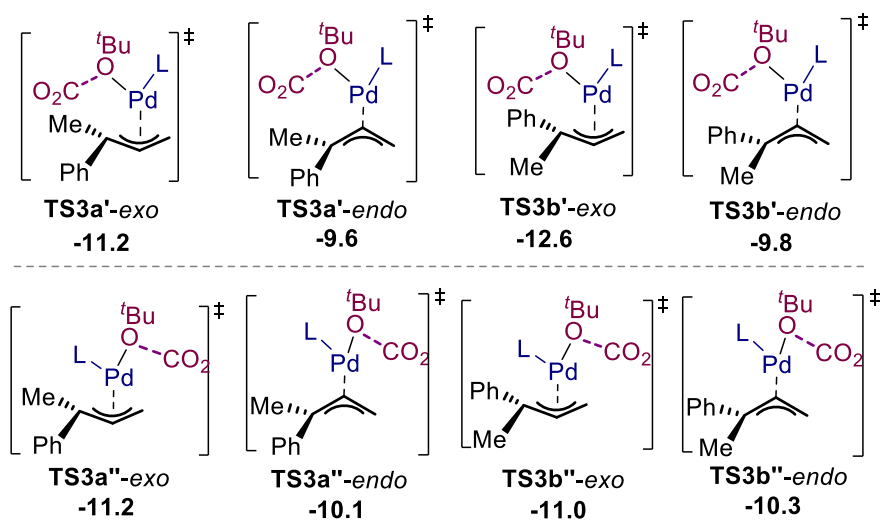
Scheme S5. S_N2 back-side and front-side attack transition states in the absence of sodium benzenesulfonate. Gibbs free energies are given in kcal/mol.

The isomerization of IM2a-*exo* to IM2a'-*exo*



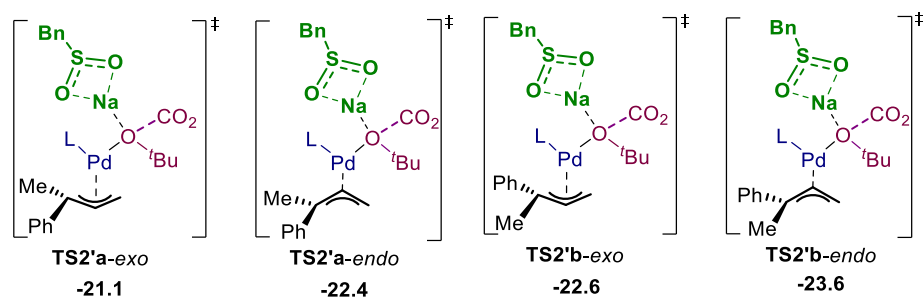
Scheme S6. The dissociation and association processes between **IM2a-*exo*** and **IM2a'-*exo***. Gibbs free energies are given in kcal/mol.

CO₂ extrusion without sodium benzyldisulfinate



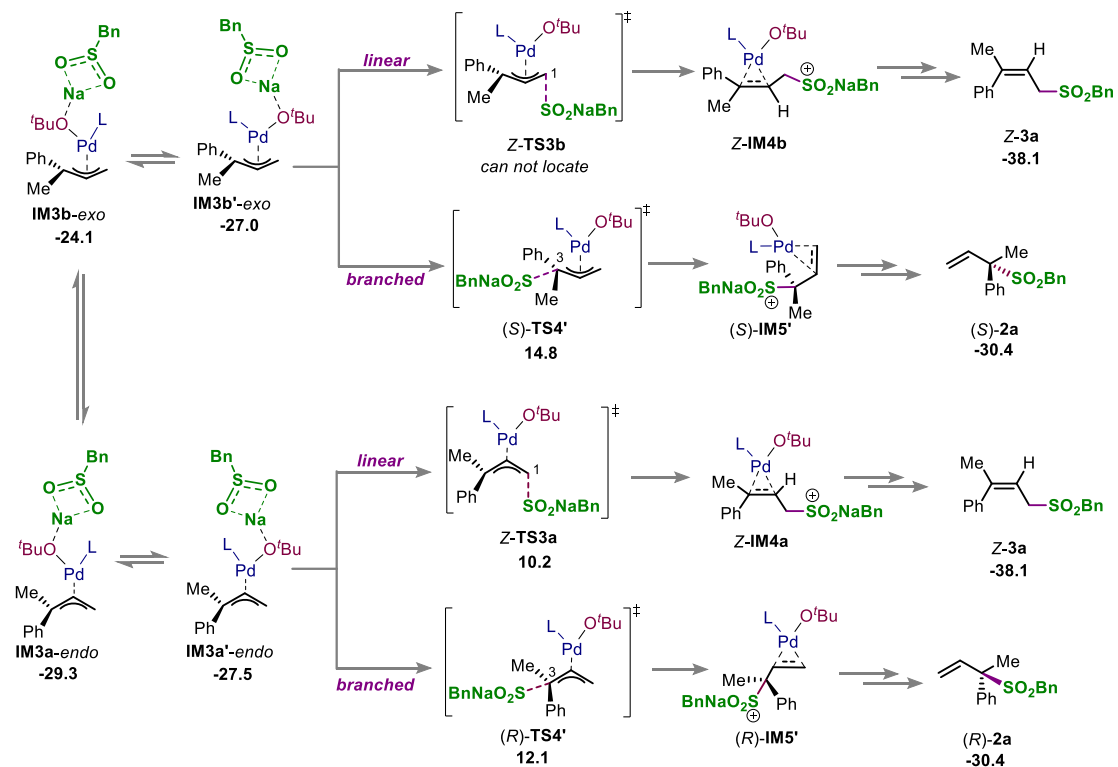
Scheme S7. CO₂ extrusion without sodium benzyldisulfinate. Gibbs free energies are given in kcal/mol.

The CO₂ extrusion process leading to **IM3a'**-*exo* and **IM3b'**-*endo*.



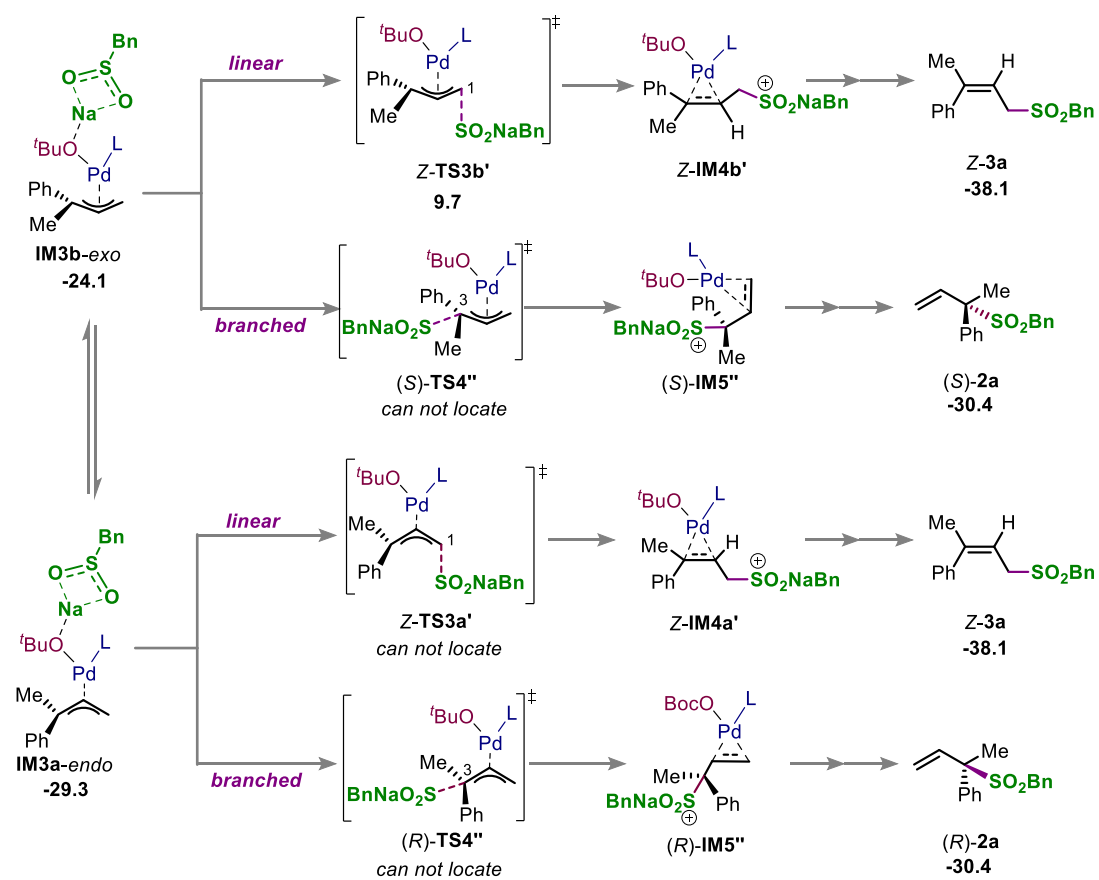
Scheme S8. The CO₂ extrusion process leading to **IM3a'**-*exo* and **IM3b'**-*endo*. Gibbs free energies are given in kcal/mol.

C-S bond formation via outer-sphere nucleophilic attack of IM3a'-endo and IM3b'-exo



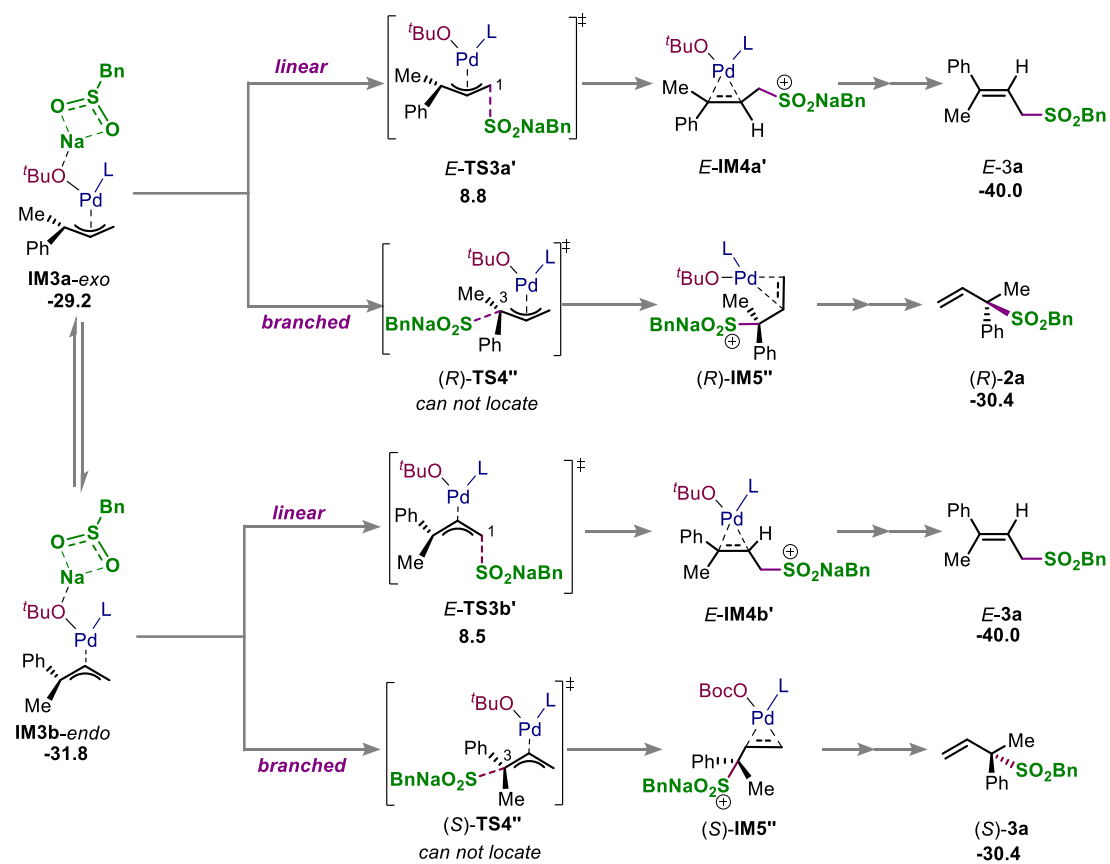
Scheme S9. Outer-sphere nucleophilic attack of **IM3a'-endo** and **IM3b'-exo**. Gibbs free energies are given in kcal/mol.

C-S bond formation via outer-sphere nucleophilic attack of **IM3a-endo** and **IM3b-exo**



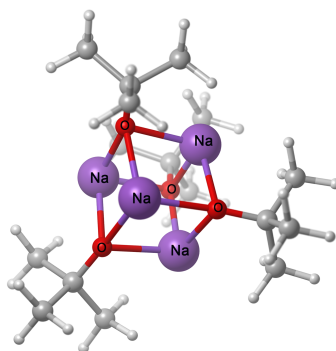
Scheme S10. outer-sphere nucleophilic attack of **IM3a-endo** and **IM3b-exo**. Gibbs free energies are given in kcal/mol.

C-S bond formation via outer-sphere nucleophilic attack of IM3a-*exo* and IM3b-*endo*



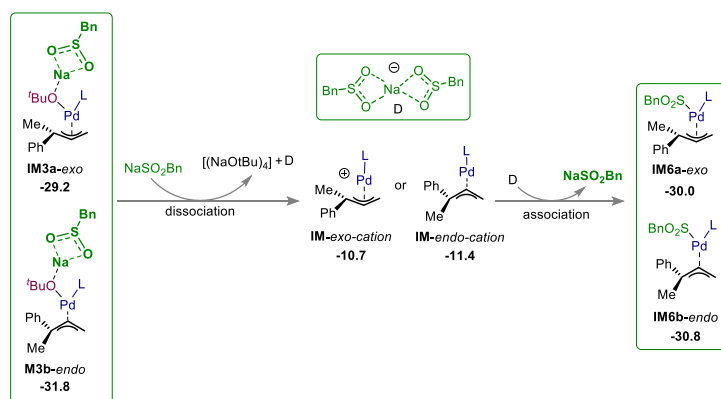
Scheme S11. outer-sphere nucleophilic attack of **IM3a-*exo*** and **IM3b-*endo***. Gibbs free energies are given in kcal/mol.

The tetramer form of NaOtBu



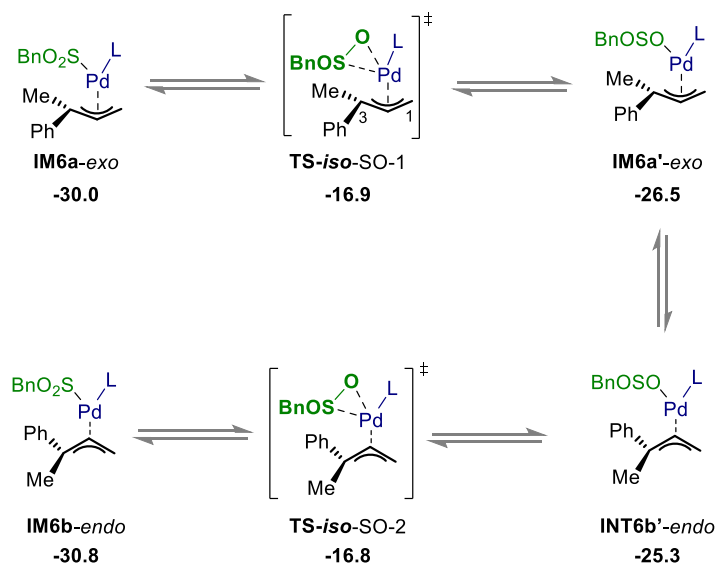
Scheme S12. The tetramer form of NaOtBu.

The isomerization of IM3a-*exo* and IM3b-*endo* to IM6a-*exo* and IM6b-*endo*



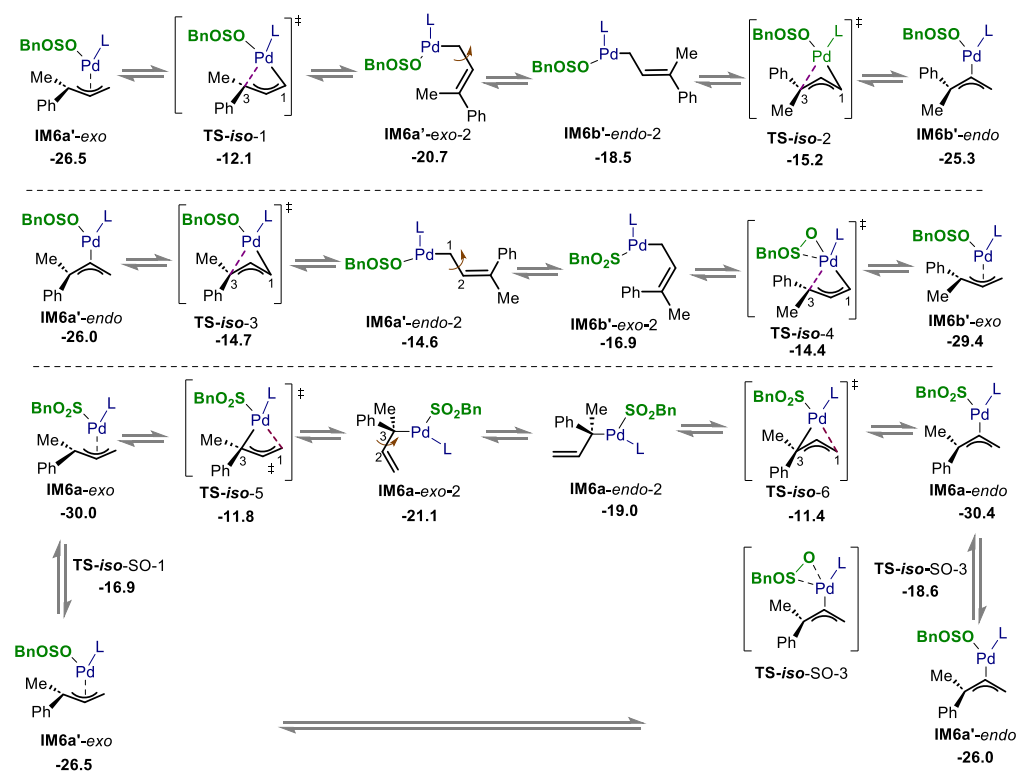
Scheme S13. The isomerization for the rearrangement of **IM3a** to **IM6a**. Gibbs free energies are given in kcal/mol.

The isomerization of **IM6a-exo** and **IM6b-endo** to **IM6a'-exo** and **IM6b'-endo**



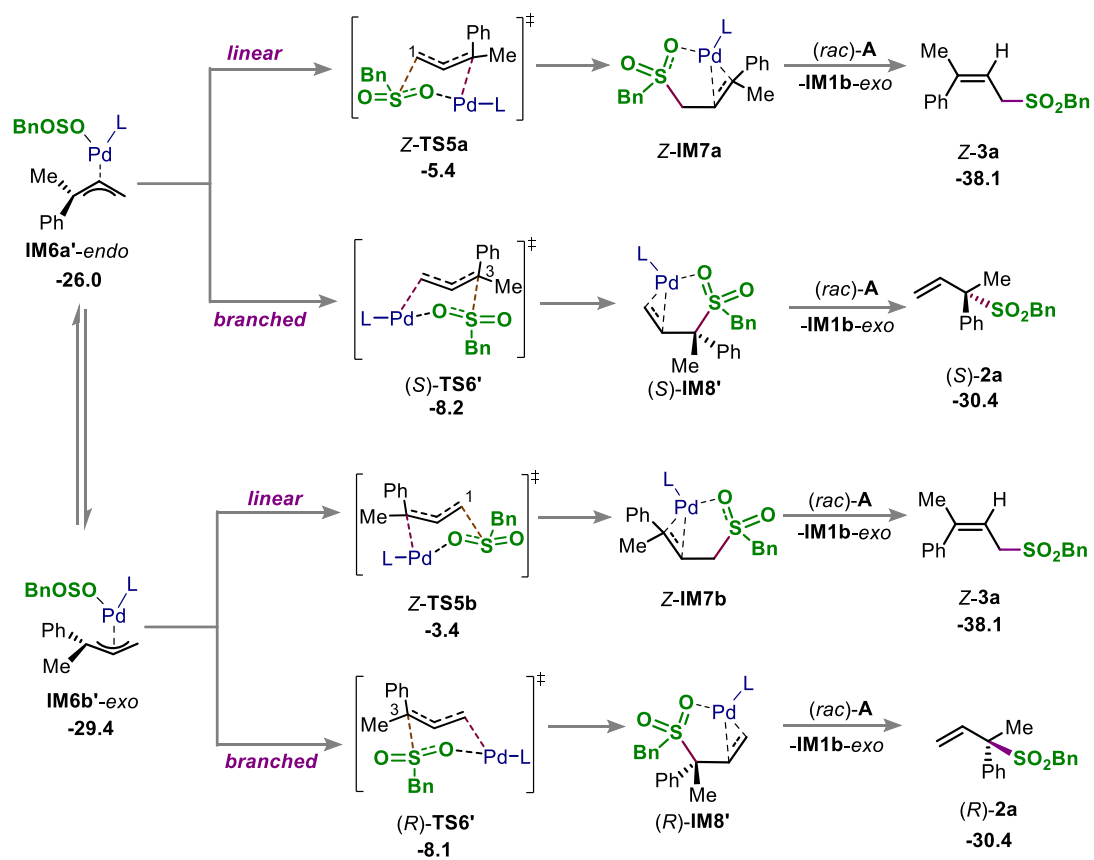
Scheme S14. The isomerization for the rearrangement of **IM6a** to **IM6a'**. Gibbs free energies are given in kcal/mol.

π - σ - π isomerization



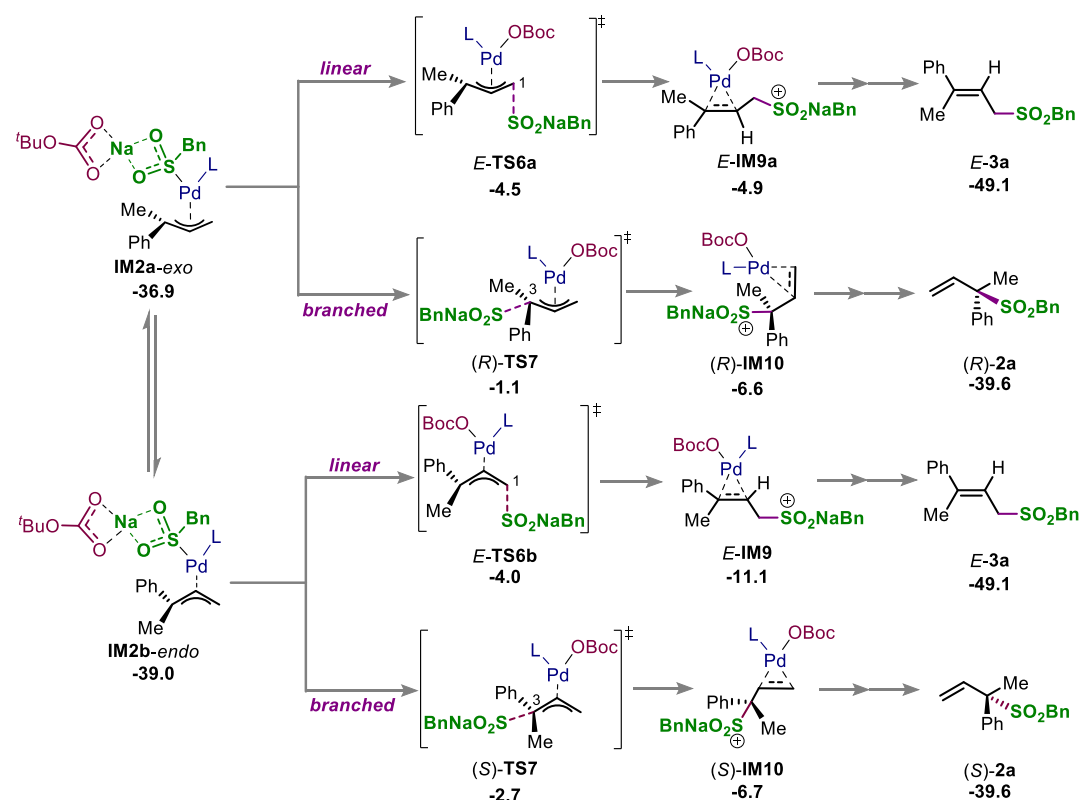
Scheme S15. The interconversion between **IM6a'-exo** and **IM6b'-endo**, **IM6a'-endo** and **IM6b'-exo**. Gibbs free energies are given in kcal/mol.

C-S bond formation via inner-sphere nucleophilic attack of **IM6a'**-endo and **IM6b'**-exo



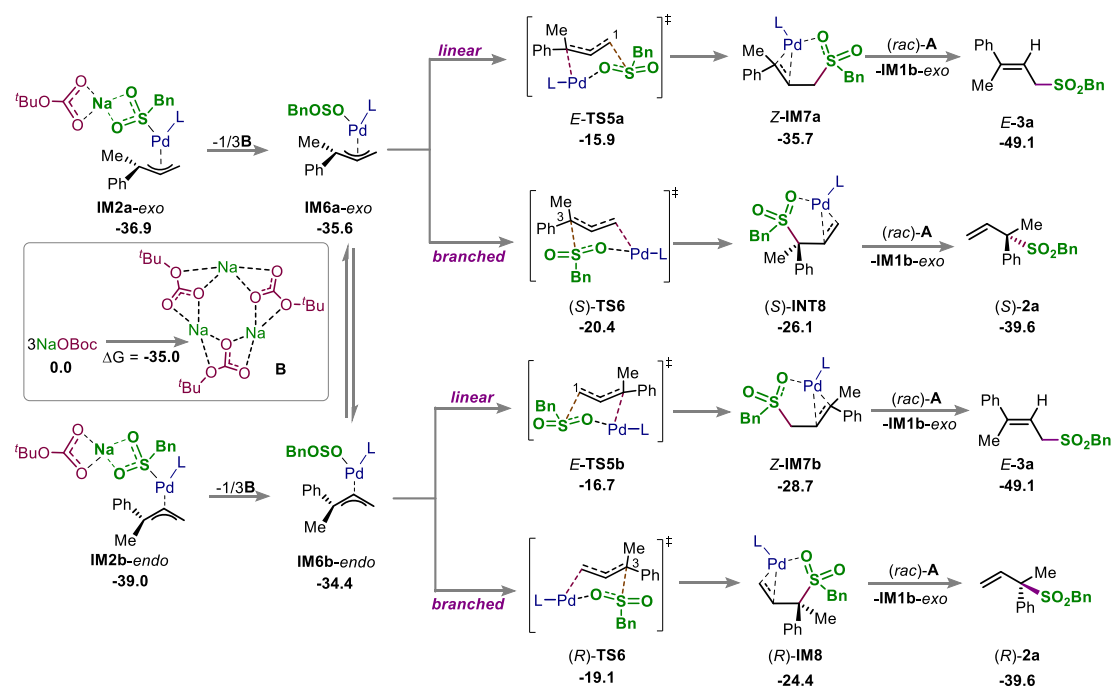
Scheme S16. inner-sphere nucleophilic attack of **IM6a'**-endo and **IM6b'**-exo. Gibbs free energies are given in kcal/mol.

C-S bond formation via outer-sphere nucleophilic attack of **IM2a-*exo*** and **IM2b-*endo***



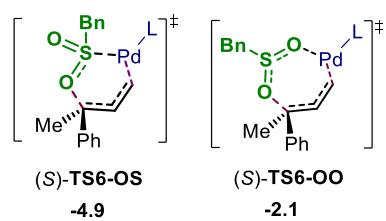
Scheme S17. outer-sphere nucleophilic attack of **IM2a-*exo*** and **IM2b-*endo***. Gibbs free energies are given in kcal/mol.

C-S bond formation via inner-sphere nucleophilic attack of **IM2a-exo** and **IM2b-endo**



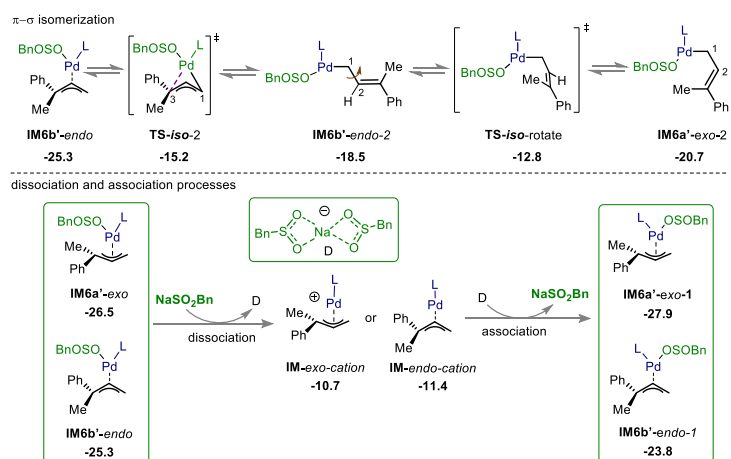
Scheme S18. inner-sphere nucleophilic attack of **IM2a-exo** and **IM2b-endo**. Gibbs free energies are given in kcal/mol.

Inner sphere C-O reductive elimination



Scheme S19. Inner sphere C-O reductive elimination. Gibbs free energies are given in kcal/mol.

The isomerization of **IM6a'**-*exo* and **IM6b'**-*endo* to pre-complexes



Scheme S20. The isomerization of **IM6a'**-*exo* and **IM6b'**-*endo* to **IM6a'**-*exo-1*, **IM6b'**-*endo-1*, **IM6a'**-*exo-2* and **IM6b'**-*endo-2*. Gibbs free energies are given in kcal/mol.

The optimized geometries of IM6a'-*exo* and IM6b'-*endo*

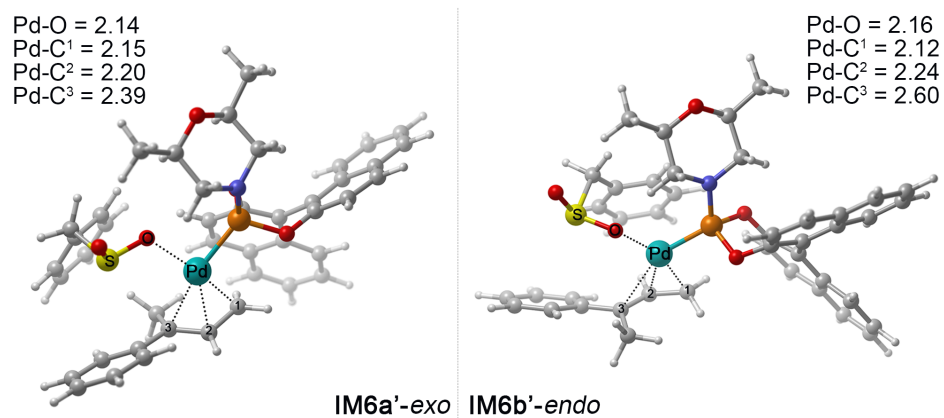
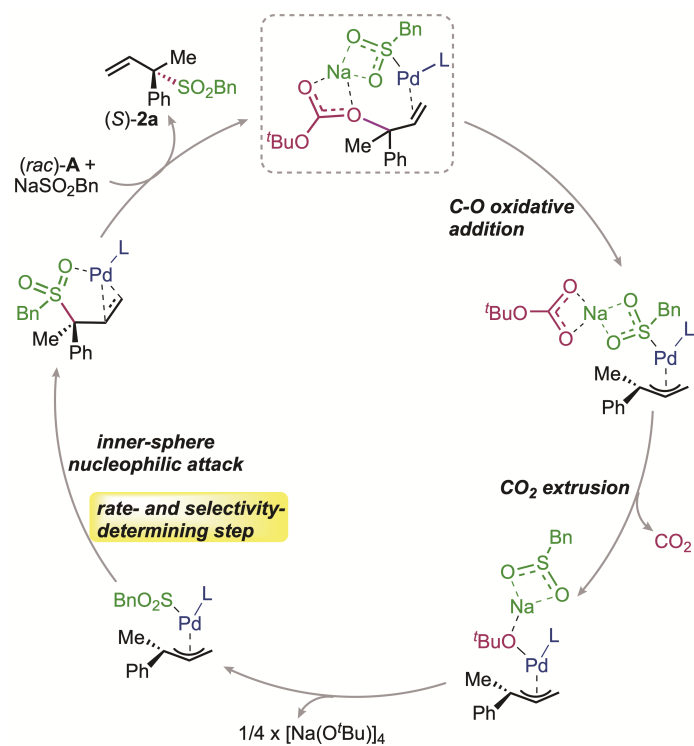


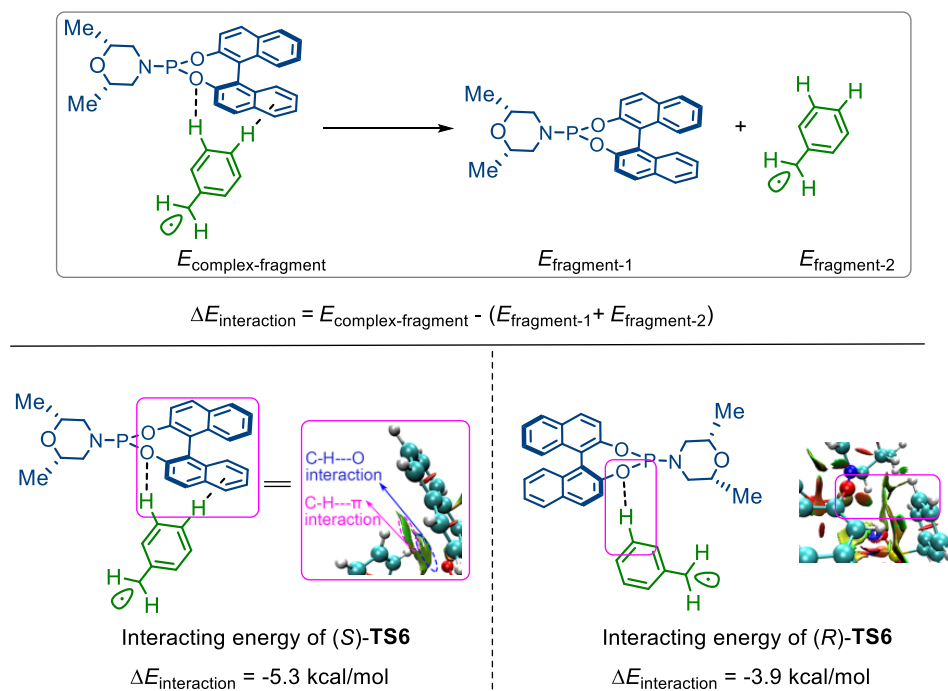
Figure S1. The optimized geometries of IM6a'-*exo* and IM6b'-*endo*. Selected bond distances are given in Å.

Overall catalytic cycle



Scheme S21. Overall catalytic cycle based on DFT Calculations

The interacting energy of ligand fragment and substrate fragment



Scheme S22. The interacting energy between the phosphoramidite ligand fragment and benzyl radical of benzylsulfinate.

