

Supporting information

SI_DFT

Parahydrogen Hyperpolarized NMR Detection of Underivatized Short Oligopeptides

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DFT calculations

1. Conformational sampling

The preliminary selection of the most favored binding pattern between Ir-parahydrogen complex and alanine oligopeptides was based on the energy evaluation of Ir complex ligated with deprotonated L-alanine as a model system in three possible bidentate binding configurations: a) N-axial/O-equatorial coordination; b) N-equatorial/O-axial coordination; and c) N-equatorial/O-equatorial coordination. The respective molecular structures were constructed for each of these diastereomeric pairs of Ir-ligand coordination, with equatorial hydrogen atoms being fixed in adjacent positions. Full geometry optimizations of the whole complex have been carried out starting from a variety of initial geometries altered manually in respect to contact characteristics of complexation (distance to Ir atom and associated angles) and torsional degrees of freedom in alanine backbone. For the peptide structures, N-axial/O-equatorial binding mode was considered as a primary contact pattern following the study on single alanine and subsequent investigation of complexation of alanine trimer methyl ester (see below) suggesting that this coordination pattern was most relevant for complexation.

Therefore, the optimized structure of N-axial/O-equatorial alanine complex served as a template for construction of all peptide complexes of gradually increased chain length, starting from two alanine units. Variations in multiple dihedral angles of peptide backbone associated with the size of the molecular cycle incorporating Ir-atom, possibility of hydrogen bond formation within peptide moiety, as well as directional preference of peptide tail position in respect to the Ir parahydrogen complex were selected manually. The resulting molecular structures were taken as input for subsequent geometry optimizations to achieve full relaxation of intramolecular forces according to standard convergence thresholds. All final structures were characterized by lack of imaginary eigenvalues during harmonic normal modes analysis, thus corresponding to true minima conditions on potential energy hypersurface.

2. Energetics

The calculated energies of deprotonated L-alanine Ir parahydrogen complexes, expressed as the ZPE-corrected total energies (E^0) and Gibbs free energies at 298.15 K (G^{298}) in hartrees using LANL2DZ/ECP representation of Ir-atom are shown in **Table S1**. One can notice that while the values of E^0 strongly favored N-axial/O-equatorial coordination, the respective values of G^{298} suggested rather similar probability for both N-axial/O-equatorial and N-equatorial/O-axial binding modes. The N-equatorial/O-equatorial binding pattern remained the least favored using both energy metrics. To get further insight on the binding mode preference, alternative single-point energy values were calculated for converged geometries within each coordination subspace using all-electron TZVP representation of Ir-atom along with DKH-2 Hamiltonian to account for respective relativistic effects. The SCF energy values, expressed in hartrees and designated as E_{DKH} , indicated that N-axial/O-equatorial coordination indeed dominated complexation events as was observed in the experimental study.

Further evidence supporting the prevalence of bidentate N-axial/O-equatorial coordination pattern was obtained by comparing N-coordinated monodentate binding in equatorial plane with three respective bidentate *ax-eq* and *eq-eq* binding modes of Ala-Ala-Ala methyl ester (A-A-A-OMe), with molecular composition of the latter configurations amended with one unbound pyridine cosubstrate molecule, to maintain comparable stoichiometry with the former complex. The calculated energies, shown in **Table S2**, suggested that even if monodentate binding appeared to be strongly stabilized in respect to both N-equatorial/O-axial and *eq-eq* coordination, the N-axial/O-equatorial pattern of peptide complexation led

to even stronger stabilization when supported by extra interactions between peptide chain and adjacent cosubstrate molecule. Therefore, this binding topology was eventually selected for all considered alanine-peptide complexes. The E^0 and G^{298} values for the most abundant conformers of latter complexes of various Ir-cycle sizes are collected in **Table S3**. The closer inspection of structure and energy relationships across the series of studied peptide complexes revealed some general trends that are worth noting. Firstly, irrespectively of the size of the interacting peptide, the molecular configuration of nhPHIP complex was largely preserved and some minor structural variations had very limited effect on binding preferences. Secondly, possibility of formation of intrapeptide hydrogen bond(s), facilitated by helix-like folding of the peptide backbone, provided an advantage over more linear counterparts. Thirdly, the most efficient peptide folding pattern contributing to enhanced stability of the complex was substantially conserved and was not particularly dependent on the size of peptide chain.

Table S1. Calculated energies of deprotonated L-alanine nhPHIP complexes. All values in hartrees.

Coordination	Diastereomer	E^0	G^{298}	E_{DKH}
N-axial/O-equatorial	C	-1738.134820	-1738.209269	-19439.2892900
	A	-1738.134652	-1738.209646	
N-equatorial/O-axial	C	-1738.132751	-1738.209431	-19439.2840070
	A	-1738.132386	-1738.209379	
N-equatorial/O-equatorial	A	-1738.130183	-1738.206786	-19439.2837917
	C	-1738.129731	-1738.205938	

Table S2. Calculated energies of various binding modes for A-A-A-OMe nhPHIP complexes. All values in hartrees.

Binding mode	Position of alanine trimer	E^0	G^{298}
Monodentate binding	N-terminus in the equatorial plane	-2658.303576	-2658.403520
Bidentate binding (5-membered Ir-cycle)	N-terminus is in the equatorial and oxygen in axial position	-2658.289958	-2658.390552
	N-terminus and oxygen are in the equatorial position	-2658.293989	-2658.393477
	oxygen is in the equatorial and N-terminus in axial position	-2658.306977	-2658.408165

Table S3. Calculated energies for the most abundant conformers of nhPHIP complexes with N-axial/O-equatorial coordinated alanine oligopeptides of various Ir-cycle sizes. All values in hartrees.

nhPHIP complexes	Energy	Cycle size, N/O coordination with Ir			
		5	8	11	14
Alanine dimer					
Ir-A-A-OH	E ⁰	-1985.617373	-1985.615203	-	-
	G ²⁹⁸	-1985.701878	-1985.696164	-	-
Ir-A-A-OMe	E ⁰	-2024.844904	-2024.841580	-	-
	G ²⁹⁸	-2024.932348	-2024.925479	-	-
Alanine trimer					
Ir-A-A-A-O [−]	E ⁰	-2232.221023	-2232.208904	-2232.225488	-
	G ²⁹⁸	-2232.308326	-2232.294630	-2232.309262	-
Ir-A-A-A-OH	E ⁰	-2232.665628	-2232.662058	-2232.662372	-
	G ²⁹⁸	-2232.755501	-2232.750243	-2232.747953	-
Ir-A-A-A-OMe	E ⁰	-2271.894133	-2271.890119	-2271.889595	-
	G ²⁹⁸	-2271.986247	-2271.979900	-2271.976621	-
Alanine tetramer					
Ir-A ₄ -OMe	E ⁰	-2518.940934	-2518.947955	-2518.938185	-2518.935768
	G ²⁹⁸	-2519.037521	-2519.043040	-2519.033014	-2519.028875
Alanine pentamer					
Ir-A ₅ -OMe	E ⁰	-	-2765.992500	-2765.990132	-2765.984019
	G ²⁹⁸	-	-2766.096119	-2766.090267	-2766.083261

3. Molecular Cartesian coordinates of the optimized nhPHIP complexes of deprotonated L-alanine (Å)

N-axial/O-equatorial (C)

Ir	-0.55006200	0.61101600	0.42288200
H	-0.92814700	0.09045700	1.87224300
C	-0.89639800	-1.19336500	-0.25276000
C	-2.01928000	-3.04860700	-1.03030000
C	-0.69279000	-3.26773300	-1.23352500
H	-2.89051800	-3.65559100	-1.24986500
H	-0.15748500	-4.10916400	-1.65926700
N	-2.13179400	-1.79649000	-0.43373600
N	-0.02372400	-2.14106800	-0.75947400
C	1.40512200	-2.04264000	-0.75802000
C	2.06545100	-1.61579800	-1.92309400
C	2.09363700	-2.41239600	0.40797800
C	3.46704300	-1.58536400	-1.90173900
C	3.49397600	-2.35178600	0.38867200
C	4.19564700	-1.94683800	-0.75671500
H	4.00055900	-1.24523500	-2.79458200
H	4.04859100	-2.61455700	1.29421500
C	-3.39473400	-1.20653100	-0.10273700
C	-3.94513300	-1.45259700	1.16397500
C	-4.02643200	-0.39328600	-1.05856100
C	-5.19044000	-0.87739400	1.45775600
C	-5.26952500	0.16083100	-0.72380700
C	-5.87006100	-0.07767800	0.52430400
H	-5.63444200	-1.04997600	2.44315900
H	-5.77445800	0.80629700	-1.44932800
C	-7.22581500	0.50097300	0.84850400
H	-8.03031200	-0.18253700	0.52469400
H	-7.34406400	0.65860700	1.93157400
H	-7.38374600	1.46074000	0.33272900
C	5.70091900	-1.84986100	-0.74978100
H	6.01641200	-0.79915500	-0.86134900
H	6.12226800	-2.23966000	0.18906000
H	6.14198900	-2.41212200	-1.58904500
C	1.28298800	-1.14048000	-3.11821200
H	0.51378800	-1.87168900	-3.41556100
H	0.76151900	-0.19951400	-2.86570700
H	1.95093300	-0.96126200	-3.97344800
C	1.32590500	-2.81385800	1.63847500
H	0.59937500	-2.02499100	1.89923000
H	0.74805800	-3.73716100	1.46217900
H	2.00377300	-2.97887700	2.48807400

C	-3.17333000	-2.25360000	2.17848000
H	-2.95603900	-3.26995200	1.80978800
H	-2.20104900	-1.76540500	2.36841200
H	-3.72926600	-2.33273700	3.12382900
C	-3.32486000	-0.07429700	-2.35088700
H	-2.36548000	0.42755400	-2.12705100
H	-3.08657400	-0.99046200	-2.91697400
H	-3.94172500	0.58083800	-2.98300700
N	1.58882700	0.53103700	0.90246900
C	2.50960600	0.88927000	-0.02066900
C	2.02022700	0.32515500	2.17195500
C	3.85037700	1.01998700	0.31036400
H	2.14710900	1.06307100	-1.03423500
C	3.35478900	0.45433400	2.54733000
H	1.24463400	0.04494200	2.88440800
C	4.33318900	0.80406000	1.60426400
H	3.64273600	0.27263800	3.58486500
C	5.79242300	0.92139400	1.93054600
H	5.95324200	0.87729700	3.01642000
H	6.35772300	0.09959800	1.45974500
H	6.20979000	1.86280900	1.54061700
F	4.72469500	1.35453100	-0.67776500
N	-0.30444000	2.72162400	0.90367200
H	-0.89925600	3.04019300	1.67449000
H	0.66172100	2.91997100	1.19859000
C	-0.60745600	3.54638100	-0.31038900
H	-1.70695400	3.52938400	-0.40255000
C	-0.10555800	4.97901300	-0.17641500
C	-0.08272700	2.83399800	-1.58899800
H	0.98581500	4.98715500	-0.01667800
H	-0.31443500	5.52552600	-1.10637000
H	-0.59141400	5.49324100	0.66768500
O	-0.01962100	1.53715200	-1.52702100
O	0.20001800	3.51100000	-2.58981900
H	-2.08798200	0.88207000	0.16520000

N-axial/O-equatorial (A)

Ir	0.43742200	0.48312400	0.62160900
H	1.92486200	0.25307100	1.10297900
C	0.57190400	-1.30155800	-0.16903600
C	0.13195500	-3.37899300	-1.06092400
C	1.48120900	-3.21031500	-1.08340700
H	-0.49777800	-4.20006100	-1.38518300
H	2.28095500	-3.85721700	-1.42643800
N	-0.40662300	-2.22150000	-0.50216000

N	1.73825800	-1.95344400	-0.54354300
C	3.06335600	-1.43139500	-0.37468700
C	3.66025300	-0.72678000	-1.43171100
C	3.71062300	-1.64123800	0.85532800
C	4.95483300	-0.22326000	-1.22816300
C	5.00061900	-1.11842100	1.01504900
C	5.63899800	-0.40924100	-0.01678200
H	5.43548500	0.33722600	-2.03615000
H	5.51509200	-1.26009700	1.97065300
C	-1.81705800	-2.01799100	-0.36021800
C	-2.44295200	-2.37653400	0.84552200
C	-2.52994600	-1.50591000	-1.45562100
C	-3.83295800	-2.21772700	0.93282500
C	-3.91795800	-1.35803200	-1.32215900
C	-4.58565200	-1.71269800	-0.14065200
H	-4.33762400	-2.48466400	1.86645900
H	-4.48899300	-0.94477900	-2.15882000
C	-6.07472600	-1.51327200	-0.00510500
H	-6.56133600	-2.40839400	0.41464900
H	-6.28759600	-0.67487000	0.67866000
H	-6.53719300	-1.28775700	-0.97785400
C	7.04053300	0.12018400	0.16624000
H	7.22871300	0.39626700	1.21538100
H	7.78774700	-0.64391700	-0.11141300
H	7.21952800	1.00197500	-0.46794000
C	2.90424500	-0.47016500	-2.70733600
H	2.44837800	-1.39386200	-3.09937900
H	2.09079900	0.24792400	-2.50237800
H	3.56877000	-0.04780400	-3.47559400
C	2.98857500	-2.34485500	1.97220000
H	2.07070700	-1.78163900	2.21732300
H	2.67624700	-3.35948200	1.67298300
H	3.62303500	-2.41944500	2.86722500
C	-1.62454200	-2.88679200	2.00114400
H	-1.07665500	-3.80408300	1.72730300
H	-0.86845400	-2.13343700	2.28274100
H	-2.26321500	-3.10343100	2.86950800
C	-1.80531600	-1.11181600	-2.71496400
H	-0.94224200	-0.46971700	-2.47516600
H	-1.41064700	-1.99797000	-3.24084400
H	-2.47510800	-0.56981300	-3.39764800
N	-1.62379400	1.02422000	0.08782300
C	-2.61723800	0.83938100	0.98687600
C	-1.92723200	1.68365000	-1.05688600
C	-3.90599000	1.28952900	0.74349500

H	-2.36467000	0.30482600	1.90152200
C	-3.20946800	2.14876200	-1.34162600
H	-1.08859600	1.82430700	-1.73975100
C	-4.26170200	1.95236400	-0.43536600
H	-3.39790400	2.66388400	-2.28604500
C	-5.67387300	2.38496400	-0.69551900
H	-5.73103400	3.00646300	-1.59954400
H	-6.07771600	2.95074100	0.15864600
F	-4.85760600	1.05116000	1.68685700
N	0.52459400	2.52707800	1.38825000
H	-0.39316400	2.97818800	1.29156400
H	0.75731300	2.57905500	2.38557100
C	1.53753100	3.30941800	0.60684000
H	1.29877900	4.38358800	0.65822100
C	2.93505800	3.05974400	1.17603800
C	1.52001100	2.88712200	-0.88400200
H	3.16144300	1.98280700	1.13006300
H	3.67406600	3.61465400	0.58033300
H	2.99903900	3.39743900	2.22385400
O	1.07329000	1.69567500	-1.13984800
O	1.96875900	3.68292800	-1.72518200
H	-0.04200500	-0.21750300	1.95596500
H	-6.32409100	1.50450500	-0.83377100

N-equatorial/O-equatorial (A)

Ir	0.21957200	0.20525500	-0.41403200
H	0.31339200	0.01340600	-1.98324200
C	-0.16169000	-1.71814000	-0.22282300
C	-1.17515400	-3.78196600	-0.04391600
C	0.16598200	-3.98091700	0.06082200
H	-2.01209300	-4.47082800	-0.01612200
H	0.75010800	-4.88417500	0.19696900
N	-1.35861100	-2.41268700	-0.22031400
N	0.76789000	-2.73153900	-0.04698200
C	2.18520500	-2.54708100	0.07020500
C	2.96763200	-2.57695800	-1.09533300
C	2.73137900	-2.33215900	1.34592700
C	4.35176900	-2.40550200	-0.95731500
C	4.12151000	-2.16748200	1.43695300
C	4.94607800	-2.20825100	0.30056500
H	4.97889400	-2.41393800	-1.85427400
H	4.56933900	-1.99166900	2.42004800
C	-2.64789700	-1.79927000	-0.27224800
C	-3.30933100	-1.54070000	0.94382000
C	-3.18758100	-1.44314300	-1.51932700

