

Computational details

All density functional theory (DFT) calculations were performed using Gaussian 16.¹ The popular B3LYP²⁻³ method was chosen as the functional for all calculations. Geometry optimizations were carried out with Ahlrichs def2-SVP⁴ basis set in gas phase. Frequency calculations at the same level were carried out to confirm each stationary point to be either a minimum or a transition state geometry. The single-point energies were calculated at the level of B3LYP-D3⁵/def2-TZVP⁶ with Truhlar's SMD solvation model⁷. Tetrahydrofuran was chosen as the solvent to be consistent with the experiment. The electronic energies with ZPE and thermal free energies (at 298.15K) corrections are shown in kcal/mol.

Table S1. The free energies of different spin states for Fe species. The free energy of sextet and quintet spin state is chosen as the reference point for each kind of Fe species. (kcal/mol)

spin state	doublet	quartet	sextet
Fe(acac)₃	14.1	16.6	0.0
FeH(acac)₂	3.2	0.6	0.0
TS1	1.1	-4.5	0.0
FeO<i>t</i>Bu(acac)₂	28.8	17.2	0.0
spin state	singlet	triplet	quintet
Fe(acac)₂	42.4	18.4	0.0

Another two popular DFT functionals M06-2X⁸ and ω B97xD⁹ were also used to challenge the reliability of our computations for the energy difference between (**Z**)-**2a** and (**E**)-**2a**, and all the computational results are consistent with each other (see **Figure S1**). These results confirm that thermodynamics determines the selectivity.

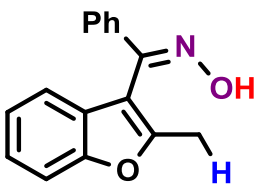
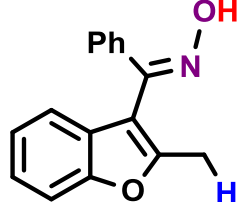
		
	(Z)-2a	(E)-2a
B3LYP-D3	0.0	1.0
M06-2X	0.0	1.3
ωB97-xD	0.0	1.1

Figure S1. The energy differences between **(Z)-2a** and **(E)-2a** by different DFT functionals. The free energy of **(Z)-2a** is chosen as the reference point. (kcal/mol)

Without NO radical catalyzing, the energy barrier for the isomerization is more than 50 kcal/mol (see **Figure S2**), this is in accordance with previous theoretical work.¹⁰ To the best of our knowledge, it is the first time to locate the transition state of NO-catalyzed *Z/E* oxime isomerization by computations.

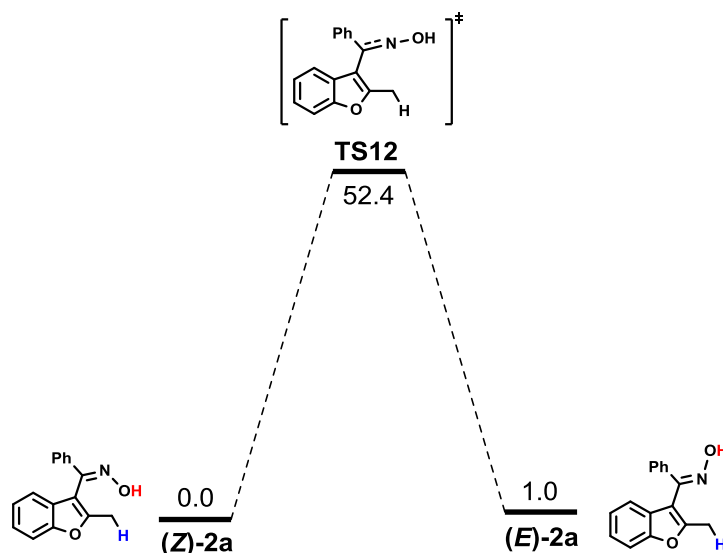


Figure S2. The energy barrier for the *Z/E* Oxime isomerization without NO catalyst. The free energy of **(Z)-2a** is chosen as the reference point. (kcal/mol)

Reference

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Cartesian Coordinates

Fe(acac)₃ (doublet)

Fe	0.08200700	-0.00024900	0.00006400
O	-1.28785800	0.55941100	-1.21488200
C	-1.98764400	1.61412500	-1.09324900
C	-3.07646100	1.77447100	-2.12958500
H	-3.71863500	0.87958600	-2.12353300
H	-3.69078000	2.66941500	-1.96447300
H	-2.61620300	1.82978600	-3.12944700
C	-1.80000500	2.60584300	-0.11381300
H	-2.47035400	3.46475000	-0.11757000
C	-0.73913700	2.59569400	0.81336900
O	0.13100100	1.67816600	0.92036700

C	-0.56001400	3.75710700	1.76414100
H	-0.61322200	3.38454900	2.79977100
H	0.44669900	4.18382100	1.62997900
H	-1.31247700	4.54373400	1.62080500
O	-1.28846600	-0.55721600	1.21532000
C	-1.99098100	-1.61019800	1.09395800
C	-3.07952900	-1.76795900	2.13093300
H	-3.72037900	-0.87211600	2.12434900
H	-3.69530800	-2.66209400	1.96686700
H	-2.61891000	-1.82305000	3.13062800
C	-1.80645200	-2.60203200	0.11408600
H	-2.47899900	-3.45922000	0.11780200
C	-0.74586000	-2.59416200	-0.81347900
O	0.12682500	-1.67901700	-0.91982200
C	-0.57004200	-3.75543200	-1.76500100
H	-0.62217900	-3.38194200	-2.80034800
H	0.43547400	-4.18509600	-1.63122900
H	-1.32473000	-4.54001800	-1.62221400
O	1.41104200	0.63238100	-1.24273200
C	2.67003400	0.55881500	-1.10433000
C	3.46851600	1.13439300	-2.25216500
H	3.16866900	2.18224700	-2.41248400
H	4.55213300	1.08503700	-2.08222500
H	3.21844000	0.58639800	-3.17490600
C	3.33744800	-0.00308600	-0.00045100
H	4.42678000	-0.00396100	-0.00061900
C	2.66945600	-0.56411100	1.10366200
O	1.41051300	-0.63572800	1.24244700
C	3.46755200	-1.14099400	2.25113900
H	3.21961700	-0.59186400	3.17378600
H	3.16530600	-2.18802500	2.41225900
H	4.55114400	-1.09430200	2.08026200

Fe(acac)₃ (quartet)

Fe	-0.14221400	-0.00181200	-0.00024900
O	-0.10421900	1.88913700	-0.86096300
C	0.80279700	2.75368300	-0.71846100
C	0.71384000	3.96951000	-1.61695100
H	-0.26447200	4.45492300	-1.47071700
H	1.51419200	4.69952300	-1.43562100
H	0.75101300	3.64028100	-2.66797600
C	1.86031800	2.65931600	0.21956300
H	2.58424800	3.47253800	0.26577900
C	1.99042600	1.61190700	1.14296700

O	1.22719600	0.59312500	1.22618100
C	3.09760400	1.64654100	2.17314700
H	2.65297900	1.64188700	3.18140800
H	3.70185600	0.72928600	2.08735600
H	3.74689200	2.52562600	2.06647200
O	-1.48546700	0.55240500	1.27415800
C	-2.74754600	0.49020700	1.13157100
C	-3.54158700	1.01280900	2.30553100
H	-3.25174600	2.05789500	2.49900700
H	-4.62588900	0.95626100	2.14362800
H	-3.27363100	0.43590300	3.20509700
C	-3.41494300	-0.01388300	0.00120600
H	-4.50417000	-0.01713200	0.00144400
C	-2.74500400	-0.51473700	-1.12916700
O	-1.48268400	-0.56945600	-1.27219700
C	-3.53647700	-1.04323800	-2.30223200
H	-3.27294800	-0.46514000	-3.20234000
H	-3.23994300	-2.08652400	-2.49528100
H	-4.62100700	-0.99370600	-2.13956400
O	1.22977900	-0.58336800	-1.22922000
C	2.00537300	-1.59288000	-1.14556700
C	3.11111000	-1.61584900	-2.17756300
H	3.70384500	-0.69082900	-2.09495500
H	3.77158100	-2.48645700	-2.07004000
H	2.66472600	-1.61916600	-3.18506300
C	1.88917600	-2.64024700	-0.22041600
H	2.62262800	-3.44490300	-0.26649900
C	0.83383000	-2.74599700	0.71898700
O	-0.08305500	-1.89204600	0.86150300
C	0.76013000	-3.96191500	1.61873500
H	0.79357600	-3.63118100	2.66940500
H	-0.21217700	-4.45948100	1.47328700
H	1.56932900	-4.68222100	1.43785400

Fe(acac)₃ (sextet)

Fe	0.00077000	-0.00239300	0.00083200
O	-0.92547600	1.37132200	-1.15985000
C	-1.00858900	2.63271600	-1.04894800
C	-1.78528500	3.33391600	-2.14048700
H	-1.31052800	3.12056500	-3.11187400
H	-2.80296700	2.91394800	-2.18591800
H	-1.84404800	4.42069500	-1.99402600
C	-0.43709200	3.38337800	-0.00230600
H	-0.57694300	4.46410900	-0.00326500

C	0.30652300	2.80474700	1.04543400
O	0.54736800	1.56396100	1.15838700
C	0.87888100	3.68238800	2.13563200
H	0.66073500	4.74827400	1.98633600
H	0.47217100	3.35814700	3.10722300
H	1.96964800	3.53382800	2.18300900
O	-1.62346600	-0.31237000	1.16567300
C	-2.58206400	-1.13623700	1.05300100
C	-3.62500000	-1.07723100	2.14623100
H	-3.13916100	-1.27250900	3.11595600
H	-4.03648400	-0.05638900	2.19760900
H	-4.44301900	-1.79460700	1.99716500
C	-2.71863500	-2.06611600	0.00317100
H	-3.58777700	-2.72346900	0.00279500
C	-1.78538400	-2.18835800	-1.04549100
O	-0.73149500	-1.49042100	-1.15728200
C	-2.01101000	-3.20901000	-2.13807500
H	-2.92512200	-3.79949100	-1.99064500
H	-2.06329700	-2.68949500	-3.10857900
H	-1.14153000	-3.88413600	-2.18625600
O	1.64956500	0.10692000	-1.16603200
C	2.78504300	-0.44842000	-1.05391200
C	3.77747400	-0.13145400	-2.14981900
H	3.35419400	-0.44418600	-3.11809200
H	3.91939800	0.95991200	-2.20345900
H	4.74971700	-0.62017000	-2.00184900
C	3.15361500	-1.31107500	-0.00245900
H	4.16036400	-1.72819600	-0.00299200
C	2.28356800	-1.66146100	1.04908700
O	1.08802500	-1.25130300	1.16222000
C	2.76139600	-2.58903100	2.14346000
H	3.79423900	-2.93113800	1.99451500
H	2.68384000	-2.06993900	3.11250400
H	2.08973800	-3.46092400	2.19616100