Table of calculated energies and energy corrections

Stationary point	Single-point energy PBE0-D3(BJ)-SMD 6-311+G(d,p), LANL2TZf (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)
PdL	-1752.61837	0.374533
CO ₂	-188.4434532	-0.009504
[(NaO ^t Bu) ₄]	-1580.567838	0.424291
(<i>R</i>)-A	-1790.012535	0.369107
(<i>S</i>)-A	-1790.012535	0.369107
(<i>S</i>)-2a	-1206.404181	0.253013
(<i>R</i>)-2a	-1206.404181	0.253013
<i>E</i> -3a	-1206.420577	0.254186
IM1a- <i>exo</i>	-3542.711061	0.778532
IM1a- <i>endo</i>	-3542.715406	0.777652
IM1b- <i>exo</i>	-3542.717693	0.778515
IM1b- <i>endo</i>	-3542.708357	0.775403
TS1a- <i>exo</i>	-3542.689978	0.774942
IM2a- <i>exo</i>	-3542.726565	0.780491
IM2a'- <i>exo</i>	-3542.708335	0.781837
TS2a- <i>exo</i>	-3542.704897	0.77773
IM3a- <i>exo</i>	-3354.251929	0.771145
IM3a- <i>endo</i>	-3354.251314	0.770335
IM3b- <i>endo</i>	-3354.25311	0.768195
IM3b- <i>exo</i>	-3354.2474713	0.774801
IM3a'- <i>exo</i>	-3354.25395	0.772853
IM3b'- <i>endo</i>	-3354.254213	0.772734
<i>E</i> -TS3a	-3354.187068	0.76519
(<i>R</i>)-TS4	-3354.185138	0.767521
<i>E</i> -TS3b	-3354.186966	0.76437
(<i>S</i>)-TS4	-3354.189316	0.765778
<i>E</i> -IM4a	-3354.199694	0.769187
(<i>R</i>)-IM5	-3354.194598	0.766203
<i>E</i> -IM4b	-3354.196868	0.767114
(<i>S</i>)-IM5	-3354.192829	0.766525
IM6a- <i>exo</i>	-2959.102096	0.655903

IM6b-endo	-2959.102694	0.655124
IM6a'-exo	-2959.094553	0.653919
IM6b'-endo	-2959.091731	0.653064
IM6a'-exo-1	-2959.097848	0.655022
IM6a'-exo-2	-2959.08612	0.654732
IM6b'-endo-1	-2959.093525	0.657232
IM6b'-endo-2	-2959.084200	0.656221
E-TS5a	-2959.064086	0.654878
(S)-TS6	-2959.067502	0.651196
E-TS5b	-2959.065312	0.654799
(R)-TS6	-2959.067673	0.653401
E-IM7a	-2959.099666	0.65892
(S)-IM8	-2959.083038	0.657529
E-IM7b	-2959.088716	0.659167
(R)-IM8	-2959.080448	0.657704
TS-iso-1	-2959.071871	0.654176
TS-iso-2	-2959.07648	0.65388
TS-iso-rotate	-2959.07208	0.653339
TS-iso-3	-2959.07361	0.651698
TS-iso-4	-2959.074862	0.653456
TS-iso-5	-2959.072358	0.655151
TS-iso-6	-2959.072792	0.65615
TS-iso-SO-1	-2959.078015	0.652583
TS-iso-SO-2	-2959.076853	0.651636
TS-iso-SO-3	-2959.078733	0.650711

Cartesian coordinates

PdL			
Pd	0.74453400	-0.49993400	0.14428400
P	-1.12243400	0.42938700	0.54297400
O	-2.33656800	0.37078100	-0.65088300
O	-1.00334100	2.13816900	0.67979300
C	-2.30738900	2.47714400	-1.81730800
C	-2.07334300	1.09921800	-1.80394400
C	-1.59972600	0.39099900	-2.93826700
C	-1.35526700	1.07372300	-4.11633700
C	-1.23723000	3.20620600	-5.38357600
C	-1.35972900	4.58584600	-5.43481400
C	-1.77307300	5.30174900	-4.27771700
C	-2.07996500	4.63197600	-3.10224100
C	-1.99349200	3.20852400	-3.01996000
C	-1.53274600	2.48698600	-4.18693900
C	-2.81535900	3.13440300	-0.58116400
C	-2.13127000	2.94403800	0.62582300
C	-2.52050000	3.59412800	1.82732400
C	-3.63022100	4.41755400	1.83743300
C	-5.59979600	5.38729300	0.67535600
C	-6.38752000	5.51486200	-0.45825700
C	-6.02006700	4.83654200	-1.65269400
C	-4.86757100	4.06561700	-1.70431100
C	-4.01823400	3.93053600	-0.56372900
C	-4.41578500	4.59161300	0.65997400
H	-1.44887100	-0.68573100	-2.85424800
H	-1.00467000	0.54154000	-5.00334900
H	-0.90073200	2.64274000	-6.25723000
H	-1.12703600	5.12571400	-6.35496700
H	-1.84422900	6.39092100	-4.31190600
H	-2.38662100	5.19538600	-2.22245500
H	-1.92621400	3.42465100	2.72589900
H	-3.93356400	4.92843300	2.75397600
H	-5.87687700	5.88624800	1.60725300
H	-7.29383700	6.12328400	-0.43400800
H	-6.65376600	4.91830100	-2.53831100
H	-4.60425400	3.54625900	-2.62451000
C	-1.49935400	-0.98837500	2.85722200
C	-3.44531900	0.30807800	2.11447700
C	-2.42612000	-2.19789600	3.07064800
H	-1.40645400	-0.43301400	3.80987000
H	-0.49990900	-1.32776100	2.53942000

C	-4.32208600	-0.93421700	2.35501200
H	-3.45380600	0.93884000	3.02188300
H	-3.84405700	0.88755600	1.27469400
H	-2.45938900	-2.76997700	2.12083900
H	-4.34997000	-1.51785000	1.41290300
N	-2.06297200	-0.11152700	1.82186500
O	-3.75736600	-1.75439300	3.39444300
C	-5.73272100	-0.54810400	2.78830000
H	-6.21694400	0.05305200	2.00237300
H	-6.33831000	-1.44980800	2.96872600
H	-5.69834900	0.04494700	3.71658400
C	-1.94699000	-3.08425700	4.21539500
H	-2.64361700	-3.92354600	4.36546100
H	-0.94820500	-3.48944500	3.98721900
H	-1.88874000	-2.50358300	5.15028800
CO ₂			
C	-0.83769600	0.56282700	0.00000000
O	0.33990400	0.56282700	0.00000000
O	-2.01529700	0.56282700	0.00000000
[(NaO ^t Bu) ₄]			
O	3.39251300	2.27845900	4.45995000
C	2.98319900	3.53020800	4.89775400
C	1.43624300	3.62856400	4.89807600
C	3.50371600	3.79802500	6.34140200
C	3.55321100	4.64608800	3.97114600
H	1.05756900	3.45291800	3.87604400
H	1.01907400	2.84855500	5.55843600
H	1.07213200	4.61290900	5.24285600
H	4.61070000	3.81870800	6.34780400
H	3.15806100	4.76309100	6.75111600
H	3.15319900	2.99447000	7.01551700
H	3.19255400	5.65356600	4.24192200
H	4.65808900	4.66931200	4.03436900
H	3.25661000	4.44485300	2.92525600
Na	3.38540900	0.19808100	3.72402700
O	6.76893100	2.00322700	4.52095800
C	8.00169300	2.43822100	4.05545100
C	8.85495800	1.23240000	3.55757200
C	7.81580800	3.41295800	2.85436500
C	8.78267800	3.17002800	5.17625600
H	8.93617600	0.48018300	4.36373800
H	8.37925700	0.76498200	2.67315700

H	9.87570300	1.52487800	3.25578500
H	7.17699700	4.26207000	3.15974000
H	8.77100400	3.82168700	2.48134900
H	7.33356700	2.88413400	2.00994700
H	9.76658100	3.53954700	4.83615000
H	8.18976300	4.02904200	5.53542400
H	8.94012500	2.48152100	6.02460400
Na	5.05990700	1.49286600	5.83961200
O	4.83351900	-0.63980200	5.29872300
C	4.69416100	-2.01956300	5.34663500
C	4.69679800	-2.51841300	6.81404100
C	3.35985600	-2.45781100	4.67097000
C	5.86201800	-2.71227300	4.58145800
H	5.64358200	-2.22449600	7.29964100
H	3.86593500	-2.04448700	7.36500300
H	4.58820300	-3.61520000	6.89011000
H	3.37863700	-2.20967800	3.59222100
H	3.17587000	-3.54346100	4.74925900
H	2.51286200	-1.93073400	5.14793300
H	5.82580000	-3.81356500	4.64780400
H	5.82141400	-2.44815200	3.50708000
H	6.82871800	-2.37606000	5.00051800
Na	6.38364600	-0.10653500	3.68937800
O	4.97093800	0.43954200	2.07149200
C	4.32947500	0.54157700	0.84442200
C	5.04806900	-0.32323700	-0.22249600
C	2.85082300	0.06493900	0.96141300
C	4.31170900	2.02207800	0.35864300
H	6.09635400	0.00895600	-0.31961400
H	5.05053100	-1.37938700	0.09860900
H	4.56650200	-0.25971800	-1.21467100
H	2.28864700	0.73149700	1.64395300
H	2.32087200	0.07121500	-0.00682500
H	2.82490400	-0.96513000	1.36138100
H	3.86452000	2.13949900	-0.64370800
H	3.71584800	2.64329100	1.05461700
H	5.34471300	2.41397600	0.32038200
Na	5.14303500	2.53783100	2.99835600
 (R)-A			
C	-2.41334800	-1.14430200	2.66267600
H	-1.80132700	-1.95275700	2.23377100
H	-3.46281600	-1.26248900	2.35181300
C	-2.25772200	-1.01439000	4.13951000

C	-1.06366600	-1.41545600	4.78042500
C	-3.26804900	-0.40853300	4.92073600
C	-0.89102700	-1.22981600	6.16013600
H	-0.27360300	-1.88140300	4.18802700
C	-3.09675100	-0.22027000	6.30073300
H	-4.19500100	-0.08993900	4.43637700
C	-1.90696600	-0.63145500	6.92698700
H	0.03620900	-1.55369000	6.63913900
H	-3.89226400	0.24479700	6.88792900
H	-1.77351700	-0.48957900	8.00180000
S	-1.79285800	0.41982700	1.70601900
O	-1.92736700	-0.08424800	0.23768600
Na	0.42455100	-0.44399200	0.03788800
O	-0.28619200	0.46049700	2.09523700
C	4.53481100	-0.61050700	-4.10997500
C	3.81611900	-0.44351200	-2.99168000
H	5.61969900	-0.73078100	-4.06208700
H	4.07514100	-0.63503300	-5.10041600
H	4.31265700	-0.40953200	-2.01735200
C	2.31883900	-0.23006200	-2.93408400
C	1.56939200	-0.57226800	-4.22869800
H	0.48480600	-0.50876000	-4.06161500
H	1.84385600	0.16264300	-4.99944100
H	1.83076500	-1.57824300	-4.57835300
C	1.92957000	1.17363900	-2.43415700
C	0.59010500	1.41793600	-2.05401600
C	2.86135500	2.22194800	-2.33790700
C	0.20057500	2.66699400	-1.55037000
H	-0.15890800	0.62862900	-2.15140700
C	2.46771200	3.48088300	-1.85070000
H	3.89535300	2.06007800	-2.64429900
C	1.14297700	3.70503200	-1.44563900
H	-0.83505400	2.82295600	-1.24379100
H	3.20467300	4.28358800	-1.78165500
H	0.84430200	4.67978100	-1.05541200
O	1.79588200	-1.07651300	-1.80536800
C	1.79914300	-2.43796800	-1.82980100
O	2.28237300	-3.16114400	-2.67582700
O	1.14626800	-2.77627100	-0.69276500
C	0.89269700	-4.20962300	-0.31859500
C	0.03000700	-4.86976200	-1.39809900
C	2.23164600	-4.92052300	-0.10459400
C	0.11911800	-4.06410600	0.99466600
H	-0.88637800	-4.28186700	-1.56530200

H	0.57903100	-4.96829400	-2.34337600
H	-0.25917500	-5.87368400	-1.05029600
H	2.83776200	-4.37964100	0.63925800
H	2.03399900	-5.93393300	0.27793900
H	2.79395000	-5.00170000	-1.04399900
H	-0.11960400	-5.06563800	1.38325900
H	0.72226200	-3.53139900	1.74679400
H	-0.82259600	-3.51782500	0.83060000

(S)-A

C	-2.41334800	-1.14430200	-2.66267600
H	-1.80132700	-1.95275700	-2.23377100
H	-3.46281600	-1.26248900	-2.35181300
C	-2.25772200	-1.01439000	-4.13951000
C	-1.06366600	-1.41545600	-4.78042500
C	-3.26804900	-0.40853300	-4.92073600
C	-0.89102700	-1.22981600	-6.16013600
H	-0.27360300	-1.88140300	-4.18802700
C	-3.09675100	-0.22027000	-6.30073300
H	-4.19500100	-0.08993900	-4.43637700
C	-1.90696600	-0.63145500	-6.92698700
H	0.03620900	-1.55369000	-6.63913900
H	-3.89226400	0.24479700	-6.88792900
H	-1.77351700	-0.48957900	-8.00180000
S	-1.79285800	0.41982700	-1.70601900
O	-1.92736700	-0.08424800	-0.23768600
Na	0.42455100	-0.44399200	-0.03788800
O	-0.28619200	0.46049700	-2.09523700
C	4.53481100	-0.61050700	4.10997500
C	3.81611900	-0.44351200	2.99168000
H	5.61969900	-0.73078100	4.06208700
H	4.07514100	-0.63503300	5.10041600
H	4.31265700	-0.40953200	2.01735200
C	2.31883900	-0.23006200	2.93408400
C	1.56939200	-0.57226800	4.22869800
H	0.48480600	-0.50876000	4.06161500
H	1.84385600	0.16264300	4.99944100
H	1.83076500	-1.57824300	4.57835300
C	1.92957000	1.17363900	2.43415700
C	0.59010500	1.41793600	2.05401600
C	2.86135500	2.22194800	2.33790700
C	0.20057500	2.66699400	1.55037000
H	-0.15890800	0.62862900	2.15140700
C	2.46771200	3.48088300	1.85070000

H	3.89535300	2.06007800	2.64429900
C	1.14297700	3.70503200	1.44563900
H	-0.83505400	2.82295600	1.24379100
H	3.20467300	4.28358800	1.78165500
H	0.84430200	4.67978100	1.05541200
O	1.79588200	-1.07651300	1.80536800
C	1.79914300	-2.43796800	1.82980100
O	2.28237300	-3.16114400	2.67582700
O	1.14626800	-2.77627100	0.69276500
C	0.89269700	-4.20962300	0.31859500
C	0.03000700	-4.86976200	1.39809900
C	2.23164600	-4.92052300	0.10459400
C	0.11911800	-4.06410600	-0.99466600
H	-0.88637800	-4.28186700	1.56530200
H	0.57903100	-4.96829400	2.34337600
H	-0.25917500	-5.87368400	1.05029600
H	2.83776200	-4.37964100	-0.63925800
H	2.03399900	-5.93393300	-0.27793900
H	2.79395000	-5.00170000	1.04399900
H	-0.11960400	-5.06563800	-1.38325900
H	0.72226200	-3.53139900	-1.74679400
H	-0.82259600	-3.51782500	-0.83060000

(R)-2a

C	0.81845200	-5.08461900	-16.57841200
C	0.04739300	-3.97022800	-15.84832200
H	1.89365400	-4.86932700	-16.60631900
H	0.66149300	-6.02995400	-16.03717600
C	-1.45129500	-4.13783700	-15.89414100
C	-2.10938600	-5.16770200	-16.44899000
H	-2.03007800	-3.33906400	-15.42317500
C	0.59610400	-3.71224800	-14.44298200
C	1.97982000	-3.49623200	-14.24542100
C	-0.24767900	-3.69829300	-13.31052600
C	2.49614300	-3.26016100	-12.96380000
H	2.65228300	-3.48936700	-15.10078700
C	0.27128100	-3.46860000	-12.02622300
H	-1.31572100	-3.88491500	-13.41971600
C	1.64453500	-3.24376800	-11.84639000
H	3.56789000	-3.09084500	-12.83989800
H	-0.40321400	-3.46919500	-11.16735400
H	2.04822100	-3.06303200	-10.84801100
H	-1.59671000	-6.00323300	-16.92911200
H	-3.20151100	-5.19956400	-16.43207500

H	0.45203200	-5.20124200	-17.60875700
C	-0.24621200	-0.98597800	-15.85410900
H	0.31827700	-1.06282900	-14.91611900
H	-1.30568800	-1.21618000	-15.67723100
C	-0.04796700	0.33002400	-16.54813500
C	1.15761000	1.04220700	-16.38580500
C	-1.04414500	0.84252200	-17.40331400
C	1.35666600	2.25853500	-17.05592500
H	1.93255700	0.63933300	-15.73091700
C	-0.84498700	2.05938400	-18.07279300
H	-1.97395100	0.28604400	-17.53675600
C	0.35568600	2.76973300	-17.90032800
H	2.29132200	2.80661900	-16.91962800
H	-1.62503200	2.45225400	-18.72833000
H	0.51013800	3.71753200	-18.42040600
S	0.39219300	-2.37435300	-16.92667700
O	1.86549700	-2.20473700	-17.07720500
O	-0.44506600	-2.45021200	-18.15579400

(S)-2a

C	0.81845200	-5.08461900	16.57841200
C	0.04739300	-3.97022800	15.84832200
H	1.89365400	-4.86932700	16.60631900
H	0.66149300	-6.02995400	16.03717600
C	-1.45129500	-4.13783700	15.89414100
C	-2.10938600	-5.16770200	16.44899000
H	-2.03007800	-3.33906400	15.42317500
C	0.59610400	-3.71224800	14.44298200
C	1.97982000	-3.49623200	14.24542100
C	-0.24767900	-3.69829300	13.31052600
C	2.49614300	-3.26016100	12.96380000
H	2.65228300	-3.48936700	15.10078700
C	0.27128100	-3.46860000	12.02622300
H	-1.31572100	-3.88491500	13.41971600
C	1.64453500	-3.24376800	11.84639000
H	3.56789000	-3.09084500	12.83989800
H	-0.40321400	-3.46919500	11.16735400
H	2.04822100	-3.06303200	10.84801100
H	-1.59671000	-6.00323300	16.92911200
H	-3.20151100	-5.19956400	16.43207500
H	0.45203200	-5.20124200	17.60875700
C	-0.24621200	-0.98597800	15.85410900
H	0.31827700	-1.06282900	14.91611900
H	-1.30568800	-1.21618000	15.67723100

C	-0.04796700	0.33002400	16.54813500
C	1.15761000	1.04220700	16.38580500
C	-1.04414500	0.84252200	17.40331400
C	1.35666600	2.25853500	17.05592500
H	1.93255700	0.63933300	15.73091700
C	-0.84498700	2.05938400	18.07279300
H	-1.97395100	0.28604400	17.53675600
C	0.35568600	2.76973300	17.90032800
H	2.29132200	2.80661900	16.91962800
H	-1.62503200	2.45225400	18.72833000
H	0.51013800	3.71753200	18.42040600
S	0.39219300	-2.37435300	16.92667700
O	1.86549700	-2.20473700	17.07720500
O	-0.44506600	-2.45021200	18.15579400

E-3a

C	4.12986700	-3.99208800	2.80454800
C	3.13132700	-3.32232000	1.91789600
C	2.68705100	-3.75339700	0.70961200
H	2.76727500	-2.36938700	2.30511100
C	2.39638000	-5.63764500	4.54913400
H	2.05347800	-5.66854300	5.59533800
H	3.04721900	-6.50224200	4.35829500
C	1.26198300	-5.54999300	3.56630600
C	1.24149200	-6.40094300	2.44487100
C	0.21362200	-4.62438100	3.74927800
C	0.19787800	-6.32164100	1.51035900
H	2.04914700	-7.12299200	2.30617000
C	-0.82470700	-4.54015500	2.81095000
H	0.22646100	-3.96427100	4.61737500
C	-0.83320100	-5.38520200	1.68729500
H	0.19358600	-6.98549600	0.64358700
H	-1.62690700	-3.81344700	2.95406200
H	-1.63960700	-5.31310100	0.95486300
S	3.53646300	-4.16786600	4.56244500
O	4.71417000	-4.54884000	5.39076100
O	2.75199500	-2.95530400	4.92539000
H	5.03562600	-3.37726000	2.94692800
H	4.44077800	-4.99787900	2.49359800
C	1.67144600	-2.95815700	-0.03655100
C	0.73085800	-2.13987400	0.63742600
C	1.59669500	-3.02178500	-1.44882600
C	-0.22707800	-1.40367200	-0.07074900
H	0.72940100	-2.11187400	1.72709800

C	0.63797400	-2.28276600	-2.15900100
H	2.30109500	-3.64595500	-2.00023100
C	-0.27863900	-1.46852400	-1.47482200
H	-0.94637300	-0.78979600	0.47625300
H	0.60859500	-2.34575200	-3.24919800
H	-1.03025600	-0.89931800	-2.02604500
C	3.19835800	-5.00818700	0.03092300
H	2.36786300	-5.56542700	-0.42811100
H	3.90411900	-4.75074300	-0.77875400
H	3.72118300	-5.67922900	0.72406700

IM1a-exo

C	-0.82386300	-0.55160600	-5.29263300
C	0.55771800	-0.96294700	-4.77351100
H	-1.35727600	-1.40191800	-5.73686400
H	-1.39743900	-0.14354600	-4.44758600
O	0.34186000	-1.79265700	-3.52601800
C	1.38231300	0.22433900	-4.27088000
C	1.60324100	1.35994800	-5.09795600
H	2.17881800	-0.07407200	-3.58115600
C	1.42423600	-1.75600000	-5.75580000
C	1.18429200	-1.71196900	-7.14099900
C	2.52852700	-2.49278400	-5.27919200
C	2.02508500	-2.39929700	-8.03308000
H	0.33628400	-1.14848000	-7.53075300
C	3.36151300	-3.18734600	-6.16704900
H	2.72602400	-2.53142100	-4.20650800
C	3.11300800	-3.14393400	-7.55080700
H	1.82182500	-2.35623100	-9.10543300
H	4.20640600	-3.76076600	-5.77913000
H	3.76245100	-3.68280600	-8.24386300
C	-0.20060700	-3.03001200	-3.52716700
O	-0.48883900	-3.49890100	-4.73179600
O	-0.37717000	-3.59033000	-2.43958600
H	1.12776200	1.42925900	-6.08005600
H	2.55455600	1.89696200	-5.01959900
H	-0.72103300	0.23526700	-6.05223500
C	-0.95747000	-4.91204300	-4.95625100
C	0.10617000	-5.88379700	-4.43725800
C	-2.32525100	-5.10615000	-4.29730800
C	-1.05873900	-4.97400400	-6.48292900
H	1.08534400	-5.64408000	-4.87974800
H	0.18057800	-5.84930900	-3.34262400
H	-0.17505300	-6.90436400	-4.74042900

H	-3.03411500	-4.34333400	-4.65574200
H	-2.71072900	-6.09886100	-4.57810100
H	-2.25199200	-5.05058500	-3.20364000
H	-1.40166200	-5.97829600	-6.77474400
H	-1.78247000	-4.23311600	-6.85606700
H	-0.07897100	-4.78378600	-6.94573100
Pd	0.30580600	1.94772300	-3.50121800
P	-0.08978900	4.15805400	-3.70298900
O	1.27320700	5.08488100	-3.25190000
O	-1.21659100	4.88286200	-2.63469900
C	0.95009700	5.57455500	-0.91871800
C	1.61820500	4.86493600	-1.91976200
C	2.62791300	3.90812500	-1.64102300
C	2.97739800	3.65148400	-0.32775000
C	2.60606200	3.99108100	2.10381600
C	1.89798600	4.57174000	3.14485000
C	0.83862900	5.47607900	2.86087600
C	0.52449000	5.81014700	1.55152400
C	1.25440700	5.25899900	0.45533500
C	2.29846500	4.30068100	0.74528600
C	-0.08306200	6.57073300	-1.31504700
C	-1.11938500	6.18573600	-2.17590500
C	-2.15472400	7.07946600	-2.56093700
C	-2.14796600	8.38258400	-2.10070100
C	-1.04482500	10.21127400	-0.83233900
C	0.01063400	10.67870000	-0.06459900
C	1.07271700	9.79985400	0.28353800
C	1.05403900	8.47157500	-0.11711600
C	-0.02983800	7.94703500	-0.88578200
C	-1.08922000	8.85410600	-1.26989900
H	3.10262900	3.39044100	-2.47439200
H	3.75640200	2.92284600	-0.09400000
H	3.40272900	3.27064900	2.30335400
H	2.13687500	4.32113900	4.18032500
H	0.25849100	5.90449200	3.68058800
H	-0.29814100	6.49404600	1.34878700
H	-2.94294100	6.70861100	-3.21718100
H	-2.94489600	9.07416000	-2.38290000
H	-1.86002200	10.87730800	-1.12562600
H	0.03567500	11.72017100	0.26236100
H	1.91588000	10.17446800	0.86783600
H	1.88029900	7.81468500	0.14969600
C	-0.50313100	3.96239400	-6.38298100
C	-0.21362800	6.24983500	-5.55170500

C	0.76129500	4.13648600	-7.23915900
H	-1.38695500	4.24953900	-6.98027200
H	-0.61037000	2.91708200	-6.06086800
C	1.03381000	6.37895000	-6.44897300
H	-1.09808400	6.61946300	-6.10048000
H	-0.08407500	6.84795000	-4.64165000
H	1.62901800	3.82444700	-6.62404000
H	1.91123700	6.05926900	-5.85349200
N	-0.43562000	4.83500000	-5.19882300
O	0.91790600	5.52242800	-7.60229200
C	1.22057900	7.80590100	-6.95336200
H	1.35484800	8.49104800	-6.10113000
H	2.10746000	7.87046100	-7.60280800
H	0.33742000	8.12652500	-7.52964400
C	0.69996400	3.31965900	-8.52464700
H	1.60087000	3.49325600	-9.13338200
H	0.63911900	2.24642600	-8.28239700
H	-0.18601500	3.59971200	-9.11767000
Na	-0.37935600	-1.63024200	-1.05598800
C	-1.34944700	2.60925100	-0.38484100
H	-2.21040800	2.97936400	-0.95757700
H	-0.55404600	3.36523700	-0.39113600
C	-1.69921400	2.14451500	0.98683600
C	-2.94138200	1.52591300	1.24726400
C	-0.75701900	2.24847300	2.03231100
C	-3.23967500	1.03536400	2.52835600
H	-3.67092000	1.43797800	0.44015800
C	-1.05573500	1.76289800	3.31401100
H	0.20448200	2.72266900	1.83539800
C	-2.29771500	1.15253400	3.56672100
H	-4.20830100	0.56666900	2.71896300
H	-0.32024400	1.86374900	4.11590600
H	-2.53277600	0.77707600	4.56550500
S	-0.65644000	1.19506900	-1.45455700
O	-1.84757700	0.22389100	-1.62927400
O	0.42482800	0.54599000	-0.56065700
IM1a-endo			
Pd	3.53571100	-3.25946800	-12.75357700
P	2.01852400	-1.66660800	-13.22751100
O	1.43890300	-1.37676700	-14.81133000
O	2.72177600	-0.13306700	-12.95570200
C	2.80958900	0.36155300	-15.76081300
C	2.38986300	-0.97132100	-15.73874900
C	2.86540600	-1.93719700	-16.66287500

C	3.78856200	-1.56889600	-17.62320600
C	5.32259500	0.12520600	-18.59067400
C	5.88828400	1.39063000	-18.56812000
C	5.45993400	2.33789900	-17.59733800
C	4.46136400	2.01754200	-16.68875100
C	3.84166100	0.73127900	-16.69718000
C	4.31095400	-0.24329700	-17.65572700
C	2.19618900	1.33130600	-14.81146300
C	2.17174400	1.04215000	-13.44212000
C	1.64436500	1.94770700	-12.48311500
C	1.10160700	3.14939600	-12.89608200
C	0.41576300	4.68463300	-14.72267300
C	0.30097100	4.97609100	-16.07305100
C	0.78996400	4.05246300	-17.03688000
C	1.40326500	2.87221200	-16.64144300
C	1.56389600	2.54974700	-15.25890500
C	1.02954300	3.47430100	-14.28276200
H	2.48276800	-2.95553400	-16.59608800
H	4.15509900	-2.29834200	-18.34832200
H	5.65534700	-0.62175200	-19.31530700
H	6.66890900	1.65841500	-19.28312700
H	5.92378100	3.32597600	-17.56334500
H	4.14848600	2.74995300	-15.94593700
H	1.68107500	1.66930200	-11.42931100
H	0.70070300	3.85665700	-12.16665900
H	0.02751500	5.37263700	-13.96769300
H	-0.17458000	5.90347900	-16.39870800
H	0.67667900	4.26990000	-18.10111700
H	1.76195800	2.17229400	-17.39420900
C	0.16419000	-2.81584100	-11.60274400
C	-0.60653000	-0.79662100	-12.76257100
C	-0.97559100	-3.60161300	-12.27259900
H	-0.17650600	-2.45743500	-10.61418700
H	1.04017500	-3.46882300	-11.46411300
C	-1.73148700	-1.63401800	-13.40012800
H	-0.98269600	-0.33166200	-11.83353800
H	-0.29154300	-0.00624700	-13.45289600
H	-0.59219800	-3.99832500	-13.23555500
H	-1.34959500	-2.04185800	-14.35652400
N	0.54305900	-1.65610100	-12.42577200
O	-2.09049400	-2.72998500	-12.53721900
C	-2.98825800	-0.80316300	-13.63611500
H	-2.76698200	0.02589300	-14.32717800
H	-3.78380400	-1.42622200	-14.07372700

H	-3.35312500	-0.38285800	-12.68473400
C	-1.47653900	-4.73751900	-11.38726200
H	-2.30755500	-5.26855900	-11.87690300
H	-0.66077000	-5.45342400	-11.19707400
H	-1.83176400	-4.34099000	-10.42211300
C	6.82005200	-5.93443700	-14.40827500
C	6.25931400	-4.71934200	-13.64924600
C	8.16640800	-4.46598000	-11.99436400
H	7.89343700	-5.82997600	-14.61462200
H	6.64716300	-6.84158600	-13.80982300
O	8.90209400	-4.23145300	-13.07153700
O	8.54158700	-4.45762100	-10.81666100
O	6.87467300	-4.75897900	-12.25530200
C	4.77055600	-4.94817500	-13.38883000
C	3.81464800	-4.61766400	-14.38623500
H	4.58202900	-5.82184100	-12.75451600
C	6.53307800	-3.36511800	-14.29985200
C	6.85615500	-3.25333500	-15.66274300
C	6.39242600	-2.19086800	-13.53247800
C	7.02473100	-1.98857100	-16.25348300
H	6.97591000	-4.14794800	-16.27420000
C	6.56137500	-0.93029300	-14.12241000
H	6.16328200	-2.26503800	-12.46916500
C	6.87222200	-0.82252500	-15.48846800
H	7.26175600	-1.91624200	-17.31660700
H	6.43663000	-0.03208700	-13.51377600
H	6.97960400	0.15780100	-15.95513700
H	4.12590200	-4.08681300	-15.28971000
H	2.91824100	-5.23852400	-14.49591500
H	6.28009700	-6.04625100	-15.35919300
C	10.27579200	-3.62094100	-12.98579400
C	10.18365400	-2.27433600	-12.26188100
C	11.23354500	-4.60484600	-12.30922500
C	10.62857900	-3.42452500	-14.46277200
H	9.43474100	-1.63219900	-12.74984400
H	9.91934200	-2.40382900	-11.20400200
H	11.16511100	-1.77869900	-12.32194700
H	11.20475800	-5.57971600	-12.82108500
H	12.25691200	-4.20417600	-12.38303100
H	10.98163200	-4.74208600	-11.25001200
H	11.63033800	-2.97381500	-14.53146000
H	10.63979800	-4.39001000	-14.99218500
H	9.90279800	-2.75595300	-14.94907400
C	2.94038000	-1.65243400	-9.55770100

H	1.94258300	-2.09037700	-9.69204900
H	3.02157100	-0.71862500	-10.13128200
C	3.32536000	-1.50142800	-8.12628600
C	2.81352400	-2.38198400	-7.14851900
C	4.28136600	-0.53735100	-7.73875200
C	3.23228300	-2.28930700	-5.81229900
H	2.08158900	-3.13648300	-7.44355800
C	4.70158700	-0.44345900	-6.40318600
H	4.68870000	0.13823100	-8.49309200
C	4.17842300	-1.31943200	-5.43500700
H	2.82002000	-2.97161000	-5.06509300
H	5.43548800	0.31353000	-6.11656000
H	4.50196500	-1.24387900	-4.39434300
S	4.11970500	-2.85403200	-10.46276300
O	4.01098200	-4.16993500	-9.65734500
Na	6.41502800	-4.41088300	-9.74275900
O	5.51107500	-2.21757600	-10.24467500

IM1b-exo

C	2.06712800	-1.76531600	-5.74764900
C	1.07830100	-0.93833000	-4.90741600
H	1.57798200	-2.61648200	-6.23974200
H	2.51992200	-1.11895100	-6.51263200
O	0.68827200	-1.80136800	-3.71928500
C	1.82275100	0.23488700	-4.26982100
C	2.03216800	1.42862300	-5.01148300
H	2.58908600	-0.08323900	-3.55456300
C	-0.17384600	-0.47451900	-5.65132100
C	-1.31504600	-0.08718300	-4.91696500
C	-0.18681900	-0.34232100	-7.04946100
C	-2.44722600	0.41487900	-5.57448700
H	-1.32216800	-0.18771700	-3.83083100
C	-1.32035300	0.16905800	-7.70878200
H	0.68378200	-0.63385200	-7.63654200
C	-2.45388500	0.54859200	-6.97463800
H	-3.32183100	0.70667500	-4.98900800
H	-1.31010800	0.27006700	-8.79587900
H	-3.33319100	0.94594100	-7.48612200
C	-0.11823000	-2.88164600	-3.80650900
O	-0.48364500	-3.19265400	-5.04178400
O	-0.42462500	-3.47104700	-2.76464200
H	1.58712500	1.54392800	-6.00302000
H	2.94503300	2.01049400	-4.84414000
H	2.87199400	-2.13191600	-5.09288200

C	-1.58738500	-4.17862200	-5.32563300
C	-1.14532500	-5.57958000	-4.89659800
C	-2.86977100	-3.71190700	-4.63017300
C	-1.72045800	-4.07694000	-6.84756600
H	-0.18406100	-5.83769000	-5.36807600
H	-1.04762400	-5.64983300	-3.80587700
H	-1.90309400	-6.30434700	-5.23372500
H	-3.10646000	-2.67747800	-4.92218600
H	-3.69651700	-4.36569100	-4.94898300
H	-2.77761100	-3.76962200	-3.53756600
H	-2.51884300	-4.75772100	-7.17997200
H	-1.97983900	-3.05064500	-7.14700800
H	-0.78095900	-4.37006700	-7.34147900
Pd	0.63040100	1.86141200	-3.44130200
P	0.01636700	4.01684200	-3.64071100
O	1.24307600	5.12442600	-3.20885300
O	-1.19506800	4.61081000	-2.57428000
C	0.86212600	5.64028100	-0.89083500
C	1.60676300	4.98102800	-1.87157500
C	2.71018500	4.14303800	-1.56716800
C	3.08927600	3.96924200	-0.24876800
C	2.69868400	4.35852500	2.17131100
C	1.92914200	4.88362900	3.19762900
C	0.77139700	5.64958800	2.89129400
C	0.42007500	5.90698200	1.57406100
C	1.20598900	5.40955100	0.49101000
C	2.35220600	4.58443300	0.80562700
C	-0.29414700	6.47746200	-1.31306800
C	-1.27352800	5.92613000	-2.15149900
C	-2.42431000	6.65840300	-2.55080600
C	-2.59168900	7.96502300	-2.13354400
C	-1.73791100	9.96895600	-0.94071400
C	-0.75164000	10.60088900	-0.19922800
C	0.42049800	9.88532900	0.16892400
C	0.57996100	8.55378100	-0.18737300
C	-0.42634000	7.86154900	-0.92873100
C	-1.60079300	8.60388900	-1.33142700
H	3.23010200	3.64603300	-2.38612300
H	3.94039400	3.33370400	0.00447100
H	3.57433500	3.74225200	2.38835200
H	2.19688800	4.69458400	4.23910100
H	0.14702200	6.03364400	3.70050300
H	-0.47417200	6.48809700	1.35446300
H	-3.15972100	6.16234900	-3.18544600

H	-3.47756200	8.53177700	-2.42864500
H	-2.63688100	10.50835200	-1.24910300
H	-0.86564300	11.64712800	0.09178300
H	1.20789700	10.38986800	0.73290700
H	1.48871700	8.02458200	0.09540900
C	-0.45979300	3.72775000	-6.31223000
C	-0.46273800	6.04685400	-5.50280300
C	0.65107400	4.10503600	-7.30550700
H	-1.44137800	3.84262700	-6.80582200
H	-0.34577000	2.68600900	-5.98511300
C	0.64187000	6.36794200	-6.52880700
H	-1.44904200	6.26732600	-5.94959900
H	-0.33199600	6.66503800	-4.60666600
H	1.62429700	3.94709000	-6.79771400
H	1.61955200	6.19666700	-6.03576500
N	-0.40744600	4.61980400	-5.14314500
O	0.53740200	5.49564100	-7.66944600
C	0.54254800	7.80278500	-7.03603900
H	0.66057600	8.50766400	-6.19763400
H	1.32992200	8.00187900	-7.77962600
H	-0.43880600	7.97450800	-7.50751100
C	0.57856400	3.28490100	-8.58876000
H	1.35730100	3.61211800	-9.29542400
H	0.72646700	2.21818200	-8.36190500
H	-0.40661600	3.40759900	-9.06760700
Na	0.18547200	-1.80293400	-1.17400900
C	-0.82191700	2.42082300	-0.23139400
H	-1.68948900	2.82068300	-0.77216300
H	-0.01269200	3.16089000	-0.24685600
C	-1.14429600	1.93972300	1.14178400
C	-2.39687100	1.35357400	1.42665700
C	-0.17520500	2.00611500	2.16505800
C	-2.67739800	0.85680100	2.70911800
H	-3.14860300	1.29661100	0.63735900
C	-0.45609900	1.51503900	3.44879700
H	0.79161400	2.46176100	1.95038200
C	-1.70791200	0.93643900	3.72537200
H	-3.65371400	0.41266000	2.91820700
H	0.30009200	1.58872400	4.23429400
H	-1.92907000	0.55651900	4.72562100
S	-0.19108200	1.02836600	-1.35652200
O	-1.37969600	0.03917500	-1.44696200
O	0.96452000	0.38077800	-0.55730800

IM1b-endo

Pd	3.47559900	-3.37879200	-12.75768500
P	1.97717300	-1.76624300	-13.22966500
O	1.41118500	-1.48849100	-14.82015400
O	2.67613900	-0.22435500	-12.96582500
C	2.82999300	0.21398800	-15.76291300
C	2.39926500	-1.11520800	-15.72471500
C	2.91718600	-2.11114400	-16.59214500
C	3.90958500	-1.78144200	-17.49744000
C	5.50637400	-0.12271400	-18.43000900
C	6.05112500	1.15196500	-18.43910500
C	5.55376400	2.13977700	-17.54511000
C	4.51195600	1.84876600	-16.67642300
C	3.90980800	0.55393200	-16.65548200
C	4.44248300	-0.45930800	-17.54093200
C	2.18560600	1.20390300	-14.85574100
C	2.12762300	0.93911500	-13.48263700
C	1.56441900	1.85630000	-12.55577300
C	1.02101600	3.04403500	-13.00773500
C	0.37676100	4.54021400	-14.88246100
C	0.30361900	4.80704500	-16.24087300
C	0.83413700	3.87312900	-17.17259600
C	1.44467100	2.70570600	-16.73716600
C	1.56030800	2.40825400	-15.34469200
C	0.98744600	3.34401100	-14.40161100
H	2.51814400	-3.12270300	-16.52380100
H	4.31195700	-2.53558700	-18.17750600
H	5.88895000	-0.89842200	-19.09789300
H	6.86813200	1.39671800	-19.12090400
H	6.00017200	3.13635900	-17.53715600
H	4.14841500	2.61201100	-15.99008200
H	1.57391500	1.59878400	-11.49607700
H	0.59161700	3.76003500	-12.30355900
H	-0.04153300	5.23786400	-14.15291800
H	-0.16971000	5.72394500	-16.59789500
H	0.75568200	4.07295800	-18.24338300
H	1.83731800	1.99717500	-17.46476600
C	0.15466400	-2.86642200	-11.53281200
C	-0.65554400	-0.91196500	-12.77724000
C	-1.00427200	-3.68754400	-12.12322000
H	-0.15449900	-2.45221700	-10.55562200
H	1.03603400	-3.51014500	-11.38568700
C	-1.79583300	-1.78372600	-13.33578700

H	-1.00441800	-0.39992700	-11.86243300
H	-0.36231200	-0.15878500	-13.51716400
H	-0.64829500	-4.13746700	-13.07305300
H	-1.43888100	-2.24307800	-14.27880800
N	0.50228700	-1.75610600	-12.43421300
O	-2.12751900	-2.83128400	-12.40405700
C	-3.06142300	-0.96930600	-13.58174500
H	-2.86129600	-0.17701700	-14.32063700
H	-3.86583800	-1.61626900	-13.96495700
H	-3.40265900	-0.50062100	-12.64431200
C	-1.47791300	-4.77112700	-11.16091200
H	-2.32114900	-5.32937300	-11.59633600
H	-0.65564300	-5.47451700	-10.95325000
H	-1.80682200	-4.32043600	-10.21036100
C	6.20487200	-4.82271800	-13.49695900
C	8.04573000	-5.19805700	-11.80398900
O	8.85861100	-5.00060700	-12.83017800
O	8.35462000	-5.41074300	-10.62599200
O	6.73313600	-5.15301900	-12.11899900
C	4.70054900	-5.07587700	-13.35548000
C	3.80434900	-4.71684000	-14.39657200
H	4.47134500	-5.96405700	-12.75720700
H	4.17060100	-4.18878200	-15.28057400
H	2.91234600	-5.32977800	-14.56693300
C	10.35457200	-5.11586200	-12.70848500
C	10.87327800	-4.04206700	-11.74846700
C	10.71345100	-6.53921500	-12.27327100
C	10.81032200	-4.84680400	-14.14539600
H	10.52568100	-3.04623700	-12.06519300
H	10.54158100	-4.23306700	-10.71986600
H	11.97429400	-4.05122900	-11.77471500
H	10.25346800	-7.27097100	-12.95523400
H	11.80748900	-6.65477600	-12.32141300
H	10.38249600	-6.73747000	-11.24557200
H	11.90851600	-4.90693300	-14.18726600
H	10.38676700	-5.59320700	-14.83389800
H	10.50019200	-3.84170300	-14.47055100
C	3.14608700	-1.56098500	-9.65966800
H	2.10270100	-1.89752500	-9.73718500
H	3.30389800	-0.68320000	-10.30134500
C	3.59584600	-1.35888500	-8.25397700
C	3.03728400	-2.12166300	-7.20513000
C	4.65592400	-0.47352700	-7.96036500
C	3.51369100	-1.98927300	-5.89176400