C	-4.56624100	-0.92217900	0.88232400
C	-4.44387900	-0.81528600	-1.52967500
C	-5.14629900	-0.55002500	-0.34340500
H	-5.09341900	-0.70439300	1.81599000
H	-4.87774100	-0.51735600	-2.48874000
C	-6.47513700	0.16210200	-0.37024400
H	-7.21363600	-0.35013500	0.26683300
H	-6.36997900	1.19030900	0.01724600
H	-6.87548100	0.22354000	-1.39287100
C	6.44268300	-2.06171300	0.42958000
H	6.70990000	-1.45139200	1.30591400
H	6.92282600	-3.04804400	0.55560800
H	6.87720400	-1.59783700	-0.46938800
C	2.30396900	-2.70476200	-2.43948300
H	1.71716000	-3.63555700	-2.51384700
H	1.59810300	-1.86529200	-2.57298300
H	3.04687900	-2.68964000	-3.24993200
C	1.83301200	-2.21351900	2.54819600
H	1.17731800	-1.32980800	2.44423100
H	1.17542000	-3.09357500	2.64529300
H	2.42625800	-2.11449300	3.46913300
C	-2.63678100	-1.85133200	2.25462600
H	-1.64478100	-1.36890400	2.28933300
H	-3.24012400	-1.48717800	3.09788600
H	-2.47490300	-2.93524900	2.37629100
C	-2.39613500	-1.66789300	-2.77854700
H	-1.45833700	-1.08613400	-2.72732900
H	-2.11186200	-2.72758500	-2.88674000
H	-2.97030300	-1.36074600	-3.66423300
N	0.82463100	2.22191600	-0.62020600
C	1.52036000	2.81869700	0.38035600
C	0.53553500	2.96414200	-1.71947200
C	1.92851300	4.14109100	0.28315900
H	1.72023800	2.21643700	1.26690100
C	0.92405300	4.29519000	-1.85104200
H	-0.01923900	2.44397500	-2.50038700
C	1.64745000	4.93686300	-0.83458900
H	0.66160900	4.84300000	-2.75814300
C	2.10144300	6.36382100	-0.91122100
H	1.77776000	6.82628900	-1.85335500
H	1.69585300	6.94704300	-0.06856800
H	3.19977600	6.42618800	-0.84232900
F	2.62074400	4.67805400	1.31839100
N	-1.82166600	1.18037000	-0.20049700
H	-2.02985300	1.78101100	-1.00447500

H	-2.59694400	0.51390700	-0.14820800
C	-1.82412300	2.01321500	1.03796600
H	-1.24324000	2.91859800	0.79218300
C	-3.22934400	2.41635200	1.47295900
C	-1.00657200	1.31817200	2.16448600
H	-3.84114100	1.51943300	1.66157900
H	-3.17475800	2.99704800	2.40429300
H	-3.72193500	3.02046900	0.69409200
O	-0.00073100	0.59052500	1.77539600
O	-1.30584800	1.52788700	3.35127900
H	1.72242600	-0.26573700	-0.44698800

N-equatorial/O-equatorial (C)

Ir	-0.17382600	0.18816400	-0.40238100
H	-1.70960400	-0.14305100	-0.52978600
C	0.02115200	-1.75493100	-0.14956600
C	-0.51289400	-3.96788900	0.19918300
C	0.84304300	-3.89194400	0.12248000
H	-1.17771900	-4.81084400	0.35104400
H	1.61416100	-4.65076000	0.19517300
N	-0.99879700	-2.67476500	0.03452600
N	1.15132000	-2.55150300	-0.09349000
C	2.48791400	-2.05412000	-0.17946000
C	3.05185400	-1.83714700	-1.44899500
C	3.16478900	-1.74754400	1.01421600
C	4.34811500	-1.30266000	-1.50233800
C	4.46106500	-1.21933200	0.91236600
C	5.06810300	-0.99370400	-0.33463400
H	4.80031200	-1.10921800	-2.47957100
H	4.99798600	-0.95534100	1.82833200
C	-2.39850200	-2.36429700	0.07211500
C	-2.99068600	-2.06711700	1.30981000
C	-3.11753800	-2.35708200	-1.13424100
C	-4.36358000	-1.77901500	1.32013500
C	-4.48623100	-2.06083600	-1.07702000
C	-5.12680100	-1.77787900	0.14109200
H	-4.84521500	-1.53749800	2.27284100
H	-5.06281800	-2.03848800	-2.00702800
C	-6.60894900	-1.49624100	0.18384100
H	-7.18072400	-2.43009800	0.32615600
H	-6.86363800	-0.82474500	1.01823400
H	-6.95532800	-1.03882900	-0.75572400
C	6.46810500	-0.43987100	-0.41934600
H	6.70067100	0.19069200	0.45213700
H	7.20767500	-1.25911200	-0.44201500

H	6.60696600	0.15453800	-1.33517800
C	2.24421500	-2.10360800	-2.68995100
H	1.89593300	-3.14920800	-2.72105600
H	1.34412500	-1.46345000	-2.68484400
H	2.83391300	-1.89795500	-3.59454900
C	2.47112900	-1.90874200	2.34052600
H	1.48537200	-1.41506400	2.31222500
H	2.29291400	-2.97234800	2.57158300
H	3.06926700	-1.46946700	3.15117600
C	-2.15073600	-1.99190200	2.55681400
H	-1.57016900	-2.91744300	2.70645000
H	-1.42461600	-1.16305100	2.46920500
H	-2.78185900	-1.82488800	3.44206900
C	-2.39789900	-2.57719600	-2.43694900
H	-1.62488600	-1.79652800	-2.55553200
H	-1.87968000	-3.55053800	-2.45340400
H	-3.09536300	-2.53299100	-3.28581300
N	-0.54395300	2.25539800	-0.66451800
C	-1.21674800	2.94845200	0.28791500
C	-0.07948000	2.94575500	-1.73782500
C	-1.42462300	4.31549500	0.17128100
H	-1.55946700	2.38557300	1.15605000
C	-0.26258500	4.31845900	-1.88680200
H	0.44666100	2.34885800	-2.48322100
C	-0.95382600	5.06042800	-0.91738200
H	0.13783300	4.81977900	-2.77001200
C	-1.19010200	6.53786800	-1.01298500
H	-0.74779000	6.94544600	-1.93194000
H	-2.26980800	6.75941800	-1.00759500
H	-0.75370700	7.05795200	-0.14472000
F	-2.10425900	4.94836000	1.15906500
N	1.93641600	0.97392600	-0.09362400
H	2.67671600	0.29889800	-0.29625400
H	2.07192100	1.73392600	-0.76935800
C	2.12823000	1.51852900	1.28786600
H	3.01786900	1.03801000	1.72508300
C	2.34748000	3.03460200	1.25008400
C	0.95943700	1.18785400	2.25656300
H	1.48744700	3.53418400	0.77393800
H	2.44598100	3.41228400	2.27707200
H	3.25872700	3.28340000	0.68297300
O	-0.10204600	0.61741600	1.77305400
O	1.11303800	1.49751300	3.45035900
H	-0.17068700	-0.02305900	-1.97273300

N-equatorial/O-axial (C)

Ir	0.33013200	0.20774500	0.90436400
H	1.30827200	-0.51176000	1.93522100
C	0.24934100	-1.45962300	-0.10525300
C	-0.49438400	-3.41086500	-1.08543800
C	0.84074600	-3.32607100	-1.32900000
H	-1.22685000	-4.16307000	-1.35651200
H	1.51865900	-3.98409800	-1.86123900
N	-0.84380400	-2.28426500	-0.34452500
N	1.28128000	-2.14918500	-0.72878800
C	2.59092200	-1.60189300	-0.90425200
C	2.84220300	-0.85404600	-2.07004300
C	3.56063900	-1.78481700	0.09576900
C	4.10498700	-0.25822100	-2.21032600
C	4.80354000	-1.15609600	-0.07828300
C	5.09136300	-0.38537200	-1.21747500
H	4.31248200	0.33843000	-3.10344800
H	5.56643100	-1.27329200	0.69705400
C	-2.19427600	-1.98101800	0.02858600
C	-2.63007100	-2.28098100	1.32984700
C	-3.04124400	-1.39954400	-0.93166500
C	-3.94254900	-1.92634800	1.67718100
C	-4.35175700	-1.08467900	-0.54735400
C	-4.81229800	-1.31913500	0.75732200
H	-4.29228300	-2.12838200	2.69418900
H	-5.01419300	-0.60739500	-1.27554400
C	-6.20502600	-0.89994000	1.15746700
H	-6.96356300	-1.35452800	0.49910000
H	-6.42802600	-1.18829600	2.19532800
H	-6.31423000	0.19432300	1.07052000
C	6.41577700	0.32301200	-1.35432200
H	7.20738300	-0.19889100	-0.79593800
H	6.71885800	0.40290600	-2.40938200
H	6.34886400	1.34959700	-0.95249600
C	1.75834600	-0.66034000	-3.09690100
H	1.50200200	-1.61124000	-3.59298800
H	0.83481000	-0.29923700	-2.61438600
H	2.06824800	0.06280200	-3.86430800
C	3.25677000	-2.61887600	1.30985300
H	2.36081000	-2.22702800	1.81786400
H	3.04341500	-3.66265600	1.02446500
H	4.10325300	-2.61256900	2.01127500
C	-1.69910900	-2.94182700	2.31010100
H	-1.37031600	-3.92668300	1.93737500
H	-0.79583600	-2.32231300	2.44016000

H	-2.18946700	-3.08036100	3.28449100
C	-2.53825100	-1.09203600	-2.31703800
H	-1.56793500	-0.57361200	-2.26994700
H	-2.38023600	-2.01442900	-2.90097300
H	-3.25329400	-0.45634900	-2.85856400
N	-1.06041000	1.29523200	-0.37470000
C	-2.34858500	1.41502300	0.02058000
C	-0.71210900	1.87114000	-1.55019600
C	-3.28309900	2.08992500	-0.75244000
H	-2.62746700	0.92788400	0.95453400
C	-1.61417300	2.56268300	-2.35546400
H	0.32622700	1.74387500	-1.85701800
C	-2.95928500	2.68661200	-1.97556200
H	-1.27272800	2.99846700	-3.29644800
C	-3.99583400	3.38660600	-2.80239400
H	-3.54928600	3.81136900	-3.71148200
H	-4.79596200	2.68591500	-3.09282900
H	-4.47372200	4.19500300	-2.22596300
F	-4.56675300	2.13823700	-0.31135300
N	2.13838100	1.32307400	0.15934000
H	2.87139500	0.73138300	-0.24166100
H	1.92171400	2.02230900	-0.56191700
C	2.69855700	2.04291400	1.33805300
H	3.12664100	1.25172100	1.97815200
C	3.77344500	3.05514900	0.95884800
C	1.53583300	2.65662300	2.15849200
H	3.36432000	3.80718300	0.26344200
H	4.11891900	3.58102400	1.85999400
H	4.62979100	2.55612600	0.47716500
O	0.40881800	2.00584400	2.09872900
O	1.72352900	3.67886200	2.83511700
H	-0.92589800	-0.36403800	1.66661500

N-equatorial/O-axial (A)

Ir	-0.33358900	0.27229900	0.86999100
H	0.89132200	-0.34895000	1.64031100
C	-0.31649600	-1.40278100	-0.12888600
C	0.35510700	-3.38848900	-1.09164800
C	-0.97178400	-3.24673600	-1.35325800
H	1.05777700	-4.17270400	-1.35066200
H	-1.67063900	-3.87637600	-1.89271300
N	0.74324200	-2.27522100	-0.35001500
N	-1.36855600	-2.04926100	-0.76293500
C	-2.65609100	-1.45534100	-0.95253600
C	-3.65006600	-1.62390300	0.02671700

C	-2.86676600	-0.69423700	-2.11644500
C	-4.87919300	-0.97963500	-0.17428200
C	-4.11571200	-0.07346500	-2.27960800
C	-5.12877900	-0.19752000	-1.31540700
H	-5.66031400	-1.08856700	0.58406600
H	-4.29264200	0.53450600	-3.17164000
C	2.09940800	-2.03061300	0.04474200
C	2.98799400	-1.49213100	-0.90281700
C	2.49876400	-2.34227700	1.35515300
C	4.30369400	-1.23155300	-0.49622300
C	3.81922800	-2.04374300	1.72409100
C	4.73056200	-1.47915700	0.81741000
H	4.99943100	-0.78835800	-1.21487600
H	4.14204500	-2.25622100	2.74785600
C	6.13294900	-1.11885700	1.24060100
H	6.32870600	-1.42167000	2.27985200
H	6.88230200	-1.59976200	0.59052200
H	6.28754500	-0.02935900	1.16233800
C	-6.44588800	0.51897000	-1.47814200
H	-6.59041900	0.85905600	-2.51425900
H	-7.28960200	-0.13163500	-1.19921600
H	-6.48842400	1.40592900	-0.82239500
C	-3.37950100	-2.45049400	1.25319700
H	-3.12613700	-3.48877100	0.98157000
H	-2.51493000	-2.03499300	1.79682800
H	-4.25469500	-2.46298600	1.91827800
C	-1.76117500	-0.52342300	-3.12422800
H	-2.02102600	0.24392700	-3.86705700
H	-0.82328200	-0.23626900	-2.62115200
H	-1.55608700	-1.46832100	-3.65497400
C	2.52477500	-1.17384800	-2.29957000
H	1.57886800	-0.61080500	-2.27499900
H	3.27823800	-0.57681600	-2.83292200
H	2.33483100	-2.09320600	-2.87878600
C	1.52209900	-2.95350300	2.32309800
H	0.65630900	-2.28183300	2.45082000
H	1.13739000	-3.91388500	1.94046900
H	1.99528700	-3.12750600	3.30028400
N	1.11253200	1.29627600	-0.40994700
C	2.39580100	1.36987600	0.01175100
C	0.81497700	1.86662900	-1.60151200
C	3.37445500	1.99230100	-0.75041700
H	2.63400300	0.88762600	0.95943500
C	1.76220500	2.50722100	-2.39734700
H	-0.21947500	1.77761800	-1.93375800

C	3.10266800	2.58167000	-1.98974800
H	1.45945500	2.94053200	-3.35262500
C	4.18538600	3.22401800	-2.80407800
H	3.77757100	3.64885000	-3.73115100
H	4.68177800	4.02372700	-2.23112000
H	4.96332700	2.48671900	-3.06233600
F	4.64904800	1.99421900	-0.28147800
N	-2.07823000	1.48020400	0.07780000
H	-1.81027700	2.07480500	-0.71288000
H	-2.85645600	0.90602400	-0.26091000
C	-2.56149500	2.36172600	1.18133800
H	-3.03851400	3.26502800	0.76738400
C	-3.56896700	1.60057600	2.04533600
C	-1.37976300	2.82568400	2.06378600
H	-3.09972900	0.67979900	2.42647100
H	-3.88015600	2.23329800	2.88906800
H	-4.45728700	1.32324500	1.45503400
O	-0.31881200	2.07212500	2.05551100
O	-1.51775700	3.84872700	2.75203800
H	-1.33190300	-0.40924800	1.90271400