PMHS

Si	0.02385500	1.48174900	0.49861800
H	-0.22600900	1.68355100	1.95612000
C	-0.06451900	3.10285900	-0.42738200
H	-1.04459000	3.58712200	-0.28542000
H	0.71525000	3.79744300	-0.07491700
H	0.08411900	2.94113800	-1.50750500
O	1.53285000	0.83650500	0.31328600
O	-1.11054500	0.43333400	-0.09969000

Si	2.53103300	-0.46245700	-0.03922200
Si	-2.50683100	-0.48772900	-0.03504800
C	-3.96546500	0.59796100	-0.52732100
H	-4.09357300	1.43813000	0.17527900
H	-3.82040000	1.02142100	-1.53484400
H	-4.90667500	0.02280800	-0.53620800
C	-2.30001100	-1.90381800	-1.25685500
H	-1.44039500	-2.53918400	-0.98693800
H	-3.19707800	-2.54493800	-1.28325400
H	-2.12821700	-1.52165700	-2.27653300
C	-2.73881900	-1.14655700	1.71549200
H	-3.65063400	-1.76281900	1.79038900
H	-1.88484200	-1.77267500	2.02282100
H	-2.82981000	-0.32360700	2.44354700
C	4.29880000	0.11969200	0.23077100
H	4.53511900	0.97619900	-0.42172800
H	4.45371200	0.44027100	1.27405100
H	5.02341000	-0.68247600	0.01186800
C	2.11924700	-1.89194300	1.11899000
H	1.07675300	-2.22471100	0.98355800
H	2.77487200	-2.75946300	0.93378700
H	2.24369900	-1.59528000	2.17357200
C	2.26058800	-0.97068800	-1.83286900
H	2.89694800	-1.82824400	-2.10921900
H	1.21021000	-1.25797400	-2.00428600
H	2.49796000	-0.14067400	-2.51874200

FeH(acac)₂ (doublet)

Fe	-0.00372000	0.00007300	-0.07888400
O	1.30316200	1.36350100	0.10774800
C	2.56734100	1.23391000	0.01571400
C	3.35097200	2.52409900	0.05932800
H	3.13082600	3.05138000	1.00164500
H	4.43437200	2.36569900	-0.02319300
H	3.01291300	3.18117400	-0.75798700
C	3.23587600	-0.00006100	-0.08306100
H	4.32363400	-0.00011700	-0.14940100
C	2.56722800	-1.23394900	0.01584700
O	1.30303700	-1.36340400	0.10809200
C	3.35068000	-2.52425100	0.05917800
H	3.12888300	-3.05271100	1.00043200
H	3.01387100	-3.18026200	-0.75952800
H	4.43422400	-2.36589500	-0.02148000
O	-1.30317400	-1.36904200	-0.00831500

C	-2.57099800	-1.23558500	0.01912500
C	-3.35125300	-2.52806100	0.04699000
H	-3.03098300	-3.12790400	0.91393700
H	-4.43643900	-2.36788400	0.09506900
H	-3.10893900	-3.11682500	-0.85251600
C	-3.24354200	-0.00002700	0.02471800
H	-4.33315000	-0.00005500	0.04177000
C	-2.57107200	1.23557400	0.01900900
O	-1.30326600	1.36911600	-0.00862400
C	-3.35141200	2.52799700	0.04711400
H	-3.03235900	3.12692700	0.91515800
H	-3.10787700	3.11772400	-0.85141400
H	-4.43665400	2.36773900	0.09364600
H	0.20338800	-0.00012600	-1.53012300

FeH(acac)₂ (quartet)

Fe	-0.00001800	0.00002000	0.80602600
O	1.64041100	-1.00000400	0.91888200
C	2.75243400	-0.79013700	0.33591700
C	3.81157800	-1.83652900	0.59300500
H	3.42172500	-2.82449000	0.30028600
H	4.74612400	-1.63645400	0.05262900
H	4.01813600	-1.88385800	1.67443600
C	3.03940800	0.31299100	-0.49076500
H	4.03466800	0.38160200	-0.92904700
C	2.11205500	1.33617900	-0.76952700
O	0.92681300	1.37487600	-0.30988600
C	2.50777000	2.48968300	-1.66177600
H	1.81653600	2.53590100	-2.51883200
H	2.38530600	3.43316700	-1.10564800
H	3.53976200	2.41347800	-2.02912000
O	-1.64043300	1.00006800	0.91886800
C	-2.75243600	0.79014300	0.33585400
C	-3.81164400	1.83646000	0.59299400
H	-3.42164900	2.82454300	0.30089400
H	-4.74598300	1.63665600	0.05215400
H	-4.01866200	1.88327500	1.67436200
C	-3.03935500	-0.31297400	-0.49084700
H	-4.03459300	-0.38157500	-0.92918100
C	-2.11201400	-1.33620500	-0.76952000
O	-0.92680500	-1.37489900	-0.30980100
C	-2.50769600	-2.48971300	-1.66177200
H	-1.81630200	-2.53608200	-2.51868900
H	-2.38548900	-3.43317700	-1.10555700

H	-3.53960400	-2.41338300	-2.02933100
H	0.00001700	0.00015000	2.32808600

FeH(acac)₂ (sextet)

Fe	0.00003700	0.00000900	0.68615700
O	1.36722800	-1.36019500	0.14359700
C	2.58920900	-1.23593000	-0.18701500
C	3.34489900	-2.52743400	-0.39121700
H	2.83322500	-3.12686500	-1.16129400
H	4.39086100	-2.36860500	-0.68510500
H	3.31079700	-3.11437000	0.54085300
C	3.24016600	0.00002600	-0.36520800
H	4.29089700	0.00003600	-0.65366600
C	2.58915300	1.23597000	-0.18714000
O	1.36716900	1.36021500	0.14347200
C	3.34481300	2.52748800	-0.39136500
H	2.83306000	3.12693800	-1.16137100
H	3.31079500	3.11439500	0.54072900
H	4.39075200	2.36867800	-0.68534500
O	-1.36749000	1.36025000	0.14467900
C	-2.58913000	1.23594400	-0.18716100
C	-3.34491600	2.52742300	-0.39119000
H	-2.83086600	3.12897800	-1.15798400
H	-4.38976700	2.36858600	-0.68899500
H	-3.31458500	3.11221400	0.54238800
C	-3.23982500	-0.00003600	-0.36619300
H	-4.29026900	-0.00005200	-0.65569900
C	-2.58908500	-1.23599300	-0.18718800
O	-1.36743400	-1.36026300	0.14463400
C	-3.34478400	-2.52749700	-0.39137800
H	-2.83074100	-3.12889700	-1.15830100
H	-3.31434600	-3.11242900	0.54210600
H	-4.38966400	-2.36869200	-0.68909900
H	0.00011000	0.00002800	2.34996900

PMacacS

Si	0.16232500	-0.24384800	1.32435300
C	0.31093100	-0.72952000	3.11763500
H	1.22149400	-0.30205300	3.56661600
H	-0.55725500	-0.38076500	3.69896200
H	0.36824000	-1.82558700	3.21441000
O	-1.29129000	-0.72327900	0.75260200
O	1.44756600	-0.83987000	0.51490400
Si	-2.36605700	-1.56904200	-0.22026300

Si	2.83190300	-0.69319100	-0.42982700
C	4.12403800	-1.81509800	0.36156100
H	4.34451000	-1.50345900	1.39593500
H	3.77328000	-2.85992600	0.39373900
H	5.07016400	-1.79561600	-0.20535300
C	2.45797700	-1.25599100	-2.18170400
H	1.68810200	-0.60547300	-2.62358300
H	3.36274400	-1.21353100	-2.81150600
H	2.08355200	-2.29257800	-2.19690700
C	3.41675600	1.09625500	-0.40133300
H	4.35312800	1.21573900	-0.97215800
H	2.65551900	1.75525800	-0.84625100
H	3.60366000	1.43867400	0.62980700
C	-3.73090800	-0.37502200	-0.72680500
H	-4.21220200	0.07204300	0.15845300
H	-3.33193500	0.44554100	-1.34415000
H	-4.51125000	-0.89009500	-1.31198500
C	-1.46740500	-2.25252500	-1.72116300
H	-0.67253300	-2.95403100	-1.41969800
H	-2.15886800	-2.78956800	-2.39208200
H	-0.99504100	-1.43177300	-2.28281600
C	-3.08694600	-2.96269500	0.82404900
H	-3.83039500	-3.54486900	0.25372300
H	-2.29891900	-3.65926300	1.15514900
H	-3.58660500	-2.56812700	1.72416300
O	0.21605900	1.45600900	1.34779400
C	-0.46991600	2.52944300	0.96973500
C	-0.87454500	2.81183400	-0.30313600
H	-1.41261100	3.75151000	-0.44284000
C	-0.60653100	2.01870400	-1.50290300
O	-0.01361500	0.94378400	-1.49430600
C	-1.10241900	2.61298200	-2.81278700
H	-2.19537800	2.75748100	-2.77998800
H	-0.65308800	3.60579400	-2.98138300
H	-0.84393600	1.94638800	-3.64565700
C	-0.73212600	3.47450500	2.11028100
H	-1.33429900	2.96704800	2.88274900
H	0.22412500	3.74947600	2.58539500
H	-1.25180600	4.38650400	1.78903200
1a			
C	3.95918700	0.28874700	0.24594800
C	2.56914800	0.42357800	0.18750800
C	1.74338300	-0.71302600	-0.00982100