H	2.22386600	-2.81506300	-7.42750900
C	5.13384800	-0.34025500	-6.64766200
H	5.09795500	0.11178900	-8.76873100
C	4.56428100	-1.09795700	-5.60846700
H	3.06450400	-2.57849900	-5.08869700
H	5.94852400	0.35584700	-6.43426400
H	4.93280300	-0.99118300	-4.58564600
S	4.15542800	-2.93917500	-10.51700900
O	3.94006100	-4.17996300	-9.61913000
Na	6.28999600	-4.65431400	-9.64286200
O	5.61530800	-2.44920600	-10.40552800
C	6.76597000	-5.83119300	-14.50350700
C	6.91744700	-7.18588100	-14.14288700
C	7.06742200	-5.44188900	-15.82172800
C	7.38341900	-8.12599900	-15.07259900
H	6.68317000	-7.50094800	-13.12457200
C	7.52365000	-6.38565200	-16.75747800
H	6.95451700	-4.40009400	-16.12286200
C	7.68954400	-7.72957600	-16.38666400
H	7.50534400	-9.16893000	-14.77146400
H	7.75628300	-6.06480000	-17.77541800
H	8.05145500	-8.46094000	-17.11234200
C	6.53684400	-3.35500500	-13.79040900
H	5.92870600	-2.99505100	-14.63191400
H	6.27682600	-2.76361600	-12.90104400
H	7.59882100	-3.22286800	-14.03542600

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C	0.46981400	-0.34770400	-6.50477000
C	1.14244000	-0.78039800	-5.21694700
H	-0.10260300	-1.16639400	-6.94865700
H	-0.19589600	0.50233900	-6.30843400
O	-0.37961800	-1.29812400	-4.19540500
C	1.80097200	0.27651300	-4.44013200
C	1.93504000	1.61798800	-4.93836300
H	2.53827100	-0.06473100	-3.71079600
C	1.87865500	-2.08696000	-5.21139400
C	2.21070100	-2.74225300	-6.41444300
C	2.27509200	-2.67419000	-3.98673000
C	2.93020200	-3.94784900	-6.39621800
H	1.91211300	-2.30973300	-7.36869400
C	2.97525900	-3.88593600	-3.96843400
H	2.01714900	-2.17792800	-3.04971300
C	3.30956000	-4.52791300	-5.17554500

H	3.18434300	-4.43723400	-7.33878300
H	3.26204700	-4.33054200	-3.01308900
H	3.85992700	-5.47078800	-5.16206900
C	-1.00355300	-2.43780000	-4.39769200
O	-0.93902100	-2.88678400	-5.66661300
O	-1.62054100	-3.02508400	-3.48269100
H	1.53996100	1.88187100	-5.92235500
H	2.84212600	2.17216100	-4.66588100
H	1.24302300	-0.02222100	-7.22006100
C	-1.39356500	-4.25155500	-6.05228800
C	-0.62436400	-5.30600200	-5.24654000
C	-2.91380000	-4.36845900	-5.88615700
C	-1.00569400	-4.32255500	-7.53435900
H	0.45908000	-5.14141900	-5.34636800
H	-0.90038900	-5.27385000	-4.18462900
H	-0.86698100	-6.30381000	-5.64579200
H	-3.41938900	-3.55827600	-6.43574100
H	-3.24553200	-5.33179700	-6.30576300
H	-3.20158900	-4.32100900	-4.82855800
H	-1.30801400	-5.30032300	-7.94018000
H	-1.51544700	-3.53216700	-8.10771000
H	0.08214500	-4.20981900	-7.65340500
Pd	0.55640300	1.82903700	-3.37151400
P	0.10158600	4.01521800	-3.51860800
O	1.37607500	5.04508100	-3.08645600
O	-1.09581700	4.63128000	-2.45746900
C	0.96658900	5.64850100	-0.78956100
C	1.71254700	4.94200200	-1.73487000
C	2.80260300	4.10470000	-1.38712400
C	3.15307000	3.96336100	-0.05602700
C	2.69193900	4.39221900	2.34493800
C	1.90302300	4.95075100	3.33794100
C	0.78031500	5.74786800	2.98460800
C	0.47568100	5.99243100	1.65363000
C	1.27616100	5.44898700	0.60402100
C	2.39682100	4.60903800	0.96619600
C	-0.15555700	6.51076800	-1.25327600
C	-1.14406500	5.96686400	-2.08219000
C	-2.26299400	6.72043300	-2.52481200
C	-2.38722800	8.04688000	-2.15707400
C	-1.47863900	10.06013100	-1.02143700
C	-0.48221700	10.68127000	-0.28447200
C	0.65679100	9.93760900	0.12922400
C	0.77424300	8.58983500	-0.17904900

C	-0.24352500	7.91028900	-0.91597800
C	-1.38470900	8.67840200	-1.36338000
H	3.33913900	3.58507800	-2.18110000
H	3.99173900	3.32585200	0.23128500
H	3.54405500	3.75753900	2.59922200
H	2.12980100	4.76645300	4.38980500
H	0.14435800	6.16399200	3.76850200
H	-0.39457000	6.59452000	1.39760300
H	-3.00986200	6.22722100	-3.14793300
H	-3.24838100	8.63356700	-2.48423700
H	-2.35307800	10.61980300	-1.36220500
H	-0.56328600	11.74007900	-0.03045800
H	1.45140300	10.43274100	0.69130600
H	1.65726000	8.03763500	0.13922300
C	-0.71392600	3.75563500	-6.10548100
C	-0.27980500	6.06343900	-5.38838100
C	0.04837100	4.04613400	-7.40792700
H	-1.79122100	3.94842200	-6.26640800
H	-0.57927700	2.70497800	-5.81008400
C	0.46459200	6.29676200	-6.71664200
H	-1.33715800	6.36292000	-5.50625500
H	0.17579900	6.66354800	-4.59180700
H	1.11709200	3.80476500	-7.23655300
H	1.53230500	6.04490100	-6.55490300
N	-0.20226600	4.63322200	-5.04107900
O	-0.06426000	5.44114700	-7.74697600
C	0.31962200	7.73714300	-7.19670400
H	0.74855300	8.42732500	-6.45306200
H	0.84552800	7.87587400	-8.15397800
H	-0.74424800	7.98674200	-7.33942100
C	-0.50218800	3.23811800	-8.57806900
H	0.04467100	3.48112600	-9.50220300
H	-0.39481600	2.16066800	-8.37517500
H	-1.56994700	3.46402600	-8.73061500
Na	-0.95536200	-1.66064000	-1.72301300
C	-0.33990500	2.47105500	-0.01789200
H	-1.00787600	3.23720500	-0.42854600
H	0.69732100	2.82221300	-0.06522600
C	-0.73046700	2.01256000	1.34564400
C	-2.08878200	1.96434800	1.72624700
C	0.24901900	1.56752800	2.25870200
C	-2.45783400	1.49525400	2.99632900
H	-2.85002100	2.30299300	1.02110100
C	-0.11779500	1.10204100	3.53027900

H	1.29973300	1.60496700	1.96715600
C	-1.47318600	1.06393700	3.90330400
H	-3.51244500	1.47021400	3.28092800
H	0.65241600	0.77182900	4.23149500
H	-1.75988100	0.70475300	4.89444300
S	-0.39451900	1.07695300	-1.30147300
O	-1.85949600	0.59942500	-1.33091300
O	0.51923000	-0.02275300	-0.71003400

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C	0.10612200	1.28589200	-7.79193500
C	1.28759900	1.05912800	-6.86501800
H	-0.81852200	0.93373000	-7.31169100
H	-0.01608200	2.34250500	-8.05834100
O	-1.85031900	-3.32181600	-3.82624100
C	2.31440300	2.02708600	-6.71078900
C	2.14408600	3.42160000	-6.95193500
H	3.22725000	1.72567700	-6.19339900
C	1.47919900	-0.31704300	-6.33814500
C	0.71997600	-1.39821100	-6.85643200
C	2.39276300	-0.60101200	-5.29087500
C	0.89784400	-2.70734100	-6.38236800
H	-0.01357000	-1.22470100	-7.64149800
C	2.56782900	-1.90625500	-4.81533500
H	2.93550900	0.20702800	-4.80568200
C	1.82784700	-2.97106900	-5.36139100
H	0.29515900	-3.51610400	-6.79811100
H	3.26042800	-2.08849400	-3.99208500
H	1.94599200	-3.98172400	-4.97005600
C	-1.16479300	-3.77667400	-2.86412200
O	-1.76522100	-4.89507800	-2.26080300
O	-0.05648800	-3.33867700	-2.43383000
H	1.47847500	3.78998100	-7.73551500
H	2.97889800	4.08096500	-6.70683500
H	0.24870300	0.71198500	-8.72455100
C	-1.12434300	-5.62694000	-1.16952800
C	0.22567900	-6.21642500	-1.61680900
C	-0.97149700	-4.74186900	0.08013500
C	-2.11620300	-6.76607800	-0.88068100
H	0.08503700	-6.82297900	-2.52736100
H	0.94279900	-5.41347800	-1.82901600
H	0.63146900	-6.86857100	-0.82501300
H	-1.95646900	-4.35552200	0.38820100
H	-0.55686700	-5.33725900	0.91146800

H	-0.30608600	-3.89551900	-0.13009200
H	-1.74201900	-7.39354500	-0.05524700
H	-3.09867500	-6.35710200	-0.59421800
H	-2.24695300	-7.39969800	-1.77291500
Pd	0.82810300	2.87196500	-5.29269800
P	0.57452900	4.91658300	-4.38597600
O	1.82547600	5.36263900	-3.37272900
O	-0.73699600	4.98958100	-3.32645700
C	1.07975000	4.72404900	-1.16419900
C	1.93863000	4.52853700	-2.24604500
C	2.93727300	3.52579100	-2.27659700
C	3.06554200	2.66997500	-1.19800300
C	2.25280400	1.83349800	0.99226800
C	1.35068100	1.88856700	2.04317400
C	0.32737300	2.87535200	2.04650000
C	0.23365300	3.80251500	1.01901100
C	1.16048800	3.79153100	-0.06642700
C	2.17827000	2.76430800	-0.08625300
C	0.08412300	5.83124600	-1.20954500
C	-0.79019000	5.93013600	-2.29517300
C	-1.79707900	6.92372700	-2.38381300
C	-1.91830500	7.86141300	-1.37521500
C	-1.10540000	8.85347600	0.75119500
C	-0.20536400	8.87207400	1.80517800
C	0.82611200	7.89581200	1.87112800
C	0.93166100	6.90919600	0.90140300
C	0.00763500	6.84408600	-0.18528300
C	-1.01997300	7.85864200	-0.26761200
H	3.58027400	3.44763100	-3.15359200
H	3.82696200	1.88766500	-1.19954500
H	3.02807900	1.06476300	0.96085200
H	1.41140600	1.16513500	2.85833500
H	-0.40034200	2.89707400	2.85992400
H	-0.56348600	4.54390800	1.02687200
H	-2.46144700	6.92216700	-3.24835800
H	-2.69508500	8.62729500	-1.42341500
H	-1.89363100	9.60626000	0.67607800
H	-0.27868600	9.63933200	2.57838500
H	1.54694600	7.92480200	2.69078200
H	1.73157500	6.17288600	0.96233600
C	-0.08037200	6.12906400	-6.72333700
C	0.65588400	7.64189200	-4.93754600
C	0.71921700	6.97063600	-7.73069200
H	-1.11563500	6.51368500	-6.67142300

H	-0.10914500	5.07657000	-7.03612800
C	1.42928500	8.45181000	-5.99403500
H	-0.35706200	8.06605200	-4.82012800
H	1.17762400	7.68185000	-3.97439500
H	1.74504300	6.55385500	-7.78582400
H	2.45377900	8.03343600	-6.06029300
N	0.56005400	6.23826100	-5.39750800
O	0.79391300	8.33532800	-7.28040600
C	1.47541800	9.93357700	-5.63630500
H	1.99281900	10.07372400	-4.67419200
H	2.01462000	10.49542200	-6.41432100
H	0.45410100	10.33847300	-5.55194800
C	0.06477100	6.97254900	-9.10792800
H	0.64089800	7.60333000	-9.80198100
H	0.02658300	5.94753800	-9.51026900
H	-0.96239900	7.36594900	-9.04334200
Na	-0.22450600	-1.55819600	-4.06935800
C	-1.42077100	2.12588800	-2.44692400
H	-2.23834200	2.67243800	-2.93498300
H	-0.75657700	2.82020700	-1.91931300
C	-1.86817000	0.98131900	-1.59790300
C	-2.99907200	0.21636900	-1.95374300
C	-1.08502900	0.57861800	-0.49599700
C	-3.34473500	-0.92538000	-1.21496900
H	-3.59686200	0.51407800	-2.81656000
C	-1.43566300	-0.55698400	0.24738800
H	-0.20089500	1.15671400	-0.22921200
C	-2.56287800	-1.31540400	-0.11432500
H	-4.21683000	-1.51580800	-1.50334200
H	-0.82296800	-0.85680100	1.10058200
H	-2.82935700	-2.20658000	0.45635600
S	-0.37675600	1.41807400	-3.86883900
O	-1.36479600	0.59259100	-4.69374600
O	0.66116300	0.55612700	-3.15526500

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Pd	1.50906700	-1.98523600	-11.17637200
P	0.51081500	-0.65251100	-12.63937900
O	1.23426500	-0.65314200	-14.15304900
O	0.68759100	0.97658600	-12.23704800
C	2.73862000	1.23009000	-14.14668200
C	2.54485400	-0.15135700	-14.14692200
C	3.60962300	-1.08439300	-14.15330700
C	4.91295700	-0.61956600	-14.15019000

C	6.52622400	1.26599700	-14.01861000
C	6.78285000	2.62407100	-13.90753200
C	5.70321300	3.54760000	-13.83834600
C	4.38899300	3.10941500	-13.90627900
C	4.09041600	1.72207300	-14.05821700
C	5.18687200	0.77846600	-14.08496300
C	1.54869900	2.12136200	-14.18535400
C	0.55287500	1.96762600	-13.22390800
C	-0.57741000	2.81225900	-13.13847500
C	-0.74162200	3.81845200	-14.07162600
C	0.02329000	5.00355800	-16.11637800
C	0.93150500	5.15460200	-17.15298100
C	2.05583600	4.28868600	-17.23959100
C	2.26582200	3.30302600	-16.28586600
C	1.36425300	3.13373900	-15.19192900
C	0.20528900	3.99609500	-15.12314800
H	3.37833500	-2.14929800	-14.16164600
H	5.75006900	-1.32070700	-14.16675000
H	7.34453100	0.54261700	-14.04660200
H	7.81167700	2.98602500	-13.85554900
H	5.91024700	4.61247500	-13.71504400
H	3.56763600	3.81498200	-13.80885800
H	-1.27877500	2.66900600	-12.31826900
H	-1.60179200	4.48894900	-14.01597900
H	-0.85350000	5.65148900	-16.04370400
H	0.78166700	5.92914200	-17.90782700
H	2.75976100	4.39671400	-18.06744800
H	3.12784400	2.64269200	-16.37101500
C	-1.81486800	-0.32654600	-14.13759400
C	-1.86761500	-1.93804400	-12.27125100
C	-3.07449100	0.33056500	-13.54408800
H	-2.11726500	-1.08149700	-14.88455900
H	-1.18454700	0.42435000	-14.62827100
C	-3.11149800	-1.21542300	-11.73093300
H	-2.18702300	-2.77166300	-12.92168300
H	-1.26550600	-2.34085200	-11.44404500
H	-2.75241200	1.11578700	-12.83569200
H	-2.76969700	-0.40174400	-11.06030400
N	-1.04890900	-1.00826200	-13.07241200
O	-3.85340600	-0.64301000	-12.82384000
C	-4.03849500	-2.16830600	-10.98515800
H	-3.52182100	-2.58542600	-10.10579300
H	-4.93869100	-1.63424400	-10.64455400
H	-4.34791700	-2.99742700	-11.64199300

C	-3.95618300	0.92868600	-14.63401400
H	-4.86517300	1.36456100	-14.19167300
H	-3.40599800	1.72074800	-15.16609500
H	-4.25196300	0.15291900	-15.35868600
C	1.27181700	-4.96983000	-9.68288200
C	2.51791600	-4.37861400	-10.30925900
C	3.48154500	-0.68782800	-9.28491000
H	1.32232700	-6.07218500	-9.74017900
H	1.19798600	-4.70033900	-8.62092700
O	1.92498000	-0.48947100	-9.53455600
O	3.81059900	-1.07545600	-8.17156300
O	4.04548400	-0.38536700	-10.35145900
C	2.53897500	-3.95434400	-11.64716800
C	1.37619500	-3.66079400	-12.43918500
H	3.50937300	-3.72728200	-12.09373500
C	3.77728200	-4.44072900	-9.54217700
C	3.91856800	-5.35611500	-8.46746100
C	4.88048000	-3.60659300	-9.85890300
C	5.12778100	-5.46223400	-7.76838400
H	3.08770600	-6.00642500	-8.19356300
C	6.08447700	-3.71313000	-9.15569400
H	4.77362700	-2.83004000	-10.61512600
C	6.21847900	-4.64578600	-8.11237500
H	5.21783900	-6.18405300	-6.95397600
H	6.91258300	-3.04718500	-9.40627700
H	7.15799900	-4.72340600	-7.56140900
H	0.42072800	-4.15363300	-12.23148900
H	1.53914500	-3.44337300	-13.49795800
H	0.35624300	-4.64737700	-10.19291700
C	0.94043100	-0.47756100	-8.43154900
C	0.81431900	-1.88375300	-7.83478500
C	1.35091000	0.56730900	-7.38404800
C	-0.37913900	-0.05112300	-9.09134200
H	0.48580700	-2.58941500	-8.61548300
H	1.77708700	-2.21904500	-7.42891000
H	0.05970200	-1.88478800	-7.03054600
H	1.44753200	1.55397700	-7.85980900
H	0.56315500	0.62748600	-6.61480000
H	2.29651900	0.29054600	-6.90286600
H	-1.16736500	0.01383100	-8.32300300
H	-0.26559800	0.93006600	-9.57370200
H	-0.69110200	-0.79372700	-9.84278900
C	2.78692900	5.22429800	-9.37605000
H	2.33307200	5.53813800	-8.42487800

H	3.11938800	6.09490200	-9.96027300
C	3.81258000	4.17135900	-9.23424300
C	3.75726800	3.24952000	-8.16222200
C	4.72222300	3.91520500	-10.29000800
C	4.61757600	2.14214200	-8.11880500
H	3.03646200	3.41222400	-7.35955400
C	5.57262200	2.79959300	-10.25491100
H	4.74880200	4.59356000	-11.14187900
C	5.52845500	1.91326000	-9.16471100
H	4.55632700	1.43587800	-7.29092200
H	6.25143700	2.61209000	-11.08901500
H	6.17013600	1.03309600	-9.14453100
S	1.31594200	4.43559600	-10.44741400
O	2.10183000	3.94435600	-11.68346700
Na	2.67208700	1.74728600	-10.60686000
O	0.90940000	3.22185800	-9.57494500

TS2a-exo

Pd	1.47923500	-2.09094600	-11.11655300
P	0.40647300	-0.77207900	-12.53252000
O	1.09893200	-0.75941700	-14.06822200
O	0.57336600	0.85659500	-12.14327600
C	2.61476700	1.11796600	-14.05649600
C	2.41109100	-0.26294200	-14.07993300
C	3.47156000	-1.20093800	-14.12090300
C	4.77813900	-0.74492400	-14.11666300
C	6.40380300	1.12644700	-13.94101300
C	6.66908300	2.47951000	-13.79436500
C	5.59506200	3.40798400	-13.70404300
C	4.27801900	2.98002600	-13.78517500
C	3.97050500	1.59844700	-13.96729200
C	5.06130500	0.64935200	-14.01888600
C	1.42848900	2.01526800	-14.08207500
C	0.42544700	1.84196900	-13.13134600
C	-0.73211700	2.65038200	-13.06412900
C	-0.89774400	3.66580500	-13.98731300
C	-0.11562600	4.89874100	-15.99611100
C	0.80294400	5.07756700	-17.01894200
C	1.94026700	4.22856000	-17.10385400
C	2.15292600	3.23272500	-16.16142200
C	1.24165500	3.03589400	-15.07995100
C	0.06826500	3.87984600	-15.01462500
H	3.23363300	-2.26306500	-14.16107400
H	5.61043500	-1.45084300	-14.16025700

H	7.21758800	0.39885600	-13.98866000
H	7.70019600	2.83363800	-13.73334600
H	5.80875800	4.46849100	-13.55638300
H	3.46084500	3.68750700	-13.66897000
H	-1.45979600	2.46200900	-12.27510100
H	-1.77769500	4.31130500	-13.94808500
H	-1.00334100	5.53195900	-15.92622200
H	0.65110400	5.86035900	-17.76483500
H	2.65238100	4.35782300	-17.92162100
H	3.02554000	2.58654500	-16.24573400
C	-1.90193900	-2.19194200	-12.24500100
C	-1.91546200	-0.49631100	-14.03578700
C	-2.28175100	-3.25170900	-13.29277300
H	-2.81913000	-1.79321000	-11.77727000
H	-1.26658700	-2.63450600	-11.46414400
C	-2.29991500	-1.60801500	-15.02878700
H	-2.82974300	-0.01105500	-13.65317000
H	-1.29446600	0.25713500	-14.53337800
H	-1.34405600	-3.66878600	-13.71225300
H	-1.36391200	-2.04019000	-15.43516600
N	-1.18083200	-1.08223500	-12.89460200
O	-3.03847600	-2.64488100	-14.35649500
C	-3.17670000	-1.07235900	-16.15544700
H	-2.63016000	-0.30386400	-16.72474700
H	-3.45867000	-1.88724500	-16.83988600
H	-4.09480700	-0.62264100	-15.74412400
C	-3.13794800	-4.35935200	-12.68912700
H	-3.42281100	-5.08694000	-13.46447600
H	-2.57648500	-4.88526000	-11.89994700
H	-4.05474400	-3.93652900	-12.24766700
C	1.62827500	-4.99406000	-9.61721200
C	2.74426900	-4.31460800	-10.38868100
C	3.89659500	-0.82564800	-9.25094900
H	1.81790100	-6.08204900	-9.57382500
H	1.57880100	-4.62761600	-8.58312000
O	1.79532600	-0.64638200	-9.56207800
O	4.03714300	-1.27042400	-8.15790600
O	4.20239100	-0.39788500	-10.32630200
C	2.58619000	-3.96112700	-11.74134300
C	1.33450300	-3.77280700	-12.41083300
H	3.47496500	-3.67542800	-12.30521100
C	4.08425700	-4.25867300	-9.76161300
C	4.35227800	-4.98522600	-8.57291400
C	5.14821100	-3.49728900	-10.31566200

C	5.62278800	-4.96920400	-7.98078200
H	3.56683700	-5.58257900	-8.11099800
C	6.41344900	-3.47874400	-9.72073300
H	4.97907600	-2.87544500	-11.19281200
C	6.66282100	-4.21859700	-8.55113000
H	5.79748000	-5.54572500	-7.06984900
H	7.20503300	-2.87191800	-10.16565700
H	7.65061400	-4.20010200	-8.08626400
H	0.43828400	-4.31931600	-12.10120200
H	1.37430400	-3.55091000	-13.47948400
H	0.64791500	-4.83963800	-10.08376800
C	0.83471600	-0.62078900	-8.49698200
C	0.68895300	-2.02025800	-7.87068400
C	1.31182200	0.39557100	-7.43994500
C	-0.52201500	-0.15448900	-9.06465700
H	0.30745300	-2.72754000	-8.62617300
H	1.66448700	-2.38106100	-7.51242400
H	-0.01875900	-2.00569700	-7.02396800
H	1.40973700	1.39338500	-7.89309400
H	0.57398000	0.46239200	-6.62204600
H	2.27758700	0.08894500	-7.01567500
H	-1.28129800	-0.10692700	-8.26474300
H	-0.41797300	0.84328700	-9.51581500
H	-0.87265500	-0.86073400	-9.83518100
C	2.77189500	5.08192300	-9.25208900
H	2.30941300	5.45028300	-8.32484700
H	3.15272300	5.91883500	-9.85630900
C	3.77221900	4.01426800	-9.03239000
C	3.69902500	3.16796000	-7.90171500
C	4.71987600	3.70442600	-10.03933800
C	4.59174900	2.09523700	-7.74566900
H	2.95064100	3.37065600	-7.13383700
C	5.60569900	2.62774700	-9.88878400
H	4.76040900	4.32085500	-10.93668200
C	5.55618200	1.82850100	-8.73271100
H	4.53075200	1.46503500	-6.85690800
H	6.32638300	2.40725700	-10.67896400
H	6.24549200	0.99080800	-8.61306500
S	1.29500200	4.33047500	-10.32318400
O	2.07846200	3.73146800	-11.51418700
Na	2.38804600	1.53462000	-10.40378700
O	0.79017800	3.18925600	-9.40514600

IM3a-*exo*

Pd	2.15427900	-1.91369900	-11.03346900
P	1.13507300	-0.65088900	-12.53904000
O	1.64768800	-0.55553600	-14.14278200
O	1.26436100	0.97493400	-12.10996100
C	2.68976500	1.60531900	-14.45906900
C	2.76681800	0.21012800	-14.46622500
C	3.93828900	-0.49083400	-14.84823800
C	5.07673100	0.21698000	-15.19009900
C	6.28823800	2.37663400	-15.37898600
C	6.31641400	3.75573400	-15.24675900
C	5.14557400	4.45186300	-14.83782500
C	3.96464200	3.76788000	-14.58964300
C	3.89371000	2.34868100	-14.73347200
C	5.09472900	1.64039800	-15.11662200
C	1.40067800	2.27672600	-14.13418600
C	0.73629200	1.95861200	-12.95145500
C	-0.46715600	2.58020600	-12.54158400
C	-1.04443300	3.53287300	-13.35921500
C	-1.08178900	4.80114800	-15.49339500
C	-0.53645100	5.08751300	-16.73529300
C	0.65493200	4.43332900	-17.15196100
C	1.29254300	3.52471800	-16.31942700
C	0.77224600	3.22205300	-15.02469300
C	-0.45908900	3.86304500	-14.61750400
H	3.91362800	-1.58007100	-14.86867100
H	5.98559600	-0.30828900	-15.49046100
H	7.18429900	1.82454200	-15.67182500
H	7.23745900	4.30837200	-15.44199200
H	5.17722600	5.53560200	-14.70967500
H	3.08001800	4.31199800	-14.26325600
H	-0.90593400	2.29510000	-11.58623100
H	-1.96772400	4.03308100	-13.05998700
H	-2.00561100	5.28296800	-15.16450700
H	-1.02384500	5.80491100	-17.39851100
H	1.07120200	4.64368000	-18.13931900
H	2.19978700	3.02614900	-16.65680200
C	-1.12999500	-2.13179900	-12.12563700
C	-1.28243400	-0.46685900	-13.92453200
C	-1.53917000	-3.21426100	-13.13782100
H	-2.02838500	-1.75090600	-11.60886500
H	-0.44710400	-2.55887500	-11.37902200
C	-1.69137100	-1.59682200	-14.88548300
H	-2.18702600	-0.00430200	-13.49404300
H	-0.71724200	0.29767900	-14.46728700

H	-0.61262200	-3.61369900	-13.60076400
H	-0.76801000	-2.00913100	-15.33897200
N	-0.46706200	-1.01388200	-12.81842600
O	-2.36626300	-2.64730500	-14.16864700
C	-2.63956700	-1.09125200	-15.96758400
H	-2.14208400	-0.31449400	-16.56963400
H	-2.93819100	-1.91759900	-16.63096900
H	-3.54508400	-0.65963600	-15.51117000
C	-2.32854900	-4.33440900	-12.46894500
H	-2.63653100	-5.08349800	-13.21443200
H	-1.70789300	-4.82925000	-11.70482800
H	-3.23031900	-3.92843700	-11.98281900
C	1.49328800	-4.96930300	-10.18583500
C	2.75883200	-4.16401900	-9.96573600
H	1.71297900	-6.04173400	-10.03316400
H	0.71710800	-4.68698800	-9.46117300
O	1.89496900	-0.87934200	-9.24644700
C	3.52210700	-3.67516700	-11.04516800
C	2.98511100	-3.38979400	-12.34765900
H	4.53414500	-3.32131100	-10.83058600
C	3.25883800	-4.04769200	-8.58200600
C	2.86282400	-4.96455900	-7.57667400
C	4.09626500	-2.96846400	-8.20638800
C	3.31693700	-4.82469400	-6.25776000
H	2.20911100	-5.79913100	-7.83058000
C	4.54916100	-2.82962100	-6.89030300
H	4.34400900	-2.21198200	-8.94509700
C	4.16302800	-3.75834500	-5.90747800
H	3.00674800	-5.54893700	-5.50156600
H	5.18155100	-1.97938200	-6.62532000
H	4.50599000	-3.64403800	-4.87711600
H	2.16698900	-3.98363500	-12.76536100
H	3.68154200	-3.00189400	-13.09499300
H	1.09372000	-4.85214800	-11.19988100
C	0.69552800	-0.78846200	-8.50138200
C	0.06306100	-2.18073900	-8.30333100
C	1.07702800	-0.19104800	-7.12678400
C	-0.32199900	0.14955600	-9.19486500
H	-0.19685700	-2.61286300	-9.28207200
H	0.78289100	-2.85084400	-7.80864300
H	-0.85406500	-2.12679700	-7.69116300
H	1.51720500	0.81066900	-7.25784400
H	0.18831800	-0.10054500	-6.47837800
H	1.81386700	-0.84283000	-6.63060700

H	-1.25369400	0.22944300	-8.60855000
H	0.08905300	1.16781600	-9.29832600
H	-0.57287200	-0.22916700	-10.19660500
C	4.50049000	4.14285800	-9.46132900
H	4.95778200	4.46247300	-8.51408600
H	4.65718000	4.88815900	-10.25386100
C	4.83096800	2.76311500	-9.85555000
C	5.04471500	1.77053700	-8.86472700
C	4.68062800	2.34109700	-11.20043000
C	5.11850100	0.41284400	-9.20551400
H	5.13721000	2.07550000	-7.82180300
C	4.74926600	0.98109400	-11.53926100
H	4.49262700	3.08344600	-11.97550300
C	4.96116700	0.00880900	-10.54466800
H	5.27439300	-0.32760100	-8.42055200
H	4.61759200	0.67634900	-12.57472300
H	4.98272300	-1.04916700	-10.81089700
S	2.52006600	4.17407400	-9.11600600
O	1.96994500	3.69600400	-10.47700800
Na	2.42811200	1.28156500	-9.89301100
O	2.36929400	3.04448900	-8.07002200

IM3a-endo

Pd	1.76317900	-2.05452500	-10.98939600
P	0.80178100	-0.76743300	-12.50238300
O	1.51846400	-0.77342000	-14.02265200
O	0.93814300	0.88388200	-12.14505900
C	2.75967400	1.28317600	-14.24674400
C	2.74462800	-0.10873300	-14.13580700
C	3.92042500	-0.89803400	-14.15905600
C	5.14918600	-0.27953000	-14.30222700
C	6.51129700	1.79026100	-14.45079500
C	6.60368800	3.17294500	-14.43804600
C	5.42289000	3.96066400	-14.35020100
C	4.17299500	3.36121000	-14.29948300
C	4.03840100	1.94030100	-14.32954700
C	5.24282900	1.14028700	-14.38236200
C	1.47047000	2.02674800	-14.20464400
C	0.59945000	1.81372900	-13.13697900
C	-0.63049900	2.49828700	-12.99117000
C	-1.01796700	3.40304200	-13.96064700
C	-0.62371000	4.52264500	-16.14263800
C	0.14718100	4.70900000	-17.27980100
C	1.36800700	3.99617800	-17.43146800

C	1.80837700	3.12795100	-16.44262600
C	1.05166100	2.92852500	-15.24860800
C	-0.20585300	3.63019600	-15.11136900
H	3.83640200	-1.97976200	-14.06517500
H	6.06488200	-0.87278900	-14.32287000
H	7.40988500	1.17021700	-14.49246400
H	7.57997900	3.65975100	-14.48015300
H	5.50005700	5.04910800	-14.31359200
H	3.27886400	3.97627000	-14.21570900
H	-1.23959100	2.30037700	-12.11017500
H	-1.95915600	3.94829500	-13.86440700
H	-1.57169900	5.05138200	-16.01771200
H	-0.18464200	5.39300800	-18.06351700
H	1.96353400	4.12925700	-18.33708200
H	2.74137700	2.58207900	-16.57541000
C	-1.58333400	-2.03051000	-12.12084400
C	-1.47091700	-0.59667200	-14.12165300
C	-2.12425700	-3.16473600	-13.00621600
H	-2.43054500	-1.47014500	-11.68683900
H	-0.97382300	-2.44416600	-11.30370300
C	-2.02239300	-1.77470900	-14.94472600
H	-2.30690000	0.04303300	-13.79021500
H	-0.78508300	0.00156100	-14.73146300
H	-1.25695600	-3.73980700	-13.39030600
H	-1.16045800	-2.36755700	-15.31148400
N	-0.76215400	-1.11724800	-12.93510700
O	-2.84965600	-2.61872900	-14.12235800
C	-2.87571600	-1.28796200	-16.11121800
H	-2.26783000	-0.66946200	-16.79025900
H	-3.27710400	-2.14446600	-16.67453200
H	-3.71865400	-0.68281400	-15.74029600
C	-3.07306500	-4.07628100	-12.23568100
H	-3.47188200	-4.85974000	-12.89827300
H	-2.53942300	-4.55749700	-11.40020400
H	-3.91644000	-3.49525500	-11.82913500
C	3.34779800	-4.01574900	-8.70237000
C	3.32399700	-3.85697600	-10.20527000
H	4.21552300	-4.61710400	-8.38192500
H	3.43058300	-3.02592300	-8.22317300
O	1.95767600	-0.73043900	-9.35994900
C	2.17841600	-4.24296700	-10.92845300
C	1.86137800	-3.78405300	-12.25356000
H	1.38218100	-4.73223600	-10.35803500
C	4.59482300	-3.44677900	-10.85834900

C	5.02224700	-4.03735600	-12.07272700
C	5.44766500	-2.50316600	-10.23877000
C	6.23906600	-3.67041000	-12.66275000
H	4.40719100	-4.80820800	-12.53709000
C	6.66120700	-2.13147000	-10.83338600
H	5.14592500	-2.04559600	-9.29677600
C	7.06115100	-2.70789100	-12.05096900
H	6.55119200	-4.14637200	-13.59482900
H	7.29428000	-1.38822800	-10.34460800
H	8.00921700	-2.42094900	-12.51022600
H	2.64291200	-3.59165700	-12.98897700
H	0.90955300	-4.11344000	-12.67940600
H	2.42262700	-4.48674000	-8.34077000
C	0.86194100	-0.67191800	-8.45392100
C	0.39278500	-2.08451400	-8.03503300
C	1.35880500	0.08373700	-7.19954400
C	-0.34292500	0.08813200	-9.06351500
H	0.02273600	-2.63943900	-8.91543100
H	1.23022100	-2.64695100	-7.59629000
H	-0.42276300	-2.02962900	-7.29320900
H	1.67797900	1.10244200	-7.46531900
H	0.55456000	0.16347000	-6.44755000
H	2.20905100	-0.45533500	-6.74993000
H	-1.20258200	0.07800500	-8.37089700
H	-0.09956900	1.14377700	-9.26058200
H	-0.65149700	-0.39302700	-10.00424700
C	3.14058700	4.90329900	-9.07690100
H	3.13441700	5.26711400	-8.03964400
H	3.36369200	5.71449000	-9.78461100
C	3.93606400	3.68227200	-9.28834400
C	4.08033600	2.72896500	-8.24830100
C	4.33265300	3.30992600	-10.59726500
C	4.61913600	1.45919200	-8.50405900
H	3.75017700	2.98946000	-7.24189400
C	4.87184400	2.03983600	-10.85196700
H	4.20226200	4.01653700	-11.41615600
C	5.01391000	1.10841100	-9.80811600
H	4.70498600	0.73338900	-7.69344200
H	5.16726600	1.77195100	-11.86509000
H	5.40880700	0.11661300	-10.01729300
S	1.24215800	4.39250100	-9.46826100
O	1.37467200	3.80816500	-10.88975000
Na	2.15104700	1.55038400	-9.99136800
O	1.02166800	3.24370200	-8.45543700

IM3b-exo

Pd	1.86648400	-1.86115000	-10.69441900
P	0.96920300	-0.69906100	-12.35470300
O	1.71082300	-0.64121200	-13.86808600
O	0.99641900	0.93713800	-11.97551300
C	2.74268100	1.53551800	-14.10785900
C	2.84955900	0.14333200	-14.05503700
C	4.07573500	-0.53916700	-14.25504700
C	5.23331900	0.18640000	-14.47381700
C	6.41462800	2.36929000	-14.56628800
C	6.39666700	3.75142100	-14.46688300
C	5.16826700	4.42916000	-14.23419700
C	3.97877400	3.72355100	-14.12673200
C	3.95718400	2.30032600	-14.24069200
C	5.21213800	1.61167900	-14.44334300
C	1.40687000	2.18360300	-13.99805200
C	0.57984700	1.88344700	-12.91869000
C	-0.68138700	2.48913600	-12.70764600
C	-1.14778700	3.40728200	-13.62917200
C	-0.89248400	4.61517600	-15.78305600
C	-0.17548900	4.87938400	-16.93954300
C	1.07516400	4.23931200	-17.15689600
C	1.59894100	3.36766500	-16.21294900
C	0.89984700	3.09001400	-14.99952500
C	-0.38891600	3.71550000	-14.79720700
H	4.07791000	-1.62895500	-14.24237600
H	6.18403000	-0.32479700	-14.63767100
H	7.35304000	1.83247200	-14.72337600
H	7.32404900	4.32105600	-14.55231400
H	5.16089700	5.51587500	-14.12979600
H	3.04849300	4.25321700	-13.92996600
H	-1.25208800	2.22031100	-11.81939200
H	-2.11366800	3.89527300	-13.48378200
H	-1.86297200	5.08520500	-15.60751500
H	-0.57233900	5.56778500	-17.68826100
H	1.62831200	4.43110000	-18.07864100
H	2.55369300	2.87876500	-16.40007000
C	-1.18841100	-2.35608200	-12.30365900
C	-1.20721600	-0.67023000	-14.08606200
C	-1.14636700	-3.45020800	-13.38337200
H	-2.23694600	-2.14220900	-12.03533700
H	-0.65362900	-2.68775500	-11.40266000
C	-1.18298800	-1.80949800	-15.12013100