4. Molecular Cartesian coordinates of the optimized nhPHIP complexes of A-A-A-OMe (Å)

Monodentate binding, N-terminus in the equatorial plane

Ir	-0.99564600	0.48759700	0.41906500
H	-1.62214500	0.19097200	1.84578500
C	-2.52544600	1.69866900	0.07083200
C	-4.64648700	2.56623300	-0.12463400
C	-3.77855300	3.60341800	-0.25936300
H	-5.72953400	2.52401700	-0.15259100
H	-3.94144500	4.66246200	-0.42479600
N	-3.87767100	1.42285800	0.07342000
N	-2.49773600	3.07083000	-0.13962000
C	-1.31254200	3.87565100	-0.21807000
C	-0.68308400	4.27116300	0.97834700
C	-0.84297400	4.27741100	-1.48193500
C	0.49615300	5.01885200	0.87737300
C	0.34528800	5.02626200	-1.53168000
C	1.03625700	5.38851400	-0.36726500
H	1.00689700	5.32281100	1.79598000
H	0.73653700	5.32969500	-2.50713800
C	-4.46145000	0.11815900	0.19189300
C	-4.71140500	-0.60505100	-0.98477100
C	-4.80882700	-0.36376700	1.46496500
C	-5.32299400	-1.86057100	-0.86202400
C	-5.42251600	-1.62185100	1.53912200
C	-5.68627800	-2.38304800	0.38804000
H	-5.50991100	-2.44849900	-1.76527900
H	-5.69205200	-2.01990200	2.52206700
C	-6.31203400	-3.75061600	0.50173900
H	-6.57444600	-4.15262900	-0.48832600
H	-5.61275500	-4.45299700	0.98448800
H	-7.22372700	-3.72190500	1.12010700
C	2.34325400	6.13609300	-0.44498100
H	3.19207300	5.43124400	-0.40056900
H	2.42724200	6.69907800	-1.38662200
H	2.45408300	6.83546400	0.39796600
C	-1.28090600	3.90864500	2.31106700
H	-2.29028200	4.34185800	2.41456800
H	-1.38277900	2.81429000	2.39567400
H	-0.65336900	4.28090300	3.13342500
C	-1.59984000	3.95400200	-2.74929600
H	-2.12958100	2.99045500	-2.68544400
H	-2.36697800	4.72253800	-2.94446900
H	-0.91992900	3.93231700	-3.61341800
C	-4.31419700	-0.04358800	-2.32383000
H	-4.93196300	0.83179200	-2.58711800

H	-3.26696300	0.29905000	-2.30369600
H	-4.42466600	-0.79998400	-3.11348700
C	-4.51400300	0.45112300	2.69587000
H	-3.43750500	0.68696900	2.74414900
H	-5.05431200	1.41257800	2.67482500
H	-4.80540900	-0.09433100	3.60475500
N	-1.84773000	-1.43853700	-0.26921200
C	-1.78050800	-1.91696100	-1.53422900
C	-2.31096200	-2.27763900	0.68539600
C	-2.17907000	-3.20581100	-1.88205900
H	-1.36317800	-1.25052900	-2.28638500
C	-2.71545200	-3.56935400	0.38498400
H	-2.36411500	-1.89079400	1.70152700
C	-2.67839600	-4.08730000	-0.91306400
C	-3.16117100	-5.47272000	-1.22007100
H	-2.71353400	-6.20718200	-0.53256300
H	-4.25463700	-5.53335600	-1.08743000
H	-2.91853400	-5.75017100	-2.25476300
N	-0.09358600	1.07469500	-1.58060300
H	-0.49280000	0.54351600	-2.36497900
H	-0.42562100	2.03682500	-1.69241700
C	1.37492000	1.11621700	-1.82484500
H	1.54852600	1.71600600	-2.74067200
C	2.11900800	1.78914100	-0.67697800
C	1.80987400	-0.29857800	-2.23411000
H	2.09318800	1.18105000	0.23431200
H	3.16732700	1.97549100	-0.95634100
H	1.64442200	2.75745400	-0.45866500
O	1.04263900	-1.01473300	-2.89981400
H	-0.25624700	1.74959800	1.00396800
N	3.07026900	-0.67151100	-1.90950600
H	3.58842600	-0.14928700	-1.19480600
C	3.60063600	-1.97650500	-2.34091600
H	2.83166800	-2.74326900	-2.16286700
C	3.96862800	-1.96438100	-3.83183900
C	4.78869700	-2.31925500	-1.43398200
H	4.73020000	-1.19855600	-4.04538500
H	4.35881500	-2.94831900	-4.13318700
H	3.06660100	-1.74206000	-4.41889700
O	4.80958400	-3.32147600	-0.71572500
N	5.80469600	-1.40015000	-1.47207100
H	5.66307500	-0.57663000	-2.05663500
C	6.67819000	-1.20748300	-0.32713600
H	6.81741500	-2.19002500	0.14973000
C	8.03465300	-0.62571000	-0.73928900

C	5.94954500	-0.30328500	0.68474700
H	7.90474700	0.35068600	-1.23270600
H	8.66840100	-0.48813100	0.14687700
H	8.53121900	-1.31340700	-1.43818300
H	-2.10090800	-3.52921500	-2.92189300
F	-3.18218700	-4.34474800	1.39894700
O	6.68094600	-0.13371400	1.79472400
C	6.10800200	0.75276300	2.79949100
H	5.16885800	0.32994600	3.18155800
H	6.86251100	0.81224700	3.59098100
H	5.91853100	1.74142100	2.35867000
O	4.84837000	0.19854900	0.50127100
C	2.94451000	-2.11325200	1.99788500
C	2.23237400	-2.50443200	0.85638600
C	1.12246000	-1.78374100	0.42190700
C	1.31941800	-0.29865600	2.19078200
C	2.42473200	-0.99252500	2.65477000
H	2.58596800	-3.35496000	0.27245400
H	0.58976800	-2.06279900	-0.48599900
H	0.94444500	0.58420800	2.70593400
N	0.66435800	-0.68070500	1.06335300
C	4.16725100	-2.82561700	2.49138300
H	4.56113300	-3.48620900	1.70818800
H	4.94991000	-2.10828400	2.78435800
H	3.93101700	-3.42406800	3.38745000
F	3.03574500	-0.53852700	3.78130800

Bidentate binding, N-terminus is in the equatorial and oxygen in axial position

Ir	0.40540400	-0.50043600	-0.09016000
H	-0.61701900	-0.24419700	-1.25207700
C	0.20004400	-2.35587700	-0.61435600
C	-0.68627100	-4.37091100	-1.27721500
C	0.66376700	-4.52230300	-1.23022100
H	-1.47726800	-5.06378200	-1.54075000
H	1.30084400	-5.37387000	-1.44105200
N	-0.96213500	-3.05618400	-0.90741100
N	1.18989700	-3.29707000	-0.82705900
C	2.58032600	-3.07703800	-0.56336100
C	3.43282100	-2.74850800	-1.62933600
C	3.04790800	-3.24345700	0.75095700
C	4.79598100	-2.58329400	-1.34694100
C	4.41241600	-3.02979600	0.99490700
C	5.29991000	-2.69801000	-0.04134500
H	5.47771000	-2.33473400	-2.16598700
H	4.79177000	-3.13832800	2.01544000

C	-2.29299800	-2.55235000	-0.72506700
C	-3.00399700	-2.97246700	0.41872200
C	-2.85332600	-1.67787100	-1.67132500
C	-4.28154500	-2.44135100	0.63244600
C	-4.13328500	-1.16371400	-1.40379800
C	-4.85631300	-1.52071400	-0.25850500
H	-4.83212300	-2.73897500	1.53001500
H	-4.58190400	-0.46294100	-2.11264200
C	-6.22631100	-0.94510600	-0.00025600
H	-7.01300300	-1.61943200	-0.38134300
H	-6.40092800	-0.80930800	1.07775700
H	-6.34351400	0.02717500	-0.50044000
C	6.75672000	-2.43239900	0.24411300
H	6.92572400	-1.35429900	0.41496000
H	7.09276900	-2.96624100	1.14581300
H	7.39128800	-2.73315600	-0.60353400
C	2.87447100	-2.54077400	-3.01111500
H	2.35475000	-3.44140800	-3.37683400
H	2.13023100	-1.72573900	-2.98986200
H	3.67115200	-2.28012800	-3.72217800
C	2.10636000	-3.66652600	1.84945900
H	1.15079400	-3.12175400	1.77762900
H	1.85961000	-4.73837200	1.76502400
H	2.55167800	-3.49939800	2.84155300
C	-2.41676700	-3.97208600	1.38229000
H	-2.51701200	-4.99947100	0.99223400
H	-1.34285800	-3.79559000	1.54518000
H	-2.93308800	-3.92222900	2.35148400
C	-2.14812600	-1.30906600	-2.95094700
H	-1.18219800	-1.82164500	-3.04688000
H	-2.77839800	-1.56953400	-3.81746300
H	-1.95883000	-0.22483400	-2.99000000
N	-1.21984900	-0.50516900	1.36136100
C	-1.18557700	-1.22514000	2.50682200
C	-2.30329900	0.27112600	1.13574600
C	-2.21086500	-1.20277400	3.44753200
H	-0.29749100	-1.84104000	2.65227900
C	-3.35214500	0.31608000	2.04318500
H	-2.32209300	0.84227400	0.20999300
C	-3.35400900	-0.41966800	3.23287000
C	-4.51864600	-0.37932700	4.17546000
H	-4.81168700	0.65901700	4.39489000
H	-5.39535000	-0.87053700	3.72020300
H	-4.27865700	-0.89543800	5.11478900
N	1.91812000	-0.35877300	1.60584200

H	2.08767200	-1.19552200	2.16943200
H	2.81291000	-0.11926900	1.15719500
C	1.53544700	0.75669700	2.51567900
H	0.69214400	0.39239400	3.12528600
C	2.68045400	1.19624000	3.43196600
C	0.96830000	1.86539700	1.63001000
H	3.50051300	1.62469300	2.83716700
H	2.34694100	1.93013400	4.18221200
H	3.05702700	0.32117300	3.98192600
O	0.57098600	1.61901900	0.45970400
H	1.59379800	-0.40639800	-1.14682500
N	0.88747800	3.11696900	2.11398300
H	1.20237000	3.30966700	3.06251200
C	0.43600400	4.22871000	1.26802400
H	-0.51919600	3.94407700	0.79496900
C	0.25801700	5.49474200	2.10588300
C	1.42092900	4.46295400	0.09777500
H	1.20207300	5.77786100	2.59778600
H	-0.05452900	6.31870900	1.44933500
H	-0.51704500	5.34149800	2.87158200
O	1.02459200	4.89432600	-0.98736500
N	2.72835400	4.18770800	0.37715200
H	2.92265700	3.73074000	1.26812600
C	3.69002000	3.88118600	-0.67185500
H	3.23502400	4.16876700	-1.63019700
C	5.02503700	4.61260800	-0.47358700
C	3.91492600	2.36585700	-0.65296500
H	5.47228800	4.33902500	0.49482800
H	5.72736000	4.34398600	-1.27656800
H	4.85375400	5.69835600	-0.49391100
H	-2.12745300	-1.80878300	4.35155400
F	-4.42995200	1.08766600	1.74753000
O	4.22344400	1.89667300	-1.86520600
C	4.47584700	0.46199200	-1.91822800
H	3.58727400	-0.07892500	-1.56325300
H	4.67938000	0.24219500	-2.97187700
H	5.33961900	0.20978600	-1.28727800
O	3.84417000	1.68268800	0.36258400
C	-1.67006000	3.09310000	-1.67102700
C	-3.75363000	2.91123000	-0.71598800
C	-4.25026700	2.32488300	-1.87741200
C	-3.44828200	2.10984100	-3.00364300
C	-2.11227800	2.51517200	-2.86614100
H	-0.63325900	3.42031000	-1.56074400
H	-4.41225100	3.05436600	0.14462900

H	-1.41929400	2.38109700	-3.70055000
F	-5.55975700	1.94142900	-1.91932200
C	-4.00237100	1.50259200	-4.25909800
H	-4.39770700	0.49117700	-4.07053900
H	-4.84001800	2.10566300	-4.64465200
H	-3.22511500	1.43382400	-5.03229900
N	-2.46873800	3.29796400	-0.60501500

Bidentate binding, N-terminus and oxygen are in the equatorial position

Ir	-0.11599300	-0.77997000	-0.93274000
H	-0.62621700	-1.27901100	-2.34596100
C	0.03011500	-2.64863500	-0.30419600
C	-0.43513600	-4.78736500	0.40447000
C	0.91945000	-4.66092900	0.36772300
H	-1.07191300	-5.62059900	0.67973200
H	1.71365700	-5.36215400	0.59805500
N	-0.96504200	-3.56534800	-0.00116300
N	1.18846400	-3.36371000	-0.05826400
C	2.51199200	-2.85266600	-0.27229200
C	3.02582500	-2.87307600	-1.58224500
C	3.25139000	-2.36483200	0.81774500
C	4.31404700	-2.36319100	-1.78643600
C	4.54079100	-1.87034200	0.56517600
C	5.08477300	-1.85419400	-0.72774900
H	4.72847800	-2.36613700	-2.79906200
H	5.13136000	-1.49559300	1.40575500
C	-2.36937700	-3.27140700	-0.05309900
C	-3.07660400	-3.07727900	1.14513300
C	-2.99655700	-3.19113500	-1.31291100
C	-4.42426600	-2.69134800	1.05499600
C	-4.33464700	-2.78277700	-1.35155800
C	-5.05716100	-2.49959100	-0.17937600
H	-4.98378000	-2.51404700	1.97878000
H	-4.82850700	-2.69009900	-2.32358400
C	-6.46851500	-1.97271000	-0.25305800
H	-6.98513900	-2.07409400	0.71311700
H	-6.46424100	-0.90080000	-0.52095300
H	-7.05374600	-2.49645800	-1.02510500
C	6.45773300	-1.28478600	-0.98110900
H	6.41268900	-0.18413600	-1.05012600
H	7.15223900	-1.53231800	-0.16359900
H	6.87739800	-1.66208100	-1.92556000
C	2.19283600	-3.40566100	-2.71674500
H	1.87406700	-4.44349000	-2.52284400

H	1.27768300	-2.79717900	-2.81978000
H	2.75529600	-3.37914300	-3.66090600
C	2.70446700	-2.39319000	2.22353000
H	1.60700500	-2.30346200	2.23879900
H	2.94276300	-3.35004000	2.71855900
H	3.14631200	-1.58991800	2.83294900
C	-2.45411400	-3.28674500	2.50358500
H	-2.78669800	-4.24846000	2.92996400
H	-1.35645400	-3.31791600	2.46523200
H	-2.76881600	-2.49635000	3.20203000
C	-2.26879200	-3.59482400	-2.56777400
H	-1.30124000	-3.07839800	-2.64754000
H	-2.06842600	-4.68039300	-2.55960000
H	-2.87252300	-3.36241400	-3.45701900
N	-0.25257000	1.18782700	-1.67232400
C	-1.45276000	1.74477700	-1.97899500
C	0.85977800	1.93628900	-1.86395100
C	-1.56894900	3.03677300	-2.48191500
H	-2.32821300	1.12555000	-1.78952000
C	0.77931100	3.23143600	-2.35416100
H	1.81357700	1.47934900	-1.60758700
C	-0.43622200	3.84174200	-2.67932100
C	-0.50604000	5.26133100	-3.15146200
H	-0.41530100	5.94047000	-2.28587700
H	0.31681200	5.49407200	-3.84294100
H	-1.46793000	5.46133800	-3.64286400
N	0.45513700	0.04677900	1.07458700
H	1.35771100	-0.32979400	1.37646200
H	0.56239200	1.07191900	1.03351100
C	-0.58563800	-0.31843200	2.07601100
H	-0.50246900	-1.41077300	2.20337800
C	-0.40457400	0.38107000	3.42237200
C	-1.93626300	-0.09712100	1.39037600
H	-0.50817500	1.47010400	3.30678300
H	-1.12773400	0.01767300	4.17000600
H	0.59682900	0.15972300	3.82097000
O	-2.04793700	-0.25728600	0.15158000
H	1.28642500	-0.95564000	-1.59042200
N	-3.01165100	0.26648900	2.11546100
H	-2.93194900	0.38629600	3.12289300
C	-4.24899900	0.65935100	1.43174000
H	-4.47248600	-0.10929200	0.67900700
C	-5.39717100	0.78518200	2.43025600
C	-4.03055000	1.96853300	0.62916100
H	-5.16728200	1.53173400	3.20717700