C	2.37515200	-1.96741900	-0.17399700
C	3.76041700	-2.09424000	-0.12405900
C	4.55569900	-0.96310600	0.09453200
H	4.55464700	1.18848500	0.41218900
H	1.74511600	-2.84564400	-0.32835500
H	4.22134000	-3.07675300	-0.24867200
H	5.64361500	-1.05400900	0.14065200
C	0.32039200	-0.62109400	-0.00403300
C	-0.89768300	-0.55966800	0.00928300
C	-2.32152100	-0.45196700	0.02802100
C	-3.13712700	-1.59902900	-0.08402300
C	-2.93790700	0.81214500	0.15999600
C	-4.52638900	-1.48132500	-0.06385500
H	-2.66693700	-2.57935100	-0.18577400
C	-4.32793400	0.91895800	0.17928200
H	-2.30992900	1.70151400	0.24500500
C	-5.12700800	-0.22445300	0.06776700
H	-5.14616400	-2.37739800	-0.15107700
H	-4.79271300	1.90286600	0.28246900
H	-6.21622600	-0.13622700	0.08348100
O	2.05832700	1.67767300	0.39465900
C	1.19811900	2.23619400	-0.50909500
H	1.08102900	1.68040200	-1.44523900
C	0.58617100	3.39785900	-0.27034200
H	0.72512500	3.92848400	0.67406400
H	-0.05810200	3.83332600	-1.03469700

TS1 (doublet)

C	1.06492200	3.65015400	-0.05551000
C	1.72544700	2.42058000	-0.00734600
C	3.10209600	2.32080300	-0.33074500
C	3.77147700	3.50220500	-0.72455200
C	3.10952900	4.72586400	-0.77836200
C	1.75392800	4.80205500	-0.43738300
H	0.00518800	3.67313900	0.20709400
H	4.83178100	3.43576700	-0.97611300
H	3.65259500	5.62385800	-1.08177600
H	1.22910000	5.75969400	-0.47512100
C	3.81146500	1.08791700	-0.23115700
C	4.43624600	0.04405500	-0.14199000
C	5.14559600	-1.19032500	-0.03066900
C	6.52784200	-1.25833200	-0.31093900
C	4.47225000	-2.36762600	0.36373400
C	7.21164900	-2.46827500	-0.19871300

H	7.05484900	-0.35190000	-0.61597100
C	5.16497100	-3.57260900	0.47306200
H	3.40312000	-2.32007200	0.58061100
C	6.53487300	-3.62856300	0.19307100
H	8.28165500	-2.50680200	-0.41829500
H	4.63206600	-4.47626000	0.77977400
H	7.07433600	-4.57500000	0.28023100
O	0.99968300	1.33840900	0.42587000
C	0.88239100	0.23090600	-0.35365500
H	1.30268700	0.30921900	-1.36080500
C	0.12760100	-0.82532700	0.06763200
H	-0.12677300	-0.91689000	1.12543800
H	0.16067100	-1.74154800	-0.52471400
Fe	-2.93412000	-0.42985800	0.08309200
O	-3.30053600	1.13976000	-0.92643100
C	-3.24822000	2.34546700	-0.52131600
C	-3.61852000	3.38762400	-1.55231800
H	-4.64363200	3.19711000	-1.90919200
H	-3.55564600	4.41306900	-1.16393400
H	-2.95563500	3.28662400	-2.42679100
C	-2.88090200	2.74006100	0.78040300
H	-2.86612200	3.80468200	1.01547300
C	-2.55897800	1.82414400	1.80202600
O	-2.57331300	0.55767600	1.67095400
C	-2.15468400	2.32600000	3.16877600
H	-2.74581400	1.80805200	3.93995900
H	-1.09784400	2.06513200	3.34500800
H	-2.27682600	3.41213600	3.27736200
O	-2.80519800	-2.00719500	1.15428700
C	-2.91159100	-3.21366600	0.75910600
C	-2.72429800	-4.26292500	1.83171900
H	-3.48984900	-4.12390500	2.61253800
H	-2.79033800	-5.28728900	1.44121800
H	-1.74676900	-4.11895300	2.31928800
C	-3.20505100	-3.60172100	-0.56212400
H	-3.27357300	-4.66629900	-0.78635000
C	-3.49561500	-2.68141500	-1.58876900
O	-3.46345500	-1.41565900	-1.45906900
C	-3.90672000	-3.17920900	-2.95593300
H	-4.92282800	-2.81760000	-3.18348400
H	-3.23924800	-2.74562000	-3.71777900
H	-3.88812900	-4.27453700	-3.03391500
H	-1.40555900	-0.54047500	-0.28333200

TS1 (quartet)

C	1. 26085200	3. 41539900	-0. 36284000
C	1. 94264800	2. 20610400	-0. 21676200
C	3. 31640000	2. 09686500	-0. 54636000
C	3. 96279400	3. 24807900	-1. 05177800
C	3. 28018500	4. 45191000	-1. 20508400
C	1. 92773700	4. 53864000	-0. 85459500
H	0. 20495500	3. 45020700	-0. 08544300
H	5. 02097900	3. 17544200	-1. 31028600
H	3. 80526300	5. 32740800	-1. 59387300
H	1. 38771800	5. 48148100	-0. 96940700
C	4. 04223500	0. 88562900	-0. 34809800
C	4. 67667000	-0. 14183400	-0. 17543000
C	5. 40081100	-1. 35484300	0. 03378600
C	6. 77990100	-1. 43290500	-0. 25909700
C	4. 74598200	-2. 49965500	0. 53924600
C	7. 47877600	-2. 62132700	-0. 05105800
H	7. 29249900	-0. 55142800	-0. 64976000
C	5. 45372500	-3. 68333900	0. 74372400
H	3. 67937900	-2. 44467100	0. 76661800
C	6. 82033000	-3. 74955500	0. 45029200
H	8. 54613600	-2. 66815100	-0. 28152600
H	4. 93521400	-4. 56193100	1. 13589200
H	7. 37158600	-4. 67917600	0. 61232200
O	1. 24109800	1. 15157000	0. 32163400
C	1. 11110800	-0. 00908500	-0. 36915800
H	1. 55014000	-0. 01797900	-1. 37163500
C	0. 37337600	-1. 03230000	0. 12964500
H	0. 04487600	-1. 01553800	1. 17003900
H	0. 36164200	-1. 97866300	-0. 41219400
Fe	-2. 82206000	-0. 34082100	0. 04567500
O	-3. 51182500	1. 47835200	-0. 48946300
C	-3. 36319700	2. 60525200	0. 07794300
C	-4. 05532300	3. 77453700	-0. 58883500
H	-5. 14125100	3. 58571100	-0. 60709200
H	-3. 86434400	4. 73242600	-0. 08616300
H	-3. 72912800	3. 83774000	-1. 63942100
C	-2. 61262700	2. 81577200	1. 25280600
H	-2. 53617500	3. 83054400	1. 64415800
C	-1. 98012800	1. 77498000	1. 96938600
O	-2. 02573300	0. 54823900	1. 65031700
C	-1. 17413600	2. 09913300	3. 20770800
H	-1. 48448500	1. 43559100	4. 02977000
H	-0. 11291200	1. 88307100	3. 00020600

H	-1.27216700	3.14740000	3.52097500
O	-3.58492800	-1.91612400	1.02852400
C	-4.12841000	-2.96943400	0.56627400
C	-4.62381900	-3.95978200	1.59742200
H	-5.37944600	-3.47034000	2.23353100
H	-5.05803800	-4.86458900	1.15103700
H	-3.78914700	-4.24138700	2.25957000
C	-4.28816000	-3.24938800	-0.80500200
H	-4.75817600	-4.19117700	-1.08854000
C	-3.89284700	-2.36584900	-1.83300900
O	-3.34468400	-1.23682100	-1.64563600
C	-4.13057800	-2.74490600	-3.27917500
H	-4.76067600	-1.97625200	-3.75527400
H	-3.16912500	-2.74416300	-3.81786200
H	-4.60911500	-3.72714500	-3.39121300
H	-1.29988500	-0.68341800	-0.30669700

TS1 (sextet)

C	1.43276200	3.53132700	0.12790200
C	2.01999200	2.26503500	0.04435400
C	3.42376600	2.13019600	-0.11425300
C	4.19319500	3.31299400	-0.20790900
C	3.60321600	4.57135400	-0.13053500
C	2.21853000	4.68090700	0.04473300
H	0.34910100	3.58434900	0.25187500
H	5.27380800	3.21623500	-0.33051000
H	4.22328400	5.46792700	-0.20168400
H	1.74722600	5.66478400	0.10841600
C	4.06524900	0.85693800	-0.13684100
C	4.64014200	-0.21882200	-0.14704500
C	5.28091900	-1.49482100	-0.15786600
C	6.68609700	-1.59995400	-0.24842300
C	4.51391600	-2.67827400	-0.07764600
C	7.30106900	-2.85137700	-0.25794100
H	7.28539900	-0.68920800	-0.31037900
C	5.13830100	-3.92482300	-0.08775500
H	3.42687400	-2.60111700	-0.00879600
C	6.53174000	-4.01733500	-0.17773100
H	8.38979200	-2.91810900	-0.32824800
H	4.53298200	-4.83278200	-0.02473000
H	7.01732600	-4.99640600	-0.18531000
O	1.18819000	1.18696000	0.18358800
C	1.17678500	0.19472800	-0.75843500
H	1.69601300	0.42452200	-1.69323900

C	0.39267400	-0.90689500	-0.58148500
H	0.02753400	-1.16811800	0.41359300
H	0.47146900	-1.71355600	-1.31142600
Fe	-2.76685200	-0.33690400	-0.22116900
O	-3.18830000	1.42588300	-1.12208800
C	-3.04782700	2.61127600	-0.69129500
C	-3.40440000	3.71150900	-1.66549700
H	-4.45576200	3.59163200	-1.97331800
H	-3.25903300	4.71776600	-1.25022600
H	-2.79368200	3.59825500	-2.57568800
C	-2.59404300	2.94299800	0.60416800
H	-2.51107300	3.99741500	0.86809000
C	-2.26064100	1.98307400	1.58165100
O	-2.34829500	0.72498900	1.41782700
C	-1.75394200	2.42876800	2.93329300
H	-2.34879400	1.94467400	3.72364800
H	-0.71632600	2.07531300	3.05141100
H	-1.78127900	3.51880500	3.06421000
O	-2.48560900	-2.07812300	0.80605300
C	-3.18960800	-3.13381000	0.82615200
C	-2.67197000	-4.25590800	1.69770300
H	-2.57189100	-3.89039100	2.73244700
H	-3.31841300	-5.14352400	1.68467100
H	-1.66028000	-4.53594600	1.36201700
C	-4.38803400	-3.30762600	0.10055400
H	-4.91239900	-4.25879400	0.19010700
C	-4.93952200	-2.31972400	-0.73724300
O	-4.43476300	-1.16630600	-0.92776300
C	-6.22259200	-2.59842400	-1.48571500
H	-6.97556600	-1.84463700	-1.20393500
H	-6.04299200	-2.47666200	-2.56616800
H	-6.62184500	-3.60298800	-1.29274000
H	-1.25774300	-0.59702700	-1.08600500