H	-2.25153700	-0.39243800	-13.86568000
H	-0.68267600	0.20530000	-14.48157700
H	-0.07992300	-3.65610000	-13.61312000
H	-0.12425100	-2.03410800	-15.35299800
N	-0.57959900	-1.11234200	-12.81824400
O	-1.80121600	-2.99199200	-14.57972400
C	-1.94052200	-1.42870500	-16.38740300
H	-1.47028300	-0.54993500	-16.85662800
H	-1.92788600	-2.26330500	-17.10538600
H	-2.98820900	-1.18459300	-16.14833600
C	-1.84911800	-4.72455800	-12.93213200
H	-1.85091200	-5.46656500	-13.74536300
H	-1.32720200	-5.15337400	-12.06394900
H	-2.89166800	-4.50869100	-12.64811000
C	3.78505900	-3.18259600	-8.24018700
C	2.87589200	-3.69022200	-9.34754500
H	3.20868500	-2.56512900	-7.53349400
H	4.23729900	-4.01389700	-7.67219400
O	1.41872700	-0.66899700	-9.03700800
C	3.36676000	-3.49408300	-10.66450900
C	2.65609400	-3.47812600	-11.90455300
H	4.36916000	-3.05790100	-10.71247800
C	1.69754900	-4.49566100	-8.92192400
C	0.64081300	-4.89452700	-9.78400200
C	1.58571800	-4.88282900	-7.55877100
C	-0.44814100	-5.63601900	-9.31247500
H	0.62478900	-4.58333500	-10.82187600
C	0.49592200	-5.62784000	-7.08855000
H	2.35578900	-4.60141900	-6.84396100
C	-0.53252600	-6.01076300	-7.96140100
H	-1.24574000	-5.91082700	-10.00516500
H	0.45308500	-5.90189300	-6.03237700
H	-1.38723700	-6.58416300	-7.59732100
H	1.82880900	-4.15003500	-12.13645100
H	3.23913000	-3.18577000	-12.78047700
H	4.59725000	-2.56840100	-8.64878300
C	0.12787600	-0.54523000	-8.45846500
C	-0.54384500	-1.91959100	-8.27627200
C	0.34321900	0.11540800	-7.07605800
C	-0.80158800	0.35946900	-9.30387800
H	-0.69341400	-2.39836600	-9.25578200
H	0.09399100	-2.57947500	-7.67041200
H	-1.52647800	-1.82229000	-7.78268000
H	0.81074600	1.10555900	-7.19649900

H	-0.61823500	0.24410600	-6.54926900
H	1.00229900	-0.51684600	-6.45853000
H	-1.78236900	0.47630500	-8.81165300
H	-0.37508800	1.36847300	-9.42568500
H	-0.96694200	-0.07668700	-10.30021000
C	4.00942600	4.29747300	-9.06309600
H	4.26718700	4.64823600	-8.05352400
H	4.34476500	5.00815800	-9.83183000
C	4.38270200	2.89816700	-9.33214100
C	4.38446400	1.94110500	-8.28410900
C	4.47731100	2.42833100	-10.66659200
C	4.48543600	0.56919500	-8.55836700
H	4.28288200	2.28519300	-7.25407100
C	4.57479900	1.05541300	-10.93898700
H	4.45118900	3.14344300	-11.48810500
C	4.57324100	0.12023300	-9.88877100
H	4.46418100	-0.15125200	-7.73964600
H	4.62843700	0.71157300	-11.96939400
H	4.61651700	-0.94587100	-10.10831300
S	2.00248900	4.37501300	-9.14048300
O	1.73081700	3.82878500	-10.55877100
Na	2.00726800	1.44178100	-9.74391100
O	1.61213400	3.30836600	-8.08985200

IM3b-endo

Pd	1.78091900	-2.03530300	-11.04044100
P	0.79979300	-0.71926700	-12.51425200
O	1.52371300	-0.61501000	-14.02977600
O	0.88385500	0.90852800	-12.06632400
C	2.65932300	1.51401400	-14.14512100
C	2.71286600	0.11871900	-14.10834300
C	3.92699300	-0.60799100	-14.17881600
C	5.12355400	0.07900900	-14.28609300
C	6.38018100	2.22049900	-14.31936500
C	6.40153500	3.60428700	-14.24816000
C	5.18221300	4.32660700	-14.12840900
C	3.96472900	3.66246300	-14.09938300
C	3.90350300	2.23883300	-14.19164400
C	5.14629900	1.50482600	-14.28278000
C	1.33650500	2.19031400	-14.05847200
C	0.49124200	1.87903200	-12.99531700
C	-0.76229400	2.50263700	-12.79265500
C	-1.19908300	3.44896700	-13.70034900
C	-0.88225700	4.70824800	-15.81844400

C	-0.13657000	4.99091800	-16.95251700
C	1.10883500	4.33723600	-17.16141600
C	1.59736400	3.43086500	-16.23142900
C	0.86669500	3.13176600	-15.04190800
C	-0.41465400	3.77439300	-14.84688700
H	3.89031600	-1.69714900	-14.15659100
H	6.06887800	-0.46366200	-14.35212300
H	7.30925900	1.64999000	-14.38963800
H	7.35165400	4.14161400	-14.26968800
H	5.20404500	5.41506700	-14.04597100
H	3.04138600	4.22471200	-13.97880500
H	-1.35196300	2.22554300	-11.91902400
H	-2.15943300	3.94928000	-13.55943600
H	-1.84797100	5.19091400	-15.65048700
H	-0.50642500	5.70587900	-17.69017100
H	1.68525000	4.54703000	-18.06486100
H	2.54958300	2.93192500	-16.40726700
C	-1.52146700	-2.12735900	-12.26059700
C	-1.45373800	-0.55933500	-14.15684900
C	-1.88390300	-3.25182400	-13.24460500
H	-2.44772900	-1.68339900	-11.85485600
H	-0.92386600	-2.52507100	-11.42694500
C	-1.82416200	-1.72864400	-15.08620900
H	-2.37185700	-0.04057000	-13.83226100
H	-0.80929400	0.15223400	-14.68408100
H	-0.93819500	-3.70821200	-13.60275900
H	-0.88224100	-2.19693500	-15.43582100
N	-0.75786100	-1.07955000	-12.96196000
O	-2.59614500	-2.71285800	-14.37292300
C	-2.66054900	-1.25709700	-16.27120800
H	-2.08988100	-0.52842500	-16.86851300
H	-2.92872800	-2.11010800	-16.91347300
H	-3.58703700	-0.77672400	-15.91746000
C	-2.77367400	-4.30524100	-12.59405000
H	-3.03937500	-5.08502300	-13.32423200
H	-2.24527300	-4.77639400	-11.74948000
H	-3.70077400	-3.84351000	-12.21785700
C	4.63283800	-3.16932700	-10.78445500
C	3.35095600	-3.75197700	-10.19728300
H	4.63397300	-2.06835100	-10.77179800
H	5.50079300	-3.51050400	-10.19926800
O	1.89916300	-0.77541700	-9.37403200
C	2.29864300	-4.19544100	-11.02566400
C	2.10991500	-3.71300300	-12.36140800

H	1.47091600	-4.73769800	-10.56092700
C	3.30200700	-3.96226400	-8.73568300
C	3.96575600	-3.04610000	-7.88427500
C	2.57204000	-5.02030700	-8.14325600
C	3.88494800	-3.17225300	-6.49101800
H	4.51350500	-2.21212900	-8.32006500
C	2.49939400	-5.14986400	-6.75048900
H	2.07390500	-5.75582400	-8.77690700
C	3.15022200	-4.22312000	-5.91635200
H	4.39157700	-2.44443800	-5.85337300
H	1.93879300	-5.97956800	-6.31452600
H	3.08946300	-4.32347400	-4.83080200
H	2.96747100	-3.44893800	-12.98805600
H	1.23602300	-4.06995700	-12.91185200
H	4.76505900	-3.48699200	-11.82802000
C	0.79522100	-0.70938600	-8.48209300
C	0.30793800	-2.12126500	-8.09052000
C	1.29163800	0.02866400	-7.21665200
C	-0.38123700	0.08353300	-9.10045700
H	-0.03316100	-2.66275400	-8.99109500
H	1.12959700	-2.69056700	-7.63405300
H	-0.53210000	-2.07157400	-7.37574200
H	1.63367400	1.04355700	-7.47314100
H	0.47946400	0.11824700	-6.47442000
H	2.12540500	-0.52961600	-6.76294400
H	-1.23540200	0.12851000	-8.40260100
H	-0.08534900	1.11983600	-9.32927700
H	-0.71642700	-0.40174200	-10.03025800
C	3.70323200	4.60698700	-9.23591700
H	3.76241400	5.06949200	-8.24018900
H	4.04317900	5.30025200	-10.01835600
C	4.31448000	3.26762800	-9.31128000
C	4.30955900	2.41852100	-8.17549800
C	4.68552400	2.71042400	-10.56179000
C	4.70033300	1.07611700	-8.27590000
H	3.99044600	2.82362900	-7.21445900
C	5.07031200	1.36264600	-10.66226600
H	4.66166900	3.33529400	-11.45375300
C	5.08675600	0.54388000	-9.51855100
H	4.68469600	0.43926500	-7.38996400
H	5.34772400	0.95386500	-11.63462600
H	5.39552600	-0.49858500	-9.59188500
S	1.74936700	4.36695500	-9.59331300
O	1.78950500	3.70632100	-10.98649000

Na	2.26014600	1.43340400	-9.96430900
O	1.36079800	3.31120600	-8.52935100

IM3a'-exo

Pd	1.34342100	-1.88438300	-11.27136800
P	1.46464800	-0.92812000	-9.20515300
O	1.33454900	-1.77836700	-7.74654200
O	0.15260800	0.12105400	-9.00915300
C	-0.75856300	-1.15156000	-6.68498400
C	0.10239700	-2.12699500	-7.19606800
C	-0.18840100	-3.51308600	-7.10806000
C	-1.39394100	-3.93143500	-6.57484100
C	-3.65507900	-3.39457100	-5.69753800
C	-4.61443100	-2.46147100	-5.33753800
C	-4.31812500	-1.07316100	-5.42226500
C	-3.06984800	-0.63841100	-5.84341000
C	-2.05349300	-1.57178800	-6.21149700
C	-2.36740000	-2.98106900	-6.15086900
C	-0.34051200	0.27649500	-6.66202200
C	0.08365000	0.88367400	-7.84000900
C	0.46413200	2.24442300	-7.92217800
C	0.44272900	3.01819900	-6.77673500
C	0.11346400	3.22678200	-4.32482200
C	-0.19724800	2.66137600	-3.09798400
C	-0.54671300	1.28532200	-3.02195400
C	-0.60077300	0.50333500	-4.16674400
C	-0.30803500	1.05687100	-5.44995000
C	0.07933800	2.44906700	-5.52032200
H	0.54902100	-4.23114600	-7.46336200
H	-1.62643700	-4.99587100	-6.50343700
H	-3.87213800	-4.46448800	-5.65626200
H	-5.60049200	-2.78757400	-5.00103600
H	-5.08306900	-0.33950100	-5.16038900
H	-2.86481000	0.42782600	-5.91797800
H	0.76466200	2.64988000	-8.88740700
H	0.72408700	4.07256600	-6.81563200
H	0.39933200	4.27866500	-4.39895600
H	-0.16498600	3.26564700	-2.18924800
H	-0.77079100	0.83676200	-2.05190300
H	-0.86360600	-0.55049700	-4.09014500
C	3.93113600	0.02424800	-9.90121000
C	3.29874400	0.40327500	-7.55904000
C	5.21522000	-0.65802500	-9.40648200
H	4.12211400	1.09717500	-10.08051400

H	3.59729500	-0.43646300	-10.84194100
C	4.60886900	-0.28169800	-7.13229900
H	3.46141000	1.49148200	-7.64003100
H	2.51678500	0.21550100	-6.81640000
H	4.99595100	-1.72917400	-9.26911300
H	4.40556400	-1.36385100	-7.02030000
N	2.87345300	-0.10600700	-8.88054500
O	5.62018600	-0.09973500	-8.14073200
C	5.14353300	0.30250000	-5.82946000
H	4.41291600	0.14940700	-5.01932400
H	6.08937000	-0.18818700	-5.55199000
H	5.32632700	1.38358700	-5.94106800
C	6.36684200	-0.47393900	-10.38715100
H	7.27560100	-0.96046300	-10.00111700
H	6.10982300	-0.92786000	-11.35748400
H	6.57670600	0.59721300	-10.54117900
C	1.28211900	-4.84727800	-10.56448900
C	2.41511700	-3.90701000	-10.96686400
H	1.68326700	-5.86939400	-10.44184300
H	0.83258000	-4.54911400	-9.60841200
O	0.15999400	-0.39007900	-12.16065300
C	2.53077300	-3.39652400	-12.29949100
C	1.41577400	-3.11516500	-13.11486400
H	3.48980300	-2.97207600	-12.60663600
C	3.64078900	-3.97907100	-10.11523800
C	4.94054000	-4.04643100	-10.67235800
C	3.52406000	-4.03262900	-8.70712000
C	6.07539300	-4.13953600	-9.85247500
H	5.07163900	-4.05434000	-11.75499800
C	4.65710400	-4.11722400	-7.88742700
H	2.53904800	-3.97260300	-8.25131400
C	5.94189400	-4.16870700	-8.45516900
H	7.06502500	-4.19405700	-10.31058100
H	4.53495200	-4.13958000	-6.80257700
H	6.82546800	-4.23327100	-7.81739600
H	0.47538600	-3.66772700	-13.04052000
H	1.57170000	-2.55899100	-14.03885300
H	0.48647500	-4.87595400	-11.31919200
C	0.74701800	0.75506000	-12.75153200
C	2.00156900	0.39671400	-13.57763300
C	-0.32824600	1.35435400	-13.68893800
C	1.11938300	1.80908600	-11.68084900
H	2.76341100	-0.06646600	-12.92781200
H	1.73859800	-0.32287600	-14.36944100

H	2.43953900	1.29385000	-14.04803000
H	-1.22892000	1.62315900	-13.11389600
H	0.04873500	2.26205800	-14.19125300
H	-0.60923700	0.61446900	-14.45638300
H	1.54221200	2.71817600	-12.14286000
H	0.22444900	2.10698500	-11.10991300
H	1.85784400	1.40275500	-10.97469500
C	-5.06535000	0.27711300	-10.35957400
H	-5.80082800	0.45052200	-11.15808500
H	-5.54732400	0.24339800	-9.37210600
C	-4.14567600	-0.84478200	-10.61798700
C	-3.74475800	-1.15271600	-11.94464400
C	-3.44484700	-1.45863100	-9.54960000
C	-2.68797200	-2.04122900	-12.19195000
H	-4.25598000	-0.66788700	-12.77699500
C	-2.39228600	-2.35271800	-9.79972500
H	-3.71748200	-1.21613800	-8.52269800
C	-2.00252400	-2.64183500	-11.11970200
H	-2.37766800	-2.24135900	-13.21890000
H	-1.86405800	-2.80804200	-8.96488600
H	-1.16165700	-3.30969400	-11.30930900
S	-3.94942800	1.94913400	-10.32782500
O	-2.92342400	1.61699100	-9.22154100
Na	-1.56177700	0.22667300	-10.80641500
O	-3.25846700	1.88285000	-11.71016600

IM3b²-endo

Pd	1.72348000	-1.86901900	-11.58131800
P	2.88299800	-0.50767200	-10.19152800
O	2.92628400	-0.73161400	-8.52854200
O	2.17600600	1.02987900	-10.22345100
C	1.44564600	0.87632000	-7.49525500
C	1.79205300	-0.44934700	-7.76622900
C	1.08236700	-1.55557900	-7.23843600
C	-0.02168700	-1.33333400	-6.43549600
C	-1.67864600	0.22864200	-5.44372300
C	-2.16251400	1.51487300	-5.26407000
C	-1.46873400	2.61803900	-5.83334800
C	-0.29711700	2.42419800	-6.55058900
C	0.24078100	1.11514500	-6.73973900
C	-0.48500200	-0.00751600	-6.18807300
C	2.30199100	1.98150100	-8.00684400
C	2.62603100	2.03351800	-9.36185000
C	3.38727600	3.07782400	-9.93995300

C	3.86978800	4.08934300	-9.13148600
C	4.18748100	5.07276400	-6.87440700
C	4.00279000	5.02483400	-5.50143900
C	3.26772400	3.95335100	-4.92485300
C	2.71215300	2.96431900	-5.72379700
C	2.86031200	2.99437000	-7.14370600
C	3.64018800	4.06589100	-7.72392900
H	1.43071600	-2.55920900	-7.46967200
H	-0.57315000	-2.17497800	-6.01119800
H	-2.21169100	-0.63157600	-5.03193900
H	-3.08199800	1.68308600	-4.69990500
H	-1.86546200	3.62804300	-5.71300600
H	0.21493700	3.27588700	-6.99446800
H	3.56986500	3.06046800	-11.01419000
H	4.44961600	4.91042200	-9.55800200
H	4.76387100	5.87995800	-7.33257500
H	4.42872000	5.79983600	-4.86108400
H	3.14196600	3.90425300	-3.84127100
H	2.15928900	2.14630500	-5.26486100
C	5.16670400	-0.96056000	-11.63012000
C	5.46158500	0.39232200	-9.59481600
C	6.39548800	-1.78501400	-11.21142600
H	5.48943400	-0.15129900	-12.30930400
H	4.44683000	-1.59826200	-12.16056300
C	6.68146300	-0.47586300	-9.24326900
H	5.79734000	1.28306400	-10.15351000
H	4.95644400	0.71603000	-8.67831200
H	6.04922100	-2.62455000	-10.57623000
H	6.32873700	-1.33502000	-8.63767100
N	4.52515600	-0.38135800	-10.43732500
O	7.30147600	-0.97582500	-10.44239600
C	7.73015800	0.32354000	-8.47745100
H	7.30471800	0.69297000	-7.53101500
H	8.60267600	-0.30867100	-8.25174400
H	8.06450100	1.18649800	-9.07551800
C	7.15147900	-2.31324600	-12.42517200
H	8.04213600	-2.87522400	-12.10509800
H	6.50230000	-2.98209500	-13.01254100
H	7.47281000	-1.47842500	-13.06868000
C	3.51727100	-4.30894600	-11.66879500
C	2.31070900	-3.96216900	-10.80115500
H	4.43497800	-3.85512700	-11.27437300
H	3.65940800	-5.40546400	-11.65439500
O	0.96796100	-0.40043800	-12.88345400

C	0.99049000	-3.91970300	-11.34528900
C	0.73434100	-3.53482900	-12.67874000
H	0.15059800	-3.94258900	-10.64595000
C	2.49246300	-4.21818200	-9.34246500
C	3.64827300	-3.74818700	-8.67943100
C	1.55132400	-4.96427500	-8.59515500
C	3.85257100	-3.99885600	-7.31746800
H	4.36802900	-3.14251900	-9.22916300
C	1.75703800	-5.22004900	-7.23026700
H	0.66522800	-5.36791100	-9.08732300
C	2.90755700	-4.73746900	-6.58460000
H	4.74425100	-3.60530800	-6.82492900
H	1.01944700	-5.80304300	-6.67479900
H	3.06533000	-4.93310100	-5.52216300
H	1.44050400	-3.73422900	-13.48752600
H	-0.29455000	-3.33379100	-12.97924600
H	3.39355000	-3.98813400	-12.71113200
C	1.74623000	0.11035200	-13.94943600
C	2.52565800	-1.01126000	-14.67055000
C	0.74776400	0.75778400	-14.93858500
C	2.73477300	1.19297200	-13.45481600
H	3.23508400	-1.48765200	-13.97267400
H	1.82492600	-1.78055000	-15.03322100
H	3.09473000	-0.61777900	-15.53067600
H	0.18127900	1.55516000	-14.43207000
H	1.27764600	1.19489600	-15.80263000
H	0.03789700	-0.00179500	-15.30589700
H	3.32389900	1.61090200	-14.28950400
H	2.18585200	2.02175900	-12.97784800
H	3.43054100	0.76898700	-12.71754400
C	-2.89500400	3.00312800	-10.90391700
H	-3.65431100	3.25033800	-11.65954200
H	-3.12035800	3.47972500	-9.93920600
C	-2.58489700	1.56598100	-10.80670600
C	-2.66121700	0.73594600	-11.95574900
C	-1.95532600	1.04541600	-9.64754900
C	-2.13597200	-0.56444400	-11.94470200
H	-3.11670100	1.13206300	-12.86420300
C	-1.43193200	-0.25694700	-9.63834700
H	-1.86068800	1.67372400	-8.76209400
C	-1.51461400	-1.06579600	-10.78622300
H	-2.18159800	-1.17495100	-12.84769100
H	-0.94258500	-0.63559600	-8.74342800
H	-1.07516500	-2.06298400	-10.78442700

S	-1.21966400	3.91395900	-11.54120800
O	-0.20571500	3.47703800	-10.46102100
Na	0.09682000	1.23091700	-11.55910000
O	-0.93501700	3.15382100	-12.85756900

E-TS3a

C	-1.09741400	-0.05406800	-5.27247400
C	-0.60349600	0.87946600	-4.16759300
H	-0.93392900	-1.10442300	-4.98537600
H	-2.17575000	0.08527400	-5.43710300
C	-1.06361900	2.27118900	-4.16727100
C	-1.81615000	2.86709700	-5.22641600
H	-0.47566700	2.99390100	-3.59110500
C	0.81422300	0.69535000	-3.73555400
C	1.72444300	-0.08091300	-4.49947200
C	1.34862600	1.44695900	-2.65253200
C	3.11020600	-0.03079600	-4.25340600
H	1.35771900	-0.68406900	-5.32872800
C	2.72762100	1.50572200	-2.41380300
H	0.66484000	1.99592000	-2.00521000
C	3.62499000	0.78435000	-3.22979100
H	3.78602400	-0.61936500	-4.87769300
H	3.10235100	2.10391500	-1.58343400
H	4.69962000	0.83241700	-3.04535900
O	-3.59205700	1.84947800	-1.35593800
H	-2.37237900	2.23016600	-5.91862100
H	-2.27462000	3.84233500	-5.03677700
H	-0.57670400	0.13520400	-6.22778200
C	-4.34455000	2.93082000	-1.83511800
C	-5.46387700	3.21812800	-0.80250400
C	-3.46342000	4.19791400	-1.99266200
C	-5.00316700	2.60566800	-3.20198800
H	-6.11054000	2.33105600	-0.69599300
H	-5.01601400	3.43958700	0.18094900
H	-6.09157200	4.07641100	-1.10291000
H	-2.63949800	3.98336500	-2.69264300
H	-4.03488200	5.06485200	-2.37313100
H	-3.02522600	4.47270000	-1.01742900
H	-5.62701100	3.43893800	-3.57559400
H	-4.21810500	2.39141200	-3.94702800
H	-5.63817900	1.70930700	-3.10379000
Pd	-2.06005000	1.05830200	-2.63665600
P	-1.84749100	-0.73730400	-1.35282600
O	-1.68447400	-0.33170400	0.28750800

O	-0.37612500	-1.58488300	-1.51961600
C	0.66419600	-0.01550700	0.64711200
C	-0.60692900	0.53289600	0.47370900
C	-0.86100200	1.92799300	0.43782300
C	0.19493800	2.80298400	0.61836800
C	2.62618300	3.21740800	0.90825000
C	3.92911200	2.74881100	0.99361100
C	4.18059800	1.35030200	0.94639400
C	3.13266300	0.44698000	0.83816800
C	1.77757100	0.89113900	0.77920900
C	1.52642500	2.31634400	0.78773600
C	0.80626700	-1.49728100	0.60917100
C	0.26978100	-2.21879700	-0.46828500
C	0.41676900	-3.62771000	-0.58012400
C	1.08166100	-4.33579800	0.40296700
C	2.22277100	-4.39937600	2.60821200
C	2.66594200	-3.75732700	3.75413400
C	2.47689600	-2.35499900	3.89399900
C	1.87549500	-1.61674600	2.88486700
C	1.43204400	-2.23852500	1.67734500
C	1.58917200	-3.67129600	1.55763900
H	-1.87886500	2.25235000	0.20934100
H	0.02913200	3.88279300	0.59874100
H	2.41759700	4.29006600	0.92114600
H	4.76140100	3.45002500	1.08347100
H	5.20810200	0.98271600	0.98621600
H	3.34128900	-0.62029500	0.78757500
H	-0.00510200	-4.12363600	-1.45512100
H	1.20691000	-5.41750000	0.31781100
H	2.34001000	-5.47966000	2.49234300
H	3.14565900	-4.32508600	4.55398200
H	2.80188600	-1.85312300	4.80788100
H	1.72948300	-0.54528600	3.01227800
C	-4.31686500	-1.64949600	-1.97391000
C	-3.19593000	-2.84299300	-0.14482400
C	-5.36018900	-1.13904800	-0.96784900
H	-4.66950500	-2.59182300	-2.42960800
H	-4.15738300	-0.90110600	-2.76486600
C	-4.27803200	-2.31173900	0.81694200
H	-3.50739100	-3.82812800	-0.53452700
H	-2.23969500	-2.95624200	0.38163200
H	-4.98488100	-0.17751300	-0.57093800
H	-3.92212700	-1.34849800	1.22793200
N	-3.03416900	-1.92297600	-1.29076500

O	-5.51059200	-2.09191700	0.10762400
C	-4.56506500	-3.29984700	1.94320800
H	-3.65421500	-3.46623000	2.54048100
H	-5.35420300	-2.90816700	2.60403800
H	-4.89955800	-4.26567700	1.52998800
C	-6.73097800	-0.95542000	-1.60878700
H	-7.46114200	-0.61158100	-0.85923800
H	-6.67095000	-0.20444700	-2.41197200
H	-7.08842400	-1.90659700	-2.03736200
C	-0.59891600	4.54447600	-8.11851000
H	0.36772200	4.71661200	-8.61514800
H	-1.00970700	5.49159400	-7.74039700
C	-1.57228500	3.76323600	-8.94488300
C	-1.12101600	2.89056300	-9.95661200
C	-2.95316400	3.82779700	-8.65920000
C	-2.03487300	2.10861200	-10.67907100
H	-0.05272800	2.83071300	-10.17416600
C	-3.86667700	3.04284000	-9.37864500
H	-3.30687900	4.49936600	-7.87297300
C	-3.40906000	2.18111900	-10.39093200
H	-1.67499000	1.44134400	-11.46507800
H	-4.93301500	3.10474800	-9.15149200
H	-4.11922600	1.57105400	-10.95297700
S	-0.16004200	3.56292000	-6.55361600
O	0.69910300	4.47737400	-5.68546400
Na	2.18176400	2.56832000	-5.04105000
O	0.61787300	2.33584400	-7.00711100

E-TS3b

Pd	2.89527900	-2.49390800	-11.72385800
P	3.31680100	-1.38290500	-9.83528900
O	4.43349600	-0.10233900	-10.00009500
O	4.19909200	-2.31480600	-8.71188000
C	6.59815300	-1.09133800	-9.65726500
C	5.65079600	-0.53279100	-10.51830200
C	5.86379000	-0.39760600	-11.91423400
C	7.05308900	-0.83695200	-12.46600200
C	9.23175000	-2.00410100	-12.22922500
C	10.15600700	-2.68552000	-11.45220500
C	9.91393700	-2.86623000	-10.06290100
C	8.77177100	-2.34715800	-9.46970100
C	7.80967200	-1.61986100	-10.23383300
C	8.03975600	-1.47171400	-11.65436300
C	6.28419700	-1.18328200	-8.20440800

C	5.08756900	-1.78438400	-7.79194100
C	4.75715800	-1.95122200	-6.42005300
C	5.61774900	-1.49044800	-5.44210600
C	7.69059600	-0.28550900	-4.79401900
C	8.83648000	0.41364500	-5.14039700
C	9.14655500	0.62322700	-6.51202000
C	8.32695100	0.11557600	-7.50994200
C	7.15336100	-0.63442800	-7.19187200
C	6.82144300	-0.81190000	-5.79516000
H	5.07487600	0.04621400	-12.52094700
H	7.23876000	-0.73409800	-13.53748300
H	9.39216300	-1.87461300	-13.30235100
H	11.06137200	-3.09460600	-11.90515800
H	10.63099000	-3.42361600	-9.45643800
H	8.59582600	-2.50093800	-8.40611300
H	3.81952000	-2.44888100	-6.16993600
H	5.37696700	-1.62311200	-4.38498000
H	7.42516200	-0.43882000	-3.74508200
H	9.49297100	0.81487100	-4.36562100
H	10.03547200	1.19600000	-6.78462700
H	8.57392900	0.29477000	-8.55523500
C	0.75253100	-0.54394700	-9.48264300
C	2.38241300	0.35867200	-7.87536700
C	0.45121100	0.89383800	-9.93080100
H	0.04401100	-0.83833900	-8.68685100
H	0.65494900	-1.21382900	-10.34676000
C	2.03173900	1.77514200	-8.37220400
H	1.74876500	0.11199000	-7.00478800
H	3.43518400	0.31688100	-7.57093300
H	1.14277900	1.13053400	-10.76034100
H	2.71253700	2.01485800	-9.21255400
N	2.12267800	-0.63088000	-8.93918400
O	0.67417500	1.81764300	-8.84293700
C	2.16978500	2.81099400	-7.26082700
H	3.21048600	2.84165200	-6.90035400
H	1.89442600	3.81029000	-7.63278400
H	1.50950200	2.55615500	-6.41561600
C	-0.99537900	1.05212600	-10.38313600
H	-1.19179100	2.09195200	-10.68875400
H	-1.18745500	0.38890300	-11.24020800
H	-1.68641500	0.78956200	-9.56480100
C	5.52221600	-4.02149700	-11.48731200
C	4.02013200	-4.29264900	-11.52247400
H	5.80102700	-3.59600300	-10.51619900

H	6.12999200	-4.93415200	-11.64620700
O	1.57213500	-1.00052400	-12.46756900
C	3.32563900	-4.35005100	-12.81104200
C	3.92744100	-4.08484700	-14.09213700
H	2.40070400	-4.92966000	-12.86591600
C	3.49788500	-5.17354300	-10.42510700
C	2.11576500	-5.49291700	-10.32262400
C	4.37572700	-5.79135300	-9.49331300
C	1.64098300	-6.37548600	-9.34665500
H	1.41002600	-5.00884200	-10.99853200
C	3.89540000	-6.68253300	-8.51482100
H	5.44221400	-5.56478500	-9.51732200
C	2.52818300	-6.98278100	-8.43558800
H	0.57070200	-6.58645000	-9.29041000
H	4.59936300	-7.13163900	-7.81050400
H	2.15412700	-7.66889500	-7.67333400
H	4.84645500	-3.49539600	-14.13758700
H	3.23709300	-3.89721500	-14.91957200
H	5.81108100	-3.30102800	-12.25990600
C	1.32904300	-0.92111200	-13.84418600
C	0.39370000	0.29115300	-14.08791500
C	2.64375000	-0.70004800	-14.63598300
C	0.63094100	-2.20523200	-14.36459900
H	-0.55113800	0.15411900	-13.53650500
H	0.87583800	1.21411400	-13.72443000
H	0.15802300	0.41644300	-15.16007400
H	3.33359700	-1.53497000	-14.43304600
H	2.47268400	-0.63510800	-15.72650600
H	3.12590300	0.23463400	-14.30158500
H	0.43227400	-2.16795300	-15.45164700
H	1.26688500	-3.07859300	-14.14903800
H	-0.32981800	-2.34249100	-13.83864600
C	5.09784100	-6.38304000	-16.54921900
H	5.83969400	-5.61840700	-16.82109000
H	4.14499700	-6.19231300	-17.06377400
C	5.59689200	-7.78048200	-16.71464300
C	6.97494700	-8.06334000	-16.59871600
C	4.69039700	-8.84429600	-16.91274600
C	7.43954100	-9.38309700	-16.69821500
H	7.67687500	-7.24317800	-16.43630400
C	5.15587500	-10.16359200	-17.01202000
H	3.62328700	-8.62927900	-16.99359600
C	6.53135500	-10.43674300	-16.90432400
H	8.50884100	-9.58967800	-16.61629800

H	4.44682200	-10.97814800	-17.17476500
H	6.89343600	-11.46397100	-16.98389900
S	4.71249600	-6.03370500	-14.71273300
O	5.99613300	-6.26558300	-13.92851400
Na	4.55227500	-6.98770100	-11.99696100
O	3.61738300	-7.01047000	-14.30823700

(R)-TS4

C	-1.19621700	1.28639200	-2.51916200
C	-2.37046600	1.77139100	-3.21099600
C	-2.44387100	3.05530200	-3.90505400
H	-3.15150700	1.05859800	-3.49393800
O	-2.10887900	1.86430600	0.94569600
C	-0.77412500	1.66722300	1.32351100
C	-0.71737100	1.74427200	2.87153600
C	-0.26128100	0.27743500	0.87016000
C	0.14886300	2.76333200	0.73219400
H	-1.06556600	2.73447200	3.21060200
H	-1.37590400	0.97541700	3.30946400
H	0.30825200	1.58533400	3.24944800
H	-0.32466700	0.21073300	-0.22717100
H	0.78489100	0.09879800	1.17877800
H	-0.89356400	-0.51570600	1.30488800
H	1.20436600	2.63176000	1.03398000
H	0.08585900	2.73300300	-0.36845800
H	-0.19080200	3.75773000	1.06987100
Pd	-2.63367700	2.01312100	-1.10521500
P	-4.85117100	2.15278800	-0.71091200
O	-5.42844100	0.53926000	-0.41806600
O	-5.77562200	2.45104800	-2.09864300
C	-5.22398900	-0.42697500	-2.60769800
C	-4.79683300	-0.33788300	-1.27911400
C	-3.69157200	-1.07774000	-0.77586200
C	-2.99837400	-1.93576900	-1.60524800
C	-2.57553700	-2.84441200	-3.88197700
C	-2.82769700	-2.84036800	-5.25095400
C	-3.84402000	-1.99065600	-5.77634500
C	-4.62240300	-1.21056100	-4.92738200
C	-4.42148500	-1.21927100	-3.51257300
C	-3.33093700	-2.01869000	-2.99052700
C	-6.46579300	0.27841300	-3.02684900
C	-6.68802000	1.63302900	-2.72688100
C	-7.86208900	2.31279500	-3.15849200
C	-8.83196500	1.65055700	-3.88047900

C	-9.72906800	-0.44700200	-4.85145100
C	-9.63847600	-1.81396700	-5.06335000
C	-8.51618000	-2.52508500	-4.56126600
C	-7.49434700	-1.86289700	-3.89431700
C	-7.52821000	-0.44755600	-3.69607800
C	-8.70204500	0.25865900	-4.15838300
H	-3.41021300	-0.93323800	0.26593700
H	-2.16062800	-2.52362900	-1.22568300
H	-1.77737400	-3.46215200	-3.46440400
H	-2.23706400	-3.46563800	-5.92240000
H	-4.01324500	-1.95044300	-6.85343600
H	-5.40261600	-0.57404700	-5.34064200
H	-7.95124200	3.37340300	-2.92384300
H	-9.72103700	2.17992000	-4.23007500
H	-10.59864400	0.11611100	-5.19898900
H	-10.43207100	-2.34577000	-5.59185300
H	-8.45835900	-3.60795400	-4.69017400
H	-6.66020000	-2.44010100	-3.50008300
C	-4.94164200	3.46568300	1.63910000
C	-7.14338700	2.94438800	0.65685300
C	-5.31081200	2.57077700	2.83426300
H	-5.21561800	4.51071900	1.86945600
H	-3.86012600	3.39055000	1.44660100
C	-7.44433000	2.06365900	1.88533300
H	-7.53633100	3.96038500	0.83919500
H	-7.62852000	2.53324000	-0.23867300
H	-4.97696100	1.54039700	2.60082700
H	-7.09054600	1.03818700	1.66481800
N	-5.68899000	3.04539400	0.43278300
O	-6.73902300	2.56384000	3.03563500
C	-8.93181700	2.05546400	2.22235500
H	-9.50688100	1.63803800	1.38027600
H	-9.11864100	1.44129900	3.11705700
H	-9.28562500	3.08084300	2.41895700
C	-4.66401500	3.05780200	4.12608400
H	-4.96957700	2.42166200	4.97154700
H	-3.56766000	3.01878900	4.03087000
H	-4.96659300	4.09631300	4.33923300
C	-1.92730800	3.69619400	-7.28096500
H	-1.67564000	4.71990200	-6.97010500
H	-3.01390400	3.54723100	-7.24796100
C	-1.32051800	3.30749500	-8.58953600
C	-0.06742400	3.82521300	-8.98113500
C	-1.96209100	2.36282100	-9.41868700

C	0.52443000	3.41778000	-10.18593400
H	0.43671200	4.54723300	-8.33619500
C	-1.37071700	1.95644700	-10.62409000
H	-2.93008200	1.95824700	-9.11519600
C	-0.12501000	2.48218100	-11.01060600
H	1.49162800	3.82999300	-10.48196300
H	-1.88087800	1.23139100	-11.26228700
H	0.33529600	2.16672900	-11.94947000
S	-1.24363700	2.60588000	-5.87800200
O	0.23011400	2.89340600	-5.76341700
Na	-1.79583100	-0.36780900	-4.67353600
O	-1.60418100	1.17918900	-6.30263600
H	-1.08502000	0.20473400	-2.36384100
H	-0.24883800	1.82448100	-2.60092000
C	-3.75601100	3.41986600	-4.51939100
C	-4.24700800	4.74371300	-4.47111200
C	-4.51900100	2.45184000	-5.21575600
C	-5.45974600	5.08379200	-5.08926700
H	-3.69059200	5.51074000	-3.93328000
C	-5.72011300	2.79307500	-5.84528100
H	-4.14921200	1.43213000	-5.30231100
C	-6.19877300	4.11348900	-5.78475800
H	-5.82421700	6.11140800	-5.02873200
H	-6.28615600	2.02740200	-6.37915100
H	-7.13915800	4.38027600	-6.27110900
C	-1.56490700	4.18716500	-3.39904700
H	-0.54352000	3.83757200	-3.20637500
H	-1.51923300	5.01588800	-4.12064600
H	-1.98164400	4.56653800	-2.45094400

(S)-TS4

C	-0.55982300	2.50655000	-2.05073100
C	-1.50674000	2.97718800	-3.04328400
C	-1.35185800	2.79117900	-4.50610000
H	-2.15101500	3.81104100	-2.75354700
O	-2.12938000	-0.48459200	-0.76985100
C	-1.22459400	-0.48483700	0.29767800
C	-1.51984600	-1.74093600	1.15904800
C	0.24000800	-0.55403300	-0.20519800
C	-1.39278100	0.77597200	1.18350300
H	-2.55079300	-1.69662700	1.54672200
H	-1.42194400	-2.64917900	0.54045600
H	-0.82620200	-1.82369700	2.01522400
H	0.44797600	0.32406400	-0.83668500

H	0.97049300	-0.57654100	0.62489200
H	0.38147200	-1.46102200	-0.81797400
H	-0.69565900	0.78408400	2.04204800
H	-1.21421500	1.67389100	0.56951300
H	-2.42393400	0.82496400	1.57094100
Pd	-2.22620500	1.18102500	-2.13225900
P	-4.17620500	0.33450400	-2.87042900
O	-4.07648200	-1.30272900	-3.33883800
O	-4.76201900	0.94816700	-4.34645000
C	-3.33074000	-1.22388500	-5.61706500
C	-3.05634200	-1.46696100	-4.26957200
C	-1.77463900	-1.84399400	-3.78999900
C	-0.73921500	-2.00343200	-4.69222000
C	0.15621300	-1.79236500	-6.99858400
C	-0.00662600	-1.43146300	-8.32756100
C	-1.27510500	-0.98279600	-8.78633400
C	-2.35979700	-0.92614700	-7.92222200
C	-2.23456400	-1.30805600	-6.55187200
C	-0.93282100	-1.72734400	-6.07924000
C	-4.71301500	-0.83506700	-6.01000600
C	-5.36504400	0.21877300	-5.35070600
C	-6.65662300	0.66677500	-5.74343300
C	-7.32326800	0.04670600	-6.78159300
C	-7.45323400	-1.76542100	-8.47417900
C	-6.91572000	-2.89179400	-9.07794800
C	-5.64992800	-3.37989400	-8.65359600
C	-4.93418800	-2.72645600	-7.66031900
C	-5.44038000	-1.54431800	-7.03712700
C	-6.74799500	-1.07822500	-7.44210200
H	-1.64553500	-1.93677200	-2.71027600
H	0.25645400	-2.29312300	-4.34844500
H	1.13020400	-2.11723700	-6.62446800
H	0.83776000	-1.47777400	-9.01840400
H	-1.39772200	-0.67539800	-9.82707800
H	-3.32323800	-0.57229700	-8.28499500
H	-7.08936200	1.51470800	-5.21195200
H	-8.30908200	0.39724400	-7.09546000
H	-8.43570000	-1.38856800	-8.76952600
H	-7.46595600	-3.41255600	-9.86428400
H	-5.23776500	-4.28360300	-9.10766000
H	-3.97225400	-3.12408000	-7.34082500
C	-5.36937900	0.60514000	-0.44668400
C	-6.71348800	-0.52774500	-2.16404100
C	-5.36567800	-0.69810100	0.36793900