H	-6.30732100	1.10232600	1.90182500
H	-5.59003600	-0.18643200	2.90981800
O	-4.54138900	2.14011300	-0.48007000
N	-3.26291500	2.88866300	1.27680800
H	-2.79764100	2.58212400	2.12939700
C	-2.66327900	4.04698900	0.63882400
H	-2.92478900	4.00044400	-0.43033500
C	-3.16857100	5.37176300	1.23128200
C	-1.13970000	3.90150000	0.76413000
H	-2.93729400	5.42698500	2.30638800
H	-2.69361800	6.22125000	0.72135300
H	-4.25818000	5.43276200	1.09957700
H	-2.56122200	3.42795700	-2.71534500
F	1.93659400	3.93352600	-2.49751400
O	-0.49987300	4.95813700	0.24490000
C	0.95417600	4.97383100	0.37665700
H	1.35369300	3.95046400	0.41337800
H	1.32511000	5.51953800	-0.49836000
H	1.20879900	5.51295400	1.30045100
O	-0.59170600	2.94438800	1.29507200
C	4.56549800	1.07612900	2.23322200
C	3.24697400	1.42640600	1.96115100
C	3.87956300	2.36211000	-0.03670200
C	5.22744900	2.06315900	0.19059500
C	5.61221100	1.38991500	1.35940400
H	2.46351700	1.19100700	2.68861200
H	3.57732400	2.87974100	-0.95190300
H	5.98444100	2.34818200	-0.54393700
N	2.89328500	2.05555900	0.82687000
F	4.83970900	0.38510600	3.37439200
C	7.03003800	1.02029000	1.67776600
H	7.34606100	1.48050400	2.62774900
H	7.13134600	-0.07012100	1.80251800
H	7.70815100	1.34757400	0.87838000

Bidentate binding, oxygen is in the equatorial and N-terminus in axial position

Ir	-0.47580000	0.91799500	-0.66219900
H	0.76714400	1.70137800	-1.18279500
C	-0.67594500	2.34467300	0.66908000
C	-0.31777600	3.95549600	2.26630300
C	-1.64777600	3.96358100	1.97779400
H	0.27165600	4.55063100	2.95475000
H	-2.46297000	4.56584000	2.36321000
N	0.26296500	2.97269600	1.46612400
N	-1.85241200	2.98690500	1.00746100

C	-3.13765100	2.56877900	0.52427300
C	-3.66454100	3.16399200	-0.63162200
C	-3.80407000	1.54314900	1.21759300
C	-4.89677800	2.68848400	-1.10642700
C	-5.03650100	1.10829400	0.71422200
C	-5.59302500	1.66060700	-0.45112600
H	-5.31768600	3.12744000	-2.01621600
H	-5.56934000	0.30801400	1.23770300
C	1.62998000	2.55589000	1.58383100
C	1.98433200	1.75568300	2.68733100
C	2.56904300	2.97013100	0.62517500
C	3.32076500	1.35243200	2.80385100
C	3.89279600	2.52333400	0.77345100
C	4.28724100	1.72008600	1.85390300
H	3.60949900	0.72507700	3.65279700
H	4.63397400	2.82694900	0.02930400
C	5.71393900	1.25068000	1.99600600
H	6.08008500	1.40076400	3.02427300
H	5.79047400	0.17301700	1.77544700
H	6.38249400	1.78970000	1.30774700
C	-6.91246800	1.15340000	-0.97961800
H	-7.13385500	1.57479500	-1.97145400
H	-6.90684000	0.05378800	-1.06067900
H	-7.74010100	1.42368000	-0.30192000
C	-2.90219700	4.24792000	-1.34477000
H	-2.74842800	5.12369800	-0.69236900
H	-1.90409000	3.87448900	-1.62979800
H	-3.43632600	4.57393200	-2.24884500
C	-3.18032300	0.91716600	2.43564900
H	-2.14404400	0.61935600	2.21248200
H	-3.14307200	1.62775100	3.27865300
H	-3.73752900	0.02388500	2.75213000
C	0.95919200	1.35675800	3.71756800
H	0.73250200	2.19684800	4.39612600
H	0.01048800	1.06375900	3.24233900
H	1.32513200	0.51438700	4.32155200
C	2.18836800	3.91736800	-0.48275300
H	1.20533000	3.66102700	-0.90367700
H	2.12747000	4.94996000	-0.09632100
H	2.93946600	3.89555000	-1.28425000
N	0.78996100	-0.34791300	0.54562600
C	0.31257200	-1.07883400	1.58092600
C	2.10398600	-0.45611900	0.24545500
C	1.12647800	-1.90122500	2.35582600
H	-0.75788800	-0.99399800	1.77152800

C	2.94060300	-1.28060600	0.98056000
H	2.47847200	0.15474600	-0.57396500
C	2.49325400	-2.03220200	2.07168900
C	3.42409100	-2.90134200	2.86031700
H	3.96550400	-3.59681000	2.19950200
H	4.18501700	-2.28743200	3.37045500
H	2.87224300	-3.47948500	3.61331800
N	-0.50126100	-0.64326600	-2.17196700
H	0.03716800	-0.37887400	-3.01564300
H	-0.04892200	-1.50159900	-1.81903700
C	-1.92067800	-0.97283100	-2.49544200
H	-2.35484800	-0.05754600	-2.93190900
C	-2.05226300	-2.15095500	-3.45822000
C	-2.58770300	-1.15869500	-1.13287600
H	-1.62081300	-3.06443900	-3.01935400
H	-3.10383500	-2.33460900	-3.73078700
H	-1.51003700	-1.92457700	-4.38784000
O	-2.18618800	-0.49083000	-0.14832900
H	-1.39223600	1.78708300	-1.63822800
N	-3.55946700	-2.07613500	-0.96350400
H	-3.89634400	-2.61860800	-1.75613200
C	-3.98692500	-2.43083300	0.39284100
H	-4.22309400	-1.50158500	0.93054800
C	-5.20477300	-3.35198800	0.34988400
C	-2.82268800	-3.07787200	1.18686800
H	-4.97966700	-4.27568100	-0.20688500
H	-5.48985500	-3.62382500	1.37581400
H	-6.05279100	-2.83915800	-0.12857300
O	-2.73117600	-2.94341600	2.41020600
N	-1.96585600	-3.81446900	0.43106300
H	-2.08033600	-3.80543100	-0.58022300
C	-0.75322700	-4.42696200	0.93766800
H	-0.54001700	-3.96337200	1.91433700
C	-0.90121800	-5.94674200	1.12558900
C	0.39277800	-4.07298600	-0.01491700
H	-1.13755400	-6.43189500	0.16609100
H	0.02964800	-6.37382300	1.52333000
H	-1.72003200	-6.13998000	1.83311600
H	0.69323500	-2.44943100	3.19503900
F	4.25141100	-1.35639600	0.61973200
O	0.27441200	-3.37932300	-1.01762800
O	1.54022300	-4.64730800	0.36990200
C	2.67656500	-4.43442000	-0.51356800
H	2.91478800	-3.36363500	-0.57065000
H	3.50029800	-4.99724100	-0.06189500

H	2.44382400	-4.81435100	-1.51816700
C	2.61370800	1.03363100	-3.18474300
C	4.63399300	-0.02940200	-2.31055500
C	3.99600400	-1.25035900	-2.57641900
C	2.71132200	-1.26445700	-3.12823900
H	2.05785500	1.94680500	-3.41278900
H	4.50765300	-2.18734400	-2.34582100
H	2.20551600	-2.21466100	-3.32387500
N	2.02246500	-0.14826700	-3.43378800
C	5.99241300	0.07344500	-1.68587700
H	6.47013800	-0.91379800	-1.62874100
H	6.63780100	0.75952900	-2.25587800
H	5.90666100	0.47843200	-0.66450100
C	3.89636000	1.11209000	-2.64580700
F	4.44716000	2.33928200	-2.43277400

5. Molecular Cartesian coordinates of the optimized nhPHIP complexes of N-axial/O-equatorial coordinated alanine oligopeptides (Å)

Ir-A-A-OH, cycle size 5

Ir	0.01675200	-0.44783400	-1.09715600
H	-1.08084900	-1.25095000	-1.86945100
C	-0.14716800	-1.79840000	0.31319200
C	-0.93928100	-3.28090900	1.87814100
C	0.41656400	-3.39017900	1.87071700
H	-1.69905300	-3.79124500	2.45944600
H	1.09104500	-4.01732300	2.44289700
N	-1.27123300	-2.31640900	0.92863500
N	0.88555100	-2.48985400	0.91801600
C	2.27550400	-2.20630800	0.70278200
C	2.97459000	-2.91017600	-0.29037600
C	2.88447600	-1.22912800	1.50822100
C	4.32803600	-2.59537000	-0.48324300
C	4.24324100	-0.96001200	1.29151700
C	4.97832500	-1.62556900	0.29679100
H	4.88673300	-3.12121600	-1.26354100
H	4.74082500	-0.20986300	1.91477000
C	-2.59948300	-1.80037400	0.76679300
C	-3.05940600	-0.86069600	1.70859500
C	-3.40489500	-2.26854000	-0.28305300
C	-4.36451800	-0.37306100	1.56480300
C	-4.70204500	-1.74241700	-0.39316900
C	-5.19921500	-0.79890600	0.51867200
H	-4.73421900	0.36474700	2.28347700
H	-5.34447300	-2.09176400	-1.20721100
C	-6.59110000	-0.23608000	0.37343100
H	-7.10344100	-0.18690400	1.34738400
H	-6.55061900	0.78871200	-0.03068100
H	-7.19785000	-0.84596100	-0.31253700
C	6.44166400	-1.31995900	0.09161600
H	6.76425500	-1.58045600	-0.92778400
H	6.65357100	-0.25348700	0.26735900
H	7.06499300	-1.89833700	0.79568300
C	2.27225600	-3.94593000	-1.12610200
H	1.88349500	-4.76561000	-0.49891300
H	1.40807600	-3.48991800	-1.63776000
H	2.95291700	-4.37175100	-1.87718500
C	2.08474300	-0.48584700	2.54474300
H	1.21291800	-0.00697900	2.07108200
H	1.70284900	-1.16883800	3.32191300
H	2.69025900	0.29460000	3.02735000

C	-2.17255700	-0.40454500	2.83799300
H	-2.08688200	-1.18451000	3.61383200
H	-1.15260000	-0.19623400	2.47907800
H	-2.57562800	0.50557100	3.30419900
C	-2.90547200	-3.33207700	-1.22491600
H	-1.90868600	-3.07375700	-1.61455000
H	-2.81088700	-4.29938600	-0.70191600
H	-3.59923600	-3.46307500	-2.06789700
N	-1.48618600	0.94345600	-0.36006500
C	-1.23217500	1.82136300	0.63888500
C	-2.68642600	1.02187700	-0.98129400
C	-2.16162700	2.76869900	1.06193600
H	-0.24222500	1.75368900	1.08835800
C	-3.63338100	1.95934400	-0.59951000
H	-2.88694300	0.30082200	-1.77270900
C	-3.41993800	2.85996900	0.45013400
C	-4.48206500	3.82831500	0.87622800
H	-4.85991500	4.40223700	0.01555500
H	-5.34314800	3.28694200	1.30328300
H	-4.09495900	4.52425600	1.63264200
N	0.38699900	1.05695000	-2.63850000
H	0.26209100	0.68453600	-3.58507500
H	-0.28115000	1.83592600	-2.55491600
C	1.77943800	1.59797500	-2.53830900
H	2.43224100	0.79948100	-2.93044800
C	1.97278400	2.88211400	-3.34296400
C	2.12912900	1.68750000	-1.05316000
H	1.39021800	3.71071600	-2.91089600
H	3.03404500	3.17227400	-3.38645600
H	1.64066200	2.71935500	-4.37849100
O	1.58906000	0.91379200	-0.22371900
H	1.13164800	-1.37548400	-1.75476700
N	3.07605000	2.55062200	-0.65598500
H	3.44038700	3.24200900	-1.30642500
H	-1.90238200	3.44536200	1.87857800
F	-4.81853500	1.98243300	-1.26322000
C	3.51023500	2.59592600	0.73257400
H	3.64810800	1.55596300	1.07064600
C	4.83132600	3.36103900	0.85805600
C	2.41602500	3.20023800	1.62201700
H	4.71603200	4.39857600	0.50692700
H	5.14882700	3.37812900	1.90873900
H	5.60550300	2.86145500	0.25764500
O	1.41247800	3.76712300	1.23593400
O	2.72956200	3.00821800	2.92431900

H	2.01778100	3.41335000	3.46137500
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Ir-A-A-OH, cycle size 8

Ir	0.05834100	0.36022000	-0.71269400
H	-0.84724200	0.03353200	-1.93062600
C	0.07483900	-1.56357900	-0.29477500
C	0.73840100	-3.72528300	0.11572000
C	-0.61418200	-3.73812900	-0.01033400
H	1.45266700	-4.51772900	0.30911200
H	-1.33525600	-4.54557800	0.04859600
N	1.14588000	-2.40399500	-0.05932700
N	-1.00649800	-2.42677000	-0.25874000
C	-2.38524600	-2.03648500	-0.33921200
C	-3.10614700	-1.91775500	0.86222900
C	-2.98084600	-1.83654800	-1.59725000
C	-4.45716900	-1.54983500	0.78201200
C	-4.32988200	-1.45445100	-1.62448200
C	-5.08321100	-1.30485900	-0.44847500
H	-5.02922100	-1.43795900	1.70785500
H	-4.80615100	-1.27967600	-2.59423000
C	2.52189100	-2.02543000	0.09528900
C	3.35707600	-1.99342800	-1.03475500
C	3.01392800	-1.84431000	1.40129100
C	4.72230500	-1.73576200	-0.82940900
C	4.38733300	-1.60516300	1.55956400
C	5.25557100	-1.54408300	0.45716200
H	5.38736400	-1.69854900	-1.69718900
H	4.78493900	-1.45760100	2.56764100
C	6.71803900	-1.23004500	0.64558800
H	7.33093800	-1.69560200	-0.14096000
H	6.88745500	-0.14011400	0.59547400
H	7.07642800	-1.57479400	1.62722800
C	-6.52902500	-0.88034200	-0.51223500
H	-6.97593400	-0.84361900	0.49243700
H	-6.61818200	0.12082800	-0.96290800
H	-7.11945300	-1.57555700	-1.13148500
C	-2.45387900	-2.19063500	2.19288900
H	-2.36267300	-3.27587400	2.37114600
H	-1.43687100	-1.77187800	2.23409100
H	-3.04724200	-1.75658600	3.01000700
C	-2.22288200	-2.08943400	-2.87494800
H	-1.16399200	-1.81104800	-2.78027000
H	-2.26459700	-3.16182400	-3.13485600
H	-2.66731000	-1.52493400	-3.70790100
C	2.80281300	-2.27386800	-2.40528800