Fe(acac)₂ (singlet)

Fe	0.00025900	0.00086700	0.73908700
O	1.63561600	0.92447800	1.02755700
C	2.74199800	0.68960500	0.44563900
C	3.88884100	1.59945100	0.81862800
H	4.06158100	1.54287800	1.90579800
H	4.81921900	1.34873200	0.29202000
H	3.61363500	2.64280500	0.59465200
C	2.93688800	-0.35488100	-0.48307900
H	3.92321400	-0.46644900	-0.93355900

C	1.94834700	-1.29717800	-0.81626700
O	0.74931400	-1.29948500	-0.37032900
C	2.27183400	-2.43411200	-1.75742700
H	2.08254400	-3.39371500	-1.24970100
H	1.59181500	-2.39444300	-2.62383500
H	3.31121500	-2.40981000	-2.11047300
O	-1.63464900	-0.92367300	1.02876300
C	-2.74110600	-0.69007700	0.44669100
C	-3.88705900	-1.60119600	0.81947200
H	-4.05760900	-1.54774400	1.90711400
H	-4.81849000	-1.34936100	0.29527400
H	-3.61204100	-2.64386100	0.59199900
C	-2.93709300	0.35399100	-0.48235900
H	-3.92355200	0.46446400	-0.93280300
C	-1.94945700	1.29700400	-0.81597000
O	-0.75032900	1.30042000	-0.37025400
C	-2.27401500	2.43325000	-1.75761100
H	-2.08535600	3.39324400	-1.25037900
H	-1.59414600	2.39370400	-2.62415500
H	-3.31345200	2.40794600	-2.11041600

Fe(acac)₂ (triplet)

Fe	0.00002700	-0.00002300	0.00061900
O	1.33080700	-1.38457900	0.00024100
C	2.59440600	-1.23976000	-0.00035100
C	3.38912100	-2.52464000	-0.00273600
H	3.11141400	-3.11891300	-0.88825200
H	4.47411000	-2.35647700	-0.00142100
H	3.10978800	-3.12351500	0.87912700
C	3.26382400	-0.00005100	0.00102800
H	4.35351100	0.00004100	0.00135200
C	2.59438000	1.23973100	0.00115200
O	1.33094900	1.38445300	0.00011300
C	3.38929000	2.52456100	0.00033300
H	3.12325000	3.11268400	-0.89296100
H	3.09857300	3.12954000	0.87416600
H	4.47414200	2.35633800	0.01601200
O	-1.33079100	1.38457300	0.00099900
C	-2.59439500	1.23981700	-0.00024200
C	-3.38909300	2.52473600	-0.00276000
H	-3.11159400	3.11881800	-0.88848500
H	-4.47408200	2.35657800	-0.00121000
H	-3.10956100	3.12382900	0.87888900
C	-3.26386200	0.00007700	0.00049900

H	-4.35355000	0.00002000	0.00014100
C	-2.59441600	-1.23975500	0.00123600
O	-1.33093700	-1.38454400	0.00112100
C	-3.38936600	-2.52455700	0.00019100
H	-3.12284600	-3.11284800	-0.89285100
H	-3.09920400	-3.12942100	0.87429300
H	-4.47421800	-2.35626100	0.01520900

Fe(acac)₂ (quintet)

Fe	0.00000000	-0.00000600	0.00021000
O	1.39051700	-0.99077400	-0.99039600
C	2.65583800	-0.88336100	-0.88250700
C	3.46763600	-1.78541500	-1.78372900
H	3.19931800	-1.58493400	-2.83377700
H	4.55061000	-1.65761000	-1.65497200
H	3.19813200	-2.83516000	-1.58330700
C	3.31242000	0.00008600	0.00035900
H	4.40241800	0.00014500	0.00037700
C	2.65569200	0.88328400	0.88337700
O	1.39035700	0.99062700	0.99103900
C	3.46733400	1.78519400	1.78487000
H	3.19763600	2.83497400	1.58489500
H	3.19909200	1.58423200	2.83484600
H	4.55032400	1.65762600	1.65602300
O	-1.39014500	0.99073200	-0.99094400
C	-2.65550600	0.88329600	-0.88355500
C	-3.46696500	1.78547500	-1.78495700
H	-3.19825300	1.58511800	-2.83492500
H	-4.54998700	1.65766600	-1.65661300
H	-3.19753300	2.83519800	-1.58431000
C	-3.31242000	-0.00009500	-0.00087800
H	-4.40241800	-0.00009900	-0.00121500
C	-2.65602300	-0.88329600	0.88238300
O	-1.39072900	-0.99063500	0.99052400
C	-3.46800500	-1.78515500	1.78362100
H	-3.19825700	-2.83494900	1.58378200
H	-3.20013200	-1.58415900	2.83368400
H	-4.55094600	-1.65757000	1.65438400

tBuONO

C	-0.74978300	0.00678100	-0.00000400
C	-0.91473300	0.84627400	-1.27021300
H	-1.93645900	1.25305700	-1.32552100
H	-0.20739300	1.68792800	-1.28435700

H	-0.74074700	0.22937400	-2.16528200
C	-0.91477700	0.84687300	1.26980200
H	-1.93650700	1.25367600	1.32488700
H	-0.74081300	0.23039700	2.16516900
H	-0.20744200	1.68853800	1.28356900
C	-1.69948800	-1.19104100	0.00026200
H	-1.53629400	-1.81536700	-0.89092200
H	-1.53632200	-1.81494900	0.89174300
H	-2.74522100	-0.84713600	0.00016500
O	0.57480500	-0.62387100	0.00017300
N	1.62085200	0.29467100	-0.00003500
O	2.66443500	-0.24882100	0.00004100

B

C	-3.98669100	0.18257500	-0.22433700
C	-2.60397900	0.38206900	-0.15700300
C	-1.72649400	-0.72254000	0.00448200
C	-2.29972500	-2.00981300	0.12013000
C	-3.67766700	-2.20012800	0.06279700
C	-4.52423200	-1.10000500	-0.11838500
H	-4.62344100	1.05892700	-0.35930600
H	-1.62967600	-2.86312400	0.24294300
H	-4.09197200	-3.20695000	0.15190300
H	-5.60679900	-1.23969800	-0.17008300
C	-0.30710600	-0.57821800	0.00022000
C	0.91132600	-0.51280500	-0.01596000
C	2.33739800	-0.43391200	-0.03214000
C	3.12280400	-1.59150200	0.16372800
C	2.99138000	0.79987800	-0.24419600
C	4.51474100	-1.51296200	0.14764400
H	2.62572900	-2.54976500	0.32803000
C	4.38390500	0.86886000	-0.25857600
H	2.39277300	1.69990600	-0.39769900
C	5.15106100	-0.28478900	-0.06309100
H	5.10868200	-2.41767600	0.30064700
H	4.87525500	1.83099600	-0.42443000
H	6.24231000	-0.22692900	-0.07533900
O	-2.14972000	1.66095600	-0.31302400
C	-1.35595100	2.24813900	0.64238800
H	-1.04084200	1.61375700	1.47491400
C	-0.58450200	3.42714800	0.18280500
H	-1.23024700	4.13097500	-0.37011500
H	-0.14748400	3.95796300	1.04209300
H	0.24586200	3.15198700	-0.50241000

TS2

C	-1.09932800	2.01204800	-0.48045700
C	-0.36173300	-0.17753200	-0.05630200
C	-1.75251000	-0.55267400	-0.02772700
C	-2.74235400	0.45539900	0.00060700
C	-4.10131900	0.13857300	0.06357500
C	-4.49007900	-1.20114600	0.09895300
C	-3.52835100	-2.22002700	0.07096500
C	-2.17320500	-1.89668200	0.01290500
H	-4.83091700	0.95026200	0.08479500
H	-5.55272200	-1.45231000	0.14543000
H	-3.83711900	-3.26758800	0.09511500
H	-1.41468600	-2.68209100	-0.00164600
H	-1.00071100	1.85940500	-1.56365900
C	-0.35362400	3.10913900	0.18575200
H	0.68688700	3.12829000	-0.17309700
H	-0.79878200	4.10298700	-0.02307700
H	-0.34762000	2.97291400	1.27901500
C	0.86593800	-0.32781600	-0.01829000
C	2.28569600	-0.35336700	0.00208100
C	3.02740400	-0.46597300	-1.19971000
C	2.99642700	-0.27279800	1.22497400
C	4.42022000	-0.49353200	-1.17353500
H	2.49163500	-0.53208500	-2.14902200
C	4.38929100	-0.30031100	1.23863200
H	2.43625000	-0.18867400	2.15858000
C	5.10886100	-0.41057300	0.04259500
H	4.97567300	-0.58072500	-2.11105800
H	4.92063500	-0.23592200	2.19182900
H	6.20130900	-0.43275600	0.05834300
O	-2.35973000	1.76274000	0.01229300

C

C	-1.61722100	-0.43654000	-0.03139100
C	-2.77862600	0.34245700	-0.16416800
C	-4.05278700	-0.21564400	-0.06608800
C	-4.13876900	-1.59262900	0.17365900
C	-2.98823800	-2.38453800	0.31122300
C	-1.71703500	-1.80826400	0.21049800
C	-1.09463900	1.86244200	-0.44882400
H	-4.94143200	0.40875600	-0.17385000
H	-5.12478100	-2.05775000	0.25416500
H	-3.08684800	-3.45640900	0.49749500