H	-6.21251700	1.24262400	-0.12399500
H	-4.42179200	1.14110100	-0.29304200
C	-6.66584300	-1.80808200	-1.30784500
H	-7.62218300	0.04543300	-1.90708800
H	-6.74661400	-0.78327400	-3.23111100
H	-4.46863300	-1.26728900	0.06270600
H	-5.77091800	-2.38455800	-1.60943600
N	-5.53529900	0.31662500	-1.88568900
O	-6.55607100	-1.46615600	0.08515300
C	-7.92674400	-2.64978900	-1.47772600
H	-8.02753500	-2.97150100	-2.52676900
H	-7.87929300	-3.54425900	-0.83696700
H	-8.81887100	-2.06497400	-1.19919700
C	-5.34923600	-0.43285700	1.86927700
H	-5.36199000	-1.38301400	2.42628200
H	-4.44051000	0.12411400	2.14423500
H	-6.23132000	0.15905000	2.16542600
C	-0.11197900	4.84488500	-6.86497600
H	-1.17947500	5.03356900	-7.04021800
H	0.19738700	3.92077200	-7.37342200
C	0.76131600	6.01908800	-7.17166800
C	0.24442300	7.32901000	-7.08571300
C	2.12319800	5.83325500	-7.48989400
C	1.07208800	8.43433100	-7.33184500
H	-0.80781600	7.47323900	-6.83283700
C	2.94998900	6.93959800	-7.73539300
H	2.52557100	4.82020600	-7.55065300
C	2.42675900	8.24237100	-7.65652800
H	0.66081300	9.44423200	-7.27201900
H	4.00084000	6.78577800	-7.98975000
H	3.07014200	9.10312700	-7.85079900
S	-0.02028100	4.41358100	-5.02735100
O	-0.47671800	5.62911700	-4.23912800
Na	0.84668100	4.70177400	-2.32212000
O	1.40642900	4.01114500	-4.69190400
H	-0.52227300	3.02680700	-1.08230700
H	0.37834000	2.02469200	-2.34561800
C	-2.55449200	3.12105900	-5.35502600
C	-2.89525400	2.32704600	-6.47121700
C	-3.34587400	4.26122200	-5.08145600
C	-3.99849900	2.64697200	-7.27455600
H	-2.32324100	1.43245300	-6.70520600
C	-4.44546200	4.58428700	-5.88751400
H	-3.08427700	4.91886200	-4.25368000

C	-4.78066100	3.77588500	-6.98770000
H	-4.25055200	2.00307500	-8.11929300
H	-5.03905600	5.47170800	-5.65715700
H	-5.64108300	4.02436700	-7.61261200
C	-0.52375700	1.59256900	-4.95537200
H	-0.27948500	1.64047100	-6.02646500
H	0.41249700	1.52733000	-4.38978100
H	-1.10522800	0.68099000	-4.76586100

E-IM4a

C	-0.78393100	-0.01732700	-5.44495000
C	-0.34656200	0.88751900	-4.29269800
H	-0.58532000	-1.07210700	-5.19710200
H	-1.86461300	0.08554600	-5.62183000
C	-0.88714400	2.24595800	-4.20776100
C	-1.58268300	2.90135800	-5.35187600
H	-0.29016000	2.97000900	-3.63869400
C	1.06995000	0.74428500	-3.84422900
C	2.03934500	0.10080300	-4.65867400
C	1.54470900	1.44311400	-2.69732500
C	3.41703100	0.24071800	-4.40050000
H	1.72122400	-0.46119000	-5.53594500
C	2.91468200	1.58762000	-2.44440300
H	0.81653600	1.89120400	-2.02150500
C	3.86623300	1.00878700	-3.31198600
H	4.13762300	-0.24149800	-5.06494000
H	3.24057300	2.14161900	-1.56378800
H	4.93398200	1.12537700	-3.11792500
O	-3.42700500	1.82854600	-1.57504100
H	-2.13307700	2.22709800	-6.01760000
H	-2.21296300	3.75490700	-5.06414900
H	-0.25919900	0.22473200	-6.38678900
C	-4.12914400	2.92874300	-2.07561500
C	-5.29807400	3.23108200	-1.10207600
C	-3.21889200	4.18262300	-2.16818100
C	-4.72227200	2.63314900	-3.47965800
H	-5.96751700	2.35658600	-1.04049800
H	-4.89944200	3.43216700	-0.09315500
H	-5.89232000	4.10572100	-1.42423700
H	-2.35581100	3.95753400	-2.81400300
H	-3.75090800	5.06332100	-2.57460000
H	-2.83741600	4.44240600	-1.16525100
H	-5.28631700	3.49140800	-3.89179600
H	-3.90596900	2.37667900	-4.17430000

H	-5.40247000	1.76688900	-3.41821700
Pd	-1.82920200	0.97512700	-2.77565700
P	-1.76223300	-0.81428000	-1.44355700
O	-1.66394800	-0.37385900	0.19993500
O	-0.31919600	-1.74176400	-1.49189100
C	0.67452600	-0.08870700	0.64145600
C	-0.58065700	0.47522000	0.40709800
C	-0.80805000	1.87436000	0.33477700
C	0.25388700	2.73613500	0.54152600
C	2.68011400	3.11733800	0.91441400
C	3.97189100	2.62956600	1.04983600
C	4.20261300	1.22694700	1.02382900
C	3.14396300	0.33897000	0.89275500
C	1.79864400	0.80341400	0.78556400
C	1.57093900	2.23237800	0.76488800
C	0.78747800	-1.57305500	0.67209000
C	0.26560600	-2.33379900	-0.38658500
C	0.37724000	-3.75091600	-0.41964100
C	0.99305900	-4.42494400	0.61747800
C	2.06995900	-4.40555200	2.85540200
C	2.49669100	-3.71860500	3.98141400
C	2.33811500	-2.30720700	4.04670600
C	1.78434100	-1.60600800	2.98518500
C	1.36171100	-2.27503600	1.79517400
C	1.48563900	-3.71558300	1.75182900
H	-1.81017200	2.20951300	0.05593200
H	0.10585300	3.81802800	0.49839200
H	2.48812500	4.19328000	0.90818300
H	4.81168700	3.31875000	1.16123500
H	5.22236300	0.84379000	1.10049300
H	3.33579600	-0.73250100	0.86316000
H	-0.03126300	-4.27997400	-1.28159100
H	1.09093300	-5.51259600	0.59092700
H	2.16248400	-5.49287500	2.79629600
H	2.93915700	-4.25735200	4.82185500
H	2.64797400	-1.76824000	4.94464800
H	1.65986300	-0.52696100	3.05848400
C	-4.21550100	-1.67276300	-2.17850600
C	-3.26941700	-2.81392000	-0.22417100
C	-5.30257100	-1.07243900	-1.27442700
H	-4.57522800	-2.62248400	-2.61402400
H	-3.97109400	-0.97067200	-2.99031600
C	-4.39236800	-2.19804900	0.63627400
H	-3.59281100	-3.80636400	-0.58590600

H	-2.35525100	-2.93307300	0.37154000
H	-4.91569600	-0.10519900	-0.90276300
H	-4.02407600	-1.23202300	1.02949500
N	-2.99587700	-1.95755800	-1.39495900
O	-5.56403400	-1.96268200	-0.16590700
C	-4.79712200	-3.12226700	1.78030600
H	-3.93700100	-3.29747100	2.44634200
H	-5.61251100	-2.67098800	2.36710400
H	-5.14281100	-4.09183000	1.38533300
C	-6.61997500	-0.87366900	-2.01528300
H	-7.38249800	-0.45771100	-1.33784800
H	-6.47561500	-0.17457400	-2.85389500
H	-6.98931200	-1.83384700	-2.41280700
C	-1.08275200	4.59263300	-7.80554100
H	-0.25783100	4.93032700	-8.45088000
H	-1.55844000	5.45668400	-7.32032300
C	-2.06690800	3.69336800	-8.49949700
C	-1.63449700	2.78260000	-9.48469200
C	-3.42345500	3.70644300	-8.11512300
C	-2.54836200	1.89858700	-10.07740900
H	-0.58363900	2.76729200	-9.77880800
C	-4.33640400	2.82184000	-8.70815100
H	-3.75771800	4.40919600	-7.34880300
C	-3.89930400	1.91428200	-9.68866900
H	-2.20630100	1.19708100	-10.84082600
H	-5.38507300	2.84062200	-8.40532800
H	-4.60870400	1.22407300	-10.14952100
S	-0.23351100	3.68129100	-6.42169700
O	0.52530300	4.66692700	-5.56828400
Na	2.21659400	2.82663800	-4.97092000
O	0.63890300	2.59793500	-6.99617800

E-IM4b

Pd	2.68621200	-2.80034400	-11.33828400
P	3.19886200	-1.46748600	-9.61584700
O	4.36350900	-0.29705700	-10.08469800
O	4.14399700	-2.22483000	-8.39984000
C	6.50143000	-1.34853800	-9.78056800
C	5.49827400	-0.87975900	-10.63143300
C	5.58218500	-0.97740500	-12.04439700
C	6.69405400	-1.56191100	-12.62313800
C	8.82582000	-2.81633100	-12.39465600
C	9.78366900	-3.43069600	-11.60220100
C	9.66943400	-3.37536900	-10.18618200

C	8.61904900	-2.69414700	-9.58687500
C	7.62517600	-2.03396200	-10.37003800
C	7.72523400	-2.12216700	-11.81084800
C	6.33251500	-1.17089500	-8.31160300
C	5.15135800	-1.59883700	-7.68805500
C	4.95590000	-1.48480500	-6.28434400
C	5.93371400	-0.91504600	-5.49176800
C	8.12087700	0.23951000	-5.27115100
C	9.26022900	0.78301100	-5.84409300
C	9.44101400	0.71392800	-7.25248100
C	8.50090500	0.08790200	-8.05870700
C	7.32794700	-0.50889600	-7.50188300
C	7.13022900	-0.40142300	-6.07295400
H	4.75780500	-0.58891100	-12.64001300
H	6.78046800	-1.63405200	-13.70977300
H	8.88747500	-2.86736400	-13.48469900
H	10.61735400	-3.96602800	-12.06122100
H	10.41186600	-3.87845900	-9.56300100
H	8.53834800	-2.66829200	-8.50118300
H	4.02272300	-1.85827400	-5.86097100
H	5.79325500	-0.83205400	-4.41169700
H	7.95374500	0.30121400	-4.19296000
H	10.01046800	1.27444300	-5.22120300
H	10.32577400	1.16433500	-7.70751800
H	8.65232100	0.05540300	-9.13641300
C	0.74173400	-0.38154700	-9.27463900
C	2.52701500	0.67096900	-7.95297400
C	0.54387400	0.95299100	-10.00842200
H	0.05483200	-0.43444700	-8.41008800
H	0.53674000	-1.20625100	-9.97037300
C	2.27727900	1.98212100	-8.72481700
H	1.91979000	0.67349000	-7.03004800
H	3.58642100	0.59022000	-7.68031500
H	1.20663000	0.93654400	-10.89313200
H	2.93168500	1.97643600	-9.61818400
N	2.12706400	-0.48893800	-8.77270700
O	0.90577800	2.05748800	-9.14964300
C	2.56319700	3.20733000	-7.86208700
H	3.62010900	3.21156700	-7.55053000
H	2.35743700	4.13022500	-8.42679300
H	1.92853700	3.19842900	-6.96064200
C	-0.90451300	1.15613700	-10.43590500
H	-1.02310700	2.12503400	-10.94644400
H	-1.19797700	0.35331300	-11.12869400

H	-1.57313900	1.13710000	-9.55901600
C	5.22118500	-4.45733200	-10.80265800
C	3.73414000	-4.63818700	-11.09092600
H	5.36170800	-4.07494700	-9.78384700
H	5.80114100	-5.39888900	-10.89072900
O	1.32350100	-1.39283200	-12.22554500
C	3.22367300	-4.55370100	-12.46020800
C	4.08208200	-4.28711400	-13.65482400
H	2.34474300	-5.15642000	-12.70783300
C	3.00337500	-5.55443100	-10.15091400
C	1.60520100	-5.79026500	-10.27904200
C	3.69673500	-6.30235900	-9.15952700
C	0.94348700	-6.71619900	-9.46606600
H	1.03889500	-5.20740100	-11.00672100
C	3.02703300	-7.23590500	-8.34471800
H	4.76604500	-6.14692500	-9.00881300
C	1.65007800	-7.45214300	-8.49341200
H	-0.13280700	-6.86035800	-9.58512000
H	3.59182300	-7.78611700	-7.58845800
H	1.12988200	-8.17138300	-7.85783600
H	4.94530700	-3.63241000	-13.47909900
H	3.50157500	-3.93170600	-14.51764200
H	5.66526300	-3.73732800	-11.49430200
C	1.18193700	-1.31025500	-13.61202000
C	0.16149400	-0.18481100	-13.92779800
C	2.53310800	-0.95702500	-14.28748600
C	0.65518200	-2.64031900	-14.21223600
H	-0.81325900	-0.42211900	-13.46926800
H	0.51605300	0.77180900	-13.50913200
H	0.01205000	-0.05829200	-15.01550500
H	3.27207300	-1.73572600	-14.04169300
H	2.45257000	-0.87294900	-15.38760500
H	2.90399500	0.00349500	-13.89038900
H	0.54968300	-2.59769500	-15.31237900
H	1.34999400	-3.45241300	-13.94887900
H	-0.33068300	-2.87890900	-13.77632400
C	5.46036000	-5.64695500	-15.98612600
H	6.16755700	-4.80968500	-15.88864900
H	4.57538500	-5.32665300	-16.55491100
C	6.09263700	-6.89610700	-16.52436800
C	7.46491300	-7.14342500	-16.31577600
C	5.30727300	-7.85662300	-17.19435900
C	8.04728700	-8.33035500	-16.78474100
H	8.07050100	-6.40123500	-15.79196000

C	5.89138400	-9.04304600	-17.66228800
H	4.24367500	-7.66642900	-17.35048300
C	7.26167400	-9.28225700	-17.45786300
H	9.11226100	-8.51172900	-16.62623500
H	5.27883500	-9.77900300	-18.18703900
H	7.71598200	-10.20501100	-17.82453300
S	4.82890700	-5.92144100	-14.25568200
O	5.97719600	-6.29464900	-13.35619900
Na	4.23262300	-7.23332000	-11.74492300
O	3.72335200	-6.94303100	-14.27499800

(R)-IM5

C	-1.25183100	1.17786300	-2.56897700
C	-2.45351700	1.67512000	-3.19993800
C	-2.47017100	2.95127100	-4.01108200
H	-3.23386000	0.96719500	-3.49806800
O	-2.04344600	2.03729000	0.93072100
C	-0.73256700	1.72845500	1.30435900
C	-0.61059100	1.93756000	2.83692100
C	-0.38644200	0.25359000	0.97207600
C	0.29286800	2.65042400	0.59181100
H	-0.84965200	2.98420300	3.09191200
H	-1.32496800	1.28127400	3.36249000
H	0.40692900	1.71274800	3.20481500
H	-0.49933100	0.09584100	-0.11287800
H	0.64499600	-0.01443400	1.26771300
H	-1.08571300	-0.42105800	1.49585100
H	1.33479300	2.44082000	0.89841800
H	0.20904000	2.51010600	-0.49863300
H	0.06559000	3.70568800	0.82321800
Pd	-2.65013300	1.92099700	-1.11447700
P	-4.85519800	2.03602300	-0.72814000
O	-5.42632200	0.41575700	-0.41355500
O	-5.81224400	2.31259600	-2.10564300
C	-5.25935700	-0.56222700	-2.60040600
C	-4.81405300	-0.46785700	-1.27736100
C	-3.71481500	-1.22504200	-0.78541500
C	-3.03556700	-2.08745700	-1.62221800
C	-2.62912000	-2.98067900	-3.90893800
C	-2.89157900	-2.96629700	-5.27613000
C	-3.91417500	-2.11516100	-5.78777600
C	-4.68540100	-1.34058600	-4.92702800
C	-4.46941300	-1.35534600	-3.51428100
C	-3.37680500	-2.16083600	-3.00574100

C	-6.51086800	0.13410400	-3.00341000
C	-6.73425700	1.48887400	-2.70522200
C	-7.92486000	2.15654400	-3.11170300
C	-8.90621500	1.48380300	-3.80764400
C	-9.80762200	-0.62383300	-4.75291800
C	-9.71066500	-1.99058100	-4.96414700
C	-8.57141000	-2.69096700	-4.48600600
C	-7.54049200	-2.01866200	-3.84339600
C	-7.58115800	-0.60307200	-3.64744400
C	-8.77107400	0.09209200	-4.08517400
H	-3.43371900	-1.10541100	0.25989000
H	-2.20394900	-2.68799400	-1.24910200
H	-1.82741700	-3.60117600	-3.50239700
H	-2.30618100	-3.58705000	-5.95633000
H	-4.09393300	-2.06985700	-6.86302500
H	-5.47021800	-0.70182200	-5.32814400
H	-8.01767700	3.21706300	-2.87824200
H	-9.80826100	2.00431600	-4.13695300
H	-10.68962600	-0.06876100	-5.08175000
H	-10.51160200	-2.53009700	-5.47347000
H	-8.50734300	-3.77368900	-4.61359700
H	-6.69392100	-2.58882300	-3.46593800
C	-4.95076900	3.40594900	1.59440200
C	-7.14881800	2.78664800	0.66624900
C	-5.27351800	2.54304600	2.82563100
H	-5.25471900	4.44946600	1.79450100
H	-3.87009000	3.35836500	1.38822600
C	-7.40357400	1.93619200	1.92613500
H	-7.57090900	3.79540000	0.82417100
H	-7.63521200	2.33254900	-0.20747300
H	-4.90778600	1.51675500	2.62386900
H	-7.02057700	0.91581200	1.73151800
N	-5.70250800	2.92194200	0.41674200
O	-6.69823100	2.49420700	3.04927900
C	-8.88494900	1.89140000	2.28701100
H	-9.45875800	1.42822000	1.46830100
H	-9.03853700	1.30165100	3.20427100
H	-9.26891500	2.91092900	2.45570600
C	-4.62692200	3.09791400	4.09003700
H	-4.89481700	2.48030100	4.96170400
H	-3.53152400	3.09832900	3.97815100
H	-4.96669800	4.13078100	4.27277900
C	-1.81670400	3.84700600	-6.91936300
H	-1.57153200	4.80238800	-6.43508100

H	-2.90250100	3.75693600	-7.04514600
C	-1.05692100	3.61429700	-8.19057200
C	0.24088600	4.14016500	-8.35490000
C	-1.61831100	2.82466100	-9.21496800
C	0.96065300	3.89083000	-9.53294900
H	0.67969300	4.74334500	-7.55808600
C	-0.89801300	2.57593500	-10.39283100
H	-2.62252400	2.41609700	-9.08501400
C	0.39333100	3.10816900	-10.55371400
H	1.96296800	4.30675400	-9.65459700
H	-1.34386000	1.96998300	-11.18444200
H	0.95363300	2.91616900	-11.47122500
S	-1.36049200	2.54842700	-5.64808300
O	0.09331100	2.67165200	-5.33307700
Na	-1.89329600	-0.48223000	-4.67172100
O	-1.81464200	1.22152400	-6.21892700
H	-1.14306400	0.09849900	-2.39132700
H	-0.30589100	1.70794800	-2.69766600
C	-3.84076400	3.30688000	-4.56291200
C	-4.35755300	4.61564100	-4.47138400
C	-4.61287700	2.33257800	-5.23485100
C	-5.60299800	4.93867300	-5.03350200
H	-3.79683500	5.39196700	-3.95285300
C	-5.84900300	2.65490200	-5.80632100
H	-4.23418500	1.31818200	-5.33736100
C	-6.35113000	3.96315800	-5.70997200
H	-5.98430300	5.95798000	-4.94268200
H	-6.42485400	1.88130200	-6.31775000
H	-7.31802300	4.21555700	-6.14992600
C	-1.70870600	4.11421400	-3.36466900
H	-0.70910700	3.79610400	-3.04890300
H	-1.60853300	4.97200600	-4.04758800
H	-2.26846100	4.43043400	-2.47130900

(S)-IM5

C	-0.57126200	2.54008300	-2.01817900
C	-1.52431600	2.99794100	-3.01165700
C	-1.32875000	2.86002200	-4.49639100
H	-2.16588600	3.83537500	-2.72436500
O	-2.11708400	-0.49112800	-0.77036500
C	-1.21308100	-0.49837800	0.29595700
C	-1.49181800	-1.76797800	1.14338900
C	0.25264300	-0.54514100	-0.20865100
C	-1.39049000	0.74914000	1.20007500

H	-2.52339200	-1.74061400	1.53168700
H	-1.38389300	-2.66782500	0.51403100
H	-0.79754200	-1.85396800	1.99903000
H	0.45040600	0.34448500	-0.82727600
H	0.98514700	-0.57284800	0.61979500
H	0.40240000	-1.44130400	-0.83541900
H	-0.68752000	0.75614500	2.05416300
H	-1.22879500	1.65720400	0.59609400
H	-2.41929800	0.77987600	1.59569100
Pd	-2.22632900	1.20498900	-2.10873100
P	-4.16626600	0.36227100	-2.86732700
O	-4.06028600	-1.27349900	-3.34623200
O	-4.75401500	0.97837000	-4.34364300
C	-3.31292100	-1.18077800	-5.62259800
C	-3.03911400	-1.42955700	-4.27574100
C	-1.75612300	-1.80368400	-3.79692600
C	-0.71839900	-1.95072200	-4.69862100
C	0.17995000	-1.71639700	-7.00184700
C	0.01704900	-1.34722400	-8.32860600
C	-1.25404900	-0.90534500	-8.78684800
C	-2.34072600	-0.86318000	-7.92433900
C	-2.21510000	-1.25303000	-6.55625700
C	-0.91123300	-1.66620000	-6.08403900
C	-4.69661600	-0.79650000	-6.01484300
C	-5.35347300	0.25117500	-5.35035500
C	-6.64719100	0.69470400	-5.74179000
C	-7.31064300	0.07661500	-6.78312800
C	-7.43074000	-1.72711500	-8.48559300
C	-6.88703800	-2.84720200	-9.09555500
C	-5.61881300	-3.33095100	-8.67348400
C	-4.90706700	-2.67942600	-7.67605700
C	-5.41975900	-1.50358900	-7.04626000
C	-6.72956900	-1.04196400	-7.44941000
H	-1.62849500	-1.90123000	-2.71721500
H	0.27854300	-2.23661200	-4.35520700
H	1.15568000	-2.03662900	-6.62818700
H	0.86316000	-1.38230600	-9.01804800
H	-1.37719100	-0.59190100	-9.82575000
H	-3.30632900	-0.51448200	-8.28637400
H	-7.08391800	1.53817600	-5.20653200
H	-8.29816200	0.42381100	-7.09546500
H	-8.41510000	-1.35383300	-8.77925400
H	-7.43425200	-3.36642600	-9.88502300
H	-5.20161200	-4.22980600	-9.13258700

H	-3.94312900	-3.07364900	-7.35834200
C	-5.37559500	0.60855300	-0.44882500
C	-6.70191200	-0.52348000	-2.17874200
C	-5.36147600	-0.70041400	0.35658700
H	-6.22650300	1.23498200	-0.12449500
H	-4.43435800	1.15368500	-0.28788200
C	-6.64662500	-1.80968400	-1.33170400
H	-7.61686900	0.03970600	-1.92133300
H	-6.72886200	-0.77200300	-3.24760400
H	-4.45749800	-1.25800800	0.05016800
H	-5.74639500	-2.37677100	-1.63486500
N	-5.53263300	0.32940600	-1.89034900
O	-6.54380000	-1.47774800	0.06424300
C	-7.90023200	-2.66021200	-1.51163700
H	-7.99622300	-2.97343800	-2.56371100
H	-7.84688700	-3.55994000	-0.87871500
H	-8.79772100	-2.08519800	-1.22986400
C	-5.35317200	-0.44660300	1.85995100
H	-5.35689500	-1.40113200	2.40962800
H	-4.45188000	0.11855300	2.14255000
H	-6.24299500	0.13284800	2.15771900
C	-0.13030200	4.71031200	-6.81482300
H	-1.19496100	4.87647400	-7.02489700
H	0.19976500	3.76337900	-7.26476600
C	0.73837500	5.87643400	-7.17183900
C	0.20996400	7.18394800	-7.15096700
C	2.10126100	5.68437100	-7.47921300
C	1.02981500	8.28233800	-7.44859100
H	-0.84395100	7.33109500	-6.90709700
C	2.91998100	6.78400100	-7.77705400
H	2.51075400	4.67240200	-7.49041500
C	2.38642300	8.08475000	-7.76148200
H	0.61100000	9.29077500	-7.43851600
H	3.97226800	6.62628500	-8.02255100
H	3.02355800	8.94005700	-7.99598200
S	-0.06743800	4.39295100	-4.96524300
O	-0.55411200	5.63013900	-4.24396600
Na	0.74532200	4.78533600	-2.24804000
O	1.34387200	4.00609900	-4.57891200
H	-0.54722000	3.05188500	-1.04402200
H	0.37533500	2.07300100	-2.30880600
C	-2.55858900	3.16250500	-5.33521000
C	-2.88854900	2.37070300	-6.45509600
C	-3.37796000	4.27626700	-5.04194500

C	-4.00732500	2.66874000	-7.24550800
H	-2.29451700	1.49575000	-6.70677800
C	-4.49510500	4.57648900	-5.83323900
H	-3.12995000	4.93055200	-4.20768900
C	-4.81780600	3.77193800	-6.93925400
H	-4.24866800	2.02732300	-8.09515500
H	-5.11190300	5.44323800	-5.58579100
H	-5.69104900	4.00260900	-7.55311900
C	-0.53848900	1.62482200	-4.93161200
H	-0.26452100	1.66086000	-5.99604900
H	0.37754700	1.51693400	-4.34089600
H	-1.16996500	0.74494900	-4.75677300

IM6a-exo

C	-0.79952400	-0.95481300	-5.09364700
C	-0.13115600	0.22518500	-4.40721700
H	-1.11465300	-1.69053300	-4.34043500
H	-1.67447800	-0.64782200	-5.68002400
C	-0.26683500	1.55814100	-4.90199600
C	-1.41726400	2.03228500	-5.56884800
H	0.44999400	2.30417700	-4.54987000
C	0.98193900	-0.06685300	-3.46484400
C	1.62185600	-1.32739600	-3.45935600
C	1.42697000	0.90807300	-2.53847900
C	2.68273100	-1.59340700	-2.58117700
H	1.29548000	-2.10556900	-4.14894900
C	2.48345800	0.64292800	-1.66099600
H	0.90520500	1.86425700	-2.47797600
C	3.12154300	-0.61068400	-1.67973400
H	3.16357700	-2.57395200	-2.60008600
H	2.79670500	1.40771700	-0.94701900
H	3.94133700	-0.82160500	-0.98982500
H	-2.05409100	1.38342000	-6.17275900
H	-1.49204900	3.09917200	-5.77619800
H	-0.08376700	-1.44566300	-5.77793000
Pd	-1.97787900	1.35310300	-3.50913400
P	-3.81606200	2.67880900	-3.38525000
O	-5.15221700	2.05109300	-4.15936600
O	-3.54427400	4.06318800	-4.33891900
C	-4.86114600	2.67055100	-6.46375100
C	-4.85452700	1.68346200	-5.47927400
C	-4.53465900	0.32743700	-5.72896100
C	-4.20523900	-0.05522000	-7.01676600
C	-3.73299300	0.53007900	-9.38357100

C	-3.60979600	1.47621300	-10.38882800
C	-3.88263200	2.84399300	-10.11162200
C	-4.29354200	3.24215000	-8.84785600
C	-4.45279700	2.29262500	-7.79383600
C	-4.13967700	0.90634500	-8.06865900
C	-5.23060500	4.06491800	-6.08801500
C	-4.56596400	4.70427400	-5.03408500
C	-4.83706800	6.04855600	-4.66823300
C	-5.81129200	6.76101000	-5.34117800
C	-7.62175300	6.85652400	-7.03804300
C	-8.39138900	6.24313700	-8.01428200
C	-8.14507400	4.88568600	-8.35713800
C	-7.12779300	4.17150000	-7.74033000
C	-6.29821300	4.77743900	-6.74808500
C	-6.57487000	6.14760900	-6.37732600
H	-4.54695100	-0.37929500	-4.90245100
H	-3.96314800	-1.09691400	-7.23663600
H	-3.50884000	-0.52179700	-9.57574000
H	-3.29252100	1.17714200	-11.38977600
H	-3.76292800	3.59006500	-10.89977600
H	-4.49262700	4.29379700	-8.64793000
H	-4.26117600	6.49414400	-3.85650800
H	-6.02176600	7.79863600	-5.07373500
H	-7.80874200	7.89346000	-6.74871600
H	-9.19237200	6.79380700	-8.51140300
H	-8.76623000	4.39638400	-9.11021900
H	-6.95978800	3.12993200	-8.00936400
C	-3.63752000	3.48934900	-0.82118200
C	-5.77507100	3.97221800	-1.94336100
C	-4.40985100	3.35336300	0.50021900
H	-3.27788200	4.53101100	-0.91841000
H	-2.77923200	2.80356600	-0.81782800
C	-6.47708600	3.81573200	-0.58411500
H	-5.52388200	5.03656000	-2.09849600
H	-6.43867000	3.63886500	-2.75037300
H	-4.72377900	2.29746200	0.61418300
H	-6.76321800	2.75108100	-0.46352900
N	-4.53845300	3.15414300	-1.95077900
O	-5.58640400	4.18261800	0.48284600
C	-7.70805300	4.71154300	-0.49026500
H	-8.43696400	4.43507200	-1.26836700
H	-8.18350400	4.60070600	0.49640700
H	-7.42427900	5.76718700	-0.62921500
C	-3.55267700	3.77603100	1.68777300

H	-4.13124300	3.69724300	2.62107000
H	-2.67054700	3.12116400	1.75923700
H	-3.21535600	4.81826000	1.56761000
C	-3.82169600	-0.27770600	-1.03808000
H	-4.24421000	0.69197500	-0.74689300
H	-3.70196600	-0.90786500	-0.14118100
C	-4.66965300	-0.93966400	-2.09271900
C	-5.91641900	-0.37385000	-2.43081900
C	-4.27591800	-2.13659600	-2.73182100
C	-6.76021200	-0.99138900	-3.36645200
H	-6.22122300	0.55804100	-1.95252400
C	-5.11288000	-2.74770400	-3.67870900
H	-3.31159900	-2.57743200	-2.48134800
C	-6.36075900	-2.18167900	-3.99561200
H	-7.72176400	-0.53564500	-3.61256800
H	-4.79228900	-3.67171100	-4.16561500
H	-7.01140900	-2.66080000	-4.73043200
S	-2.03252300	0.06997900	-1.51474700
O	-1.42714300	-1.30695600	-1.68547900
O	-1.50964200	0.87170300	-0.33574700

IM6b-endo

Pd	0.34310800	-3.29363500	-13.94258800
P	-1.58486800	-2.48249500	-14.84415100
O	-2.49473200	-3.72853300	-15.48152100
O	-1.22048500	-1.62263000	-16.26784400
C	-1.60969400	-4.06605700	-17.69066800
C	-1.75455600	-4.51063200	-16.37759700
C	-1.16951400	-5.70073300	-15.88270900
C	-0.40075600	-6.47280700	-16.73437900
C	0.68859200	-6.81131100	-18.94024400
C	0.96738700	-6.37450200	-20.22591200
C	0.40939500	-5.15421100	-20.69627700
C	-0.43110400	-4.40206900	-19.88825400
C	-0.75766200	-4.83153800	-18.56674200
C	-0.16039100	-6.05611000	-18.07746100
C	-2.28248700	-2.80197000	-18.10446900
C	-2.07117200	-1.62860900	-17.37018100
C	-2.64284000	-0.38451100	-17.74304400
C	-3.46764600	-0.31201400	-18.84951000
C	-4.67593000	-1.42842600	-20.71016500
C	-5.01136900	-2.57620000	-21.41160900
C	-4.46652300	-3.82883500	-21.01756600
C	-3.58395700	-3.91422500	-19.95036800

C	-3.19644300	-2.74983700	-19.21957000
C	-3.77987600	-1.48269800	-19.60169200
H	-1.33646700	-5.97527000	-14.84339000
H	0.05776900	-7.39777900	-16.37856700
H	1.12459800	-7.73739500	-18.55831100
H	1.62321200	-6.95833100	-20.87475100
H	0.64817900	-4.80226300	-21.70190300
H	-0.84650600	-3.46586800	-20.25778200
H	-2.41204600	0.49600200	-17.14257200
H	-3.90630900	0.64156200	-19.15072600
H	-5.09992800	-0.46034400	-20.98735900
H	-5.70078100	-2.52389500	-22.25658800
H	-4.74892800	-4.73547900	-21.55669700
H	-3.18360700	-4.88319400	-19.65624800
C	-2.39918200	-0.59485600	-13.09725500
C	-4.12635000	-1.41311000	-14.64433500
C	-3.49848000	-0.38328800	-12.04506700
H	-2.25827600	0.34645700	-13.66123200
H	-1.46312200	-0.87146600	-12.59382900
C	-5.16961100	-1.18700600	-13.53751100
H	-4.06967500	-0.50671800	-15.27299300
H	-4.41824800	-2.26569900	-15.26830500
H	-3.59466200	-1.31236200	-11.45022200
H	-5.24513900	-2.11642400	-12.93725600
N	-2.80687900	-1.68188500	-14.02088400
O	-4.76157500	-0.10907600	-12.67928800
C	-6.52874300	-0.82269100	-14.12694200
H	-6.90096000	-1.64618900	-14.75664400
H	-7.25481800	-0.63693700	-13.32056900
H	-6.44654000	0.08635700	-14.74434000
C	-3.17030300	0.79150300	-11.13048000
H	-3.98055900	0.94279300	-10.40061500
H	-2.23487400	0.58878300	-10.58631300
H	-3.04847900	1.71513300	-11.71929000
C	3.30054900	-2.93583000	-13.27733500
C	2.52165700	-4.14298400	-13.77676600
H	3.13453500	-2.78878200	-12.20047400
H	4.38258000	-3.09769300	-13.43330300
C	1.99477400	-4.20150100	-15.10420600
C	1.52473400	-3.08249200	-15.82265100
H	1.72168000	-5.18284500	-15.49691500
C	2.67752500	-5.42224300	-13.03699500
C	1.76712800	-6.48877700	-13.23598600
C	3.72858200	-5.61157000	-12.11163400

C	1.91841300	-7.70475800	-12.56280900
H	0.90583800	-6.33907200	-13.88713500
C	3.87980700	-6.83046200	-11.43298200
H	4.44002000	-4.80732000	-11.92387700
C	2.97976300	-7.88443500	-11.65681500
H	1.19233900	-8.50403900	-12.72567400
H	4.70276900	-6.95344900	-10.72546900
H	3.09436600	-8.82996500	-11.12247100
H	1.92631500	-2.07574600	-15.67719700
H	1.00730700	-3.25890600	-16.76434800
H	3.01522200	-2.01676600	-13.80587400
C	-1.92340500	-3.99128900	-11.38224500
H	-2.56210400	-3.16973400	-11.72907500
H	-2.00011600	-4.08097200	-10.28599100
C	-2.26220200	-5.27418400	-12.09499900
C	-3.38751000	-5.31972000	-12.94373900
C	-1.48881400	-6.44468000	-11.93243000
C	-3.74794500	-6.50631300	-13.60049600
H	-3.97895700	-4.41429200	-13.08858000
C	-1.84038000	-7.62788100	-12.60043100
H	-0.60599100	-6.41317500	-11.29497900
C	-2.97361200	-7.66602000	-13.43242400
H	-4.62351500	-6.52019500	-14.25325300
H	-1.22864800	-8.52289200	-12.46637800
H	-3.24606300	-8.58886100	-13.94929600
S	-0.15288200	-3.40006100	-11.62514200
O	0.68119400	-4.37853300	-10.83089600
O	-0.15796100	-1.97964900	-11.08087500

IM6a^{3-exo}

Pd	0.97661100	-5.46774000	-14.21853100
P	-0.56694100	-3.88903400	-14.72470500
O	-0.50707200	-3.52650700	-16.37664100
O	-0.14347300	-2.37821900	-14.10051700
C	1.24107600	-1.87898300	-16.55498300
C	0.78581500	-3.17839000	-16.78160600
C	1.58219800	-4.18591200	-17.37835900
C	2.88127100	-3.89068800	-17.74813300
C	4.79942500	-2.31399100	-17.79450300
C	5.35307700	-1.08144100	-17.48579000
C	4.55954000	-0.08913500	-16.84720900
C	3.22695600	-0.33248400	-16.54734000
C	2.61709300	-1.58250400	-16.86902000
C	3.43638800	-2.60297100	-17.48728100

C	0.30838700	-0.88157100	-15.96129900
C	-0.36238200	-1.17575800	-14.76904700
C	-1.23419900	-0.25205500	-14.13551100
C	-1.46306200	0.98208600	-14.71408400
C	-1.13342700	2.57387000	-16.59107600
C	-0.58334200	2.88429000	-17.82493700
C	0.25414500	1.94136200	-18.48106000
C	0.54646700	0.72041100	-17.89039100
C	0.02094900	0.37687600	-16.60745700
C	-0.86062700	1.32351200	-15.96045600
H	1.16071800	-5.17984000	-17.51786000
H	3.50937900	-4.65467500	-18.21049600
H	5.40052100	-3.09383000	-18.26810500
H	6.39906200	-0.87397600	-17.71988300
H	5.00425500	0.87303100	-16.58513100
H	2.63312100	0.43408700	-16.05187500
H	-1.70641400	-0.54050500	-13.19593100
H	-2.12475400	1.70494000	-14.23227000
H	-1.79537600	3.27813700	-16.08156100
H	-0.80089300	3.84293000	-18.30002600
H	0.66754000	2.17630300	-19.46406600
H	1.18085100	0.00661300	-18.41317700
C	-2.77075600	-5.34809700	-14.01619000
C	-3.20605900	-3.16857100	-15.07520400
C	-3.49005600	-6.02570100	-15.19396400
H	-3.49761700	-5.13922400	-13.21221800
H	-1.97618600	-6.00378500	-13.64209900
C	-3.91126200	-3.91042100	-16.22685000
H	-3.94785200	-2.90051100	-14.30369500
H	-2.73209700	-2.25150500	-15.44574500
H	-2.72669100	-6.24279800	-15.96575200
H	-3.14851300	-4.14241200	-16.99561800
N	-2.19646300	-4.05479500	-14.45185900
O	-4.48431900	-5.13772800	-15.74879200
C	-5.03747500	-3.07375500	-16.82624100
H	-4.63217000	-2.13969400	-17.24702700
H	-5.54217800	-3.63367700	-17.62880000
H	-5.78084700	-2.82136200	-16.05255600
C	-4.19243300	-7.30760500	-14.76568900
H	-4.73768200	-7.74359700	-15.61819900
H	-3.44349000	-8.02931900	-14.40448400
H	-4.91486400	-7.09844100	-13.95899800
C	3.61224200	-6.60260500	-15.30585600
C	3.08392600	-6.53854100	-13.88370100