H	2.47622600	-3.32518300	-2.48189200
H	1.92013800	-1.64448500	-2.60094200
H	3.56091400	-2.08868200	-3.17943300
C	2.08678500	-1.92186200	2.58563700
H	2.61052300	-1.64251300	3.51069900
H	1.22052100	-1.25568600	2.44174300
H	1.68608200	-2.94185500	2.70868500
N	-1.68107300	0.88982900	0.48262700
C	-2.82492500	1.23544200	-0.15439500
C	-1.66778400	0.94995800	1.83513800
C	-3.95164900	1.62841200	0.55003800
H	-2.83961100	1.15686400	-1.24099100
C	-2.78319600	1.32586600	2.58073400
H	-0.72202100	0.68564500	2.30679600
C	-3.98469500	1.67418000	1.94814200
H	-2.72095800	1.33964700	3.67061500
C	-5.23537300	2.04679000	2.68464700
H	-5.05064100	2.10314500	3.76573400
H	-5.62432400	3.01549500	2.33308100
H	-6.02432900	1.29884900	2.49763100
F	-5.06756100	1.95136500	-0.15048300
H	1.30380000	0.06287400	-1.66107500
N	-0.09182000	2.47580000	-1.34518900
H	-0.81890500	2.52733400	-2.06845500
H	-0.45705700	3.02819400	-0.55532500
C	1.11177200	3.20589300	-1.86851300
H	1.45504000	2.64124000	-2.74758000
C	0.79905300	4.65288900	-2.22292500
C	2.12477000	3.08768800	-0.72436700
H	0.51864700	5.20613900	-1.31359100
H	1.68315500	5.13632200	-2.66575400
H	-0.02624000	4.70137500	-2.94960100
O	2.07846600	3.82841300	0.26301800
N	2.97110300	2.02581900	-0.83293000
H	2.72045700	1.34260300	-1.54943600
C	3.57355700	1.46031300	0.36721900
H	3.89998700	0.44651600	0.08626000
C	4.78424700	2.25328800	0.86364300
C	2.48887300	1.23161400	1.41869600
H	4.47753000	3.26365800	1.16588900
H	5.25143400	1.74316800	1.71738100
H	5.51634500	2.32520100	0.04670100
O	1.31739300	0.92769100	1.17440900
O	2.92903100	1.33223500	2.67591400
H	2.18420800	1.11167900	3.27401700

Ir-A-A-OMe, cycle size 5

Ir	-0.00586800	-0.64013500	-1.11432300
H	-1.09903500	-1.52403300	-1.80034800
C	-0.17604200	-1.83759200	0.42735700
C	-0.96826200	-3.14171300	2.14352700
C	0.38422600	-3.28503500	2.12102100
H	-1.72707100	-3.57404000	2.78615100
H	1.05610800	-3.86960800	2.73949700
N	-1.29835600	-2.26529900	1.11116500
N	0.85335300	-2.49348700	1.07643500
C	2.24370700	-2.24469100	0.82331000
C	2.93220500	-3.04999600	-0.09717300
C	2.86057100	-1.18952500	1.51659300
C	4.28482000	-2.76158200	-0.33185000
C	4.21748700	-0.94714000	1.26089900
C	4.94317300	-1.71678000	0.33689200
H	4.83622500	-3.36746500	-1.05737900
H	4.72120600	-0.13567400	1.79615900
C	-2.61613700	-1.72609400	0.93730700
C	-3.01144100	-0.67417600	1.78343000
C	-3.47692700	-2.28390300	-0.02176700
C	-4.31068700	-0.16908900	1.63842700
C	-4.76588800	-1.74100000	-0.13501300
C	-5.20111200	-0.68818600	0.68583600
H	-4.63223000	0.65417000	2.28349200
H	-5.45099000	-2.16250600	-0.87698400
C	-6.58483000	-0.10841100	0.53022500
H	-6.93924000	0.33422100	1.47370600
H	-6.58243100	0.68762200	-0.23262100
H	-7.30486000	-0.87610100	0.20743100
C	6.40590300	-1.44044400	0.09004000
H	6.71946500	-1.80648000	-0.89932200
H	6.62315200	-0.36261400	0.15298900
H	7.03270300	-1.94575000	0.84540800
C	2.21803200	-4.16031500	-0.81936000
H	1.83461400	-4.91399800	-0.11133800
H	1.34916900	-3.75279900	-1.36304800
H	2.88871300	-4.65955600	-1.53331000
C	2.06968000	-0.34270200	2.47747300
H	1.19999100	0.09444400	1.96105800
H	1.68502500	-0.94445500	3.31787600
H	2.68135900	0.47770300	2.87777200
C	-2.06549700	-0.12035700	2.81680500
H	-1.95155700	-0.81828900	3.66385100

H	-1.06143300	0.03086900	2.39058200
H	-2.43333600	0.83999800	3.20490300
C	-3.03574000	-3.44997200	-0.86607000
H	-2.06434100	-3.24135500	-1.34130600
H	-2.90622900	-4.35322200	-0.24542100
H	-3.77898200	-3.67022800	-1.64581600
N	-1.51563900	0.82276200	-0.55034100
C	-1.26269600	1.82258700	0.32683100
C	-2.71796000	0.81703000	-1.17240800
C	-2.19486800	2.81226300	0.62981000
H	-0.27034700	1.81898500	0.77515100
C	-3.66787900	1.79141500	-0.90935800
H	-2.91647200	0.00257400	-1.86773800
C	-3.45597200	2.81871900	0.01709400
C	-4.52353400	3.82570000	0.32252200
H	-4.91467800	4.27831900	-0.60215100
H	-5.37507800	3.33643400	0.82509000
H	-4.13733700	4.61812100	0.97771100
N	0.38171400	0.68462600	-2.80849900
H	0.24448000	0.21675400	-3.70981900
H	-0.26880100	1.48274100	-2.80646200
C	1.78544100	1.20279200	-2.76786000
H	2.42151600	0.34680600	-3.05120100
C	2.01123200	2.37170800	-3.72466900
C	2.12523500	1.47180300	-1.30248500
H	1.43676300	3.25668500	-3.40887300
H	3.07772500	2.63871400	-3.78470300
H	1.69282800	2.08445400	-4.73740700
O	1.56882300	0.81184400	-0.38882400
H	1.11360600	-1.63243200	-1.65877000
N	3.07178700	2.37377100	-1.00506500
H	3.44836400	2.97492700	-1.73361400
H	-1.93491700	3.58836800	1.35250400
F	-4.85369400	1.72662200	-1.56941000
C	3.47667300	2.60237800	0.37597600
H	3.69552800	1.62289300	0.82991500
C	4.71834200	3.49685700	0.42664800
C	2.32022200	3.21980300	1.17625600
H	4.50886800	4.47605800	-0.03214600
H	5.01517400	3.65330800	1.47215900
H	5.54812100	3.01629500	-0.11212800
C	1.53161800	3.59418600	3.37714200
H	1.92403700	3.45671000	4.39051000
H	1.36483000	4.65819600	3.15852800
H	0.59239400	3.03679100	3.24454700

O	1.35055800	3.78500600	0.70559100
O	2.55110400	3.05445000	2.49399700

Ir-A-A-OMe, cycle size 8

Ir	0.12166300	0.17205100	-0.76766800
H	-0.46084900	-0.43251800	-2.08050600
C	0.19098700	-1.64983200	-0.01968600
C	0.96036800	-3.69986000	0.68299400
C	-0.39565700	-3.72523900	0.77423100
H	1.71168600	-4.44769900	0.91011900
H	-1.08296800	-4.49737700	1.10126300
N	1.30640400	-2.44166900	0.19904600
N	-0.84728400	-2.48057500	0.34623800
C	-2.23520500	-2.12308700	0.35942900
C	-2.75171500	-1.50999200	1.51073400
C	-3.02922900	-2.43502300	-0.75620300
C	-4.12180500	-1.21332600	1.53120100
C	-4.39539400	-2.13075900	-0.68783200
C	-4.95743600	-1.52216500	0.44731300
H	-4.54307100	-0.71694400	2.41010300
H	-5.03055200	-2.35403500	-1.55021500
C	2.67070500	-2.05693200	-0.01595100
C	3.19850900	-2.12578800	-1.31973500
C	3.44897700	-1.68892700	1.09240000
C	4.53666300	-1.75390000	-1.50149700
C	4.79386400	-1.34892600	0.86482600
C	5.34792300	-1.35617800	-0.42404600
H	4.96067300	-1.78791100	-2.50954800
H	5.41606200	-1.05738200	1.71680200
C	6.77502000	-0.92601600	-0.65329700
H	7.23824800	-1.50009900	-1.47044100
H	6.81644400	0.14012600	-0.93695000
H	7.38142900	-1.05140200	0.25622300
C	-6.42302200	-1.16744900	0.47437800
H	-6.71246600	-0.74071500	1.44628600
H	-6.65351800	-0.42959000	-0.31157200
H	-7.05074900	-2.05305100	0.28279100
C	-1.83692100	-1.15297000	2.65123400
H	-1.39660800	-2.05605200	3.10699900
H	-0.99873800	-0.53661200	2.28506400
H	-2.37744400	-0.59462000	3.42856200
C	-2.40413000	-3.03005300	-1.99005900
H	-1.61295700	-2.36148900	-2.37227300
H	-1.92334700	-3.99791500	-1.77098600
H	-3.15645100	-3.18106900	-2.77699800

C	2.33812700	-2.58161200	-2.46639500
H	1.94521000	-3.59571600	-2.28225900
H	1.46902300	-1.91058200	-2.57216100
H	2.90987000	-2.58984000	-3.40527700
C	2.86133000	-1.65330000	2.48010400
H	3.45182300	-0.99943400	3.13835200
H	1.81972400	-1.29783800	2.45689500
H	2.84596500	-2.66049100	2.92988200
N	-1.86649800	0.87770500	-0.14057800
C	-2.91031800	0.72761300	-0.98741000
C	-2.06103400	1.63766400	0.96482200
C	-4.14268400	1.30880900	-0.72744300
H	-2.75092800	0.11848300	-1.87567400
C	-3.28065200	2.24071200	1.26202300
H	-1.19430600	1.74594300	1.61535200
C	-4.38464100	2.08252900	0.41198200
H	-3.37755100	2.83648400	2.17180000
C	-5.73585500	2.66919000	0.68970400
H	-5.69456900	3.35324100	1.54801800
H	-6.11759200	3.21210800	-0.18896700
H	-6.46094400	1.86865700	0.91285300
F	-5.15035500	1.09202800	-1.61210200
H	1.55718600	-0.15443200	-1.34397000
N	0.08593300	2.11764400	-1.80698800
H	-0.41288700	1.99226800	-2.69563500
H	-0.47650600	2.79643300	-1.27242600
C	1.40054000	2.77485800	-2.10410500
H	1.97817000	2.05161500	-2.69767500
C	1.23443800	4.09792300	-2.83989400
C	2.02234000	2.95584500	-0.71457000
H	0.71088100	4.81924600	-2.19391400
H	2.21845900	4.51472300	-3.10366400
H	0.65779400	3.95096100	-3.76596300
O	1.61715600	3.83415600	0.05413400
N	2.94906000	2.01711200	-0.37255900
H	2.98740200	1.19548700	-0.97741000
C	3.24860500	1.77826000	1.03303500
H	3.82044400	0.83548800	1.06246500
C	4.09941200	2.88621600	1.66365300
C	1.95085500	1.46944000	1.78385400
H	3.54889000	3.83575900	1.65934400
H	4.36427600	2.62017500	2.69562900
H	5.02108200	2.99757100	1.07473900
O	0.91699000	1.02272400	1.27706900
C	0.90821000	1.31139000	3.90516500

H	0.65700000	0.25182300	3.75646200
H	1.21507400	1.50225700	4.93855300
H	0.05258200	1.94263700	3.62747000
O	2.06514800	1.66573900	3.09578800

Ir-A-A-OH-OH-A-A, cycle size 5, dimer

Ir	1.79515300	-1.14502800	-0.81322100
H	1.89340300	-2.69109700	-1.06366700
C	1.62138900	-1.58935800	1.08790100
C	0.96628000	-2.43884400	3.11814500
C	2.07061000	-1.67652100	3.34005000
H	0.33923900	-3.01148700	3.79238500
H	2.61639100	-1.44811200	4.24875500
N	0.70613400	-2.38332700	1.74986000
N	2.46126600	-1.16682500	2.10501100
C	3.49599700	-0.18545900	1.94035500
C	4.79928600	-0.60451800	1.62914500
C	3.15470200	1.16946700	2.09380100
C	5.77474300	0.38442800	1.43485800
C	4.16330500	2.12312200	1.89454800
C	5.47495300	1.75093700	1.55739600
H	6.79296900	0.07812500	1.17605200
H	3.91844000	3.18422300	2.00862600
C	-0.52068100	-2.86029300	1.17895200
C	-1.62858600	-1.99662000	1.21045500
C	-0.59014400	-4.15732100	0.64711800
C	-2.84433800	-2.46839000	0.69488900
C	-1.83040100	-4.59585100	0.15975400
C	-2.96607200	-3.76921400	0.18270700
H	-3.70275800	-1.79029400	0.66875300
H	-1.90597900	-5.60466700	-0.25755600
C	-4.28041600	-4.25142100	-0.37922600
H	-5.10513000	-3.58405200	-0.08619800
H	-4.23913400	-4.28356300	-1.48061400
H	-4.51360200	-5.27052500	-0.03144600
C	6.54461200	2.79779400	1.36552700
H	7.35319700	2.42776200	0.71707900
H	6.12809700	3.71563000	0.92198700
H	6.99673900	3.07719700	2.33317400
C	5.11091800	-2.06861200	1.47719900
H	4.88701900	-2.62184300	2.40443700
H	4.48222300	-2.50121200	0.68076900
H	6.16988500	-2.22060700	1.22376200
C	1.74572000	1.57254100	2.43687100
H	1.06247000	1.28685900	1.62257000

H	1.39607800	1.06873100	3.35275400
H	1.67077900	2.65974400	2.58227500
C	-1.49609000	-0.60145700	1.76025000
H	-1.38013700	-0.61601500	2.85814800
H	-0.59787200	-0.11127600	1.35166000
H	-2.37875500	-0.00277700	1.49769000
C	0.64028700	-5.02299200	0.59050100
H	1.42901400	-4.51827900	0.00657900
H	1.05217000	-5.20000400	1.59799500
H	0.41612800	-5.99429400	0.12684800
N	-0.30305100	-1.16552600	-1.43355400
C	-1.09766600	-0.06976900	-1.37141300
C	-0.80980300	-2.27603600	-2.01733500
C	-2.40581300	-0.05826400	-1.84685800
H	-0.64990000	0.81156600	-0.91393000
C	-2.10536100	-2.30417900	-2.51100700
H	-0.16725100	-3.15404100	-2.06043700
C	-2.96460400	-1.20425000	-2.42782500
C	-4.38964600	-1.27821700	-2.88695000
H	-4.46764100	-1.75991200	-3.87360900
H	-4.98071800	-1.88641300	-2.18101600
H	-4.83469600	-0.27501700	-2.93280100
N	2.17176500	-0.43981400	-2.85318300
H	2.75364300	-1.08382900	-3.39779600
H	1.29210400	-0.34327200	-3.37986100
C	2.86608400	0.88714600	-2.81761900
H	3.89670800	0.66976000	-2.48939600
C	2.87429700	1.58807100	-4.17509400
C	2.24729600	1.68792600	-1.67410200
H	1.85586600	1.88287200	-4.47265500
H	3.51664700	2.48219700	-4.16008600
H	3.28384500	0.90822000	-4.93620100
O	1.70537700	1.09892300	-0.70412200
H	3.36015600	-1.11252400	-0.54794800
N	2.32832500	3.02636000	-1.67951400
H	2.67643500	3.51666800	-2.49946400
H	-3.01212500	0.83977300	-1.73035100
F	-2.55311300	-3.46248500	-3.06573200
C	1.78723100	3.79455300	-0.56484200
H	2.19599300	3.37687000	0.36823800
C	2.16718600	5.27266400	-0.69375900
C	0.26403900	3.64227700	-0.49544300
H	1.76512300	5.69571100	-1.62746200
H	1.75571800	5.83411300	0.15578700
H	3.26209700	5.37547100	-0.69070000