H	-0.81464400	-2.41556100	0.31676200
H	-0.86159100	2.18492700	-1.47895000
C	-0.69404600	2.94404300	0.54026500
H	0.38919300	3.12948500	0.47447300
H	-1.22634600	3.88183800	0.31976400
H	-0.93485200	2.63531300	1.56895400
C	-0.46503400	0.47336900	-0.18344300
C	0.81984600	0.21440900	-0.11628900
C	2.17158000	-0.05119700	-0.06023400
C	2.91001800	-0.41686400	-1.23781500
C	2.89862900	0.02528800	1.17711200
C	4.26943900	-0.68155900	-1.16915900
H	2.37907100	-0.48365000	-2.18968300
C	4.25819900	-0.24417300	1.21914000
H	2.35861400	0.29921400	2.08582000
C	4.95789400	-0.59890600	0.05316900
H	4.80945100	-0.95802500	-2.07878000
H	4.78945300	-0.17952600	2.17257400
H	6.02896000	-0.80941400	0.09674000
O	-2.52493700	1.65383000	-0.38892600

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Fe	0.01189500	-0.03687600	-0.47607400
O	-1.83688200	0.14193600	-1.03327900
C	-2.67130100	1.04511500	-0.70148200
C	-4.09365200	0.80348700	-1.14739800
H	-4.43280000	-0.17214100	-0.76419300
H	-4.78331800	1.58994500	-0.81350500
H	-4.12085100	0.73912200	-2.24734800
C	-2.33741400	2.21431500	0.00014200
H	-3.12709200	2.92640600	0.23753500
C	-1.00578600	2.56003100	0.30367400
O	0.00766100	1.83136400	0.06933200
C	-0.70223200	3.90655700	0.91916300
H	-0.15843500	3.75889200	1.86581500
H	-0.03252800	4.47028500	0.24974700
H	-1.60688200	4.49955600	1.10744500
O	-0.41515700	-0.52675000	1.29878400
C	-0.60676800	-1.72997200	1.69284900
C	-0.90066700	-1.85602700	3.16913300
H	-1.77520500	-1.23486600	3.42007900
H	-1.08867300	-2.89352000	3.47442600
H	-0.04967700	-1.45546400	3.74327400
C	-0.56261600	-2.87317300	0.88415500

H	-0.74749600	-3.83794500	1.35521000
C	-0.29863800	-2.85316100	-0.50592400
O	-0.06393400	-1.80907900	-1.18004600
C	-0.28512500	-4.14570200	-1.28740600
H	-1.01675000	-4.07907600	-2.10820300
H	0.70553600	-4.27423400	-1.75206600
H	-0.51227900	-5.02085900	-0.66478100
O	1.76404700	-0.04722900	-0.73559200
C	2.89266000	0.62609500	-0.20875600
C	3.04206300	1.99961700	-0.88703900
H	3.96599200	2.50438600	-0.55985300
H	3.08687000	1.87353200	-1.98047700
H	2.18302000	2.63961200	-0.64661000
C	2.77831600	0.77459500	1.31778500
H	1.90557900	1.38491800	1.58517300
H	2.66579600	-0.21528800	1.78739600
H	3.68299700	1.25006000	1.73055800
C	4.10156100	-0.26263100	-0.55730500
H	3.98629300	-1.25604700	-0.09670400
H	4.16840100	-0.39970300	-1.64761400
H	5.04393300	0.18439900	-0.20052000

NO

N	0.00000000	0.00000000	-0.61253700
O	0.00000000	0.00000000	0.53597000

TS3

C	-1.93884500	-0.44931800	0.00664600
C	-3.07947500	0.34174700	-0.21084800
C	-4.36685700	-0.18834500	-0.12793000
C	-4.48761600	-1.54786600	0.18508600
C	-3.35814100	-2.35077100	0.40784600
C	-2.07322700	-1.80359800	0.31928700
C	-1.35540400	1.82194900	-0.46908900
H	-5.23911300	0.44402500	-0.30253600
H	-5.48465400	-1.99041400	0.25666800
H	-3.48401800	-3.40830600	0.65097200
H	-1.18682700	-2.41985400	0.48930900
H	-1.05302900	2.15287000	-1.47732100
C	-1.01228300	2.88927300	0.55770200
H	0.07668200	3.04133400	0.58337100
H	-1.50331800	3.84004100	0.30041300
H	-1.34653500	2.57943500	1.55978900
C	-0.76605600	0.42842900	-0.17021000

C	0. 51093300	0. 11712600	-0. 10053100
C	1. 70260300	-0. 54232800	-0. 01383700
C	2. 32533100	-1. 14836500	-1. 17199000
C	2. 55078500	-0. 32654100	1. 15856300
C	3. 65224200	-1. 48529900	-1. 15655400
H	1. 71792400	-1. 30079800	-2. 06652500
C	3. 89218100	-0. 79294100	1. 16140800
H	2. 06893600	-0. 04714600	2. 09647200
C	4. 45671100	-1. 29811300	0. 01454500
H	4. 10745200	-1. 92353100	-2. 04896800
H	4. 48442700	-0. 69727400	2. 07517500
H	5. 50660700	-1. 59974900	-0. 00123500
O	-2. 79139400	1. 63149800	-0. 50268200
N	2. 48192800	1. 60125100	0. 37592200
O	3. 29697900	1. 88479900	-0. 38326800

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C	-1. 32754400	-0. 48750700	0. 01974400
C	-2. 70585800	-0. 23547900	-0. 17294900
C	-3. 66477900	-1. 24998500	-0. 10387100
C	-3. 21396600	-2. 53907900	0. 18014300
C	-1. 84841200	-2. 81326200	0. 39325200
C	-0. 89979500	-1. 79730500	0. 31307500
C	-1. 75437400	1. 82444800	-0. 30380200
H	-4. 72047300	-1. 02498600	-0. 26255200
H	-3. 93942400	-3. 35448900	0. 24308300
H	-1. 53274000	-3. 83322500	0. 62251500
H	0. 15604600	-2. 01104900	0. 47695600
H	-1. 63424100	2. 38294500	-1. 24343400
C	-1. 91672200	2. 79304200	0. 86416100
H	-1. 03961700	3. 45108500	0. 91562800
H	-2. 82168500	3. 40068400	0. 71470300
H	-2. 01537200	2. 24412600	1. 81338700
C	-0. 64675900	0. 78245200	-0. 14110100
C	0. 69324200	1. 08268700	-0. 16718400
C	1. 81539400	0. 11010300	-0. 06926900
C	2. 04875200	-0. 82181600	-1. 09477500
C	2. 70199400	0. 15297900	1. 02024700
C	3. 12692700	-1. 70754600	-1. 02119500
H	1. 37827200	-0. 84975700	-1. 95757500
C	3. 77869800	-0. 73344200	1. 09443900
H	2. 54390800	0. 88585000	1. 81418700
C	3. 99302100	-1. 66717500	0. 07571300
H	3. 29401200	-2. 42773900	-1. 82635400

H	4.45731700	-0.69146100	1.95024900
H	4.83788200	-2.35828800	0.13362700
N	0.96255200	2.46130500	-0.36201500
O	2.13448700	2.79683100	-0.35079200
O	-2.98206800	1.05297900	-0.42171900

TS4

C	-1.22669700	-0.64337700	-0.01958400
C	-2.61631100	-0.37556000	0.02976600
C	-3.58347100	-1.36277400	-0.17998500
C	-3.12343900	-2.65293600	-0.43205100
C	-1.74259100	-2.94676800	-0.49328900
C	-0.78827100	-1.95573000	-0.29712500
C	-1.63401600	1.60342300	0.35118100
H	-4.64644500	-1.11943200	-0.14309500
H	-3.84737100	-3.45636500	-0.59000000
H	-1.42348500	-3.97038300	-0.70198100
H	0.27659900	-2.18452800	-0.35305100
H	-1.28290900	2.30052100	-0.63565800
C	-1.66081200	2.67047200	1.43307400
H	-0.72436800	3.24274100	1.41603400
H	-2.49619500	3.36421400	1.25683600
H	-1.78811600	2.21006500	2.42526100
C	-0.57627000	0.62577700	0.19893900
C	0.74472600	1.04588000	-0.18333500
C	1.96785300	0.23684500	-0.00636500
C	3.04847200	0.33990100	-0.90425800
C	2.09386900	-0.62269600	1.10104000
C	4.21370800	-0.39764200	-0.69780800
H	2.95399000	1.00408700	-1.76455200
C	3.26019900	-1.36550200	1.30053400
H	1.27520200	-0.69636900	1.82137200
C	4.32524100	-1.25687500	0.40193800
H	5.04128200	-0.30796500	-1.40647800
H	3.33990000	-2.02485600	2.16880300
H	5.23852900	-1.83663400	0.55778100
N	0.82626800	2.11845300	-0.97902900
O	-0.11767900	2.95060000	-1.11953900
O	-2.87152400	0.92328900	0.26777700

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C	-1.30043600	-0.50348800	-0.27021800
C	-2.58049300	-0.31789100	0.28697900
C	-3.59917600	-1.26338400	0.21353300

C	-3.30203500	-2.45085100	-0.45951600
C	-2.03237200	-2.66513300	-1.03173000
C	-1.02462200	-1.70398900	-0.94705600
H	-4.57738700	-1.07562200	0.65973700
H	-4.06839600	-3.22506000	-0.54513900
H	-1.83501700	-3.60478000	-1.55365800
H	-0.04493600	-1.88141000	-1.39509600
C	-0.57216600	0.72078300	0.02431800
C	0.81766700	1.04638600	-0.36547000
C	1.92560700	0.11279900	-0.01368400
C	3.14296300	0.14162200	-0.72230400
C	1.78763100	-0.79837300	1.04818500
C	4.18817200	-0.71192400	-0.37341600
H	3.25158200	0.84408600	-1.54978200
C	2.83749200	-1.65278300	1.39604300
H	0.85342500	-0.83209000	1.61180300
C	4.04075000	-1.61384400	0.68757300
H	5.12466000	-0.67871900	-0.93649300
H	2.71226800	-2.35175900	2.22700500
H	4.86023100	-2.28509500	0.95712400
N	1.15969000	2.10570500	-1.02052200
O	0.10057200	2.92146600	-1.36862600
O	-2.65604600	0.90422400	0.88822000
C	-1.44637200	1.51937400	0.71878300
C	-1.31838100	2.87642200	1.30780200
H	-0.26632300	3.18508500	1.33991100
H	-1.86816600	3.61623000	0.70197400
H	-1.73634300	2.89527700	2.32673400
H	0.53498500	3.63404100	-1.85616300