H	4.68375500	-6.87241200	-15.28804300
H	3.08558900	-7.37474700	-15.88124500
C	2.91630700	-5.30536800	-13.19872400
C	2.58815100	-4.09099200	-13.86799300
H	2.81179300	-5.32657500	-12.11153800
C	3.04709500	-7.80705300	-13.11290700
C	3.70269500	-8.96652500	-13.59108500
C	2.31364000	-7.91236300	-11.90424700
C	3.64507000	-10.17401400	-12.87881100
H	4.25923200	-8.93085300	-14.52650400
C	2.26085300	-9.11424200	-11.19138600
H	1.73696600	-7.05720300	-11.54901400
C	2.92808900	-10.25470400	-11.67484900
H	4.16106600	-11.05363000	-13.26996400
H	1.67729000	-9.16937500	-10.27010000
H	2.87666100	-11.19680300	-11.12524100
H	2.35693800	-3.21880300	-13.25415100
H	2.95850800	-3.86190500	-14.87144300
H	3.50881600	-5.64536800	-15.82714600
C	-0.21144700	-9.43412800	-16.04260800
H	-1.17740900	-9.09223700	-16.44298300
H	-0.25625500	-10.50845500	-15.80859900
C	0.94803500	-9.08543800	-16.91680800
C	0.89909000	-7.96895000	-17.78069700
C	2.14969900	-9.82472900	-16.84327800
C	2.00691100	-7.61988200	-18.56790100
H	-0.01775300	-7.37935700	-17.83218700
C	3.26051200	-9.47587600	-17.62807900
H	2.20539500	-10.68235100	-16.16858900
C	3.19285800	-8.37280500	-18.49674800
H	1.94424100	-6.75954700	-19.23793700
H	4.17793900	-10.06534600	-17.56150400
H	4.05394800	-8.10286100	-19.11197700
S	-0.09334700	-8.56985000	-14.33178700
O	-1.35402100	-9.02809300	-13.60862400
O	-0.28440200	-7.07126600	-14.87968800

IM6b'-endo

Pd	2.06686700	-4.59815000	-15.24318100
P	0.29194200	-3.36691800	-15.83259200
O	0.15971500	-2.84336100	-17.42677600
O	0.40326500	-1.87672900	-15.02660900
C	0.48899500	-0.43916700	-17.44843400
C	0.83701200	-1.71925300	-17.88948600

C	1.81930700	-1.93928900	-18.88938000
C	2.51142000	-0.86727000	-19.42016800
C	3.02456500	1.56276000	-19.44271300
C	2.81576700	2.84198200	-18.95154300
C	1.84597100	3.05842900	-17.93470600
C	1.08780300	2.00610800	-17.44206600
C	1.25981800	0.67828000	-17.93901200
C	2.27135600	0.45656700	-18.94860900
C	-0.63210100	-0.25876100	-16.48353900
C	-0.62139100	-0.96256000	-15.27879900
C	-1.61344300	-0.79577500	-14.27989200
C	-2.66681100	0.07006700	-14.50759200
C	-3.90583900	1.60022200	-16.02057700
C	-4.04168200	2.23388600	-17.24592000
C	-3.05685400	2.04306900	-18.25356600
C	-1.94696300	1.24463500	-18.01788800
C	-1.76322300	0.59270900	-16.76079500
C	-2.78397800	0.76173400	-15.74952900
H	2.01075800	-2.96140700	-19.21492100
H	3.26584600	-1.02423700	-20.19385000
H	3.77826300	1.37510800	-20.21109600
H	3.40092000	3.68101700	-19.33316000
H	1.69941100	4.06254800	-17.53158500
H	0.35743100	2.18869900	-16.65561300
H	-1.52578300	-1.36244800	-13.35242900
H	-3.43864300	0.21455800	-13.74882900
H	-4.66248300	1.72159700	-15.24188700
H	-4.90747600	2.86865100	-17.44451600
H	-3.17737600	2.52502600	-19.22590400
H	-1.20671900	1.10113200	-18.80329900
C	-1.54648600	-4.97501800	-14.63800900
C	-2.47806200	-3.43112200	-16.30437800
C	-2.45587100	-6.07297200	-15.20357500
H	-2.07020100	-4.46579300	-13.80736300
H	-0.61283400	-5.42091900	-14.26303400
C	-3.36752500	-4.57880100	-16.81481400
H	-3.02858900	-2.86044200	-15.53699100
H	-2.21736200	-2.75941300	-17.12890200
H	-1.90795000	-6.58127400	-16.02228200
H	-2.81456900	-5.11251600	-17.61496900
N	-1.24799500	-3.99362800	-15.70208400
O	-3.66035800	-5.50409700	-15.75404300
C	-4.69575000	-4.04994500	-17.34784100
H	-4.52024600	-3.37112100	-18.19754100

H	-5.32935400	-4.88453200	-17.68592300
H	-5.23124500	-3.49788900	-16.55863600
C	-2.84408900	-7.07891500	-14.12607800
H	-3.49059100	-7.86395800	-14.54909200
H	-1.93634600	-7.54378200	-13.70769400
H	-3.39076900	-6.57440600	-13.31253500
C	4.51557600	-4.00723200	-13.38768900
C	4.55302600	-4.95928100	-14.56939700
H	5.50954400	-3.97675000	-12.90988700
H	4.22851100	-2.99127100	-13.68378500
C	4.21628300	-4.56186000	-15.87515400
C	3.50023100	-3.36131200	-16.20293100
H	4.33119400	-5.29303600	-16.67760200
C	5.11466100	-6.30830700	-14.32458200
C	5.02015700	-6.89952700	-13.04032300
C	5.77813700	-7.03679900	-15.34398300
C	5.53398800	-8.17892700	-12.79539700
H	4.51427200	-6.36781900	-12.23532600
C	6.29788100	-8.31316000	-15.09597100
H	5.91233800	-6.59481200	-16.33064600
C	6.17096200	-8.89521000	-13.82276700
H	5.43086100	-8.61928600	-11.80173700
H	6.81105200	-8.85008900	-15.89643700
H	6.57330700	-9.89200000	-13.63112800
H	3.61536200	-2.45013800	-15.60711200
H	3.32124300	-3.17965500	-17.26289100
H	3.79755500	-4.34990400	-12.62615400
C	0.85791200	-8.08881000	-15.59569600
H	-0.20487800	-7.81256400	-15.56044200
H	0.95577100	-9.18497900	-15.56542300
C	1.57640200	-7.48956800	-16.75616300
C	0.98999100	-6.44772200	-17.51029500
C	2.87546500	-7.92297200	-17.10781500
C	1.66786200	-5.87342900	-18.59737000
H	-0.01088500	-6.10463800	-17.24477900
C	3.55916300	-7.34117900	-18.18531100
H	3.34609400	-8.72228100	-16.53162400
C	2.95713700	-6.31499100	-18.93763400
H	1.18480100	-5.08342600	-19.17412300
H	4.56068100	-7.69270100	-18.44324300
H	3.48611800	-5.87102400	-19.78400500
S	1.53572700	-7.57651000	-13.85677600
O	0.54214000	-8.25842600	-12.92768100
O	1.23543600	-6.00068300	-13.83187800

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Pd	1.69202400	-4.54581000	-14.97874800
P	-0.08532300	-3.22495800	-15.55542200
O	-0.85711900	-3.41444600	-17.04567800
O	0.37933600	-1.61182000	-15.68066600
C	-0.27442500	-1.51278200	-18.42794600
C	-0.26324900	-2.89050200	-18.19267600
C	0.27073300	-3.81965900	-19.11992600
C	0.83889200	-3.36480200	-20.29554900
C	1.59356700	-1.48630000	-21.73072300
C	1.74169500	-0.12661000	-21.95480800
C	1.23451800	0.80453400	-21.00694500
C	0.57572900	0.36778800	-19.86709000
C	0.38836600	-1.02439900	-19.61176400
C	0.93330500	-1.96818500	-20.56148700
C	-0.91938900	-0.59855100	-17.44487900
C	-0.54985300	-0.66477600	-16.09963500
C	-1.06569100	0.21485400	-15.11493000
C	-2.00329700	1.16467600	-15.47446100
C	-3.49849700	2.17252000	-17.18091900
C	-3.99876200	2.21097000	-18.47297100
C	-3.50464000	1.30267500	-19.44893200
C	-2.50864000	0.39125900	-19.12957700
C	-1.95151300	0.33889400	-17.81559900
C	-2.48354600	1.23894100	-16.81517400
H	0.20864000	-4.88247800	-18.89103600
H	1.24250000	-4.07152300	-21.02352400
H	1.99235900	-2.21614500	-22.43915200
H	2.25482400	0.23170700	-22.84943300
H	1.37249300	1.87495500	-21.17283500
H	0.21038000	1.09348600	-19.14283800
H	-0.70944200	0.11758400	-14.08898100
H	-2.40673300	1.85483100	-14.73053800
H	-3.88017900	2.85019900	-16.41354900
H	-4.77886200	2.92645200	-18.74038000
H	-3.91711600	1.31763000	-20.45984900
H	-2.14880500	-0.30398600	-19.88611400
C	-1.38876000	-4.08364300	-13.29739800
C	-2.75463900	-2.78040600	-14.86699600
C	-2.44479100	-5.19938000	-13.35640600
H	-1.62651000	-3.39803300	-12.46368600
H	-0.39602400	-4.52220500	-13.14213000
C	-3.78652600	-3.92365200	-14.85906100
H	-3.02445900	-2.03999500	-14.09394700

H	-2.74765800	-2.28729800	-15.84473300
H	-2.17236600	-5.86903000	-14.19110100
H	-3.52059100	-4.62443000	-15.67577100
N	-1.41212200	-3.31624300	-14.55840500
O	-3.74750900	-4.62782300	-13.60670500
C	-5.20359000	-3.39156800	-15.04899500
H	-5.28709500	-2.87537800	-16.01869900
H	-5.92878300	-4.21965100	-15.02430500
H	-5.45461700	-2.67928200	-14.24605400
C	-2.51563300	-5.98477300	-12.05294900
H	-3.34611000	-6.70694300	-12.09416900
H	-1.57834900	-6.54313500	-11.91137100
H	-2.67781800	-5.31085000	-11.19501800
C	3.58645300	-5.33147600	-14.09337500
C	3.84670100	-4.25863400	-14.96418200
C	3.26637000	-2.95353400	-14.77795300
H	4.30847100	-4.48961700	-15.92691300
C	1.39018100	-8.47540700	-15.78324900
H	0.40924400	-8.54342700	-16.27710800
H	1.73044800	-9.47720000	-15.47987900
C	2.40432900	-7.74314700	-16.59426800
C	2.01280500	-6.70041500	-17.46425800
C	3.78242600	-8.02100600	-16.45722800
C	2.96731400	-5.97648900	-18.19299200
H	0.95220200	-6.47003700	-17.56580900
C	4.74114300	-7.28630500	-17.17297900
H	4.09880800	-8.82452300	-15.78696000
C	4.33661100	-6.26206600	-18.04741800
H	2.64205500	-5.18306600	-18.86783700
H	5.80205900	-7.51897700	-17.05534200
H	5.07926400	-5.69545400	-18.61336300
S	0.94528300	-7.58386100	-14.12824800
O	-0.22074600	-8.40990700	-13.61297900
O	0.36551500	-6.21424900	-14.74389900
H	3.91160400	-6.32648300	-14.39289100
H	3.36939800	-5.19127900	-13.03074100
C	3.38351200	-1.97568400	-15.90136100
C	3.35807400	-2.41382700	-17.24705300
C	3.51517400	-0.59110700	-15.65606200
C	3.48401900	-1.50784300	-18.30378600
H	3.19922300	-3.47035300	-17.45996600
C	3.63408700	0.32030800	-16.71704000
H	3.52751500	-0.21677400	-14.63282100
C	3.62299400	-0.13214400	-18.04480500

H	3.44648200	-1.86800000	-19.33207900
H	3.73358400	1.38641600	-16.50113300
H	3.70315400	0.57547700	-18.87152700
C	3.07186300	-2.37988200	-13.37982000
H	3.97252600	-1.81033900	-13.08729000
H	2.21600500	-1.69081200	-13.35950700
H	2.90887800	-3.16651400	-12.63302000

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Pd	-0.19498800	-6.98846700	-14.15053600
P	-0.58890000	-5.08838500	-15.19991900
O	0.11269200	-4.89545400	-16.70193800
O	0.03080400	-3.72061500	-14.41641300
C	2.05329200	-3.49916200	-16.40295000
C	1.50778500	-4.75518900	-16.66604900
C	2.28725500	-5.90923500	-16.91632600
C	3.66554000	-5.80225700	-16.91453000
C	5.71921200	-4.45781100	-16.57337500
C	6.33633300	-3.26758800	-16.22411800
C	5.54620900	-2.12865700	-15.90989000
C	4.16116900	-2.18720500	-15.97173600
C	3.49116400	-3.38878400	-16.35381800
C	4.29785100	-4.55669300	-16.63234900
C	1.14200500	-2.36223700	-16.09517600
C	0.17407400	-2.50939600	-15.09514200
C	-0.66454100	-1.44424000	-14.67872600
C	-0.56876700	-0.21416600	-15.30149800
C	0.39768200	1.22752600	-17.07774100
C	1.24698000	1.39979200	-18.15969200
C	2.06360900	0.32069700	-18.59589400
C	2.03733200	-0.89971700	-17.93636100
C	1.19311800	-1.10627800	-16.80330800
C	0.33720000	-0.01811800	-16.38505700
H	1.77749100	-6.85320300	-17.10140500
H	4.28896900	-6.67804000	-17.10183900
H	6.30868000	-5.35250600	-16.78258900
H	7.42499700	-3.20739700	-16.16953500
H	6.03262700	-1.19865000	-15.60840100
H	3.57216600	-1.30995600	-15.71132700
H	-1.37240700	-1.62267000	-13.86871900
H	-1.20276500	0.61688300	-14.98554700
H	-0.25000300	2.04037400	-16.74073800
H	1.28250800	2.35619300	-18.68505100
H	2.71495500	0.45101200	-19.46252800

H	2.66350400	-1.71894100	-18.28655900
C	-3.24370600	-5.29566800	-14.70867200
C	-2.62696000	-3.67129700	-16.45236500
C	-4.50466900	-5.63373200	-15.52128000
H	-3.49533200	-4.51663800	-13.96449600
H	-2.88647200	-6.19224100	-14.17877000
C	-3.89991800	-4.07133500	-17.21691600
H	-2.85151400	-2.79904800	-15.81350300
H	-1.83068600	-3.40267100	-17.15636200
H	-4.26243500	-6.46501400	-16.21229500
H	-3.64966500	-4.91635400	-17.88955900
N	-2.18371200	-4.80766800	-15.61593900
O	-4.92081100	-4.49499900	-16.29525600
C	-4.45789100	-2.89810400	-18.01580900
H	-3.72212500	-2.56780900	-18.76594700
H	-5.38309900	-3.19547500	-18.53290200
H	-4.68352300	-2.05304300	-17.34551200
C	-5.66323600	-6.02458100	-14.60992700
H	-6.56134000	-6.24167500	-15.20818800
H	-5.39933300	-6.92204400	-14.02811500
H	-5.89368100	-5.20436200	-13.91110700
C	3.08007700	-4.10321300	-12.90837500
C	3.20141300	-5.60947600	-12.98095600
H	3.52385600	-3.73150800	-11.96621100
H	3.62857500	-3.62430700	-13.73109900
C	2.15490700	-6.45397900	-12.69142300
C	0.76339700	-6.10520800	-12.45726200
H	2.36731800	-7.52291400	-12.63604400
C	4.52894500	-6.16817700	-13.31914700
C	5.71177900	-5.41484300	-13.11125100
C	4.66302600	-7.45507300	-13.90625100
C	6.97050000	-5.93159800	-13.44845400
H	5.64572800	-4.41729700	-12.67633400
C	5.92005400	-7.96877100	-14.24524600
H	3.76961800	-8.04093500	-14.12727900
C	7.08375800	-7.21128400	-14.01627500
H	7.86449600	-5.32954900	-13.27116300
H	5.99156900	-8.95820700	-14.70269500
H	8.06365700	-7.61090900	-14.28623900
H	0.26447400	-6.70680500	-11.68590500
H	0.51442300	-5.04366900	-12.39817800
H	2.03772000	-3.76828500	-12.94313700
C	-0.05860900	-10.66978400	-14.98914700
H	-0.98590600	-10.97760900	-14.48459900

H	0.51453100	-11.55138500	-15.31079400
C	-0.27493600	-9.69454700	-16.08826400
C	-1.33504800	-8.75002800	-16.03225300
C	0.61004000	-9.64263800	-17.18874800
C	-1.51803800	-7.81824300	-17.07371300
H	-2.06468900	-8.81381900	-15.22255300
C	0.41841900	-8.71776300	-18.22553000
H	1.43490300	-10.35753500	-17.23912600
C	-0.64580000	-7.80008700	-18.17096300
H	-2.33600600	-7.10230300	-17.01442000
H	1.10384000	-8.70887800	-19.07593400
H	-0.78822600	-7.07298700	-18.97179000
S	0.97274100	-9.90334100	-13.53853100
O	1.01616900	-11.01550800	-12.51087600
O	-0.09467100	-8.79670900	-13.07385300

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C	1.53835400	1.27354300	-3.19511700
C	1.18708300	2.08408800	-4.28997400
C	0.27245700	1.64142300	-5.30907500
H	1.46278400	3.14080900	-4.25768800
Pd	-0.64558900	1.69491100	-3.18759400
P	-2.88237700	2.02145500	-3.67237600
O	-3.65470900	0.94471700	-4.71596600
O	-3.04894100	3.46841000	-4.52256700
C	-4.27239800	2.17161400	-6.72732900
C	-3.66678000	1.07901200	-6.09880600
C	-3.14608000	-0.01963000	-6.83052100
C	-3.14999500	0.00478300	-8.21165100
C	-3.54982300	1.22887700	-10.33406600
C	-3.97294700	2.36460200	-11.00684000
C	-4.49289500	3.46633900	-10.27328300
C	-4.60088800	3.41007800	-8.89166700
C	-4.18748300	2.25211800	-8.16605300
C	-3.63239800	1.14701800	-8.91238800
C	-4.98691700	3.20984500	-5.93296000
C	-4.33867800	3.85388000	-4.87965700
C	-4.93182700	4.90359400	-4.13420200
C	-6.22599700	5.29448200	-4.42130200
C	-8.34094100	4.96880500	-5.67873500
C	-9.08914200	4.28105700	-6.62137800
C	-8.50011500	3.20726400	-7.34297200
C	-7.17499200	2.85359700	-7.13290600
C	-6.36593700	3.55453800	-6.18732300

C	-6.98036500	4.62131200	-5.42728600
H	-2.75649900	-0.87331000	-6.27751700
H	-2.75713500	-0.84023400	-8.78093200
H	-3.13172200	0.37921700	-10.87918500
H	-3.89891000	2.42069300	-12.09470000
H	-4.80372100	4.36991500	-10.80173900
H	-4.98666400	4.26837500	-8.34416400
H	-4.35019800	5.37718500	-3.34267300
H	-6.69731100	6.10502300	-3.86157300
H	-8.78307600	5.78355300	-5.10040400
H	-10.13132400	4.55179800	-6.80188100
H	-9.09787100	2.64972400	-8.06702400
H	-6.74410200	2.02222300	-7.68806200
C	-3.68413700	2.36892400	-1.08654500
C	-5.49196600	1.82469900	-2.64617500
C	-4.30871600	1.39639900	-0.07731000
H	-4.08948800	3.38233300	-0.90619800
H	-2.59261800	2.37549300	-0.95797700
C	-6.07013400	0.87031700	-1.58606500
H	-5.95397500	2.81968200	-2.52650300
H	-5.71432400	1.44852700	-3.64995800
H	-3.87946500	0.39121200	-0.26159500
H	-5.62450100	-0.13251800	-1.74863200
N	-4.02851000	1.93912300	-2.45713200
O	-5.73589400	1.31817800	-0.26082100
C	-7.59115100	0.79890500	-1.68074700
H	-7.89119900	0.41287400	-2.66791400
H	-7.99042500	0.13078800	-0.90196800
H	-8.03004100	1.80060800	-1.54479600
C	-4.02837200	1.83043400	1.35692200
H	-4.49697300	1.13145200	2.06745700
H	-2.94076200	1.84747400	1.53341500
H	-4.43325400	2.83973900	1.53752100
C	-0.81896600	-0.44496500	-0.03695500
H	-1.83185500	-0.13793500	0.25900800
H	-0.35293300	-1.02436600	0.77448400
C	-0.78572100	-1.16756900	-1.33888400
C	0.33900500	-1.94133700	-1.70663600
C	-1.85942000	-1.06855100	-2.25337000
C	0.37673000	-2.61839800	-2.93466600
H	1.17819400	-2.02509100	-1.01131100
C	-1.82840800	-1.75625700	-3.47777100
H	-2.73471400	-0.47614500	-1.98451300
C	-0.71330500	-2.53699800	-3.82119200

H	1.24994800	-3.22087800	-3.19537800
H	-2.67995300	-1.68089600	-4.15513600
H	-0.68888700	-3.07387600	-4.77183100
S	0.17103600	1.21101700	-0.00949200
O	-0.13042600	1.73484200	1.38509400
O	-0.67348100	2.08306000	-1.05636400
H	2.11433800	1.71705100	-2.38231100
H	1.52999000	0.18142500	-3.23896500
C	-0.24285300	2.65934800	-6.26848000
C	-0.44467500	4.00207600	-5.86646600
C	-0.54123000	2.31594500	-7.60746400
C	-0.90933500	4.96431100	-6.76789600
H	-0.29137900	4.27205600	-4.82129900
C	-1.01193800	3.27947900	-8.51081800
H	-0.41123700	1.29091400	-7.94971700
C	-1.19577700	4.60766400	-8.09764500
H	-1.07306500	5.98871000	-6.42647100
H	-1.25102200	2.98590900	-9.53381100
H	-1.57844400	5.35222200	-8.79850000
C	0.28527300	0.19300700	-5.76313600
H	-0.69988300	-0.10493300	-6.13780500
H	1.01021200	0.07922400	-6.59001400
H	0.56914400	-0.49030200	-4.95683600

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Pd	0.83809200	-5.67414600	-14.65796200
P	-0.42427700	-4.08556100	-15.52413700
O	-0.27011100	-3.84178000	-17.16706700
O	-0.05316900	-2.52690100	-14.96507200
C	1.15459100	-1.92277300	-17.45965900
C	0.97204200	-3.30307200	-17.53733800
C	1.97189800	-4.20090600	-17.98027500
C	3.19096200	-3.69446400	-18.39389100
C	4.71003400	-1.76892500	-18.76814700
C	4.97835200	-0.41236400	-18.68745600
C	4.00324900	0.47017100	-18.14866600
C	2.76952000	-0.00668600	-17.73052500
C	2.43827300	-1.39034200	-17.84708100
C	3.45216700	-2.29357800	-18.34772100
C	0.05556300	-1.08058800	-16.91049100
C	-0.49602300	-1.40405100	-15.66546200
C	-1.48210900	-0.60296300	-15.03527600
C	-1.96403800	0.52177700	-15.67840900
C	-2.05061600	1.97813300	-17.68902500

C	-1.64069200	2.27434000	-18.97971900
C	-0.67503300	1.45104600	-19.62133200
C	-0.11923700	0.36481200	-18.96107200
C	-0.49907800	0.04398200	-17.62252600
C	-1.50892300	0.86091800	-16.98663200
H	1.75166100	-5.26754600	-17.99094100
H	3.97608600	-4.36481300	-18.74950500
H	5.46209900	-2.46565200	-19.14468800
H	5.94528700	-0.02270000	-19.01114900
H	4.22935600	1.53433600	-18.05439600
H	2.03857000	0.68166700	-17.31021300
H	-1.84216800	-0.89723900	-14.04899800
H	-2.71853500	1.15116100	-15.20181800
H	-2.80598500	2.58871000	-17.18861700
H	-2.06527200	3.12935600	-19.50951800
H	-0.37144200	1.67182100	-20.64670100
H	0.61357500	-0.26188400	-19.46716900
C	-2.63334700	-5.06391400	-14.28924400
C	-3.07163600	-3.45732200	-16.10504800
C	-3.87805000	-5.84969300	-14.73522000
H	-2.92432800	-4.35831700	-13.48852300
H	-1.87090300	-5.75456500	-13.89654000
C	-4.29278800	-4.30373000	-16.50186200
H	-3.39677600	-2.65947800	-15.41448100
H	-2.62433100	-2.99876200	-16.99476700
H	-3.56631400	-6.60566700	-15.48203000
H	-3.96058900	-5.06908700	-17.23179400
N	-2.07483200	-4.32207400	-15.43882500
O	-4.83554300	-4.96590000	-15.34500300
C	-5.39703000	-3.43874100	-17.10026900
H	-5.03369100	-2.94160300	-18.01348700
H	-6.26930900	-4.05920700	-17.35714600
H	-5.71237100	-2.66774900	-16.37886100
C	-4.55960200	-6.52645200	-13.55066000
H	-5.45903000	-7.06501500	-13.88622800
H	-3.87065100	-7.24547900	-13.07962000
H	-4.85586000	-5.77564700	-12.80052400
C	4.68162100	-5.27308000	-13.34238000
C	4.15511400	-4.00303800	-13.97452000
H	5.15535300	-5.91802300	-14.09972100
H	5.46012600	-5.04226400	-12.59396400
C	2.82621200	-3.65493200	-13.93605800
C	1.75047600	-4.36158500	-13.25096100
H	2.51344500	-2.76491200	-14.48398500

C	5.14039500	-3.11313500	-14.63599700
C	6.35935700	-3.62344500	-15.15154500
C	4.91907300	-1.71456000	-14.74655300
C	7.29781000	-2.78237000	-15.76690800
H	6.57182100	-4.69066800	-15.08753500
C	5.86019000	-0.87523100	-15.35190200
H	4.01295800	-1.27843800	-14.32458900
C	7.05583700	-1.40336500	-15.86959900
H	8.22171500	-3.20853000	-16.16462600
H	5.66031000	0.19568400	-15.41746300
H	7.78952100	-0.74696400	-16.34223800
H	2.04492600	-5.07602700	-12.47381700
H	0.93939100	-3.70076000	-12.92370300
H	3.88958300	-5.86262300	-12.86891500
C	1.71991300	-9.24771900	-15.51734100
H	1.09811600	-9.69278200	-14.72715900
H	2.36778400	-10.00972600	-15.97455100
C	0.94682200	-8.47444800	-16.52305900
C	-0.27222500	-7.83486100	-16.17786300
C	1.44982600	-8.29718600	-17.83212500
C	-0.97695000	-7.07694500	-17.13356100
H	-0.70080700	-8.00294300	-15.18766900
C	0.74060200	-7.54721000	-18.78145800
H	2.39189100	-8.77739200	-18.10735200
C	-0.47624700	-6.93319600	-18.43484900
H	-1.90845500	-6.59054300	-16.85030800
H	1.13968500	-7.43718200	-19.79222300
H	-1.02324600	-6.34036200	-19.16964500
S	2.92496200	-8.09257300	-14.54089600
O	3.64216700	-9.03196900	-13.59344000
O	1.81609600	-7.27105500	-13.71194400

E-TS5a

Pd	1.52455600	-4.56086000	-14.96886500
P	-0.07854900	-3.21536400	-15.65406100
O	-0.72444900	-3.28185900	-17.23433300
O	0.38191200	-1.58787700	-15.61792600
C	-0.15301400	-1.21966600	-18.37491100
C	-0.14045900	-2.61677700	-18.30142200
C	0.36544400	-3.42283200	-19.35488500
C	0.91762500	-2.83037600	-20.47391400
C	1.71879400	-0.79428700	-21.64797500
C	1.89542000	0.58036400	-21.68964800
C	1.40212200	1.38770700	-20.62774200

C	0.73039400	0.81601600	-19.55728900
C	0.52134700	-0.59452100	-19.48612900
C	1.04553900	-1.41372600	-20.55410700
C	-0.85014700	-0.42042300	-17.32917000
C	-0.54528500	-0.61981900	-15.98106000
C	-1.14068100	0.13485700	-14.93808200
C	-2.08813200	1.09332900	-15.24447600
C	-3.52121900	2.24533900	-16.91128900
C	-3.95595900	2.41337000	-18.21657200
C	-3.38721400	1.62696200	-19.25547600
C	-2.38300700	0.70939100	-18.98248700
C	-1.88971300	0.52762700	-17.65400600
C	-2.49955500	1.30149100	-16.59383200
H	0.29547200	-4.50495800	-19.26113900
H	1.29884000	-3.44316000	-21.29380500
H	2.10641100	-1.43156300	-22.44662300
H	2.41937800	1.04363100	-22.52812900
H	1.56048100	2.46793500	-20.65071600
H	0.37067700	1.44476000	-18.74416800
H	-0.83549900	-0.06219600	-13.91004600
H	-2.55172600	1.68745200	-14.45402300
H	-3.96102900	2.82580900	-16.09671500
H	-4.74141900	3.13580900	-18.44727100
H	-3.74822300	1.74086400	-20.27977900
H	-1.96738300	0.10960400	-19.79012000
C	-1.68386300	-4.31378400	-13.73353700
C	-2.84701500	-2.87277300	-15.32177100
C	-2.52457300	-5.50154700	-14.22773800
H	-2.20022500	-3.83232800	-12.88424100
H	-0.69833600	-4.66343700	-13.39839000
C	-3.68209800	-4.08762300	-15.76841000
H	-3.37375800	-2.34583900	-14.50738300
H	-2.71312700	-2.18349400	-16.16138700
H	-1.97862300	-5.96659200	-15.07577200
H	-3.15130000	-4.56745900	-16.61423700
N	-1.53358000	-3.31601600	-14.80894000
O	-3.80614300	-5.04209600	-14.69669600
C	-5.09046400	-3.67693700	-16.18543100
H	-5.04150400	-2.97474600	-17.03297300
H	-5.67440800	-4.55967200	-16.48926700
H	-5.60869400	-3.18330600	-15.34723300
C	-2.76634600	-6.52754500	-13.12668700
H	-3.39123400	-7.35349900	-13.50086500
H	-1.80290000	-6.93574500	-12.78250800

H	-3.27825600	-6.05875400	-12.27056800
C	4.40818800	-5.21276100	-13.69297700
C	3.95764400	-4.51457300	-14.81366700
C	3.27987600	-3.23553300	-14.81650600
H	4.21424200	-4.94476200	-15.78310200
C	2.44726200	-8.22921100	-14.29047900
H	1.53640400	-8.76430500	-13.98337400
H	3.32740300	-8.87346100	-14.15442900
C	2.35361600	-7.65061500	-15.65942300
C	1.12463700	-7.12943000	-16.13574900
C	3.49422800	-7.55879300	-16.48817200
C	1.04279200	-6.54745500	-17.41475200
H	0.23145400	-7.21702800	-15.51617900
C	3.41031100	-6.97634700	-17.76030400
H	4.44658700	-7.95433100	-16.12735700
C	2.18417500	-6.46701000	-18.22778800
H	0.08638600	-6.15365300	-17.75960600
H	4.30034200	-6.92025000	-18.39083400
H	2.12168500	-6.00868500	-19.21619400
S	2.60532300	-6.89852500	-12.90052500
O	2.58593900	-7.70541000	-11.62280500
O	1.35482100	-6.01893200	-13.13612300
H	5.10342200	-6.04091900	-13.83254200
H	4.38063800	-4.76575400	-12.69876500
C	3.41679400	-2.40632400	-16.05616500
C	3.41517900	-3.00523800	-17.34054400
C	3.56236200	-1.00219700	-15.98290900
C	3.57866700	-2.23621800	-18.49565400
H	3.23764900	-4.07702400	-17.43308400
C	3.71005000	-0.22923200	-17.14466300
H	3.55777000	-0.50380800	-15.01426700
C	3.72333800	-0.84034000	-18.40722200
H	3.55806400	-2.72139000	-19.47167200
H	3.80868600	0.85530200	-17.05972800
H	3.81819400	-0.23970200	-19.31292100
C	3.11974100	-2.48445800	-13.49950600
H	4.05084300	-1.94323100	-13.24765100
H	2.30675400	-1.75101900	-13.58025600
H	2.88558800	-3.17337500	-12.67765300

E-TS5b

C	2.03919900	1.32659300	-3.20537500
C	1.18921000	2.20554300	-3.90408000
C	0.19838800	1.83511800	-4.88512500

H	1.37649900	3.27100900	-3.76008100
Pd	-1.04125400	1.88113600	-3.06107500
P	-3.16131200	2.06514800	-3.63434100
O	-4.02466200	0.98957100	-4.62826100
O	-3.40997200	3.50137000	-4.50965500
C	-4.37758400	2.07429700	-6.76275900
C	-3.84083800	1.03008000	-6.00383000
C	-3.16931500	-0.07112600	-6.59357200
C	-2.96487500	-0.09962200	-7.96048800
C	-3.09745000	1.01683000	-10.17422500
C	-3.46515000	2.10073400	-10.95653400
C	-4.13828800	3.20395300	-10.36283100
C	-4.44719100	3.20021400	-9.01079200
C	-4.09676100	2.09539900	-8.17700500
C	-3.38886600	0.98794500	-8.77810900
C	-5.18912100	3.13217800	-6.09952100
C	-4.66690100	3.81978300	-5.00126900
C	-5.35947900	4.88424000	-4.36730000
C	-6.61693000	5.24553000	-4.81164500
C	-8.56652900	4.85360200	-6.29868200
C	-9.19087100	4.12914000	-7.30221100
C	-8.50958400	3.04231700	-7.91518200
C	-7.21641600	2.71154700	-7.53618800
C	-6.53202300	3.45012900	-6.52325800
C	-7.24255600	4.53192600	-5.87639600
H	-2.82233400	-0.87442500	-5.94380000
H	-2.44919000	-0.94215000	-8.42632300
H	-2.56614900	0.16787700	-10.61123100
H	-3.23147500	2.11489600	-12.02300300
H	-4.40725900	4.06716900	-10.97508800
H	-4.94700600	4.05958400	-8.56693600
H	-4.87739600	5.39485500	-3.53282900
H	-7.15813500	6.06698200	-4.33716500
H	-9.08199700	5.67988300	-5.80331400
H	-10.20642300	4.38151500	-7.61383400
H	-9.01052600	2.45653400	-8.68879800
H	-6.71414800	1.86922500	-8.00876600
C	-3.78414000	2.26305900	-0.97623600
C	-5.71876800	2.06376300	-2.46024800
C	-4.45623400	1.26682400	-0.01753600
H	-4.05106900	3.29228700	-0.66974000
H	-2.69223900	2.14839100	-0.91847500
C	-6.34711000	1.08070900	-1.45644100
H	-6.07130900	3.08549100	-2.23151400

H	-6.02385900	1.80243100	-3.47934000
H	-4.14368500	0.24512900	-0.31391200
H	-6.03020600	0.05566900	-1.73746800
N	-4.24781700	2.01115000	-2.35115700
O	-5.88843900	1.35935800	-0.12088500
C	-7.86874600	1.18676800	-1.45173100
H	-8.26721400	0.93918400	-2.44840600
H	-8.29834900	0.49068600	-0.71470800
H	-8.17892800	2.21179200	-1.19165300
C	-4.07245200	1.53783300	1.43309500
H	-4.58120000	0.82731600	2.10285200
H	-2.98343600	1.42774900	1.55956800
H	-4.35935000	2.56198200	1.72177100
C	0.54282300	-0.71390800	-0.53832400
H	-0.01896400	-0.58709900	0.39939200
H	1.45284800	-1.30129400	-0.35207900
C	-0.28727400	-1.27763500	-1.64448000
C	0.27374400	-2.18591300	-2.56921800
C	-1.64269700	-0.90620500	-1.79434500
C	-0.50639400	-2.73226000	-3.59948500
H	1.32185500	-2.47613300	-2.46185900
C	-2.42234900	-1.44909100	-2.82798000
H	-2.08479500	-0.20425900	-1.08802000
C	-1.85811300	-2.36632900	-3.72950100
H	-0.06113000	-3.44317800	-4.29881200
H	-3.46384100	-1.14416800	-2.93221000
H	-2.46776800	-2.79482700	-4.52781700
S	1.18872200	1.06119900	-0.85474900
O	2.04271300	1.36702400	0.35003700
O	-0.11021000	1.89684900	-0.95596300
H	2.95476800	1.72824900	-2.76917200
H	2.04234000	0.25692300	-3.42060000
C	-0.26643800	2.88038100	-5.85014800
C	-0.42000800	4.23196900	-5.45257100
C	-0.59177700	2.54354500	-7.18453400
C	-0.87926700	5.20118800	-6.34864600
H	-0.22798200	4.50768000	-4.41492600
C	-1.05945500	3.51444700	-8.08253000
H	-0.49210400	1.51562700	-7.52794100
C	-1.20690400	4.84715300	-7.67088800
H	-1.00464500	6.23209300	-6.00992500
H	-1.32402500	3.22090200	-9.09942600
H	-1.58596000	5.59903100	-8.36626900
C	0.16713100	0.38821600	-5.35967100

H	-0.78920100	0.15612700	-5.83949700
H	0.97363300	0.21223700	-6.09599900
H	0.30583300	-0.30613100	-4.52250900

(R)-TS6

Pd	1.39739600	-4.45440900	-15.02155600
P	-0.33945400	-3.26315100	-15.58325200
O	-0.46670300	-2.81970300	-17.22119500
O	-0.33498500	-1.68580500	-14.90662300
C	0.35799600	-0.56746400	-17.41337200
C	0.50713000	-1.93352100	-17.66539600
C	1.60883000	-2.46812100	-18.37992200
C	2.59046800	-1.61696400	-18.85425400
C	3.55536300	0.66443600	-19.04055200
C	3.51365700	2.01819700	-18.74556700
C	2.43665700	2.54164900	-17.97854500
C	1.41173200	1.71549800	-17.54059800
C	1.40618900	0.32104100	-17.84923900
C	2.52374500	-0.21555800	-18.59644100
C	-0.84416000	-0.10378800	-16.66507300
C	-1.14537000	-0.68846700	-15.42870600
C	-2.25014300	-0.26949300	-14.64093000
C	-3.08771000	0.72725200	-15.10510200
C	-3.76830900	2.30333400	-16.90027600
C	-3.58594500	2.84036800	-18.16527600
C	-2.50107600	2.39704400	-18.97051600
C	-1.60849800	1.44664500	-18.49604500
C	-1.74980000	0.88903100	-17.18843800
C	-2.87546800	1.31649600	-16.38631900
H	1.65765300	-3.54646700	-18.52777000
H	3.44203800	-2.01000700	-19.41439900
H	4.38633100	0.24264600	-19.61119200
H	4.31054200	2.68124700	-19.08844000
H	2.41832300	3.60389000	-17.72610400
H	0.59812300	2.12850800	-16.94626500
H	-2.41403800	-0.75097800	-13.67611700
H	-3.93667800	1.06177600	-14.50484200
H	-4.60735500	2.61898700	-16.27542800
H	-4.27820300	3.59219000	-18.54962500
H	-2.37165000	2.80376100	-19.97569100
H	-0.78826200	1.11089800	-19.12875300
C	-2.12885100	-5.03895600	-14.53615900
C	-3.12553000	-3.34487300	-16.00083000
C	-2.91717400	-6.11965000	-15.29492000