O	-0.41860400	3.37194600	-1.49260600
O	-0.21018900	3.86101500	0.71284800
N	-5.36626600	-0.67072300	2.75491000
H	-5.49619200	-0.99334100	3.71843300
H	-4.43200700	-0.99122800	2.47743600
C	-5.35278100	0.79595200	2.76799100
H	-6.36185900	1.14568100	3.04767300
C	-4.32617600	1.41912000	3.74268600
C	-5.04095900	1.30307800	1.35720500
H	-3.30771900	1.10214200	3.46535400
H	-4.36381300	2.52050700	3.73219700
H	-4.53455000	1.07082700	4.76641000
O	-4.41286000	0.63318100	0.52375400
N	-5.43272900	2.57888300	1.09131300
H	-5.88717000	3.13200500	1.81408100
C	-5.01578100	3.23387600	-0.13563900
H	-5.34160200	2.63047300	-0.99732400
C	-5.61474600	4.64276200	-0.22278100
C	-3.48872600	3.33072100	-0.20622600
H	-5.27481700	5.25469200	0.62739100
H	-5.30149800	5.12791300	-1.15755500
H	-6.71265200	4.57988600	-0.20679600
O	-2.78811400	3.49617100	0.80073100
O	-3.03021200	3.27510000	-1.44468700
H	-1.23080900	3.73693000	0.72023800
H	-2.00914500	3.34968600	-1.44543000

Ir-A-A-A-O⁻, cycle size 5

Ir	0.08709300	-0.88717000	-1.02116900
H	-1.01920800	-1.62599000	-1.84114100
C	-0.09212700	-2.30216500	0.32402900
C	-0.88819300	-3.87118800	1.80282300
C	0.47092000	-3.92102500	1.85627000
H	-1.64861400	-4.43638200	2.33003400
H	1.14475400	-4.53763700	2.44067400
N	-1.21964600	-2.88999700	0.87025300
N	0.94251000	-2.97026400	0.95540700
C	2.32159100	-2.60281900	0.80216500
C	3.09013500	-3.22023700	-0.19636000
C	2.84234200	-1.60692000	1.64683000
C	4.41685900	-2.79222000	-0.35760800
C	4.17478800	-1.21858400	1.45748900
C	4.97166400	-1.78766700	0.45121500
H	5.02888400	-3.25161300	-1.13990200
H	4.59613900	-0.44087600	2.10239700

C	-2.55381900	-2.42084300	0.63482600
C	-3.14334400	-1.58230800	1.59907900
C	-3.22771000	-2.80788000	-0.53575700
C	-4.42870300	-1.08740100	1.33971700
C	-4.50610900	-2.27463300	-0.75838500
C	-5.11730400	-1.40614200	0.15961400
H	-4.89290500	-0.41824900	2.07046600
H	-5.04126700	-2.55407400	-1.67126700
C	-6.46845400	-0.80108200	-0.12880300
H	-7.04389000	-0.64863600	0.79750500
H	-6.34717500	0.18437900	-0.60929200
H	-7.05537000	-1.43679300	-0.80919900
C	6.38264200	-1.30087800	0.22899500
H	6.94301000	-1.98237300	-0.42834900
H	6.37728200	-0.30292900	-0.24334500
H	6.92721400	-1.20477500	1.18192800
C	2.48571800	-4.28204200	-1.07494900
H	2.14132400	-5.14445000	-0.48003900
H	1.60467200	-3.87326000	-1.59773600
H	3.21333300	-4.63692600	-1.81904900
C	1.97337800	-0.96250200	2.69266300
H	1.02320200	-0.63964000	2.24072600
H	1.72707700	-1.66909000	3.50326400
H	2.46820000	-0.08442200	3.13261300
C	-2.42281800	-1.23483400	2.87646700
H	-2.48436400	-2.06435400	3.60183800
H	-1.35438000	-1.04442400	2.69413600
H	-2.86443000	-0.33994800	3.33720500
C	-2.62097000	-3.80655900	-1.48666300
H	-1.56217600	-3.57778200	-1.67765800
H	-2.67029300	-4.82288400	-1.05796900
H	-3.16483400	-3.81325900	-2.44265100
N	-1.38452400	0.43707200	-0.15681100
C	-1.15871100	1.09405500	1.00332100
C	-2.53871300	0.69057000	-0.81301200
C	-2.07260800	1.98990800	1.54878600
H	-0.20010800	0.89287000	1.48093000
C	-3.45470200	1.60720000	-0.32371800
H	-2.71957200	0.13916500	-1.73507300
C	-3.26506700	2.29119500	0.87960800
C	-4.23000600	3.33339100	1.35048200
H	-4.02664600	4.25999100	0.78643500
H	-5.27221500	3.03837800	1.15874400
H	-4.09590400	3.53910500	2.42173600
N	0.53955000	0.67521100	-2.46901000

H	0.30626500	0.42880600	-3.43546600
H	0.05392300	1.57247300	-2.24253900
C	2.01092700	0.94648000	-2.39826600
H	2.50907300	0.01136200	-2.70656200
C	2.43936200	2.11178400	-3.28777000
C	2.30642600	1.10674500	-0.90837600
H	1.93615200	3.03744100	-2.96876200
H	3.53270100	2.24888300	-3.27360500
H	2.15539000	1.89830900	-4.32919300
O	1.65324600	0.43929700	-0.06824500
H	1.18990000	-1.78660900	-1.74634000
N	3.24884400	1.97642900	-0.49671800
H	3.72763200	2.55157400	-1.18674900
C	3.34232800	2.34995600	0.91648700
H	3.30785400	1.42162700	1.50486000
C	4.64489700	3.09975900	1.18894500
C	2.11490300	3.17992900	1.38612900
H	4.70741000	4.01005700	0.57055800
H	4.67123100	3.39563300	2.24696500
H	5.51289900	2.45785700	0.97511700
O	1.84893600	3.24566500	2.59523500
N	1.44004300	3.81191000	0.40213300
H	1.58851200	3.51019600	-0.56700600
C	0.11549800	4.40680600	0.53727100
H	-0.37676000	3.94926800	1.41044600
C	0.17819500	5.92457100	0.74128500
C	-0.71871400	4.02604000	-0.73722400
H	0.71046000	6.40353300	-0.09694000
H	-0.84496100	6.32533800	0.78295200
H	0.70396200	6.16900100	1.67759200
H	-1.84355800	2.48030400	2.49710000
F	-4.58230000	1.83810800	-1.04993900
O	-0.11045800	3.30693700	-1.60729300
O	-1.88669100	4.46906300	-0.79511100

Ir-A-A-A-O⁻, cycle size 8

Ir	-0.02844900	-0.49413200	1.04685400
H	0.74708600	-1.49744400	1.96347100
C	-0.09991900	-1.89237000	-0.32995600
C	-0.84439300	-3.53853700	-1.75300900
C	0.51349700	-3.55100200	-1.79996900
H	-1.58807300	-4.14308400	-2.26001300
H	1.21046700	-4.16456900	-2.35974900
N	-1.20821400	-2.53149500	-0.86144700
N	0.95229400	-2.55200200	-0.93527400

C	2.32356000	-2.13715900	-0.87833700
C	2.74550800	-1.15795600	-1.79305600
C	3.19498900	-2.74001500	0.04189300
C	4.09734800	-0.78867600	-1.77465600
C	4.53984200	-2.34380100	0.02056000
C	5.00768600	-1.37315200	-0.88113300
H	4.44369200	-0.01535700	-2.46633200
H	5.23490500	-2.79550000	0.73492100
C	-2.57797600	-2.14087000	-0.68890200
C	-3.30699900	-2.62671600	0.40999500
C	-3.16889300	-1.35909800	-1.69884500
C	-4.65696600	-2.25688100	0.51110800
C	-4.53172500	-1.04914200	-1.57664500
C	-5.28621800	-1.47231100	-0.46978100
H	-5.23695400	-2.61063400	1.36880100
H	-5.00545600	-0.43830000	-2.35108800
C	-6.72782400	-1.05588000	-0.31881600
H	-7.28850400	-1.77190100	0.30087100
H	-6.79431100	-0.06866200	0.17179100
H	-7.22333600	-0.96958100	-1.29799700
C	6.45000300	-0.93265900	-0.85225300
H	6.69880100	-0.32377100	-1.73436800
H	6.64658400	-0.32741500	0.04830400
H	7.13175600	-1.79758000	-0.81926600
C	1.75597600	-0.51292400	-2.72715300
H	1.39273800	-1.23035700	-3.48270200
H	0.87450300	-0.16187500	-2.16459900
H	2.20508200	0.34788400	-3.24215000
C	2.67724000	-3.75291800	1.02825000
H	1.86987700	-3.30922300	1.63578400
H	2.24610200	-4.62847300	0.51474200
H	3.48064200	-4.09735100	1.69494700
C	-2.66534400	-3.55136900	1.40981700
H	-2.47936200	-4.53944800	0.95425600
H	-1.69354300	-3.15199700	1.73883700
H	-3.31602700	-3.69267100	2.28494300
C	-2.35358500	-0.86833900	-2.86567300
H	-2.91587000	-0.12573600	-3.44868100
H	-1.41997200	-0.40660800	-2.50833900
H	-2.06866100	-1.69850800	-3.53358000
N	1.83434200	0.54305700	0.53289400
C	2.96546400	0.27903700	1.22713900
C	1.86171300	1.57823100	-0.33906600
C	4.11413100	1.03429600	1.04286200
H	2.94448900	-0.56109000	1.92021200

C	2.99235100	2.35956400	-0.55753600
H	0.93376700	1.76765900	-0.87149600
C	4.18130700	2.10008400	0.13809500
H	2.91166300	3.16948700	-1.28766900
C	5.45043200	2.87144200	-0.07091100
H	5.27073500	3.74621100	-0.71043100
H	5.87406800	3.20485300	0.88942700
H	6.21085500	2.23434900	-0.55359800
F	5.22017600	0.70033700	1.76320200
H	-1.37650100	-1.13801900	1.58436700
N	0.08809400	0.92582800	2.73786500
H	0.73352100	0.52037100	3.42592700
H	0.54339200	1.79528100	2.42249700
C	-1.16359700	1.32048700	3.46451400
H	-1.63751100	0.38173800	3.78713700
C	-0.87920600	2.23633600	4.64676100
C	-2.01424100	2.00943500	2.38595700
H	-0.46886400	3.19159800	4.28568800
H	-1.80778800	2.44475900	5.20004000
H	-0.16093600	1.76501100	5.33520700
O	-1.85097300	3.19964900	2.10140500
N	-2.86637000	1.17083900	1.73323200
H	-2.69100300	0.17665000	1.89821500
C	-3.32175800	1.47358400	0.37972600
H	-3.83368800	0.56144400	0.03771700
C	-4.32284400	2.63350400	0.33435200
C	-2.10653200	1.61672700	-0.55745200
H	-3.82159700	3.58841700	0.54150700
H	-4.82606200	2.67622600	-0.64449100
H	-5.09752400	2.46339600	1.09567200
O	-1.02703100	1.00433200	-0.35401500
N	-2.26390000	2.34025400	-1.67531600
H	-3.06721300	2.96073100	-1.73566000
C	-1.17878300	2.55207700	-2.63260200
H	-0.64791500	1.59385200	-2.73411300
C	-1.76294500	2.96591000	-3.98327600
C	-0.11154600	3.60984500	-2.14250300
H	-2.32603700	3.91017900	-3.88635300
H	-0.93504000	3.13042700	-4.68683600
H	-2.43650900	2.19400800	-4.38929600
O	0.97866000	3.54849200	-2.78466500
O	-0.44112500	4.38224000	-1.20818400

Ir-A-A-A-O⁻, cycle size 11

Ir	-0.21759700	0.30028300	-0.42065900
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H	-0.68781400	0.13355500	-1.91077200
C	-0.33220100	-1.66024500	-0.28367500
C	0.19844200	-3.90405000	-0.32239100
C	-1.15313900	-3.81377500	-0.22679800
H	0.85943700	-4.76176000	-0.37360300
H	-1.92601800	-4.57242900	-0.17447900
N	0.69058900	-2.60129100	-0.35546500
N	-1.46005300	-2.45658500	-0.20171400
C	-2.81261700	-1.98763000	-0.16364700
C	-3.39677500	-1.71113900	1.08087300
C	-3.51545800	-1.86974800	-1.37493200
C	-4.73848900	-1.30099400	1.09063400
C	-4.85694100	-1.47076400	-1.31637700
C	-5.48248700	-1.18014100	-0.09212300
H	-5.20926000	-1.05766400	2.04765200
H	-5.41777200	-1.35928700	-2.24937900
C	2.09666900	-2.33845500	-0.46069400
C	2.62808100	-1.94528500	-1.70305800
C	2.91327100	-2.58380400	0.65914600
C	4.00780700	-1.69963900	-1.77433700
C	4.28715300	-2.33693200	0.53421400
C	4.84960100	-1.87298700	-0.66350700
H	4.43728600	-1.38006600	-2.72948600
H	4.93139600	-2.49741900	1.40365800
C	6.31853000	-1.54137600	-0.73471500
H	6.93477300	-2.37062900	-0.35106200
H	6.63243000	-1.32125000	-1.76637700
H	6.52770100	-0.65879500	-0.10428700
C	-6.91140400	-0.69801700	-0.06272500
H	-7.27928700	-0.60068500	0.96970600
H	-6.99307400	0.28619500	-0.55336500
H	-7.57748500	-1.38769200	-0.60645200
C	-2.58674600	-1.82452800	2.34357800
H	-2.26446700	-2.86684200	2.51054400
H	-1.66762300	-1.21531200	2.29075900
H	-3.17679200	-1.49995700	3.21312400
C	-2.81364000	-2.11684600	-2.68394100
H	-1.94486200	-1.44113300	-2.77373900
H	-2.42323500	-3.14655700	-2.74421500
H	-3.49264600	-1.94696000	-3.53168900
C	1.74683300	-1.82238800	-2.91728500
H	1.21241900	-2.76885600	-3.10667400
H	0.98047600	-1.04637100	-2.75517400
H	2.34340400	-1.57163400	-3.80675200
C	2.33932700	-3.11614200	1.94732800

H	3.12151400	-3.16867100	2.71904000
H	1.52216300	-2.48141300	2.32411800
H	1.92766000	-4.12968300	1.80807500
N	-2.22020600	0.95760900	0.23168200
C	-3.17963600	1.19881700	-0.68914100
C	-2.46691600	1.33008100	1.51189600
C	-4.38511100	1.79173000	-0.34006200
H	-2.97560300	0.89196000	-1.71434000
C	-3.66003200	1.93356700	1.90100500
H	-1.64740100	1.12860900	2.20410100
C	-4.68001900	2.18019400	0.96960800
H	-3.80602700	2.21004900	2.94751400
C	-6.00260700	2.78879600	1.33022500
H	-5.98264800	3.18348100	2.35523600
H	-6.26735900	3.60013200	0.63454700
H	-6.80299600	2.03273000	1.26289400
F	-5.31546800	1.97363300	-1.31642800
H	1.25599300	0.03650900	-0.91919900
N	-0.00703000	2.44972800	-0.74211000
H	-0.90983900	2.83190400	-1.05333700
H	0.19187000	2.91031000	0.15998200
C	1.04336600	2.88606200	-1.71879400
H	1.02880800	2.15436500	-2.53859400
C	0.78412000	4.29844500	-2.23827500
C	2.37874800	2.83778600	-0.95816800
H	0.83797400	5.01452900	-1.40426900
H	1.53875500	4.57620000	-2.99026000
H	-0.21107400	4.35464200	-2.70693300
O	2.60365100	3.64878500	-0.05079800
N	3.23351800	1.84913200	-1.33263400
H	2.86453000	1.13296600	-1.95656000
C	4.49308900	1.55253100	-0.64492600
H	4.93106400	0.70685300	-1.19539900
C	5.47911700	2.72589300	-0.69308100
C	4.32061200	1.03120500	0.80946200
H	5.04381800	3.60918900	-0.20692100
H	6.39711700	2.43570100	-0.16436900
H	5.72033400	2.96834900	-1.73868100
O	5.32962600	0.86176900	1.51655000
N	3.05892200	0.77318500	1.19375100
H	2.29611100	0.87332200	0.52072400
C	2.64485800	0.28791700	2.50271700
H	3.09789600	-0.69906000	2.69112100
C	3.05423800	1.25011000	3.63232200
C	1.10044300	0.13261500	2.52608000