TS5

C	-1.87267300	-0.33321500	-0.00551400
C	-3.05704300	0.40570500	-0.16487000
C	-4.31417000	-0.18663200	-0.05145200
C	-4.35904700	-1.55759900	0.23074700
C	-3.18530000	-2.30984400	0.39307900
C	-1.93159400	-1.69939400	0.27654400
C	-1.41773900	1.96292600	-0.50107700
H	-5.22089000	0.40691200	-0.18062500
H	-5.33080400	-2.04951600	0.32463500
H	-3.25229500	-3.37817800	0.61122000
H	-1.00941900	-2.27201900	0.39727100
H	-1.19338300	2.25171800	-1.54329000
C	-1.04990600	3.09467300	0.44365300

H	0.02714000	3.31041700	0.36970600
H	-1.60963200	4.00655500	0.18550000
H	-1.28316600	2.82072600	1.48388400
C	-0.75093400	0.60354900	-0.18325000
C	0.54577600	0.39371600	-0.10558100
C	1.90520300	0.49093400	-0.08256300
C	2.63545900	0.78755700	1.13269800
C	2.67273700	-0.06944300	-1.19735800
C	3.97814700	0.53664200	1.22104800
H	2.08146100	1.18343800	1.98636300
C	4.08301200	-0.20521800	-1.09182000
H	2.19328200	-0.12098000	-2.17577200
C	4.71760700	0.02322900	0.10536100
H	4.50528300	0.74712100	2.15564800
H	4.64895200	-0.54455900	-1.96332400
H	5.79299400	-0.14190800	0.20428900
O	-2.84157400	1.71630000	-0.43225500
N	1.74861000	-1.78281700	-0.48503800
O	2.31820000	-2.38698900	0.30999200

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C	1.92804800	0.27752500	-0.04751300
C	2.62649500	-0.94964400	-0.09880900
C	4.02026700	-1.01527700	-0.16485200
C	4.71716000	0.19308300	-0.17551100
C	4.04535100	1.43035200	-0.12309700
C	2.65563400	1.48445000	-0.06063300
C	0.45266100	-1.57542500	0.04498100
H	4.52743000	-1.98041100	-0.20540700
H	5.80914500	0.17740200	-0.22590100
H	4.62290500	2.35726700	-0.13296300
H	2.11812000	2.43036100	-0.02135400
H	-0.09853300	-1.98696700	-0.81512400
C	-0.12176900	-2.13554300	1.34471900
H	-1.18353300	-1.87135600	1.44289600
H	-0.02607100	-3.23129700	1.34477400
H	0.42636200	-1.73409100	2.21043500
C	0.51212400	-0.05146700	-0.01431500
C	-0.59631400	0.76494100	-0.01206900
C	-2.00381000	0.28302900	-0.09815000
C	-2.93218100	0.58840000	0.91364200
C	-2.44585800	-0.44092700	-1.21917300
C	-4.25536100	0.15290800	0.81884300
H	-2.61164200	1.16825200	1.78095500

C	-3.77023100	-0.87701300	-1.31393600
H	-1.74877600	-0.64920300	-2.03540800
C	-4.67791600	-0.58411600	-0.29238300
H	-4.96294300	0.39447800	1.61614400
H	-4.09526500	-1.43911300	-2.19326200
H	-5.71473400	-0.92230500	-0.36513800
N	-0.32129500	2.15246400	0.05858400
O	-1.28753300	2.89541900	0.10788900
O	1.82013300	-2.02691000	-0.08553900

TS6

C	1.87262300	0.34490200	0.08907000
C	2.62733800	-0.79958400	0.42608900
C	4.01518600	-0.77742200	0.53075300
C	4.66068600	0.44153600	0.28762100
C	3.93462500	1.59325900	-0.05108500
C	2.54045100	1.55514200	-0.15762000
C	0.46589900	-1.51038900	0.54686200
H	4.56493900	-1.68205600	0.79572300
H	5.74976200	0.49359200	0.36503000
H	4.46366200	2.53055500	-0.23755300
H	1.98476500	2.45232600	-0.42984400
H	0.00040200	-2.20697600	-0.17427100
C	-0.15696200	-1.70217700	1.92982900
H	-1.23719700	-1.50419700	1.90949900
H	0.00370500	-2.73965500	2.25926700
H	0.31341200	-1.02664500	2.66037700
C	0.48082800	-0.08049200	0.01969100
C	-0.66253600	0.79018600	-0.02835900
C	-2.08996200	0.34448400	0.03846700
C	-3.03616900	1.12340200	0.73122000
C	-2.52743400	-0.83700900	-0.58787300
C	-4.37087200	0.72356700	0.80903300
H	-2.72532500	2.05083100	1.21481700
C	-3.86554200	-1.23111500	-0.51320900
H	-1.82995500	-1.45301600	-1.15411200
C	-4.79256000	-0.45582100	0.18785200
H	-5.08623300	1.34032700	1.35875700
H	-4.18378400	-2.14875900	-1.01429700
H	-5.83881600	-0.76587600	0.24568600
N	-0.41652100	2.08643300	-0.15122700
O	-1.11530900	3.07886000	-0.26196900
O	1.85991400	-1.89428700	0.62194800
N	0.57452500	-0.52681000	-2.19960500

O 0.27302500 -1.60865200 -2.47164200

E

C 1.82253800 0.25488400 -0.23566200
C 2.68953500 -0.65951000 0.37819400
C 4.07081900 -0.46522600 0.38942600
C 4.56682500 0.67708200 -0.24915800
C 3.71335600 1.59263300 -0.88227400
C 2.32983500 1.38087400 -0.88801900
C 0.62161900 -1.51021200 0.83219700
H 4.72729800 -1.18439100 0.88178700
H 5.64517300 0.85640300 -0.25386000
H 4.13023500 2.47162900 -1.37825400
H 1.66196200 2.08014900 -1.39383500
H 0.22384800 -2.42863900 0.37269100
C 0.06160100 -1.30904100 2.23147600
H -1.03659900 -1.26162600 2.21706000
H 0.36454300 -2.15496500 2.86630200
H 0.44571100 -0.38187200 2.68286700
C 0.42749500 -0.31909000 -0.15622200
C -0.69134400 0.66231100 0.13847400
C -2.12745000 0.32311400 -0.01832200
C -3.13243600 1.30275700 0.12916600
C -2.53104800 -0.99592100 -0.31862100
C -4.47988900 0.97457100 -0.02161700
H -2.85833400 2.33193800 0.35998100
C -3.88049900 -1.31860100 -0.46497200
H -1.79536200 -1.78860000 -0.44426900
C -4.86314200 -0.33629100 -0.31819900
H -5.23661200 1.75431700 0.09486400
H -4.16235100 -2.34849100 -0.69726500
H -5.91946300 -0.59050600 -0.43430800
N -0.30542700 1.83606900 0.53346000
O -0.84393400 2.87503000 0.86556000
O 2.05363500 -1.71149700 0.93494600
N 0.24043500 -0.78004500 -1.65119700
O 0.37504900 -1.94772100 -1.84110300

TS7

C 1.28301600 0.67053300 -0.28865600
C 2.55759500 0.45508900 0.25469900
C 3.38973600 1.52041900 0.59913500
C 2.90984200 2.81649700 0.37712400
C 1.63910400 3.04321800 -0.17033600

C	0.80909600	1.96477400	-0.50348800
C	1.86006500	-1.63155800	-0.27748300
H	4.37788600	1.33473100	1.02348500
H	3.54397100	3.66878700	0.63471600
H	1.29355400	4.06564800	-0.33765800
H	-0.18434300	2.13332100	-0.92342500
H	2.24225800	-1.78680000	-1.30096700
C	1.71046300	-2.98596300	0.38622000
H	0.93559100	-3.57825500	-0.12401100
H	2.66372900	-3.52984900	0.30205300
H	1.45143800	-2.90483900	1.44894200
C	0.62861300	-0.69091000	-0.48456800
C	-0.59880600	-0.83730400	0.42066200
C	-1.92188400	-0.18805800	0.14955400
C	-2.44519500	0.69769700	1.11042600
C	-2.68335600	-0.46412800	-1.00018200
C	-3.68771900	1.30384000	0.91979800
H	-1.87316900	0.90954600	2.01629300
C	-3.92970800	0.13972500	-1.18399500
H	-2.30521100	-1.15538000	-1.75209000
C	-4.43374400	1.02791300	-0.23002500
H	-4.07424900	1.99386200	1.67399300
H	-4.51105700	-0.09017800	-2.08041800
H	-5.40803600	1.50007000	-0.37961800
N	-0.39436700	-1.38063500	1.57308600
O	-1.05386700	-1.58081600	2.57818100
O	2.85935900	-0.85096400	0.41875300
N	0.12142500	-0.70433600	-1.94819500
O	0.84894900	-1.19529200	-2.75304000

F

C	1.38564100	0.26348800	-0.46720600
C	2.21272700	0.64936000	0.59654100
C	3.07185500	1.74353900	0.49162600
C	3.08252100	2.44208400	-0.72194200
C	2.26315000	2.06281000	-1.79551800
C	1.40496200	0.96302500	-1.67391700
C	1.17738200	-1.22446700	1.39032300
H	3.70486900	2.03456300	1.33153200
H	3.74706800	3.30301800	-0.83214000
H	2.29702200	2.62627900	-2.73037900
H	0.76325100	0.65720500	-2.50314500
H	1.82298400	-2.11761800	1.31377600
C	0.17821800	-1.42003600	2.51438800

H	-0.42990300	-2.31796000	2.32847800
H	0.71937800	-1.56423600	3.46152100
H	-0.49591900	-0.55967200	2.62797900
C	0.63270700	-0.97037900	-0.04775300
C	-0.86658200	-1.00869100	-0.27216400
C	-1.79779000	0.12396600	-0.05050000
C	-3.12030800	0.07990900	-0.54036400
C	-1.39285000	1.27109400	0.66474200
C	-3.99697700	1.14414600	-0.32807000
H	-3.46565400	-0.79197800	-1.09629800
C	-2.27684400	2.32917200	0.87884300
H	-0.38193300	1.34380100	1.06190900
C	-3.58217700	2.27365000	0.38310400
H	-5.01467400	1.08666100	-0.72210700
H	-1.93819500	3.20399100	1.43935500
H	-4.27218000	3.10411500	0.55153800
N	-1.28150300	-2.16118500	-0.70664800
O	-2.34544700	-2.65866000	-1.02171700
O	2.05456100	-0.11099800	1.70184100
N	1.16379900	-2.07040400	-1.07934500
O	1.98013700	-2.82072700	-0.66298200