H	-2.71895000	-4.71513800	-13.65812500
H	-1.16692400	-5.44550700	-14.18773000
C	-3.89610100	-4.46880400	-16.71841200
H	-3.75679200	-2.93127200	-15.19352300
H	-2.88404000	-2.54595900	-16.71048500
H	-2.28987600	-6.46864500	-16.14016700
H	-3.26888400	-4.82540700	-17.56055400
N	-1.88566600	-3.89114200	-15.42263800
O	-4.13872200	-5.56779000	-15.82071000
C	-5.25012200	-3.98470900	-17.22711300
H	-5.11053700	-3.16910400	-17.95427200
H	-5.79198500	-4.80834900	-17.71732300
H	-5.86045700	-3.61057900	-16.38912600
C	-3.29031500	-7.28736900	-14.38789300
H	-3.87831200	-8.03301000	-14.94517300
H	-2.37877200	-7.77092300	-14.00143300
H	-3.88987900	-6.93139700	-13.53448500
C	4.56183500	-4.54865800	-12.96933100
C	4.50452300	-5.15968100	-14.36258300
H	4.94071500	-5.25472100	-12.21950900
H	5.23927000	-3.67771600	-12.99105000
C	3.77201600	-4.41053200	-15.36901200
C	3.13211800	-3.16669400	-15.18173200
H	3.82141500	-4.78517200	-16.39148700
C	5.70729400	-5.94377600	-14.80654100
C	6.36138500	-6.82813300	-13.91187200
C	6.24227900	-5.81531400	-16.11200200
C	7.48241300	-7.56623700	-14.31177000
H	5.96713600	-6.96987400	-12.90706500
C	7.36786500	-6.55222700	-16.51005100
H	5.79860500	-5.11775300	-16.82051100
C	7.99179600	-7.43552800	-15.61521500
H	7.95685700	-8.24770300	-13.60265700
H	7.76039400	-6.42603400	-17.52130500
H	8.86727800	-8.00936000	-15.92579700
H	3.23148700	-2.62858300	-14.23349900
H	2.97376400	-2.53431800	-16.05864700
H	3.56463100	-4.20494200	-12.65873300
C	2.94421100	-8.04351900	-15.33236800
H	2.32316400	-8.87074000	-14.95637400
H	3.96851700	-8.40077600	-15.50552700
C	2.35372800	-7.37191600	-16.53208300
C	0.97194200	-7.07731600	-16.58832400
C	3.17064800	-7.02936500	-17.63006600

C	0.42384500	-6.45772100	-17.72334700
H	0.33189600	-7.34766300	-15.74827900
C	2.62082500	-6.41638100	-18.76504600
H	4.23886300	-7.25007600	-17.58581200
C	1.24417000	-6.13058600	-18.81523600
H	-0.64355600	-6.23329500	-17.75273800
H	3.26341400	-6.16581300	-19.61197600
H	0.81384300	-5.65661000	-19.69961600
S	3.08695500	-6.94472100	-13.79252700
O	3.52495000	-7.86836700	-12.68976600
O	1.71032900	-6.29239000	-13.61408500

(S)-TS6

C	1.98626100	1.16793700	-4.76031500
C	1.10757700	2.21615400	-4.28051200
C	0.00816000	2.76231000	-4.98550200
H	1.40339200	2.71921700	-3.35948000
H	-0.18835800	2.46249700	-6.01924500
H	-0.29926900	3.78184700	-4.73799900
Pd	-1.04023900	1.43146500	-3.65736500
P	-3.13302100	2.07155600	-3.57689500
O	-3.51578500	3.73406500	-3.67166900
O	-3.87117900	1.74270600	-2.06642600
C	-3.93629900	4.49526800	-1.42443400
C	-3.14985600	4.51097200	-2.58056700
C	-1.99780900	5.32863100	-2.70640400
C	-1.60169100	6.12316700	-1.64673300
C	-1.86795900	6.84845900	0.71393600
C	-2.53140500	6.77404000	1.92899200
C	-3.66943400	5.93190600	2.06289200
C	-4.13619900	5.19501800	0.98405300
C	-3.48896000	5.25948100	-0.28729100
C	-2.31394500	6.09415100	-0.41212600
C	-5.17348900	3.66644400	-1.40380700
C	-5.09401600	2.30987800	-1.73560500
C	-6.22497500	1.45225700	-1.71425700
C	-7.46503700	1.96197600	-1.37787400
C	-8.91251600	3.89428000	-0.79738200
C	-9.07552500	5.25120600	-0.56544200
C	-7.94986500	6.11773700	-0.62737500
C	-6.68368900	5.61776000	-0.89573100
C	-6.47299200	4.22211000	-1.11579000
C	-7.62666100	3.34904500	-1.08828100
H	-1.45206100	5.32065100	-3.64936600

H	-0.72053000	6.76258000	-1.73290200
H	-0.98233200	7.47815900	0.59868000
H	-2.17749700	7.35095300	2.78575300
H	-4.17771900	5.85848500	3.02651800
H	-5.00382000	4.54756500	1.10320100
H	-6.08659600	0.40056300	-1.96695100
H	-8.34238600	1.31200200	-1.35034700
H	-9.76923100	3.21642400	-0.77300400
H	-10.06509900	5.65836900	-0.34828900
H	-8.08313100	7.18988400	-0.46811800
H	-5.83496800	6.29759000	-0.95103900
C	-3.68912100	0.63223800	-5.82001800
C	-5.47017600	2.15976100	-5.12724400
C	-3.56378800	1.41180900	-7.13890000
H	-4.40423100	-0.19850500	-5.95604300
H	-2.71233400	0.21823500	-5.52738800
C	-5.31670100	2.89731200	-6.47145100
H	-6.23993700	1.37419300	-5.22638400
H	-5.77828700	2.86266400	-4.34549200
H	-2.82312500	2.22336500	-6.98036000
H	-4.57448200	3.70683800	-6.32690200
N	-4.19416600	1.51739600	-4.75601100
O	-4.83179500	1.99857700	-7.48803100
C	-6.64449400	3.46796600	-6.95833300
H	-7.02968600	4.19917000	-6.22987900
H	-6.51320600	3.97074600	-7.92918500
H	-7.38691300	2.66194600	-7.07661800
C	-3.13323200	0.51456600	-8.29406400
H	-3.08249300	1.09107600	-9.23084600
H	-2.13906100	0.08681800	-8.08619700
H	-3.85213700	-0.31026800	-8.42652400
C	1.61548900	-0.50766800	-1.68469000
H	2.70625300	-0.57821400	-1.57602600
H	1.13695900	-1.39292900	-1.23892900
C	1.06614000	0.78245600	-1.16704500
C	-0.32092200	0.94499300	-0.93560200
C	1.92934300	1.87261400	-0.92674400
C	-0.82600400	2.17612400	-0.47534300
H	-0.99582800	0.10038900	-1.08323200
C	1.42426900	3.09517200	-0.46327000
H	2.99847200	1.75418400	-1.11230400
C	0.04383600	3.25169500	-0.23871300
H	-1.89799700	2.28874400	-0.31756600
H	2.10744400	3.92646300	-0.27395600

H	-0.35119500	4.20211300	0.12120300
S	1.30751700	-0.80424600	-3.54257800
O	-0.21926300	-0.77915000	-3.69774000
O	1.97465500	-2.12027700	-3.84471700
C	3.42963700	1.21061900	-4.35971800
C	4.00033800	2.35767900	-3.75455200
C	4.28193700	0.10545100	-4.61107800
C	5.35780000	2.39058500	-3.40219200
H	3.39219300	3.24334000	-3.57688700
C	5.63522500	0.13773000	-4.25381200
H	3.87260400	-0.80243000	-5.05122000
C	6.18240300	1.28080200	-3.64515500
H	5.77043000	3.29164500	-2.94346100
H	6.26273900	-0.73439000	-4.44872100
H	7.23852300	1.30699300	-3.36930300
C	1.66559700	0.57623600	-6.12432300
H	1.91242100	1.32206700	-6.90010300
H	2.24498300	-0.33222100	-6.33325000
H	0.59459100	0.33840500	-6.19999900

E-IM7a

Pd	1.53198400	-4.48594000	-15.53688600
P	-0.27110400	-3.20186500	-15.79637700
O	-1.06478300	-3.12958100	-17.31494800
O	0.09946800	-1.54174400	-15.64380400
C	-0.26896400	-1.13855700	-18.41940100
C	-0.35129600	-2.53231600	-18.34686200
C	0.23147800	-3.37948900	-19.32399000
C	0.93917600	-2.82873700	-20.37617500
C	1.92822500	-0.84422400	-21.49542200
C	2.15909400	0.52220800	-21.54086500
C	1.60376200	1.36688400	-20.54026400
C	0.81445400	0.83981200	-19.52867400
C	0.53838700	-0.55906000	-19.46237500
C	1.13239600	-1.41930700	-20.46086000
C	-0.99655000	-0.31792200	-17.41177000
C	-0.79156000	-0.56234000	-16.04948000
C	-1.43628000	0.19302300	-15.03461600
C	-2.32103600	1.19614800	-15.38286400
C	-3.57396100	2.45336400	-17.11930300
C	-3.90060800	2.67322500	-18.44845600
C	-3.28752700	1.88908400	-19.46377700
C	-2.34794100	0.92024900	-19.14171100
C	-1.96632400	0.68275000	-17.78546500

C	-2.62046800	1.45737900	-16.75260500
H	0.09654500	-4.45563200	-19.22815100
H	1.38451800	-3.46967300	-21.14041700
H	2.36351100	-1.50878400	-22.24588700
H	2.77426100	0.95055300	-22.33493600
H	1.80660200	2.43963900	-20.56374500
H	0.40429300	1.49455600	-18.76109000
H	-1.21456400	-0.03941500	-13.99246000
H	-2.81827000	1.78899500	-14.61192100
H	-4.04935800	3.03300000	-16.32418800
H	-4.63452800	3.43580700	-18.71694900
H	-3.56273800	2.04589000	-20.50895500
H	-1.89711800	0.32250400	-19.93209900
C	-1.58210600	-4.56868400	-13.85105200
C	-2.99571300	-3.03281400	-15.13048200
C	-2.44925000	-5.74052500	-14.33697000
H	-1.98136100	-4.19923400	-12.88931200
H	-0.54419300	-4.89766500	-13.69904600
C	-3.83705900	-4.24153500	-15.58566300
H	-3.43922200	-2.60267800	-14.21485900
H	-2.98401800	-2.26720400	-15.91459100
H	-2.00673400	-6.11772800	-15.28308000
H	-3.39556500	-4.61960800	-16.52914400
N	-1.62023300	-3.46832500	-14.82933900
O	-3.79208600	-5.29091500	-14.59890800
C	-5.30146700	-3.86850800	-15.79046500
H	-5.38738700	-3.09731900	-16.57245700
H	-5.88368100	-4.75132200	-16.09753400
H	-5.72919700	-3.47278700	-14.85489900
C	-2.52875200	-6.85939600	-13.30392000
H	-3.16489100	-7.67955300	-13.67173800
H	-1.52146500	-7.25450300	-13.09681600
H	-2.95490900	-6.47827000	-12.36183500
C	4.07595700	-5.47407900	-13.76224300
C	3.69330500	-4.68108700	-14.98494500
C	3.32657200	-3.30910800	-14.94307200
H	4.13476500	-5.07790600	-15.90213400
C	2.49699900	-7.96724700	-14.10016800
H	1.62469500	-8.46874300	-13.65346000
H	3.38315000	-8.60977600	-14.00677400
C	2.26479900	-7.51495900	-15.50777300
C	1.03285500	-6.90279500	-15.86483400
C	3.28620100	-7.62659700	-16.46725500
C	0.85266500	-6.39192600	-17.17122000

H	0.20132200	-6.91111900	-15.15925600
C	3.10242400	-7.11935200	-17.76522600
H	4.23018900	-8.10046900	-16.19004200
C	1.89846100	-6.49246300	-18.11593900
H	-0.11225100	-5.97686000	-17.46058800
H	3.90386700	-7.21165800	-18.50101500
H	1.76060400	-6.08865600	-19.11969600
S	2.80390200	-6.55672100	-12.90925200
O	3.46584300	-7.13688100	-11.70674700
O	1.52606200	-5.80911300	-12.72354200
H	4.88219800	-6.18683800	-13.98797000
H	4.40193300	-4.84507900	-12.91997000
C	3.59229200	-2.42338200	-16.12771800
C	3.68564600	-2.94502600	-17.44495600
C	3.74987800	-1.02705400	-15.96843900
C	3.91753100	-2.11090400	-18.54230600
H	3.52247100	-4.01024100	-17.61145100
C	3.97920200	-0.18917200	-17.07299600
H	3.68655500	-0.58159100	-14.97615400
C	4.06228500	-0.72210500	-18.36670100
H	3.95923600	-2.54110900	-19.54452200
H	4.08437500	0.88695000	-16.91542200
H	4.21373700	-0.07011200	-19.22825500
C	3.11166100	-2.62331400	-13.59861300
H	4.05198100	-2.16849900	-13.23210400
H	2.36272200	-1.82367300	-13.68697200
H	2.75218300	-3.33917900	-12.84898600

E-IM7b

C	1.82108800	1.07860500	-3.00405700
C	0.96865800	2.03250500	-3.78990600
C	0.33345900	1.74287000	-5.01718200
H	1.17828300	3.08002200	-3.55920200
Pd	-1.22058000	1.83035100	-3.34572200
P	-3.40539600	2.05034900	-3.59839300
O	-4.31201900	1.01237200	-4.59515300
O	-3.76654600	3.53036700	-4.38643100
C	-4.48023900	2.10590600	-6.73860100
C	-3.97926600	1.07106800	-5.94433600
C	-3.15702400	0.03885600	-6.45980400
C	-2.81346700	0.04342700	-7.79917000
C	-2.81853000	1.16224100	-10.01528600
C	-3.17102500	2.23183000	-10.82403500
C	-3.94639100	3.29664000	-10.28799100

C	-4.37747300	3.26464200	-8.96983800
C	-4.05533100	2.16763400	-8.11482000
C	-3.23232000	1.10651600	-8.65124400
C	-5.39191300	3.11306100	-6.12852700
C	-4.99635700	3.78476900	-4.96550500
C	-5.79456700	4.79590100	-4.36645400
C	-7.02099600	5.12120400	-4.91292700
C	-8.80169400	4.71630900	-6.59521300
C	-9.29679900	4.00990900	-7.68049800
C	-8.51744700	2.97174000	-8.26021200
C	-7.25591800	2.67142400	-7.76611100
C	-6.70106200	3.39545200	-6.66666100
C	-7.51312500	4.42591900	-6.05667600
H	-2.80598300	-0.73236000	-5.77493900
H	-2.18771900	-0.75011800	-8.21351500
H	-2.20403600	0.34664700	-10.40452300
H	-2.84434400	2.26632300	-11.86538800
H	-4.19999300	4.15194400	-10.91776000
H	-4.96078100	4.09233600	-8.56941800
H	-5.41193100	5.30033800	-3.47835600
H	-7.63804700	5.90319100	-4.46493200
H	-9.39410000	5.50482600	-6.12444200
H	-10.28565200	4.23903900	-8.08298100
H	-8.91727500	2.39936600	-9.09999800
H	-6.67759300	1.86631300	-8.21638900
C	-3.81542100	2.18098200	-0.91968300
C	-5.87244100	2.01933800	-2.24031400
C	-4.42119100	1.19742000	0.09434000
H	-4.03146600	3.21466100	-0.58713300
H	-2.72389200	2.04895500	-0.97147800
C	-6.43212300	1.04785500	-1.18498300
H	-6.19415000	3.04677100	-1.98819400
H	-6.25958000	1.75896900	-3.23259500
H	-4.15402200	0.16964800	-0.22219900
H	-6.15615300	0.01757800	-1.48904500
N	-4.40227600	1.93768000	-2.24658800
O	-5.85648200	1.32005800	0.10634800
C	-7.94583400	1.17755700	-1.04931000
H	-8.43237600	0.93890500	-2.00837000
H	-8.32213800	0.48674000	-0.27888600
H	-8.21607400	2.20673300	-0.76244000
C	-3.92145100	1.46509100	1.50975700
H	-4.38595200	0.76289700	2.21927600
H	-2.82734500	1.34185400	1.55382700

H	-4.17210300	2.49354900	1.81633000
C	0.85406100	-0.69389500	-0.84301600
H	0.56524600	-0.65978400	0.21883300
H	1.76807600	-1.29484900	-0.95121000
C	-0.25371100	-1.18112600	-1.73263800
C	0.02340200	-2.10396800	-2.76212700
C	-1.57845100	-0.73020600	-1.55413300
C	-1.00467800	-2.57792100	-3.59151600
H	1.04798500	-2.45684000	-2.90141500
C	-2.60535600	-1.20161500	-2.38609600
H	-1.80361000	-0.02174200	-0.75787200
C	-2.32206300	-2.12645700	-3.40424000
H	-0.77685900	-3.29755200	-4.38048600
H	-3.61922900	-0.82678500	-2.24855300
H	-3.12414800	-2.49113200	-4.04871000
S	1.40544600	1.05910700	-1.16022300
O	2.66153800	1.26044300	-0.38551800
O	0.24759700	1.96768500	-0.88964500
H	2.88162500	1.37677400	-2.99474800
H	1.74240700	0.03172800	-3.32232700
C	-0.05007300	2.84709700	-5.96131000
C	-0.25460200	4.17958800	-5.51698600
C	-0.24512800	2.58438100	-7.33743700
C	-0.64141200	5.19029300	-6.40147500
H	-0.16691700	4.40964900	-4.45467700
C	-0.64309200	3.59745300	-8.22537400
H	-0.10123000	1.57913300	-7.72917900
C	-0.84565500	4.90509500	-7.76561100
H	-0.80645500	6.20122600	-6.02151000
H	-0.81160600	3.35021300	-9.27478300
H	-1.17075900	5.68943600	-8.45241500
C	0.37455100	0.33537700	-5.59452600
H	-0.52799300	0.13209400	-6.18360300
H	1.24891300	0.22035500	-6.26266600
H	0.43299100	-0.42571600	-4.80857500

(R)-IM8

Pd	1.77132200	-4.36655000	-15.68978900
P	-0.04710200	-3.12130300	-15.95941900
O	-0.42069700	-2.60545900	-17.53471000
O	0.00604400	-1.57658800	-15.20696300
C	0.25268000	-0.30218800	-17.71656900
C	0.44013100	-1.64429400	-18.05625300
C	1.46668200	-2.07888900	-18.93278500

C	2.32566800	-1.14799800	-19.48918000
C	3.12377100	1.19558400	-19.69110600
C	3.04593200	2.53058700	-19.32629100
C	2.05548500	2.95285000	-18.39731200
C	1.14816500	2.04630100	-17.86842900
C	1.17925300	0.66838400	-18.24314000
C	2.21366400	0.23458400	-19.15778400
C	-0.84899300	0.05172700	-16.77816200
C	-0.92507600	-0.60428800	-15.54316700
C	-1.91690100	-0.28833600	-14.57753300
C	-2.86863000	0.67436100	-14.85766200
C	-3.89932100	2.28344800	-16.44542800
C	-3.94052700	2.88616500	-17.69328800
C	-2.96828600	2.54636800	-18.67370800
C	-1.96414700	1.63217300	-18.38902500
C	-1.87534500	1.00930000	-17.10644200
C	-2.88699400	1.33110100	-16.12358900
H	1.55435300	-3.14363500	-19.14754400
H	3.11557200	-1.46331500	-20.17457500
H	3.89280000	0.85083600	-20.38662200
H	3.75047500	3.25596000	-19.73819900
H	2.01180200	4.00025100	-18.09146900
H	0.40166800	2.38229300	-17.15046900
H	-1.90580300	-0.82260200	-13.62679300
H	-3.63316500	0.92900000	-14.12028500
H	-4.64916400	2.51946800	-15.68642800
H	-4.72232200	3.61084400	-17.92957900
H	-3.01505500	3.00477500	-19.66381300
H	-1.23199800	1.37592900	-19.15346100
C	-1.59642100	-4.97655600	-14.70693400
C	-2.86297400	-3.29560300	-15.96664100
C	-2.47205800	-6.06976500	-15.33979600
H	-2.04492900	-4.67491500	-13.74141100
H	-0.58314700	-5.36114000	-14.51954700
C	-3.71458700	-4.43343900	-16.55990700
H	-3.36313100	-2.90479700	-15.06181600
H	-2.75849400	-2.48304000	-16.69454400
H	-1.98869700	-6.39134800	-16.28355900
H	-3.22675100	-4.76878200	-17.49800700
N	-1.53262100	-3.81761500	-15.61140200
O	-3.77815800	-5.54418900	-15.64600900
C	-5.14510300	-3.98142100	-16.83444700
H	-5.14616700	-3.15601100	-17.56404100
H	-5.73886500	-4.81485800	-17.24098700

H	-5.62021400	-3.63143500	-15.90369500
C	-2.65750600	-7.25889500	-14.40362100
H	-3.30237300	-8.01893700	-14.87146500
H	-1.68083100	-7.71328300	-14.17321100
H	-3.12428400	-6.93281600	-13.46004700
C	3.92959900	-5.00841700	-12.88503500
C	4.19506900	-5.77528700	-14.19180900
H	3.94874600	-5.67181900	-12.00980400
H	4.71023600	-4.24359600	-12.75917800
C	3.91168700	-4.93236900	-15.42353000
C	3.75250300	-3.53444000	-15.39757800
H	4.19051400	-5.37775800	-16.37872800
C	5.55394900	-6.47456500	-14.24989700
C	6.35424600	-6.60633100	-13.09346300
C	6.04216500	-7.03264500	-15.45443600
C	7.59614200	-7.25797700	-13.14131000
H	6.01716000	-6.19762900	-12.14272500
C	7.27896200	-7.69142200	-15.50201600
H	5.46050600	-6.96109200	-16.37151400
C	8.06576200	-7.80581200	-14.34477900
H	8.19402700	-7.33779800	-12.23095800
H	7.62677100	-8.11168200	-16.44805000
H	9.03114400	-8.31472500	-14.38103000
H	3.78492900	-2.96735700	-14.46456800
H	3.97489100	-2.96014600	-16.30275000
H	2.95109900	-4.51445700	-12.94042900
C	2.77533600	-8.10627000	-15.70454600
H	2.11452500	-8.94661700	-15.43803100
H	3.78507000	-8.49649400	-15.88288500
C	2.24805300	-7.31613600	-16.86848800
C	0.93596600	-6.78621000	-16.85955700
C	3.05423000	-7.12458200	-18.00868600
C	0.44871000	-6.07982000	-17.97567000
H	0.29239500	-6.95643400	-15.99778500
C	2.56567900	-6.42039900	-19.11913200
H	4.06298600	-7.54178400	-18.02532600
C	1.26188800	-5.89538800	-19.10571400
H	-0.56262000	-5.67421800	-17.94993100
H	3.20099500	-6.28647200	-19.99715900
H	0.87983200	-5.35039300	-19.97085100
S	2.86866900	-7.23090900	-14.05627200
O	3.38020300	-8.24333400	-13.08959200
O	1.52664900	-6.62401000	-13.78316000

(S)-IM8

C	1.82852500	0.80049700	-4.56998300
C	1.09470400	2.04792800	-4.10809800
C	0.14887100	2.73457400	-4.89535400
H	1.57745100	2.61581200	-3.31257800
H	-0.13914600	2.37841100	-5.88669000
H	0.00871500	3.80758300	-4.73097300
Pd	-0.98271700	1.73714700	-3.34567100
P	-3.17181900	2.07623500	-3.44488600
O	-3.63590600	3.71047200	-3.64408900
O	-4.10118800	1.75352900	-2.03879600
C	-4.01593000	4.54098600	-1.42092000
C	-3.23416900	4.50889300	-2.57822500
C	-2.04036000	5.26295600	-2.71823300
C	-1.60430300	6.05041000	-1.66855300
C	-1.82456700	6.80810100	0.68584200
C	-2.47839000	6.76826300	1.90787200
C	-3.65349600	5.98119700	2.05606400
C	-4.16625200	5.26595900	0.98328600
C	-3.52865000	5.29580400	-0.29374900
C	-2.31567400	6.07172300	-0.43301000
C	-5.28842900	3.76838100	-1.39610200
C	-5.28291700	2.40763300	-1.72927400
C	-6.46287100	1.61647300	-1.69932500
C	-7.67124700	2.19195100	-1.35480500
C	-9.00791500	4.20052800	-0.76623600
C	-9.09583300	5.56497600	-0.53728700
C	-7.92542700	6.36859900	-0.61174100
C	-6.69068100	5.79949600	-0.88881300
C	-6.55635200	4.39342900	-1.10434800
C	-7.75577100	3.58573600	-1.06519300
H	-1.49178900	5.20615900	-3.65791200
H	-0.69107300	6.64214200	-1.76160500
H	-0.90946800	7.39219500	0.56094900
H	-2.08822100	7.32927000	2.75950100
H	-4.15448300	5.93385600	3.02514900
H	-5.06236900	4.66042200	1.11196300
H	-6.38438000	0.55821200	-1.95079400
H	-8.58190900	1.58982800	-1.32043800
H	-9.89992700	3.57016800	-0.73370100
H	-10.06021300	6.02576300	-0.31391300
H	-7.99846600	7.44703700	-0.45583500
H	-5.80742400	6.43272900	-0.95346600
C	-3.30919800	0.63756900	-5.74412200

C	-5.35168600	1.86387500	-5.17663800
C	-3.16673600	1.50324000	-7.00548400
H	-3.87809500	-0.27613500	-5.99120600
H	-2.31760800	0.35033000	-5.36286300
C	-5.17529800	2.68868800	-6.46742000
H	-5.99363700	0.99029800	-5.38752600
H	-5.82885300	2.47610500	-4.40191000
H	-2.57425000	2.40001900	-6.73030300
H	-4.57857100	3.58631600	-6.21473100
N	-4.04262800	1.37628300	-4.70050500
O	-4.46662400	1.92341200	-7.46227000
C	-6.51809900	3.09017700	-7.06846200
H	-7.07625100	3.71838100	-6.35599500
H	-6.36716400	3.65916800	-7.99910600
H	-7.11820700	2.19425200	-7.29651800
C	-2.49303500	0.74893800	-8.14661100
H	-2.42893300	1.38497800	-9.04321400
H	-1.47457300	0.45067500	-7.84989000
H	-3.06660100	-0.15789500	-8.39864600
C	1.85246400	-0.11389600	-1.58877000
H	2.91886800	0.14444500	-1.58403800
H	1.71648800	-1.05998600	-1.04047000
C	0.99309600	0.98831600	-1.03638600
C	-0.40882100	0.83025400	-0.89897600
C	1.59058700	2.18648400	-0.59448200
C	-1.18373300	1.85384600	-0.31336900
H	-0.87739000	-0.11229800	-1.18364200
C	0.81309900	3.20432200	-0.02175700
H	2.67226900	2.30663300	-0.68007900
C	-0.57541400	3.04213900	0.12043300
H	-2.25936100	1.71600000	-0.21304200
H	1.29293900	4.12374200	0.32086000
H	-1.17873700	3.83229300	0.56655200
S	1.49183700	-0.69267600	-3.32788200
O	0.03791900	-1.04123000	-3.40513200
O	2.48178700	-1.77084500	-3.60986300
C	3.34729100	0.98025700	-4.57954000
C	4.00703100	1.66963100	-3.53548600
C	4.14223700	0.43969800	-5.61399400
C	5.40141200	1.81379400	-3.52564900
H	3.43669200	2.10036100	-2.71455500
C	5.53759500	0.59078400	-5.61054600
H	3.68009300	-0.10218600	-6.43703900
C	6.17628100	1.27616700	-4.56596900

H	5.87967500	2.35004100	-2.70325800
H	6.12369900	0.16549800	-6.42800100
H	7.26215000	1.39072700	-4.56221100
C	1.25001100	0.22706600	-5.87562800
H	1.49235100	0.91166400	-6.70175500
H	1.66918100	-0.76141800	-6.10686300
H	0.15979200	0.13867500	-5.79147100

TS-iso-1

P	0.43693400	-7.74068400	-12.30068600
O	0.80211000	-8.16263000	-13.89342300
O	1.87411800	-6.95784100	-11.87334500
C	3.20913200	-8.08707700	-14.09415300
C	2.01776600	-8.81719900	-14.09853300
C	1.97007800	-10.21058500	-14.34692000
C	3.14608100	-10.90374900	-14.56826000
C	5.62616600	-10.95349300	-14.67532800
C	6.84882000	-10.30884200	-14.57492500
C	6.89313000	-8.91589800	-14.29150300
C	5.72354500	-8.18673700	-14.13440100
C	4.44530100	-8.81208100	-14.25396200
C	4.40414900	-10.23614300	-14.50831600
C	3.15841000	-6.61229000	-13.89203300
C	2.48796800	-6.09444300	-12.78049300
C	2.42663700	-4.70665000	-12.49739800
C	3.02738600	-3.80889100	-13.36009900
C	4.24407100	-3.33838000	-15.47259000
C	4.82843000	-3.77804300	-16.65005800
C	4.85258200	-5.16743400	-16.95081300
C	4.31708300	-6.09364800	-16.06746500
C	3.72932200	-5.67989600	-14.83338600
C	3.67332000	-4.26267200	-14.54775300
H	1.00139000	-10.70673400	-14.36340400
H	3.12589400	-11.97738400	-14.76621600
H	5.57439600	-12.02640600	-14.87497900
H	7.77803300	-10.86793500	-14.70103200
H	7.85806000	-8.41505600	-14.19053200
H	5.77350500	-7.12235700	-13.91005100
H	1.90298600	-4.37794500	-11.59933400
H	2.99572300	-2.73710200	-13.15341400
H	4.19986900	-2.27291600	-15.23483300
H	5.25824200	-3.06135400	-17.35256400
H	5.29197400	-5.51032700	-17.88976000
H	4.33522300	-7.15307900	-16.31773500

C	-1.91616800	-6.45507700	-11.72371300
C	-0.70811600	-5.60956900	-13.69509700
C	-3.20143600	-6.46765500	-12.56571700
H	-1.83715700	-5.48751800	-11.19536300
H	-1.95859700	-7.26661100	-10.98254800
C	-2.03477100	-5.64102900	-14.47563500
H	-0.57293900	-4.60972800	-13.24650400
H	0.13123500	-5.81541700	-14.36841300
H	-3.27454800	-7.45740200	-13.05927700
H	-2.12359800	-6.63740300	-14.95417200
N	-0.74810800	-6.61738300	-12.61419300
O	-3.14639500	-5.44956200	-13.58419300
C	-2.08850800	-4.53563000	-15.52529500
H	-1.27555200	-4.66780100	-16.25683500
H	-3.05204900	-4.56247700	-16.05721500
H	-1.97762400	-3.54907900	-15.04684200
C	-4.43260600	-6.21535200	-11.70452400
H	-5.34150700	-6.22006600	-12.32635200
H	-4.50692800	-7.00400800	-10.94025200
H	-4.35441800	-5.23688400	-11.20277800
Pd	-0.13867000	-9.32977500	-10.92049100
C	1.95232300	-12.21764100	-11.35229300
C	1.64471400	-11.97135600	-9.89607900
H	2.57300400	-13.11847100	-11.48048500
H	2.45665600	-11.36732700	-11.82377000
C	1.58501700	-10.69053100	-9.37474900
C	1.82471300	-9.47595000	-10.11228000
H	1.21575600	-10.56651700	-8.35613100
C	1.30809400	-13.13626900	-9.05921900
C	0.80357800	-14.32311800	-9.65264700
C	1.47567500	-13.11618100	-7.64944600
C	0.45909600	-15.43033800	-8.86731800
H	0.64713900	-14.36284900	-10.73066500
C	1.14374000	-14.22894100	-6.86899200
H	1.89797200	-12.23179600	-7.17053000
C	0.62988600	-15.39097200	-7.47292000
H	0.05411100	-16.32490200	-9.34498100
H	1.29310100	-14.19358900	-5.78789900
H	0.36933600	-16.25790000	-6.86235300
H	2.50976700	-9.50727500	-10.96524600
H	1.93753400	-8.56443600	-9.51404700
H	1.01021000	-12.38614200	-11.90191800
C	-3.24430800	-10.26215600	-11.75711500
H	-4.32193000	-10.09021800	-11.90312200

H	-2.67885900	-9.37624100	-12.09148200
C	-2.74824000	-11.52008200	-12.38302500
C	-3.45310700	-12.73523400	-12.22451600
C	-1.51975300	-11.54427300	-13.07906700
C	-2.94176300	-13.93534800	-12.73945100
H	-4.40572500	-12.73437500	-11.68871700
C	-1.01017300	-12.74268500	-13.60364700
H	-0.97118800	-10.60854800	-13.21410000
C	-1.71685000	-13.94533900	-13.43165400
H	-3.49976200	-14.86461600	-12.60325500
H	-0.06330100	-12.73684000	-14.14851600
H	-1.32325300	-14.87870600	-13.83991000
S	-3.01470900	-10.24381700	-9.83061200
O	-3.29187400	-8.77485400	-9.50942600
O	-1.47311400	-10.59576300	-9.72288500

TS-iso-rotate

Pd	0.76738100	-5.67622200	-14.69952500
P	-0.51329000	-4.14233700	-15.64332100
O	-0.32979500	-3.93276100	-17.28508200
O	-0.16608600	-2.58454800	-15.09637200
C	1.10478200	-2.00976700	-17.56909400
C	0.91041500	-3.38791700	-17.65946300
C	1.89530800	-4.28430700	-18.13597600
C	3.10894700	-3.78237000	-18.57078600
C	4.64947300	-1.86679700	-18.90992700
C	4.94978000	-0.52337300	-18.75685300
C	4.00133200	0.34937100	-18.15810300
C	2.75760900	-0.11950000	-17.76256900
C	2.39670500	-1.48843900	-17.94386100
C	3.38909500	-2.38720500	-18.49188600
C	0.01100400	-1.14934600	-17.04081400
C	-0.57610100	-1.45965500	-15.81063500
C	-1.55636700	-0.63664100	-15.19996700
C	-1.99699200	0.49946100	-15.85196400
C	-2.00244800	1.96181700	-17.85890100
C	-1.55449900	2.25371600	-19.13788600
C	-0.59364600	1.40999000	-19.75931900
C	-0.08017700	0.30777800	-19.09105400
C	-0.49955400	-0.00967600	-17.76369300
C	-1.50409700	0.82959300	-17.14886200
H	1.66628300	-5.34792800	-18.15957500
H	3.87565200	-4.45385700	-18.96297600
H	5.38074400	-2.55874800	-19.33400000

H	5.92170000	-0.13739700	-19.06981200
H	4.25659700	1.39895700	-17.99993100
H	2.04508200	0.56066900	-17.29930500
H	-1.94279300	-0.92243300	-14.22117900
H	-2.74570700	1.14694200	-15.39093000
H	-2.75480300	2.58804400	-17.37350300
H	-1.94525700	3.12099300	-19.67374300
H	-0.25952500	1.62742500	-20.77587800
H	0.64873500	-0.33340200	-19.58409600
C	-2.71720100	-5.03494200	-14.36395400
C	-3.13767400	-3.51997000	-16.26467100
C	-4.03267700	-5.75653500	-14.70385100
H	-2.91969100	-4.26710300	-13.59390800
H	-1.98529200	-5.75444800	-13.96540200
C	-4.42262200	-4.31098800	-16.55488100
H	-3.38705500	-2.65994500	-15.61882000
H	-2.70055200	-3.14913800	-17.19933400
H	-3.81125200	-6.58042800	-15.41058800
H	-4.17068400	-5.14728700	-17.23782600
N	-2.16361900	-4.40273300	-15.58248900
O	-4.95562400	-4.85076200	-15.33209500
C	-5.49408400	-3.41859500	-17.17260200
H	-5.13829700	-3.01012600	-18.13152400
H	-6.41340000	-3.99687000	-17.35215700
H	-5.72974700	-2.58109300	-16.49644700
C	-4.70177300	-6.30703300	-13.44887700
H	-5.64567200	-6.80883000	-13.71128900
H	-4.03825400	-7.03531800	-12.95612200
H	-4.92035000	-5.49087300	-12.74169400
C	3.30305300	-2.27409500	-11.97198400
C	3.52453100	-2.63055300	-13.43111000
H	4.26295900	-2.16058100	-11.44217500
H	2.76464000	-1.31373600	-11.87509800
C	2.72952200	-3.52194500	-14.07697500
C	1.61020500	-4.27848700	-13.41215600
H	2.88970000	-3.68149500	-15.14513300
C	4.62074000	-1.92453000	-14.14630700
C	4.99123200	-0.60785000	-13.78159200
C	5.34616100	-2.55167300	-15.18807700
C	6.02813400	0.06345700	-14.44709300
H	4.45266900	-0.10109400	-12.97896500
C	6.38657300	-1.88456300	-15.84713100
H	5.10218000	-3.58002700	-15.46055100
C	6.73220200	-0.57141900	-15.48312000

H	6.28636100	1.08375300	-14.15345300
H	6.93466500	-2.39382100	-16.64229400
H	7.54499300	-0.05324100	-15.99672600
H	1.95972800	-4.91760600	-12.58538800
H	0.80373900	-3.62293500	-13.05225300
H	2.70701500	-3.04095000	-11.45527200
C	2.25990500	-8.96780000	-15.64678000
H	1.86179000	-9.62474300	-14.85983100
H	3.03704600	-9.48781700	-16.22551000
C	1.20772500	-8.36589200	-16.50504500
C	-0.04993500	-7.99039200	-15.95706400
C	1.44792200	-8.09411500	-17.87017700
C	-1.03303000	-7.38628600	-16.76728500
H	-0.28389400	-8.26356700	-14.92672700
C	0.45883100	-7.50667200	-18.67437100
H	2.41034600	-8.37361300	-18.30512200
C	-0.78172600	-7.14047400	-18.12482300
H	-1.99336300	-7.11743100	-16.33194600
H	0.66196500	-7.32423200	-19.73183600
H	-1.54468900	-6.67020400	-18.74697200
S	3.20364900	-7.62318900	-14.61203100
O	4.11722800	-8.43993700	-13.72364500
O	1.94281200	-7.11466300	-13.74409100

TS-iso-2

Pd	1.28555300	-4.61532600	-14.64683800
P	-0.30413800	-3.41423500	-15.53512500
O	-0.23801500	-3.00994800	-17.17079500
O	-0.33531700	-1.85905200	-14.85857900
C	0.55078300	-0.73147400	-17.28940100
C	0.74794400	-2.09183700	-17.53662400
C	1.91270900	-2.60351300	-18.15945900
C	2.92572400	-1.73464000	-18.52074400
C	3.88622800	0.55460500	-18.55877800
C	3.80175200	1.90162400	-18.24358300
C	2.64341000	2.40376000	-17.58922600
C	1.58374900	1.56369500	-17.27965900
C	1.62589100	0.17469500	-17.60871200
C	2.82018900	-0.33973100	-18.24404700
C	-0.71914400	-0.28407700	-16.65166400
C	-1.11869800	-0.86588700	-15.44538300
C	-2.28577900	-0.46199500	-14.74856400
C	-3.09081100	0.52675200	-15.28303200
C	-3.62979300	2.10059900	-17.12684700