H	2.59429100	2.23782600	3.46827800
H	2.70725800	0.84593700	4.59483700
H	4.14699600	1.36192500	3.64832000
O	0.44176800	0.85387000	1.67611800
O	0.60536600	-0.59433000	3.40533000

Ir-A-A-A-OH, cycle size 5

Ir	0.11159200	-0.89439000	-1.05415600
H	-0.98558400	-1.66010500	-1.85850900
C	-0.09029200	-2.27218700	0.32714000
C	-0.90462100	-3.80559300	1.83001500
C	0.45345100	-3.86137400	1.89378400
H	-1.67208300	-4.35592200	2.36260100
H	1.12051700	-4.46850700	2.49548800
N	-1.22475300	-2.84078200	0.87651400
N	0.93585400	-2.93166100	0.97730000
C	2.31896000	-2.57319100	0.83758500
C	3.10397000	-3.22786800	-0.12369000
C	2.83018800	-1.56116400	1.66939100
C	4.44218200	-2.82642100	-0.25716500
C	4.17597600	-1.20538100	1.51211000
C	4.99285200	-1.81579100	0.54642800
H	5.06765300	-3.31459300	-1.01074100
H	4.59554600	-0.42419200	2.15408000
C	-2.55972800	-2.38086600	0.62558500
C	-3.16261800	-1.54194700	1.58132000
C	-3.22901500	-2.79308700	-0.53972800
C	-4.46013300	-1.07824800	1.32181500
C	-4.51846900	-2.28782600	-0.76364600
C	-5.14764900	-1.42695900	0.14972500
H	-4.93847800	-0.41651800	2.05033400
H	-5.05134300	-2.59052000	-1.67037000
C	-6.52061400	-0.87044200	-0.13309600
H	-7.06277600	-0.65453500	0.80034700
H	-6.43992900	0.07426100	-0.69612200
H	-7.11928700	-1.56993100	-0.73647300
C	6.42532600	-1.37446000	0.37169300
H	6.95046300	-2.00213500	-0.36342500
H	6.47093500	-0.32794700	0.02431900
H	6.97536700	-1.42174800	1.32582100
C	2.50801200	-4.30435900	-0.99013100
H	2.15268300	-5.15377100	-0.38300100
H	1.63573000	-3.90515300	-1.53430500
H	3.24538200	-4.67686300	-1.71566400
C	1.94477900	-0.87411800	2.67417100

H	0.96885000	-0.64358600	2.22094300
H	1.75643400	-1.51914600	3.54947000
H	2.39251700	0.06796800	3.02185000
C	-2.44800000	-1.16671700	2.85424800
H	-2.49774000	-1.98745000	3.59024300
H	-1.38209100	-0.96278900	2.67153100
H	-2.90410400	-0.27351900	3.30413400
C	-2.61437500	-3.79928000	-1.47768200
H	-1.54407300	-3.60053000	-1.63149700
H	-2.70871700	-4.81662500	-1.05886400
H	-3.12531100	-3.78539900	-2.45159800
N	-1.36045000	0.45584600	-0.22164500
C	-1.13618300	1.13245800	0.92968500
C	-2.53415600	0.66440100	-0.85999500
C	-2.07957300	1.98778700	1.49286200
H	-0.16211000	0.97444300	1.39331600
C	-3.48682900	1.53178600	-0.34699600
H	-2.71105000	0.10256300	-1.77656400
C	-3.31060100	2.21366800	0.86148800
C	-4.36877300	3.12172900	1.40839500
H	-4.56500300	3.95143900	0.70981000
H	-5.31858600	2.57773400	1.53734100
H	-4.06070500	3.54000400	2.37598500
N	0.58845800	0.60542700	-2.56423600
H	0.38878800	0.29424700	-3.51959300
H	0.05629100	1.47681800	-2.41593400
C	2.04970100	0.93052600	-2.47675500
H	2.57734700	0.01091900	-2.78080300
C	2.44240300	2.10486700	-3.37000300
C	2.33761900	1.10920500	-0.98780300
H	1.91574100	3.02119900	-3.06130100
H	3.52913900	2.28190900	-3.35126700
H	2.17040500	1.87937100	-4.41171000
O	1.67129400	0.46785000	-0.13895500
H	1.20739100	-1.82849500	-1.74075000
N	3.28491000	1.97363700	-0.57745900
H	3.84360000	2.48460000	-1.25788700
C	3.40003500	2.29085200	0.84959600
H	3.44564000	1.34323100	1.40391800
C	4.64700900	3.13040400	1.11861900
C	2.11686900	2.99552600	1.35928700
H	4.61968200	4.07252700	0.54871500
H	4.69623700	3.37236900	2.18954300
H	5.55118000	2.56705400	0.84256700
O	1.70416000	2.82214600	2.50892900

N	1.53286400	3.82285700	0.45094200
H	1.90158500	3.82850100	-0.49765400
C	0.23810600	4.44771000	0.63493200
H	-0.21461800	3.99431800	1.53245800
C	0.34198500	5.96893800	0.83789100
C	-0.64134400	4.07937000	-0.56204100
H	0.81425600	6.44357600	-0.03575700
H	-0.65610300	6.40399900	0.98527500
H	0.95783200	6.16750400	1.72630200
H	-1.85719300	2.48443600	2.43965500
F	-4.64183200	1.70353600	-1.04087900
O	-0.29469400	3.35141200	-1.48145300
O	-1.84667600	4.67284600	-0.49551700
H	-2.35598100	4.39816700	-1.28645600

Ir-A-A-A-OH, cycle size 8

Ir	0.11913800	-0.42109300	1.01887400
H	1.08689300	-1.27778200	1.88910900
C	0.13212400	-1.88446600	-0.29365900
C	-0.49796600	-3.63346400	-1.64643700
C	0.85964800	-3.58589400	-1.65835900
H	-1.20082300	-4.29391600	-2.14175800
H	1.59798800	-4.19685900	-2.16547500
N	-0.92986800	-2.60081900	-0.81583000
N	1.23080300	-2.52570300	-0.83678100
C	2.59134200	-2.08387800	-0.72373000
C	3.09339300	-1.24434800	-1.73298000
C	3.38664200	-2.54686600	0.33762900
C	4.43494200	-0.84649400	-1.64581300
C	4.72121300	-2.11849600	0.38546500
C	5.26241400	-1.27093000	-0.59545000
H	4.84043900	-0.18283300	-2.41524100
H	5.35555200	-2.46451500	1.20727900
C	-2.32397800	-2.28026000	-0.69590600
C	-3.07778600	-2.83689900	0.35155500
C	-2.91149500	-1.52395200	-1.72647700
C	-4.45926200	-2.58663100	0.36407300
C	-4.29776300	-1.31384600	-1.68341100
C	-5.08671000	-1.83409000	-0.64429200
H	-5.06215400	-3.00382600	1.17607100
H	-4.76809700	-0.72415800	-2.47575500
C	-6.56673700	-1.55222300	-0.58539000
H	-7.11256000	-2.38292900	-0.11284400
H	-6.76401200	-0.64558500	0.01301800
H	-6.98032700	-1.38149200	-1.59072900

C	6.69536500	-0.80888700	-0.50562200
H	7.02880300	-0.36091400	-1.45374600
H	6.80405600	-0.04856300	0.28495300
H	7.36835500	-1.64424000	-0.25493100
C	2.21282100	-0.79864100	-2.87072700
H	2.01203600	-1.63229400	-3.56516300
H	1.23665300	-0.45000500	-2.49875900
H	2.68731400	0.01732300	-3.43372900
C	2.82819300	-3.50143900	1.35972200
H	1.86356400	-3.14027000	1.74911000
H	2.64441300	-4.49146100	0.90791600
H	3.52895500	-3.62964200	2.19715800
C	-2.42200100	-3.70656700	1.38990500
H	-2.09122100	-4.65954100	0.94236700
H	-1.52734900	-3.21151400	1.79949100
H	-3.12026600	-3.93273400	2.20832000
C	-2.06371200	-0.97677700	-2.84293800
H	-2.63805000	-0.27378700	-3.46272000
H	-1.17935400	-0.46532100	-2.43084400
H	-1.69070000	-1.78655100	-3.49213700
N	1.79707900	0.74856200	0.26455400
C	2.96728200	0.72275500	0.94551700
C	1.69599900	1.60237800	-0.78061500
C	4.03039200	1.53364500	0.58086700
H	3.05083000	0.02092700	1.77456000
C	2.74226500	2.42762000	-1.18520700
H	0.73396200	1.61169600	-1.28777300
C	3.97005700	2.40938400	-0.50901500
H	2.58682200	3.09517000	-2.03447800
C	5.15421800	3.23536700	-0.91156100
H	4.88132800	3.95300900	-1.69692900
H	5.56633800	3.78061800	-0.04813600
H	5.95895000	2.58422700	-1.29350300
F	5.17520900	1.45387100	1.30757900
H	-1.08135200	-1.21711400	1.69750900
N	0.22632300	1.10439700	2.62278400
H	1.00753000	0.83756900	3.23367800
H	0.51142100	2.00033200	2.20045400
C	-0.95379400	1.39177700	3.50656500
H	-1.21921900	0.43554900	3.98118600
C	-0.64858500	2.46150900	4.54502900
C	-2.05173400	1.82305900	2.52406300
H	-0.45908300	3.42306600	4.04401600
H	-1.50561300	2.58777600	5.22410800
H	0.23180600	2.17908300	5.14244900

O	-2.15221700	2.98653200	2.12395600
N	-2.80298800	0.78787800	2.05557800
H	-2.43053700	-0.13939800	2.27323600
C	-3.43838000	0.87335900	0.74586600
H	-3.67159300	-0.16563400	0.47171400
C	-4.74123500	1.67733700	0.77743500
C	-2.40669500	1.32611500	-0.30141500
H	-4.53685200	2.74092100	0.96655800
H	-5.30153300	1.56062900	-0.16409500
H	-5.37418200	1.28978800	1.58787800
O	-1.20401700	0.97255900	-0.26492700
N	-2.85233200	2.07403400	-1.32943000
H	-3.79172700	2.46125700	-1.28815100
C	-1.97928900	2.51253900	-2.41002600
H	-1.34363800	1.66571200	-2.70329400
C	-2.81992000	2.97075400	-3.60787200
C	-1.01069700	3.62946300	-2.00593300
H	-3.46948900	3.81382200	-3.32476000
H	-2.15874000	3.29236600	-4.42409700
H	-3.44543400	2.13791400	-3.96155200
O	0.07438700	3.78466400	-2.53755000
O	-1.51438100	4.43525300	-1.05028600
H	-0.84732800	5.13087900	-0.87387800

Ir-A-A-A-OH, cycle size 11

Ir	-0.17181700	0.30431000	-0.26838600
H	-0.84031100	0.56857300	-1.64389000
C	-0.45663300	-1.62337600	-0.58729100
C	-0.06806200	-3.84786100	-0.99409600
C	-1.39821700	-3.63059400	-1.17544300
H	0.53402100	-4.74546400	-1.07920600
H	-2.20609900	-4.29779000	-1.45402600
N	0.49205000	-2.62381700	-0.64075000
N	-1.62156600	-2.27950200	-0.92752200
C	-2.93055900	-1.69137100	-0.95111800
C	-3.74214500	-1.83797600	0.18661200
C	-3.37529400	-1.04748900	-2.11853200
C	-5.03267300	-1.29136100	0.14328100
C	-4.67142000	-0.51198000	-2.11199300
C	-5.51359900	-0.62472600	-0.99355500
H	-5.67615700	-1.38695100	1.02286400
H	-5.03504600	-0.00383500	-3.01026000
C	1.87770100	-2.47025900	-0.30131300
C	2.79668200	-2.12704400	-1.30788000
C	2.27241200	-2.75331300	1.01717500

C	4.14713300	-2.02607800	-0.94802900
C	3.63356300	-2.62625700	1.33285400
C	4.58225000	-2.25177000	0.36836800
H	4.88046100	-1.76156000	-1.71621300
H	3.95913400	-2.83026400	2.35742200
C	6.02780200	-2.05278200	0.74276300
H	6.28181000	-2.59653300	1.66505900
H	6.69892400	-2.38676500	-0.06393300
H	6.21958300	-0.97838000	0.91008800
C	-6.89546500	-0.02087900	-1.00720200
H	-7.52523400	-0.45099900	-0.21393900
H	-6.83962600	1.06744900	-0.84092100
H	-7.39057600	-0.18156600	-1.97770100
C	-3.24427500	-2.57522300	1.40227800
H	-3.26261900	-3.66592100	1.23550100
H	-2.20267300	-2.30346900	1.63369700
H	-3.87133600	-2.34992100	2.27640400
C	-2.50681600	-0.98480800	-3.34761600
H	-1.48450100	-0.66199100	-3.09766400
H	-2.42568000	-1.98138800	-3.81507800
H	-2.93086900	-0.29205900	-4.08855100
C	2.33152800	-1.88439300	-2.71897900
H	1.93516700	-2.81004300	-3.16944300
H	1.51174300	-1.14682400	-2.73228200
H	3.15758000	-1.52203200	-3.34817600
C	1.26332400	-3.21092300	2.03873500
H	1.71402200	-3.25271800	3.04021000
H	0.39125300	-2.53760600	2.05976600
H	0.88374200	-4.21603900	1.79005400
N	-2.03495600	0.74177500	0.76802000
C	-2.99126800	1.44038100	0.11115700
C	-2.25911400	0.43068000	2.06621100
C	-4.16665400	1.82048200	0.74070600
H	-2.81432300	1.66912200	-0.93951100
C	-3.43090200	0.78329300	2.73140500
H	-1.45902300	-0.11757500	2.56172400
C	-4.44345100	1.49576900	2.07309200
H	-3.56266000	0.49467600	3.77597000
C	-5.74425200	1.87337800	2.71384800
H	-5.72831700	1.65419300	3.78982500
H	-5.96046300	2.94257500	2.56362500
H	-6.57298500	1.31056000	2.25177400
F	-5.08176200	2.51640300	0.02112000
H	1.17269300	0.07289600	-1.07457700
N	0.10535700	2.47748400	-0.11734500

H	-0.82994500	2.88349500	0.02920900
H	0.64022100	2.77022200	0.71346400
C	0.70840100	3.18340900	-1.30729000
H	0.33032800	2.65924600	-2.19624200
C	0.33099700	4.65908900	-1.33362100
C	2.22798700	3.00142300	-1.16603900
H	0.75421100	5.16725300	-0.45431000
H	0.73181300	5.13791900	-2.23982900
H	-0.76424900	4.77371800	-1.33509400
O	2.88316800	3.71308000	-0.39550800
N	2.75495300	1.96035100	-1.86156000
H	2.10197800	1.35533400	-2.35591800
C	4.09673200	1.44339800	-1.57427800
H	4.15021800	0.45874700	-2.06667600
C	5.19963800	2.34844600	-2.12416700
C	4.29269500	1.17495400	-0.05641800
H	5.11636400	3.34758700	-1.67442300
H	6.18209000	1.92689500	-1.87187200
H	5.10368300	2.42875400	-3.21655700
O	5.40175800	1.28332500	0.48177600
N	3.17289100	0.79225300	0.60576000
H	2.30340600	0.60681000	0.08242600
C	3.17042600	0.58740100	2.03750000
H	3.96595300	-0.12554700	2.31219500
C	3.40114700	1.90368100	2.81746400
C	1.85082400	-0.01425800	2.47127000
H	2.61227600	2.63390200	2.58383300
H	3.41523200	1.70708600	3.89858400
H	4.37081100	2.31177500	2.50449700
O	0.79113900	-0.03085700	1.84051300
O	1.93142200	-0.50520400	3.71260000
H	1.04607300	-0.83399800	3.97336300