TS8

C	-1.24216000	-0.65981600	-0.04124000
C	-2.61734500	-0.45593800	0.21487600
C	-3.55521000	-1.48156000	0.13057500
C	-3.09374200	-2.75200700	-0.23451300
C	-1.73769000	-2.97687000	-0.51606900
C	-0.80631800	-1.93736500	-0.43025400
C	-1.68763200	1.59071100	0.58346000
H	-4.60805900	-1.28521500	0.33993800
H	-3.80496400	-3.57885800	-0.30641300
H	-1.40513200	-3.97424700	-0.81269700
H	0.24062800	-2.12118500	-0.66968600
H	-1.80715700	2.45346400	-0.10160100
C	-1.50624400	2.10121900	2.01174000
H	-0.63460600	2.76678500	2.08207500
H	-2.40145500	2.66688200	2.31033300
H	-1.37295700	1.26362200	2.71357300
C	-0.61051700	0.64759800	0.06573900
C	0.79027600	0.97146200	0.16259200
C	1.90423200	-0.02620600	0.14563600
C	2.93098400	0.06743200	-0.80821800
C	1.96579700	-1.03573000	1.12059900

C	3.99023700	-0.84232300	-0.79685100
H	2.89739200	0.85624900	-1.56296100
C	3.02949900	-1.94119400	1.13267400
H	1.17765100	-1.10899800	1.87305400
C	4.04189900	-1.84884900	0.17277300
H	4.77939400	-0.76396600	-1.54875300
H	3.06884400	-2.71967300	1.89872300
H	4.87319600	-2.55828700	0.18274500
N	1.10393700	2.25400600	0.23673600
O	2.15767500	2.86352000	0.30611400
O	-2.91346300	0.82615600	0.52182800
N	-0.66945900	1.18635200	-2.05849000
O	-1.09677700	2.24751800	-2.21883800

TS9

C	1.68692600	0.23528200	-0.29156100
C	2.88361600	-0.35502900	0.15455400
C	4.14717500	0.17093400	-0.09688600
C	4.19329500	1.35262600	-0.83966000
C	3.01350100	1.96562900	-1.30602700
C	1.75650600	1.42080400	-1.04278900
H	5.04837700	-0.32397100	0.26900000
H	5.16099200	1.80712900	-1.06497500
H	3.08652400	2.88763500	-1.88789400
H	0.85062400	1.90534600	-1.41140800
C	0.62773500	-0.65072900	0.17328300
C	-0.81426700	-0.48166800	-0.04218400
C	-1.45541800	0.83047800	0.19773800
C	-2.53751500	1.29733400	-0.57614800
C	-0.94908300	1.66043400	1.21894900
C	-3.09290700	2.55222800	-0.32896800
H	-2.94061100	0.67124400	-1.37114500
C	-1.51503100	2.91063000	1.46772300
H	-0.11050900	1.31429000	1.82602900
C	-2.58872300	3.36230700	0.69415800
H	-3.92791900	2.90041100	-0.94197900
H	-1.11462600	3.53526800	2.27002600
H	-3.03027100	4.34340500	0.88644100
N	-1.54485100	-1.48897800	-0.46583000
O	-1.00771400	-2.65398400	-0.81139100
O	2.61137300	-1.49887400	0.84980600
C	1.25919100	-1.66910000	0.85458900
C	0.75541300	-2.86155100	1.58202200
H	1.35192500	-3.02939000	2.49156100

H	-0.29900700	-2.73603800	1.85908100
H	0.82913800	-3.76375500	0.95172800
H	-1.86617500	-3.16342400	-1.02381100
N	-3.16502900	-1.60289600	-0.50696700
O	-3.39013200	-2.74073000	-0.90789400

G

C	1.66583700	0.29191300	-0.25088600
C	2.87190600	-0.30070000	0.16384500
C	4.12771200	0.25143500	-0.06917700
C	4.15646000	1.46385600	-0.76166700
C	2.96722100	2.07904600	-1.19947100
C	1.71843000	1.50704400	-0.95427500
H	5.03625800	-0.24780000	0.27182800
H	5.11743500	1.94006700	-0.97039600
H	3.02562900	3.02432800	-1.74450100
H	0.80555800	1.99386500	-1.30144800
C	0.61595000	-0.62879300	0.17543300
C	-0.81594000	-0.47566600	-0.03311600
C	-1.50254500	0.80001400	0.18007000
C	-2.63542900	1.20241700	-0.56690400
C	-0.99474100	1.69633500	1.14988500
C	-3.22291800	2.44654300	-0.35272100
H	-3.05007100	0.53844300	-1.32466500
C	-1.59330500	2.93630400	1.36407700
H	-0.12891700	1.40347600	1.74615300
C	-2.71023500	3.31989600	0.61434700
H	-4.09143500	2.73886400	-0.94819900
H	-1.18742400	3.60614400	2.12628400
H	-3.17965500	4.29229200	0.78241700
N	-1.53021900	-1.57215700	-0.43951900
O	-0.88866500	-2.63387500	-0.98683400
O	2.61997400	-1.48097300	0.80403800
C	1.27052000	-1.66967000	0.80909900
C	0.79116900	-2.90390800	1.48064500
H	-0.26492000	-2.81171600	1.76572400
H	0.88337900	-3.77647100	0.81202800
H	1.39091400	-3.09995100	2.38253200
H	-1.71136800	-3.20630100	-1.15131200
N	-2.87332400	-1.72044500	-0.30797300
O	-3.24145000	-2.81557900	-0.78084300

TS10

C	1.69262000	0.40754700	0.01657100
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C	2.90980200	-0.29487600	0.06176100
C	4.16236100	0.30874300	0.05097400
C	4.18326500	1.70422400	0.00206300
C	2.98659100	2.44223100	-0.02776100
C	1.74046000	1.81180500	-0.02035000
H	5.07444600	-0.28928900	0.08547600
H	5.14216500	2.22797500	-0.00724600
H	3.03169600	3.53350900	-0.05602400
H	0.82865100	2.40682800	-0.03875300
C	0.64157900	-0.62103700	0.04987100
C	-0.76175000	-0.44426000	0.04247600
C	-1.48841400	0.85485900	0.03908700
C	-1.42203400	1.69611000	-1.08796000
C	-2.29861600	1.24033200	1.12298000
C	-2.13312200	2.89785300	-1.12273600
H	-0.81390800	1.39707300	-1.94501200
C	-3.00941500	2.44252200	1.08442900
H	-2.36886000	0.58994200	1.99618600
C	-2.92722800	3.27541000	-0.03528900
H	-2.07296200	3.53752400	-2.00705000
H	-3.63046300	2.73030000	1.93657800
H	-3.48500800	4.21494700	-0.06308300
N	-1.58030700	-1.59770500	-0.01571600
O	-2.41979700	-1.86765100	1.03666100
O	2.68633900	-1.63937300	0.13839300
C	1.33954700	-1.84344600	0.14815600
C	0.91682400	-3.26201700	0.29330400
H	0.03734500	-3.35590100	0.94601800
H	0.64929100	-3.71127500	-0.67819600
H	1.74545800	-3.84134800	0.72473500
H	-2.90412500	-2.64959100	0.63237700
N	-1.66367800	-2.39428800	-1.05798000
O	-2.48162400	-3.31082000	-0.88950300

H

C	-1.57247800	-0.44698000	-0.25121400
C	-2.82292700	0.00290100	0.20913800
C	-4.02468700	-0.64907600	-0.04880800
C	-3.94921400	-1.81331200	-0.81649800
C	-2.71356000	-2.28620400	-1.30052300
C	-1.52036100	-1.61618400	-1.02867800
H	-4.97133000	-0.25952900	0.32944200
H	-4.86431400	-2.36338100	-1.04848000
H	-2.69102400	-3.19718600	-1.90355300

H	-0.57035900	-1.99290900	-1.41170200
C	-0.60843700	0.53764400	0.22753300
C	0.83356500	0.52779200	0.00650700
C	1.63475200	-0.68325100	0.18096600
C	2.81738100	-0.94816900	-0.55283300
C	1.19563800	-1.66262600	1.10451700
C	3.51489600	-2.13972100	-0.36989400
H	3.18298500	-0.21689700	-1.27181600
C	1.90410100	-2.84797200	1.28643500
H	0.29380400	-1.47743800	1.69025800
C	3.06760200	-3.09576300	0.54984200
H	4.41962800	-2.32528400	-0.95439800
H	1.54719300	-3.58275000	2.01246900
H	3.62288100	-4.02613700	0.69191200
N	1.40795500	1.69612400	-0.40771900
O	2.74524000	1.87996300	-0.34614200
O	-2.67209000	1.15823500	0.92291000
C	-1.34720600	1.47127400	0.92943100
C	-0.97383300	2.70639400	1.66301700
H	0.07664700	2.67247300	1.98182100
H	-1.09802600	3.59364500	1.01899800
H	-1.61489100	2.82882200	2.54883800
H	2.75464900	2.83644100	-0.69864400
N	0.70915200	2.76232500	-0.89610200
O	1.48697800	3.70686600	-1.15077000

TS11

C	-1.54403100	-0.48403600	-0.28267000
C	-2.79551100	-0.11812700	0.24638800
C	-3.98074900	-0.79030900	-0.03564200
C	-3.88668900	-1.88440000	-0.89875200
C	-2.64948400	-2.27281900	-1.44964400
C	-1.47272000	-1.58428600	-1.15368400
H	-4.92954100	-0.46846400	0.39702100
H	-4.78879600	-2.44590400	-1.15316300
H	-2.61308100	-3.13103000	-2.12508000
H	-0.52098800	-1.89426400	-1.58954200
C	-0.60425900	0.48832500	0.25581100
C	0.84276100	0.54880000	-0.00456600
C	1.68492300	-0.65394200	0.17672700
C	2.87730900	-0.87336500	-0.54767400
C	1.27055400	-1.63869600	1.09927400
C	3.61597100	-2.04043900	-0.35599900
H	3.22029700	-0.12996500	-1.26478400