C	-3.34285800	2.64473800	-18.36903100
C	-2.18937400	2.21408900	-19.08021800
C	-1.33375200	1.26726000	-18.53582100
C	-1.58464200	0.70253200	-17.24851800
C	-2.77657600	1.11829900	-16.54205000
H	1.98765000	-3.67768200	-18.32075000
H	3.83153600	-2.11025200	-19.00161900
H	4.77658000	0.14904500	-19.04492500
H	4.62579100	2.57604800	-18.48448300
H	2.58886500	3.46087100	-17.32139400
H	0.70819700	1.96184900	-16.76954000
H	-2.52277000	-0.94402700	-13.79954500
H	-3.98931500	0.85409700	-14.75572300
H	-4.52135300	2.40761700	-16.57505900
H	-4.00462700	3.39404300	-18.80784700
H	-1.97656800	2.62865600	-20.06771200
H	-0.45839400	0.94120400	-19.09553500
C	-2.21840200	-5.09185100	-14.53386400
C	-3.00535000	-3.51189000	-16.24213300
C	-3.05141000	-6.18892100	-15.21890500
H	-2.82726700	-4.62115000	-13.74022600
H	-1.31692300	-5.52610700	-14.07705900
C	-3.82019200	-4.65433600	-16.87224400
H	-3.64058300	-2.96854300	-15.52076900
H	-2.67155900	-2.81600000	-17.01931600
H	-2.41877700	-6.67334500	-15.98895400
H	-3.17913500	-5.15722400	-17.62440800
N	-1.83495000	-4.07659700	-15.53506800
O	-4.19919200	-5.61170100	-15.86722700
C	-5.09879600	-4.13322300	-17.52022900
H	-4.85148600	-3.42587400	-18.32748800
H	-5.67783800	-4.96774900	-17.94482000
H	-5.72172400	-3.61493100	-16.77338700
C	-3.54982700	-7.22274800	-14.21531800
H	-4.16456900	-7.98109400	-14.72416300
H	-2.69405400	-7.72389400	-13.73551600
H	-4.15950200	-6.73924400	-13.43510700
C	4.47360600	-4.59132200	-12.97749200
C	4.49944500	-4.72797900	-14.48439500
H	5.29606800	-5.13901300	-12.49980400
H	4.56161300	-3.52978400	-12.69420600
C	3.66257000	-3.94571000	-15.27114800
C	2.68759100	-3.01390500	-14.77359400
H	3.68212900	-4.08449900	-16.35257000

C	5.42105100	-5.68801200	-15.12175300
C	5.82206200	-6.86928800	-14.44604300
C	5.92654000	-5.47162500	-16.43061300
C	6.66321100	-7.80438400	-15.06130400
H	5.42631100	-7.07775700	-13.45263000
C	6.77778900	-6.40165900	-17.03996900
H	5.67445700	-4.55236200	-16.96065400
C	7.14589500	-7.57730400	-16.36255000
H	6.93859500	-8.71513300	-14.52542200
H	7.16154900	-6.20431700	-18.04319900
H	7.80669000	-8.30387500	-16.83963400
H	2.76591900	-2.66980500	-13.73459500
H	2.36175800	-2.23633200	-15.46550100
H	3.51593900	-4.95671400	-12.57065400
C	1.49603300	-8.39783900	-14.60084300
H	0.44149900	-8.48584900	-14.29935400
H	1.98017100	-9.38509900	-14.57276100
C	1.67863500	-7.70431400	-15.90142700
C	0.65809100	-6.87646000	-16.42686200
C	2.89655400	-7.80281200	-16.61381700
C	0.83302400	-6.20057800	-17.64800400
H	-0.29283900	-6.80958500	-15.89833500
C	3.07546900	-7.12290000	-17.82550100
H	3.70201800	-8.42148500	-16.21300200
C	2.04058000	-6.32498100	-18.35171400
H	0.02981900	-5.57275100	-18.03478000
H	4.02090900	-7.21788000	-18.36233400
H	2.17604800	-5.80756700	-19.30410600
S	2.30916800	-7.47587800	-13.09557400
O	1.89444900	-8.35004800	-11.92555500
O	1.47214800	-6.11824500	-13.09927700

TS-iso-3

Pd	1.44766900	-4.54573500	-14.94209000
P	-0.21878700	-3.34521000	-15.67933400
O	-0.30010600	-2.91349600	-17.30555100
O	-0.19212200	-1.79725700	-14.98170000
C	0.42692100	-0.61899400	-17.47905600
C	0.62681500	-1.97318200	-17.75509900
C	1.72915200	-2.45483800	-18.50395700
C	2.66953000	-1.55961800	-18.97936800
C	3.55115400	0.75593600	-19.13567800
C	3.46734800	2.10119900	-18.81294200
C	2.38591200	2.57143600	-18.01845500

C	1.39730500	1.70228400	-17.58049500
C	1.43538700	0.31481800	-17.91650500
C	2.55804100	-0.16729700	-18.69201800
C	-0.77636500	-0.20300800	-16.70591700
C	-1.03875900	-0.80327000	-15.47056600
C	-2.12760200	-0.41690900	-14.64802300
C	-2.99709400	0.56558200	-15.08319200
C	-3.76053200	2.13554900	-16.84955900
C	-3.62225700	2.68486200	-18.11473500
C	-2.54758100	2.27374300	-18.95006900
C	-1.62045400	1.34231800	-18.50545300
C	-1.71744700	0.77232700	-17.19962000
C	-2.83177100	1.16677700	-16.36575800
H	1.81487200	-3.52707700	-18.67402400
H	3.52313100	-1.91102800	-19.56303100
H	4.38596800	0.37414000	-19.72816300
H	4.23449900	2.79843700	-19.15538900
H	2.33518200	3.62713700	-17.74433200
H	0.58108600	2.07631900	-16.96466800
H	-2.25533800	-0.90877800	-13.68323600
H	-3.83656200	0.87792000	-14.45855100
H	-4.59073700	2.42675700	-16.20171000
H	-4.34141200	3.42236300	-18.47648000
H	-2.45316000	2.69064700	-19.95484100
H	-0.80801400	1.03190600	-19.16062500
C	-2.01020100	-5.10661900	-14.59585800
C	-2.97939600	-3.41282200	-16.09385600
C	-2.90905800	-6.15699200	-15.27018800
H	-2.52837700	-4.70898200	-13.70388100
H	-1.06446100	-5.57141300	-14.28127500
C	-3.85231600	-4.51601500	-16.71636600
H	-3.54034600	-2.92408900	-15.27791000
H	-2.72666600	-2.66390200	-16.85226500
H	-2.35855800	-6.57720900	-16.13499800
H	-3.29316300	-4.95670800	-17.56676800
N	-1.74235400	-4.00952600	-15.54686100
O	-4.12109500	-5.54695300	-15.75048100
C	-5.19341500	-3.96286600	-17.18768300
H	-5.03518100	-3.19396700	-17.96033700
H	-5.81043200	-4.77011600	-17.61157300
H	-5.73729900	-3.50959500	-16.34323700
C	-3.29744900	-7.26500100	-14.29748800
H	-3.95866900	-7.99243900	-14.79306900
H	-2.39561500	-7.78898600	-13.94284000

H	-3.82563700	-6.84331900	-13.42713900
C	5.58841500	-5.75896300	-15.12014400
C	4.62372600	-4.74850300	-14.52956900
H	5.74746200	-6.60926900	-14.44254100
H	5.22036700	-6.12934600	-16.08727200
C	3.79807700	-4.06592200	-15.42596000
C	2.87133900	-2.99401000	-15.17661500
H	3.87883700	-4.38094500	-16.47034800
C	4.75295200	-4.44705600	-13.08997100
C	6.02540400	-4.57869500	-12.47100900
C	3.66573700	-4.03487000	-12.27662000
C	6.20818700	-4.27595200	-11.11643500
H	6.88350600	-4.89717100	-13.06320400
C	3.84865000	-3.74811900	-10.91833300
H	2.66074500	-3.99193800	-12.69128500
C	5.12045100	-3.85771100	-10.33114900
H	7.20143600	-4.37175400	-10.67289900
H	2.98864800	-3.45116400	-10.31440600
H	5.25983800	-3.63267100	-9.27178800
H	2.91448700	-2.45256500	-14.22538500
H	2.64017500	-2.35749900	-16.03275400
H	6.57368800	-5.28759400	-15.29423500
C	2.02738800	-8.39946400	-15.21092400
H	1.10534900	-8.84903000	-14.81359400
H	2.80107300	-9.17217500	-15.33019900
C	1.80091000	-7.61144700	-16.45037400
C	0.55501800	-6.98176500	-16.68154500
C	2.82923100	-7.43410400	-17.40427200
C	0.32988300	-6.23540400	-17.84870400
H	-0.24167200	-7.10428200	-15.94849800
C	2.60752500	-6.68432000	-18.56911700
H	3.79828300	-7.91043900	-17.23623500
C	1.35206000	-6.09195000	-18.80129600
H	-0.64023000	-5.76276600	-18.00696800
H	3.40825100	-6.57454100	-19.30433400
H	1.17264400	-5.52459400	-19.71677800
S	2.64326200	-7.35025700	-13.69417100
O	2.55844700	-8.35642800	-12.56220100
O	1.46870600	-6.28483900	-13.60614200

TS-iso-4

Pd	0.14527800	-5.73442000	-13.96369400
P	-0.71618000	-3.88406900	-14.81165700
O	-0.33237300	-3.62288400	-16.42516500

O	-0.08322000	-2.47220500	-14.13797600
C	1.36614000	-1.91166300	-16.49874300
C	0.98366900	-3.23908700	-16.69961400
C	1.85605600	-4.23280900	-17.20304700
C	3.15142600	-3.88590900	-17.53880000
C	4.96892300	-2.19885000	-17.64560100
C	5.44657900	-0.92401900	-17.38557000
C	4.59039600	0.04420200	-16.79222700
C	3.27043400	-0.26418900	-16.49725500
C	2.73546300	-1.55771000	-16.78022900
C	3.62194900	-2.55520100	-17.33847900
C	0.37110400	-0.94339200	-15.95871400
C	-0.31790600	-1.25506400	-14.78210300
C	-1.24862800	-0.37290500	-14.17825100
C	-1.52236300	0.84222900	-14.77852500
C	-1.23353300	2.42019000	-16.67367100
C	-0.67377500	2.73939200	-17.90076400
C	0.22983800	1.83422300	-18.52224900
C	0.57673700	0.64198400	-17.90366900
C	0.03977400	0.29081800	-16.62763800
C	-0.90809900	1.19670300	-16.01549000
H	1.48430800	-5.24963100	-17.31869900
H	3.83937300	-4.63504000	-17.93341000
H	5.62006800	-2.96193800	-18.07658300
H	6.48067700	-0.66470700	-17.62132900
H	4.97588000	1.03976300	-16.56289500
H	2.62876400	0.48592000	-16.03790800
H	-1.73288600	-0.67682000	-13.24992100
H	-2.23230400	1.53650400	-14.32435900
H	-1.94423000	3.09541400	-16.19128900
H	-0.93343000	3.67630900	-18.39755000
H	0.65132200	2.07626900	-19.50004500
H	1.26230100	-0.04473800	-18.39748900
C	-3.25403200	-4.74232900	-14.25971600
C	-3.09037600	-2.85981100	-15.82974500
C	-3.94051200	-5.56232300	-15.36343600
H	-4.01775300	-4.21540900	-13.66133700
H	-2.67155700	-5.40638200	-13.60976200
C	-3.79694000	-3.72763600	-16.88813200
H	-3.84197200	-2.27944700	-15.26775300
H	-2.39255400	-2.16643300	-16.31157600
H	-3.14763800	-6.08711300	-15.92959600
H	-3.01466600	-4.26677500	-17.45862900
N	-2.37038400	-3.72761400	-14.86990400

O	-4.66093600	-4.68726100	-16.25575800
C	-4.65269700	-2.87918200	-17.82318700
H	-4.01969500	-2.15794800	-18.36417200
H	-5.16614500	-3.52007800	-18.55659800
H	-5.41152200	-2.32347900	-17.24842100
C	-4.93414000	-6.56386600	-14.78756000
H	-5.44115300	-7.10795700	-15.59975600
H	-4.39940900	-7.28765100	-14.15423700
H	-5.69642900	-6.04812500	-14.18064400
C	3.65622900	-8.04548300	-12.58412800
C	3.46894200	-6.65159200	-13.14156400
H	3.31892100	-8.79742200	-13.32315400
H	4.71448100	-8.26675100	-12.36611300
C	2.43289400	-5.87956400	-12.65516100
C	1.83401800	-4.69300400	-13.24592900
H	1.92743100	-6.26101700	-11.76143700
C	4.40335200	-6.21173800	-14.19623900
C	4.97493200	-7.14553200	-15.09809600
C	4.83898600	-4.86379800	-14.27972600
C	5.90188100	-6.74133100	-16.06889900
H	4.68345900	-8.19412700	-15.04137100
C	5.77409200	-4.46264300	-15.24067500
H	4.46699900	-4.13952000	-13.55525600
C	6.30397500	-5.39673000	-16.14796600
H	6.31745500	-7.47980400	-16.75821200
H	6.09190600	-3.41996800	-15.28044400
H	7.03405600	-5.08314800	-16.89705500
H	1.44011900	-3.95015300	-12.54058800
H	2.34898400	-4.23193600	-14.09360400
H	3.05903600	-8.19173600	-11.67152900
C	0.10688900	-9.50420300	-14.87178100
H	-0.82417600	-10.07987900	-14.98361500
H	0.88259700	-10.12594400	-14.40200900
C	0.55822900	-8.85655300	-16.13779300
C	-0.37546200	-8.47070900	-17.12456900
C	1.92247200	-8.56080800	-16.34151100
C	0.05121700	-7.83422800	-18.29888200
H	-1.43467500	-8.67698400	-16.96395100
C	2.35215400	-7.92336700	-17.51497700
H	2.64703700	-8.84665300	-15.57687300
C	1.41750600	-7.56558500	-18.50188700
H	-0.68057200	-7.54944400	-19.05811500
H	3.41205200	-7.70333200	-17.65374100
H	1.74910800	-7.07183700	-19.41776900

S	-0.34884600	-8.19988600	-13.54686200
O	-0.88389700	-9.00110600	-12.38012300
O	-1.43083900	-7.35914400	-14.32663400
TS-iso-5			
C	0.38481200	-1.43239800	-4.01311200
C	-0.00583700	0.02667000	-4.14735300
H	0.29437700	-1.78606200	-2.97997700
H	-0.26021100	-2.06467200	-4.63503200
C	-0.40672400	0.50154900	-5.49286100
C	-1.19865100	-0.19386700	-6.35918400
H	-0.07407800	1.49086200	-5.81377400
C	0.53984800	1.02090800	-3.19703200
C	1.17579900	0.61315000	-1.98804600
C	0.33323200	2.42842000	-3.38413200
C	1.55477300	1.54594000	-1.02115100
H	1.35872900	-0.44248100	-1.80435300
C	0.70028900	3.35356400	-2.39633900
H	-0.11936700	2.80609700	-4.29945700
C	1.31151800	2.92101300	-1.21042200
H	2.04012700	1.19994900	-0.10602100
H	0.51632300	4.41634200	-2.56717900
H	1.60793300	3.64254500	-0.44647500
H	-1.58718400	-1.18416100	-6.11555800
H	-1.47832500	0.23690600	-7.32165600
H	1.43216500	-1.56673400	-4.34336000
Pd	-1.99280000	0.70000900	-3.61540300
P	-3.68694700	2.20806200	-3.48636600
O	-5.15739200	1.95383900	-4.24332500
O	-3.14971000	3.55466800	-4.40130300
C	-4.76045400	2.53997000	-6.54064700
C	-4.96139500	1.55595500	-5.57261900
C	-4.95236100	0.16744900	-5.85195100
C	-4.72987900	-0.25167200	-7.15088800
C	-4.16363900	0.26280200	-9.51309100
C	-3.84745600	1.17818500	-10.50511100
C	-3.81309700	2.56701700	-10.20195400
C	-4.11267900	3.02065200	-8.92530600
C	-4.46276400	2.10882100	-7.88401500
C	-4.46515400	0.69327700	-8.18637000
C	-4.80911500	3.97106500	-6.12991600
C	-4.01033200	4.41655800	-5.06849400
C	-3.97985900	5.77709600	-4.66233700
C	-4.77863400	6.70587600	-5.30159600
C	-6.53638100	7.24600100	-6.97047500

C	-7.43067300	6.84533500	-7.95107100
C	-7.49179200	5.47728100	-8.33299000
C	-6.65067800	4.53979600	-7.75071400
C	-5.69890400	4.91961200	-6.75531300
C	-5.66527000	6.30591300	-6.34433700
H	-5.11805100	-0.53388300	-5.03641200
H	-4.72514100	-1.31636600	-7.39349700
H	-4.17653200	-0.80889600	-9.72540200
H	-3.61371800	0.83609600	-11.51530600
H	-3.54317600	3.28412300	-10.97992100
H	-4.07604300	4.08646900	-8.70476300
H	-3.31495100	6.06072000	-3.84576800
H	-4.75544300	7.75563700	-5.00134900
H	-6.48892300	8.28967500	-6.65046400
H	-8.09573100	7.57256900	-8.42109400
H	-8.21273400	5.15785900	-9.08841600
H	-6.71868500	3.49483200	-8.04902900
C	-3.28770300	2.68249200	-0.85941200
C	-5.21884400	3.84153600	-1.85987600
C	-4.09003500	2.55916700	0.44522500
H	-2.66408300	3.59452000	-0.81434400
H	-2.62923200	1.80973800	-0.98272200
C	-5.96013800	3.67816700	-0.52161700
H	-4.71009400	4.82265800	-1.87398800
H	-5.92996400	3.79496100	-2.69422000
H	-4.66155100	1.61052500	0.41359300
H	-6.50833500	2.71443500	-0.54687700
N	-4.22532100	2.75740700	-2.00174800
O	-5.01976300	3.65129500	0.56739900
C	-6.92423100	4.83318700	-0.27297500
H	-7.68577900	4.86665900	-1.06805200
H	-7.42950800	4.70505500	0.69663400
H	-6.37912500	5.79077600	-0.26355500
C	-3.17305400	2.58353100	1.66287800
H	-3.76523100	2.51216400	2.58816000
H	-2.47422900	1.73307400	1.62104900
H	-2.59168000	3.51936000	1.68589200
C	-4.12446300	-1.03459600	-1.38838500
H	-4.14996300	-0.06110700	-0.88475800
H	-4.05145400	-1.83619100	-0.63642300
C	-5.29301600	-1.22310300	-2.30783200
C	-6.24266700	-0.19243400	-2.45748100
C	-5.48776000	-2.43356800	-3.01165100
C	-7.36177700	-0.36037200	-3.28693000

H	-6.08957400	0.74890900	-1.92841700
C	-6.59948100	-2.59724700	-3.85059900
H	-4.75461300	-3.23239000	-2.90365800
C	-7.54232200	-1.56171800	-3.99007900
H	-8.08255100	0.45307300	-3.39383100
H	-6.73426800	-3.53587100	-4.39310800
H	-8.40804000	-1.69218100	-4.64314300
S	-2.39041100	-1.13929500	-2.16870700
O	-2.38325700	-2.46565000	-2.89872000
O	-1.49608600	-1.05612600	-0.94768000

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Pd	-0.11045300	-3.70941400	-13.41416500
P	-1.87254800	-2.58031300	-14.33534600
O	-1.44436100	-1.01473700	-14.78965200
O	-3.18139600	-2.22856600	-13.32575100
C	-2.36941700	0.48536000	-13.14730400
C	-1.25513600	-0.10587400	-13.74428900
C	0.07699200	0.18948200	-13.36649000
C	0.30350500	1.10030700	-12.35091300
C	-0.56092300	2.61074400	-10.58018400
C	-1.62128800	3.16390600	-9.87977100
C	-2.95594900	2.82274500	-10.23216700
C	-3.21101700	1.95732500	-11.28594800
C	-2.14490300	1.38905500	-12.04680000
C	-0.78677900	1.70859500	-11.66216400
C	-3.73131300	0.11234400	-13.62385900
C	-4.09452500	-1.23710300	-13.68347900
C	-5.38690100	-1.66817700	-14.07689800
C	-6.33458200	-0.73365600	-14.45059700
C	-6.96133100	1.62164000	-14.92555500
C	-6.62836600	2.96493900	-15.00167500
C	-5.31985000	3.39008200	-14.64220400
C	-4.37620300	2.47718300	-14.19414100
C	-4.69034500	1.08851500	-14.07969700
C	-6.01108200	0.65468200	-14.48099900
H	0.89569400	-0.31011000	-13.88243200
H	1.32380200	1.34527000	-12.04807600
H	0.47103600	2.84497200	-10.30817300
H	-1.43554600	3.84902800	-9.05009900
H	-3.78953700	3.23973700	-9.66314800
H	-4.23800100	1.69694500	-11.53690200
H	-5.60236400	-2.73710600	-14.07801800
H	-7.33642000	-1.04879300	-14.75017400

H	-7.95632900	1.27543700	-15.21548100
H	-7.36232800	3.69543600	-15.34770800
H	-5.05232500	4.44560600	-14.72409800
H	-3.37604700	2.81677600	-13.92925300
C	-2.14879900	-4.43183000	-16.34666500
C	-3.24651500	-2.27230600	-16.74571600
C	-1.41600600	-4.27182400	-17.68987200
H	-3.08237800	-5.00100800	-16.50626200
H	-1.51381800	-4.97704100	-15.63648100
C	-2.46883000	-2.15764200	-18.06851700
H	-4.22285400	-2.75131300	-16.93523400
H	-3.41317400	-1.27716400	-16.31982100
H	-0.45359600	-3.75841500	-17.48669900
H	-1.50973400	-1.64501400	-17.85350500
N	-2.48378800	-3.10904600	-15.79654700
O	-2.19104600	-3.46714500	-18.59693800
C	-3.26147000	-1.39333900	-19.12345000
H	-3.46302700	-0.36856400	-18.77337000
H	-2.69372000	-1.34124800	-20.06530300
H	-4.22224200	-1.89681700	-19.31835500
C	-1.17770800	-5.61702200	-18.36734600
H	-0.67109300	-5.47346400	-19.33417200
H	-0.55101900	-6.25860400	-17.72999000
H	-2.13858500	-6.12635500	-18.54645200
C	2.51468800	-4.93864400	-11.95714000
C	1.94247000	-4.48413600	-13.28884900
H	3.58712100	-5.18211100	-12.07554800
H	2.41348200	-4.17304600	-11.17877800
C	1.31814600	-5.56342000	-14.05918000
C	1.09305700	-5.72308100	-15.40342600
H	0.94959300	-6.37498300	-13.42488700
C	2.48732700	-3.22714300	-13.87275200
C	3.38100600	-2.42239700	-13.10578400
C	2.09501300	-2.70418900	-15.14557800
C	3.85218200	-1.19382200	-13.57549000
H	3.71368000	-2.76564500	-12.12825400
C	2.56263500	-1.46416700	-15.60545800
H	1.39436200	-3.24018200	-15.77618600
C	3.44816700	-0.70206100	-14.83118600
H	4.54070900	-0.61435800	-12.95681500
H	2.22547400	-1.09866800	-16.57762900
H	3.81746300	0.25875500	-15.19464400
H	1.49499400	-5.07954600	-16.18164300
H	0.54598100	-6.60718000	-15.73409500

H	1.98826800	-5.83210400	-11.60075400
C	-2.27214900	-4.72801500	-11.13337900
H	-3.04991300	-4.09089300	-11.57097200
H	-2.46963500	-4.91323400	-10.06703800
C	-2.02015400	-5.97110100	-11.92380700
C	-2.50270500	-6.08371000	-13.24521700
C	-1.20851700	-7.00450100	-11.40684400
C	-2.19010400	-7.20436000	-14.03087900
H	-3.13325300	-5.29056600	-13.64998100
C	-0.88955300	-8.12134900	-12.19262200
H	-0.81515100	-6.91268800	-10.39401300
C	-1.37722500	-8.22375000	-13.50894200
H	-2.57518200	-7.27627800	-15.04993500
H	-0.25996100	-8.91280600	-11.78004300
H	-1.12962900	-9.09533200	-14.11880200
S	-0.69426600	-3.64856600	-11.10408800
O	0.22344600	-4.39878300	-10.16580400
O	-1.13235000	-2.28735200	-10.63137300

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C	-2.40804900	-0.20620000	-7.58099600
C	-1.00384200	-0.06150300	-7.02199300
H	-3.07551400	-0.64854400	-6.82776200
H	-2.82555000	0.75366000	-7.90691100
C	-0.16443800	1.03895100	-7.35523200
C	-0.68475700	2.33231600	-7.64932800
H	0.90916900	0.94483700	-7.17838200
C	-0.40504400	-1.24129100	-6.35542300
C	-0.95809500	-2.53320400	-6.52723600
C	0.72658000	-1.10601400	-5.51216000
C	-0.38078500	-3.65033400	-5.90821900
H	-1.83630700	-2.66931200	-7.15774500
C	1.29824600	-2.22059300	-4.89053400
H	1.12755500	-0.11254600	-5.31030400
C	0.75026200	-3.50060400	-5.08932700
H	-0.81946800	-4.63816900	-6.06290900
H	2.16194500	-2.08946000	-4.23535600
H	1.19355900	-4.37004200	-4.59949200
H	-1.64991700	2.47191300	-8.14375300
H	0.02608100	3.14904600	-7.78428900
H	-2.38229100	-0.88412400	-8.45326800
Pd	-1.19673200	1.88503700	-5.60720400
P	-1.45585300	4.00875900	-4.92855100
O	-2.95746500	4.66134100	-5.30227600

O	-0.45815700	5.04019800	-5.83310700
C	-2.69615400	5.56061500	-7.52106600
C	-3.24060100	4.59640300	-6.67297000
C	-4.05890600	3.53222400	-7.12404400
C	-4.32534000	3.41558800	-8.47632200
C	-3.97365100	4.17771600	-10.81347500
C	-3.37820100	5.03641300	-11.72414400
C	-2.52746700	6.07817900	-11.26298700
C	-2.30224500	6.26073100	-9.90624600
C	-2.91645200	5.40994700	-8.93831000
C	-3.75329100	4.32841900	-9.41185800
C	-1.88299300	6.66416800	-6.93699800
C	-0.79840200	6.36415500	-6.10606200
C	0.04697300	7.36501200	-5.56201200
C	-0.21179500	8.69684700	-5.82494900
C	-1.65070300	10.45103700	-6.83442900
C	-2.77656400	10.81808100	-7.55508900
C	-3.64536100	9.81566800	-8.06633100
C	-3.36783400	8.47010400	-7.87200800
C	-2.20390500	8.05392500	-7.15673900
C	-1.34235000	9.07703400	-6.60656700
H	-4.45687100	2.82999400	-6.39323700
H	-4.96027700	2.60794500	-8.84609700
H	-4.61574400	3.36131500	-11.15228500
H	-3.55086400	4.90874200	-12.79458300
H	-2.04237000	6.73943200	-11.98381600
H	-1.64275700	7.05857100	-9.56852000
H	0.89129200	7.05642800	-4.94496300
H	0.43634700	9.47672500	-5.41968600
H	-0.98248600	11.20826900	-6.41744600
H	-3.00507900	11.87279300	-7.72049000
H	-4.54456000	10.10643000	-8.61333300
H	-4.04953700	7.71602500	-8.26195900
C	-0.51764700	3.64646800	-2.41589200
C	-1.59609700	5.82861300	-2.86059400
C	-1.06254100	3.72777900	-0.98069500
H	0.51130300	4.05196300	-2.43328700
H	-0.51655700	2.59873800	-2.74816700
C	-2.11128100	5.81963400	-1.41165300
H	-0.63924100	6.37894100	-2.89882500
H	-2.32277300	6.32409400	-3.51596900
H	-2.06157400	3.25258500	-0.96052300
H	-3.09491900	5.30879400	-1.39920400
N	-1.39208900	4.43445600	-3.31591000

O	-1.19793200	5.10066600	-0.56602900
C	-2.23745200	7.23653100	-0.86133500
H	-2.96078300	7.81176000	-1.46053100
H	-2.58466600	7.20827000	0.18293100
H	-1.26198100	7.74812300	-0.89588200
C	-0.12937700	3.03094700	0.00311000
H	-0.52377700	3.11746600	1.02730000
H	-0.04454400	1.96372300	-0.25580900
H	0.87387500	3.48604600	-0.02901900
C	-3.70848900	1.56686500	-2.72616300
H	-3.16298900	2.51849600	-2.68850100
H	-3.54019700	0.98801900	-1.80490900
C	-5.14928300	1.74632200	-3.06765400
C	-5.58183800	2.91169800	-3.73944900
C	-6.09115500	0.72657900	-2.80570000
C	-6.92176900	3.05864600	-4.13195500
H	-4.85841200	3.70137400	-3.94925200
C	-7.43060900	0.87384200	-3.19552700
H	-5.76065300	-0.18352500	-2.30214300
C	-7.85171500	2.03998100	-3.86069200
H	-7.23863400	3.96804700	-4.64832000
H	-8.14794700	0.07786400	-2.98179300
H	-8.89550800	2.15346400	-4.16218000
S	-2.77007100	0.55693500	-4.05845000
O	-3.42609200	-0.81367200	-4.04250800
O	-1.31725000	0.57064600	-3.46146200

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C	1.30884100	-0.27945600	-6.47507800
C	0.06787100	0.21086000	-7.19860400
H	1.88419500	-0.94863000	-7.13961300
H	1.96520500	0.54603300	-6.17331800
C	0.00148800	1.49306200	-7.81481000
C	0.71864100	2.61864100	-7.32302000
H	-0.77946500	1.67695700	-8.55568000
C	-0.97879500	-0.78754000	-7.53180100
C	-2.28324800	-0.37452500	-7.90591600
C	-0.71219800	-2.17642200	-7.47253800
C	-3.26905600	-1.30986700	-8.23386300
H	-2.53312200	0.68607900	-7.89379300
C	-1.70121100	-3.11313000	-7.80610900
H	0.27533300	-2.53022500	-7.17755100
C	-2.98198300	-2.68619700	-8.19120300
H	-4.27007100	-0.96682100	-8.50427600

H	-1.46924000	-4.17916200	-7.76006200
H	-3.75405600	-3.41705900	-8.44013500
H	0.51565100	3.59026300	-7.77499000
H	1.69705200	2.52097600	-6.84267600
H	1.02761600	-0.84978200	-5.57844300
Pd	-0.66217100	1.99254400	-5.78617300
P	-1.18685600	4.03270200	-4.99919700
O	-2.75728000	4.48131600	-5.38867600
O	-0.32916300	5.23939300	-5.82585300
C	-2.56273900	5.42368200	-7.59773100
C	-2.98818400	4.38553600	-6.76944600
C	-3.62927100	3.21655400	-7.24788300
C	-3.83399100	3.07146300	-8.60820900
C	-3.50454900	3.88063800	-10.93225900
C	-2.99972800	4.81573400	-11.82235400
C	-2.32341300	5.96649500	-11.33259800
C	-2.18049400	6.17750200	-9.96860800
C	-2.70589500	5.24686100	-9.02234500
C	-3.36281000	4.05879000	-9.52385200
C	-1.94451000	6.63274800	-6.98505300
C	-0.86219800	6.49467200	-6.10897200
C	-0.20268900	7.60909500	-5.52918000
C	-0.64666800	8.88822700	-5.80581200
C	-2.28415100	10.41220400	-6.88387600
C	-3.41876900	10.61028700	-7.65522300
C	-4.10446400	9.49130500	-8.20174800
C	-3.63909800	8.20135600	-7.99022000
C	-2.45913700	7.96012000	-7.22266000
C	-1.78514700	9.09855400	-6.63835400
H	-3.94865100	2.46095700	-6.53197700
H	-4.33622500	2.18473000	-8.99980600
H	-4.01114300	2.98236200	-11.29284700
H	-3.10945500	4.66597300	-12.89821300
H	-1.90756200	6.69000100	-12.03665800
H	-1.65334900	7.05938500	-9.60773400
H	0.65094900	7.42804800	-4.87541500
H	-0.14150800	9.75438400	-5.37326200
H	-1.75556800	11.25886100	-6.43948300
H	-3.79433500	11.61976700	-7.83369900
H	-5.01161900	9.64667800	-8.78935000
H	-4.18300400	7.35591100	-8.40837100
C	-0.29846300	3.64607700	-2.46788200
C	-1.60295300	5.71780800	-2.85207100
C	-0.92499100	3.57326900	-1.06556800

H	0.67714000	4.16258500	-2.39962000
H	-0.15910200	2.62912400	-2.86067100
C	-2.18923400	5.55466900	-1.43943300
H	-0.72026600	6.38044100	-2.80394000
H	-2.35092400	6.16246300	-3.52000000
H	-1.86092200	2.98749800	-1.13243300
H	-3.10290200	4.93188800	-1.51691700
N	-1.20536100	4.39052500	-3.37149000
O	-1.24162900	4.89358400	-0.58413700
C	-2.51577200	6.90686900	-0.81436300
H	-3.26650400	7.43395300	-1.42414800
H	-2.91781500	6.76818300	0.20099800
H	-1.60829000	7.52910300	-0.75280000
C	0.03034400	2.92838800	-0.06772400
H	-0.42755900	2.90059000	0.93304100
H	0.25875400	1.89773100	-0.38203500
H	0.97090700	3.49996400	-0.01021400
C	-3.33510600	1.43851700	-3.04999400
H	-2.86603200	2.43021000	-3.03350700
H	-3.09231500	0.88525400	-2.12971800
C	-4.79776400	1.50206400	-3.33897600
C	-5.35332100	2.63710100	-3.97148900
C	-5.64070400	0.40327300	-3.05919000
C	-6.71614500	2.67782000	-4.30597700
H	-4.70721900	3.48750900	-4.19521600
C	-7.00265300	0.44373600	-3.39245400
H	-5.21490200	-0.48352200	-2.58700500
C	-7.54665300	1.58117000	-4.01689200
H	-7.12921100	3.56595400	-4.79047300
H	-7.64177200	-0.41293100	-3.16542600
H	-8.60804200	1.61217500	-4.27335800
S	-2.36409800	0.47401200	-4.39383800
O	-2.91818500	-0.93675700	-4.31969800
O	-0.90265600	0.58076700	-3.81090800

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C	-0.10881000	-0.00684300	-6.98662500
C	-0.64237000	1.06246700	-7.74710400
C	-0.15762300	2.39913000	-7.61352500
H	-1.59979300	0.90134700	-8.24917200
C	-0.88623700	-1.29725800	-6.87287100
H	-0.70507900	3.19652400	-8.11761200
H	0.89350300	2.60646900	-7.40210500
Pd	-0.95356300	1.80791500	-5.69788300

P	-1.38547100	3.89041600	-4.96457000
O	-2.88571700	4.48274700	-5.42747000
O	-0.37582600	4.99103000	-5.76720400
C	-2.50404500	5.43214000	-7.60786500
C	-3.05941000	4.42607200	-6.81777700
C	-3.77254600	3.32196300	-7.34503400
C	-3.92353800	3.21268200	-8.71568700
C	-3.42861300	4.02913700	-11.00827200
C	-2.80721200	4.93101900	-11.85789300
C	-2.05505400	6.00995400	-11.31759900
C	-1.95407500	6.18604600	-9.94515300
C	-2.60002900	5.29078100	-9.03998300
C	-3.33285600	4.17134500	-9.59177800
C	-1.79379300	6.56424200	-6.94908700
C	-0.76139500	6.30128900	-6.04228900
C	-0.01122500	7.33205900	-5.41981600
C	-0.31565500	8.65428100	-5.68222300
C	-1.75366600	10.35525900	-6.78002300
C	-2.83348200	10.68090100	-7.58599300
C	-3.60773400	9.64736800	-8.18046700
C	-3.28297400	8.31325400	-7.98045200
C	-2.16267400	7.94036900	-7.17704700
C	-1.39849500	8.99373000	-6.54580900
H	-4.18716400	2.58622000	-6.65673600
H	-4.47793300	2.37574900	-9.14535400
H	-3.99446500	3.18404500	-11.40734200
H	-2.88315400	4.80898800	-12.94012900
H	-1.54759300	6.70540400	-11.98917100
H	-1.36926300	7.01285000	-9.54520200
H	0.79835000	7.05420200	-4.74436900
H	0.25916300	9.45719600	-5.21596400
H	-1.15889400	11.13619600	-6.30029300
H	-3.09831300	11.72633100	-7.75610600
H	-4.47176400	9.90470200	-8.79650700
H	-3.89305900	7.53460100	-8.43571800
C	-0.53540000	3.54753900	-2.42530400
C	-1.77370100	5.64103200	-2.86975100
C	-1.12104300	3.55998700	-1.00438500
H	0.45505300	4.03952500	-2.40908000
H	-0.43529700	2.50968700	-2.77323200
C	-2.32599200	5.56570800	-1.43684600
H	-0.86174400	6.26428600	-2.87322000
H	-2.51879600	6.08976300	-3.53783000
H	-2.07695200	3.00282700	-1.01504000

H	-3.26438600	4.97593500	-1.46101400
N	-1.44970000	4.27379300	-3.33969400
O	-1.38104700	4.91006800	-0.57455800
C	-2.58506100	6.95746500	-0.86893900
H	-3.33035300	7.48475900	-1.48513800
H	-2.96645100	6.88149900	0.16098100
H	-1.65345800	7.54590500	-0.85754200
C	-0.15637500	2.92849300	-0.00685700
H	-0.58315300	2.96097700	1.00749200
H	0.02837900	1.87789400	-0.28115700
H	0.80358300	3.46980700	-0.00399900
C	-3.49394400	1.24460900	-2.87436300
H	-3.01949400	2.23346200	-2.83345500
H	-3.32702300	0.69444000	-1.93551300
C	-4.92728000	1.31947400	-3.28155700
C	-5.39651100	2.42746800	-4.02269700
C	-5.81887200	0.25652600	-3.01615700
C	-6.72285800	2.47619800	-4.48017300
H	-4.71322100	3.25191100	-4.23297400
C	-7.14552100	0.30620600	-3.46994800
H	-5.46064300	-0.60967100	-2.45687300
C	-7.60310500	1.41534200	-4.20471500
H	-7.06817900	3.34287000	-5.04913300
H	-7.82417800	-0.52183900	-3.25179400
H	-8.63662400	1.45255600	-4.55634300
S	-2.43947500	0.27736600	-4.15028300
O	-2.94186300	-1.15483400	-4.05935200
O	-1.00069600	0.44931000	-3.53886900
C	1.30641100	-0.03458700	-6.52196400
C	2.35175800	0.41141300	-7.36346900
C	1.62576500	-0.55331900	-5.24569200
C	3.68490500	0.34962100	-6.93333700
H	2.11327600	0.78487700	-8.36039000
C	2.95873000	-0.60316700	-4.81664400
H	0.81758400	-0.85650000	-4.58097800
C	3.99273400	-0.15420800	-5.65784900
H	4.48320600	0.68821700	-7.59713400
H	3.19089800	-0.99046400	-3.82226900
H	5.03113900	-0.20050900	-5.32321400
H	-0.37231000	-2.09161700	-7.44320400
H	-0.94469800	-1.62974800	-5.82599300
H	-1.91121000	-1.18090800	-7.25353900