C	2. 02245700	-2. 79603900	1. 29646300
H	0. 35350700	-1. 48570000	1. 67042900
C	3. 19760900	-3. 00403200	0. 56776900
H	4. 53077500	-2. 19685500	-0. 93311000
H	1. 68735500	-3. 54028700	2. 02308200
H	3. 78541600	-3. 91286400	0. 71905600
N	1. 31550100	1. 70585800	-0. 39882100
O	2. 60338700	1. 95698100	-0. 58314600
O	-2. 66093100	0. 97468700	1. 05408800
C	-1. 34533000	1. 33236800	1. 05158100
C	-0. 99068600	2. 50854900	1. 88427400
H	-1. 53839200	2. 47759100	2. 83879000
H	0. 08803000	2. 53561800	2. 08419600
H	-1. 25440400	3. 44302600	1. 36187800
H	2. 52897100	2. 92458600	-0. 90502100
N	0. 43590600	3. 02318300	-0. 83956300
O	1. 27482500	3. 85532100	-1. 16506700

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C	1. 37200500	-0. 40075800	-0. 25866700
C	2. 70294500	-0. 12436900	0. 10973200
C	3. 73669900	-1. 05335500	0. 03561500
C	3. 40284700	-2. 32322600	-0. 44020700
C	2. 08283600	-2. 63055600	-0. 82471700
C	1. 06076800	-1. 68452300	-0. 74130500
H	4. 75344200	-0. 79078600	0. 33320300
H	4. 17874300	-3. 08874100	-0. 51802300
H	1. 85606300	-3. 63260300	-1. 19730000
H	0. 04358600	-1. 93799300	-1. 04417700
C	0. 64574800	0. 84185900	-0. 03685600
C	-0. 78478600	1. 10464500	-0. 29379300
C	-1. 78273100	0. 04490500	0. 04392700
C	-1. 64525500	-0. 67361500	1. 24520500
C	-2. 85231000	-0. 27317300	-0. 81369400
C	-2. 55767600	-1. 67330300	1. 58862100
H	-0. 81519100	-0. 44191900	1. 91634500
C	-3. 75250700	-1. 28544300	-0. 47682800
H	-2. 97491400	0. 27702300	-1. 74617700
C	-3. 61267500	-1. 98506500	0. 72637400
H	-2. 43989600	-2. 21458100	2. 53082900
H	-4. 57278800	-1. 52698400	-1. 15777400
H	-4. 32364800	-2. 77241400	0. 98995900
N	-1. 05874100	2. 27166300	-0. 77776800
O	-2. 41309300	2. 51979900	-0. 93063700

O	2.81408700	1.16774700	0.53134700
C	1.57509600	1.73984300	0.43627800
C	1.49090700	3.16138600	0.85810000
H	1.95654400	3.82160700	0.10617300
H	0.44343400	3.46693000	0.96355100
H	2.02817800	3.31163100	1.80827500
H	-2.42178900	3.41531700	-1.29289400

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C	-2.33282500	-0.97702100	-0.44732800
C	-3.44419800	0.00459600	-0.29318500
C	-4.78475000	-0.43039800	-0.28533200
C	-3.18134800	1.38158100	-0.17504500
C	-5.82764500	0.48568500	-0.16437100
H	-4.99096100	-1.49793200	-0.37455600
C	-4.23171600	2.29691000	-0.05671900
H	-2.15132600	1.74284900	-0.19495800
C	-5.55636600	1.85487700	-0.04875100
H	-6.86153400	0.13032800	-0.15581700
H	-4.00820200	3.36358600	0.02660000
H	-6.37583700	2.57173400	0.04843400
N	-2.63791700	-2.11967800	-0.95695300
O	-1.56094600	-2.97913200	-1.07319800
H	-1.95527900	-3.76107500	-1.48175900
C	-0.40221500	-0.84352100	1.38859800
C	0.92758000	-0.02393900	1.36037000
C	-0.95008500	-0.60003200	-0.02715400
C	-0.05837200	-0.01020800	-0.83067600
H	-0.20803900	0.23533000	-1.88284800
H	1.75705700	-0.54925800	1.84875200
C	-1.34919800	-0.32806400	2.48743200
H	-2.29590200	-0.89100300	2.49803000
H	-0.88015400	-0.44698600	3.47825200
H	-1.59247000	0.73666300	2.35059600
C	-0.12982600	-2.34498600	1.62141100
H	-1.05500800	-2.93453700	1.54227700
H	0.58224800	-2.73875000	0.88331500
H	0.29149900	-2.49729500	2.62923200
H	0.77611900	0.92379100	1.89894000
C	1.25099400	0.29476800	-0.13107100
C	2.36158400	-0.52833300	-0.80360300
C	1.61222700	1.77883200	-0.27997100
O	0.84258300	2.64487700	-0.61356500
O	2.69483800	-0.34682600	-1.94935200

O	2. 88752100	-1. 47839200	-0. 01891300
O	2. 88589300	2. 00428200	0. 07488500
C	3. 35608600	3. 36345400	0. 00371400
H	2. 73596200	3. 98825100	0. 66699700
H	3. 20746800	3. 73448000	-1. 02286200
C	4. 81492400	3. 37604200	0. 40852900
H	5. 20682000	4. 40422400	0. 36700600
H	4. 94351400	2. 99883800	1. 43488500
H	5. 41606600	2. 74948500	-0. 26806900
C	3. 90740600	-2. 30850200	-0. 60783200
H	4. 72150100	-1. 66110900	-0. 97078000
H	3. 48323800	-2. 81675300	-1. 48862500
C	4. 38299100	-3. 28832300	0. 44380100
H	3. 55828400	-3. 92941000	0. 79141200
H	5. 16838800	-3. 93562500	0. 02338600
H	4. 80136600	-2. 76105700	1. 31507000

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C	-2. 29346200	-1. 12995700	-0. 32436900
C	-3. 36720600	-0. 09372200	-0. 29645200
C	-3. 02963800	1. 24543000	-0. 58078600
C	-4. 70818400	-0. 39637200	0. 01777500
C	-4. 00469400	2. 24468100	-0. 56947500
H	-1. 99477200	1. 50752400	-0. 81045300
C	-5. 67406700	0. 61071500	0. 04567600
H	-4. 98933700	-1. 42326400	0. 24201300
C	-5. 33005600	1. 93254100	-0. 25453800
H	-3. 72266400	3. 27447800	-0. 80313100
H	-6. 70704900	0. 35838100	0. 29954500
H	-6. 09215400	2. 71621200	-0. 24007800
N	-2. 39593600	-2. 36857500	-0. 66750300
O	-3. 66640600	-2. 76372900	-1. 05577200
H	-3. 52601700	-3. 68315500	-1. 31677200
C	-0. 42977400	-0. 59577200	1. 51177500
C	1. 11340800	-0. 45995500	1. 32558000
C	-0. 90201600	-0. 73644700	0. 05639000
C	0. 06631400	-0. 46348100	-0. 82533000
H	-0. 03558800	-0. 47630200	-1. 91140600
H	1. 56479100	0. 24649700	2. 03790800
C	-0. 77847300	-1. 84610300	2. 33861100
H	-1. 86662100	-1. 94004100	2. 48096100
H	-0. 31329600	-1. 78905500	3. 33687600
H	-0. 42595500	-2. 76388600	1. 84303000
C	-1. 02431900	0. 65375800	2. 19659900

H	-2.12044900	0.58966000	2.26820300
H	-0.77663900	1.57311900	1.64617900
H	-0.62630300	0.74482600	3.22121100
H	1.59638400	-1.43158000	1.48852400
C	1.35924200	-0.04567000	-0.15580400
C	2.55687300	-0.69518900	-0.86534400
C	1.54249500	1.48061300	-0.27284200
O	0.67490100	2.26681100	-0.56341000
O	2.77581600	-0.53029500	-2.04113700
O	3.30991500	-1.46444800	-0.07028100
O	2.79561600	1.84003800	0.04230300
C	3.11147900	3.24453700	-0.01452800
H	2.45993000	3.78226200	0.69329300
H	2.87311400	3.61843800	-1.02286200
C	4.57803500	3.40887400	0.32331900
H	4.85237100	4.47479300	0.29192000
H	4.79683800	3.02577500	1.33202400
H	5.21079500	2.86814500	-0.39706700
C	4.44378200	-2.10978600	-0.68030900
H	5.09534600	-1.33628600	-1.11763100
H	4.08788100	-2.73851300	-1.51223000
C	5.15296900	-2.91883900	0.38493400
H	4.48819200	-3.68932900	0.80512000
H	6.03112600	-3.42160600	-0.04933100
H	5.49664400	-2.27320600	1.20775200

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C	0.85903700	0.98412500	-0.30132800
N	1.20852500	2.05306100	-0.86316400
O	1.57273700	3.16719300	-1.45047500
C	-1.41749900	-0.41078600	-0.27746400
C	-2.69615200	-0.10602300	0.23169600
C	-3.80013900	-0.94396500	0.10010500
C	-3.59577300	-2.14533000	-0.58246500
C	-2.33135000	-2.47764300	-1.10846000
C	-1.23727400	-1.62398100	-0.96573400
H	-4.77228600	-0.66604400	0.51136600
H	-4.43130000	-2.83764500	-0.71196000
H	-2.20744000	-3.42477900	-1.63944700
H	-0.26246900	-1.89386900	-1.37660300
C	-0.58098900	0.72968300	0.06405000
C	1.87102700	-0.08529200	0.04174000
C	3.13757500	-0.05228600	-0.56685100
C	1.60496600	-1.09276400	0.98402700

C	4.10794800	-1.00218600	-0.25157700
H	3.34559500	0.73912600	-1.29122600
C	2.58080800	-2.04083700	1.30851600
H	0.63149600	-1.13152000	1.47655500
C	3.83294200	-2.00184800	0.69016000
H	5.08543200	-0.96505900	-0.74006300
H	2.35972500	-2.81295600	2.05025200
H	4.59375300	-2.74572500	0.94077500
O	-2.67827200	1.11028900	0.84635500
C	-1.40212600	1.60098700	0.73243200
C	-1.16593000	2.93237700	1.35137600
H	-0.11588700	3.22972800	1.23399900
H	-1.80695400	3.70341800	0.89037600
H	-1.40866500	2.91479100	2.42713300
H	0.77117600	3.71386700	-1.59738300