Ir-A-A-A-OMe, cycle size 5

Ir	0.36168200	-0.90322300	-1.05290100
H	-0.54200700	-1.86741600	-1.88585900
C	0.49239800	-2.34561400	0.26871000
C	0.06182500	-4.07199900	1.71984900
C	1.40375900	-3.84822800	1.74745400
H	-0.55826700	-4.78855400	2.24671100
H	2.20129400	-4.32752500	2.30415800
N	-0.48161400	-3.15802800	0.81868000
N	1.65366500	-2.80323800	0.86268000
C	2.92469500	-2.15365900	0.70954000
C	3.80181400	-2.58505400	-0.29632400

C	3.22929800	-1.08527600	1.57187800
C	5.01454300	-1.89380000	-0.44442300
C	4.45604600	-0.43299600	1.39550600
C	5.35522400	-0.81467300	0.38581600
H	5.70692400	-2.20460300	-1.23270200
H	4.71278600	0.40082000	2.05687600
C	-1.89080700	-2.96422000	0.63518100
C	-2.59996300	-2.27907000	1.63957600
C	-2.52021400	-3.47651800	-0.51169600
C	-3.97425400	-2.07792800	1.45113300
C	-3.89438400	-3.23619400	-0.66301800
C	-4.63618000	-2.53694700	0.30208000
H	-4.53803800	-1.53829600	2.21819000
H	-4.40038300	-3.62127900	-1.55368500
C	-6.10558900	-2.26314900	0.10031400
H	-6.64010900	-2.23028600	1.06224400
H	-6.24780900	-1.28656200	-0.39177700
H	-6.57119400	-3.03021800	-0.53708900
C	6.65372200	-0.06833800	0.20069900
H	7.23429900	-0.47891200	-0.63862700
H	6.46602100	1.00034600	0.00145200
H	7.27548600	-0.12250600	1.10984500
C	3.42524100	-3.73072700	-1.19635800
H	3.26545700	-4.65630100	-0.61845200
H	2.47827200	-3.50208900	-1.71381900
H	4.20904600	-3.91563300	-1.94489600
C	2.24487600	-0.65116700	2.62430500
H	1.25013300	-0.51541900	2.17267400
H	2.14431600	-1.41077000	3.41792000
H	2.54707400	0.30031300	3.08462900
C	-1.90891900	-1.79298900	2.88758700
H	-1.73697700	-2.62484400	3.59192600
H	-0.92374300	-1.35952800	2.65722800
H	-2.51782900	-1.03165000	3.39533700
C	-1.75964400	-4.31091900	-1.50890100
H	-0.78343200	-3.86068600	-1.74142500
H	-1.57073300	-5.31867300	-1.09938200
H	-2.33414100	-4.42384800	-2.43985600
N	-1.36627600	0.06073100	-0.17441500
C	-1.28593800	0.76099400	0.98164600
C	-2.55997000	0.01957700	-0.80790100
C	-2.38379300	1.40308900	1.54795000
H	-0.30048400	0.80342100	1.44594200
C	-3.66941900	0.66774900	-0.28882900
H	-2.61814100	-0.56007900	-1.72837200

C	-3.63450000	1.37838700	0.91518300
C	-4.85300200	2.05689800	1.46115300
H	-5.27078900	2.76159400	0.72418000
H	-5.64126600	1.31772200	1.68000600
H	-4.61288300	2.60521000	2.38173300
N	0.47182600	0.73108700	-2.49683900
H	0.33490100	0.42536800	-3.46512200
H	-0.24016400	1.45414700	-2.30810300
C	1.82433500	1.37208700	-2.39835900
H	2.54074300	0.61201800	-2.75251300
C	1.92798600	2.64988200	-3.22837200
C	2.08638700	1.53743400	-0.90318700
H	1.21189700	3.40527100	-2.86922000
H	2.94673500	3.06739200	-3.20323800
H	1.69756500	2.42379200	-4.27964200
O	1.58558600	0.72688900	-0.08583400
H	1.63469400	-1.53597400	-1.77451600
N	2.82502200	2.56741300	-0.44932700
H	3.24786900	3.22375200	-1.10224500
C	2.86379100	2.84441700	0.99009900
H	3.10447000	1.90635600	1.50940600
C	3.90599300	3.91477500	1.30625300
C	1.45965100	3.24929900	1.50890700
H	3.68565200	4.85081500	0.76903300
H	3.89598900	4.12179000	2.38551900
H	4.90960500	3.56286100	1.02356400
O	1.10044400	2.98151900	2.65864100
N	0.70705700	3.93510100	0.60889500
H	1.06656100	4.04016600	-0.33715600
C	-0.67795200	4.31007700	0.81494700
H	-1.03902700	3.74221400	1.68783400
C	-0.83909400	5.81433200	1.09213800
C	-1.47931000	3.85364000	-0.41045900
H	-0.46513800	6.40520500	0.24168200
H	-1.89663700	6.05969700	1.26000900
H	-0.25934400	6.07596800	1.98872500
H	-2.26739600	1.93092400	2.49665900
F	-4.83455100	0.60964100	-0.98942100
O	-1.01060000	3.22607500	-1.35170700
O	-2.75317400	4.26358100	-0.33368600
C	-3.58896100	3.97400300	-1.48864500
H	-3.79615700	2.89681300	-1.54432900
H	-4.51300000	4.53766600	-1.32104900
H	-3.08521300	4.30238600	-2.40786400

Ir-A-A-A-OMe, cycle size 8

Ir	0.10159500	-0.49802600	1.00799900
H	1.06752100	-1.32870000	1.90529400
C	0.11497000	-1.98981900	-0.27155300
C	-0.51708800	-3.74859100	-1.60952200
C	0.84114800	-3.71715200	-1.60333000
H	-1.22096100	-4.40780800	-2.10505000
H	1.57878800	-4.34368600	-2.09209300
N	-0.94805200	-2.69982300	-0.79879500
N	1.21374200	-2.65098400	-0.79026600
C	2.57672300	-2.22083100	-0.66201300
C	3.11057400	-1.41911500	-1.68651200
C	3.34257100	-2.65455900	0.43238300
C	4.45196500	-1.02711700	-1.57907900
C	4.67879800	-2.23235800	0.49960800
C	5.25003700	-1.42075200	-0.49392000
H	4.88173400	-0.39446100	-2.36140900
H	5.29107700	-2.55723600	1.34638000
C	-2.34053900	-2.36700800	-0.69220600
C	-3.10380300	-2.90582000	0.35782500
C	-2.91684100	-1.61739100	-1.73392800
C	-4.48347900	-2.64570400	0.36062400
C	-4.30167100	-1.39599200	-1.69902600
C	-5.09998100	-1.89925200	-0.65875900
H	-5.09334400	-3.04966600	1.17409700
H	-4.76379700	-0.81143200	-2.49993200
C	-6.57821500	-1.60591000	-0.61085500
H	-7.13275900	-2.42759000	-0.13269200
H	-6.77203400	-0.69163200	-0.02303100
H	-6.98513300	-1.44266200	-1.62016700
C	6.68176300	-0.95947200	-0.38385700
H	7.09277900	-0.69852800	-1.37087100
H	6.74689300	-0.06294800	0.25462400
H	7.31711100	-1.73591100	0.06980500
C	2.26545100	-1.01063700	-2.86475200
H	2.10965500	-1.86015300	-3.55158900
H	1.26820600	-0.67569500	-2.53925000
H	2.74618700	-0.19586100	-3.42422700
C	2.75711100	-3.57926200	1.46677900
H	1.77398900	-3.21862500	1.80635500
H	2.60521300	-4.58740800	1.04390100
H	3.42719200	-3.66798100	2.33399200
C	-2.45939400	-3.76605500	1.41105100
H	-2.11747800	-4.72039500	0.97507600
H	-1.57301900	-3.26400600	1.83033900

H	-3.16844900	-3.98952600	2.22087800
C	-2.06102800	-1.08703200	-2.85263000
H	-2.63645400	-0.40637800	-3.49594000
H	-1.18950400	-0.55250600	-2.44209300
H	-1.66924900	-1.90750800	-3.47683500
N	1.78231100	0.64130900	0.22262900
C	2.94377700	0.65910100	0.91844600
C	1.68729500	1.44288700	-0.86307600
C	4.00236300	1.46569200	0.53111500
H	3.02402300	-0.00407500	1.77915900
C	2.72833800	2.26289400	-1.29091700
H	0.73261000	1.41022000	-1.38271400
C	3.94621300	2.29192400	-0.59703100
H	2.57588600	2.89075900	-2.17035300
C	5.12367100	3.11740600	-1.01944500
H	4.84820400	3.80377600	-1.83139200
H	5.52292800	3.69701500	-0.17262400
H	5.93852900	2.46305300	-1.37328200
F	5.13735800	1.43308700	1.27616300
H	-1.10118800	-1.27551900	1.70568000
N	0.21123900	1.07889100	2.56242600
H	1.00357300	0.83719200	3.16957300
H	0.48458500	1.96243100	2.10723300
C	-0.95561300	1.38793500	3.45698400
H	-1.21590400	0.44212400	3.95492800
C	-0.63059100	2.47645500	4.46937400
C	-2.07123000	1.80249900	2.48601800
H	-0.43775000	3.42612000	3.94740500
H	-1.47955000	2.62467500	5.15406400
H	0.25314700	2.19843100	5.06396300
O	-2.20166400	2.96532000	2.09437500
N	-2.80554500	0.75095400	2.02400500
H	-2.41233000	-0.16775000	2.24449900
C	-3.44330000	0.81050000	0.71298200
H	-3.67614500	-0.23412300	0.46092500
C	-4.74632500	1.61369400	0.72878700
C	-2.41093200	1.24034900	-0.34334400
H	-4.54324000	2.67981900	0.90472600
H	-5.30132400	1.48368900	-0.21412400
H	-5.38264900	1.23748600	1.54201700
O	-1.21684000	0.85708100	-0.31433000
N	-2.84362600	2.00472100	-1.36365100
H	-3.77057900	2.41868500	-1.30581700
C	-1.95636700	2.46802800	-2.42308100
H	-1.41120300	1.59774700	-2.81975600

C	-2.76963600	3.11580700	-3.54811000
C	-0.86229500	3.43181400	-1.94053700
H	-3.33478100	3.98180100	-3.16821000
H	-2.08821900	3.45857500	-4.33819200
H	-3.47322000	2.38517100	-3.97316600
O	0.12076500	3.68654100	-2.61811000
O	-1.12127100	3.94253800	-0.73069500
C	-0.08900200	4.79367300	-0.16869000
H	0.04962700	5.68665100	-0.79497500
H	-0.45566100	5.05781200	0.82891100
H	0.85639300	4.23447300	-0.10459700

Ir-A-A-A-OMe, cycle size 11

Ir	-0.19292800	0.32296200	-0.40675700
H	-0.75543800	0.48043500	-1.84909000
C	-0.42069500	-1.63034400	-0.58349000
C	0.02747100	-3.86975500	-0.82377300
C	-1.31923900	-3.71538400	-0.92408800
H	0.65820600	-4.74978400	-0.87848700
H	-2.11820800	-4.43132800	-1.08074100
N	0.56199500	-2.60111300	-0.61918000
N	-1.57758500	-2.35579500	-0.77890000
C	-2.91245100	-1.83126000	-0.75038800
C	-3.59735600	-1.83843800	0.47513900
C	-3.50256800	-1.38831900	-1.94564500
C	-4.92114600	-1.37697300	0.48536100
C	-4.82956000	-0.93968600	-1.88819300
C	-5.55381200	-0.92963000	-0.68429400
H	-5.46832500	-1.36049700	1.43236200
H	-5.30627700	-0.58504700	-2.80692500
C	1.97204800	-2.38928700	-0.45579700
C	2.73882400	-2.05059100	-1.58525800
C	2.55118500	-2.64428700	0.79860100
C	4.12461600	-1.93359600	-1.41780900
C	3.94127900	-2.49757700	0.92063500
C	4.74282400	-2.13543900	-0.17180700
H	4.74135900	-1.68780000	-2.28825500
H	4.40846400	-2.68338600	1.89251000
C	6.22797100	-1.93832300	-0.01040100
H	6.62903100	-2.56902200	0.79767500
H	6.76533300	-2.17049900	-0.94274200
H	6.43566100	-0.88581100	0.24925700
C	-6.96926400	-0.41052300	-0.64598800
H	-7.45597000	-0.64929800	0.31145700
H	-6.97947600	0.68474700	-0.77209500

H	-7.57269100	-0.83842400	-1.46237000
C	-2.91234800	-2.31563800	1.72825800
H	-2.74458000	-3.40564700	1.69968100
H	-1.92219600	-1.84202800	1.83025200
H	-3.51266800	-2.07756100	2.61751200
C	-2.72173200	-1.39596900	-3.23281300
H	-1.79971500	-0.80005100	-3.12675500
H	-2.41037100	-2.41922100	-3.50194700
H	-3.32173100	-0.98399300	-4.05646600
C	2.07969400	-1.84689500	-2.92334800
H	1.61577000	-2.78227500	-3.27984900
H	1.27264400	-1.09948900	-2.84173800
H	2.81165500	-1.51386700	-3.67326700
C	1.71257500	-3.11899800	1.95731000
H	2.21432600	-2.91610400	2.91390200
H	0.72449700	-2.63538900	1.95592100
H	1.53689400	-4.20614400	1.88954800
N	-2.12323900	0.86808900	0.47228000
C	-3.07703300	1.38297600	-0.33847800
C	-2.36472400	0.86596800	1.80466400
C	-4.26890900	1.87631300	0.17144900
H	-2.88194300	1.37574700	-1.41009200
C	-3.54922200	1.34608200	2.35684100
H	-1.56624500	0.45886500	2.42244400
C	-4.56211800	1.86739400	1.53900200
H	-3.69115800	1.30783700	3.43861500
C	-5.87907300	2.35716400	2.06012700
H	-5.86597100	2.42115600	3.15645800
H	-6.12665000	3.34442700	1.64045800
H	-6.68598900	1.66774800	1.75869600
F	-5.18453300	2.36303200	-0.70385300
H	1.20834000	0.07742300	-1.09999500
N	0.05209000	2.50372300	-0.39601300
H	-0.89392800	2.90939300	-0.42111900
H	0.46664000	2.86780500	0.47509900
C	0.82516100	3.10650200	-1.53891600
H	0.57532600	2.51056800	-2.42790800
C	0.47527800	4.57667800	-1.74148200
C	2.30304400	2.94281500	-1.15826900
H	0.77298100	5.15486500	-0.85383100
H	1.00902300	4.97828600	-2.61632200
H	-0.60671000	4.69210500	-1.91086700
O	2.80896800	3.66180500	-0.28763000
N	2.96033900	1.92449500	-1.76967400
H	2.42019100	1.30973200	-2.37457100

C	4.28583500	1.48562900	-1.32694200
H	4.47927600	0.53621500	-1.84855800
C	5.38145300	2.49124200	-1.69041600
C	4.31068900	1.15150100	0.18797900
H	5.16749600	3.46148500	-1.22139700
H	6.35038100	2.12485200	-1.32566600
H	5.42282700	2.61317600	-2.78250500
O	5.36195100	1.22476000	0.83907100
N	3.12830800	0.76172500	0.72564700
H	2.30288100	0.62425600	0.12539900
C	2.98404700	0.56315000	2.15274700
H	3.72029900	-0.18206800	2.49956700
C	3.19627800	1.87813300	2.94277600
C	1.60008600	0.04176800	2.48433100
H	2.45636900	2.62949400	2.62889400
H	3.10205100	1.69013900	4.02116900
H	4.20397000	2.25058100	2.71952800
O	0.59585700	0.06448800	1.76775700
O	1.55988900	-0.40395000	3.74108900
C	0.25520400	-0.78440500	4.25907800
H	0.45413200	-1.20354400	5.25058300
H	-0.38322600	0.10736000	4.33561400
H	-0.21283700	-1.53243600	3.60432400

Ir-A₄-OMe, cycle size 5

Ir	-1.07990700	-0.85369900	1.01075500
H	-0.87858700	-2.23136000	1.72135700
C	-2.02508000	-1.85946900	-0.38379900
C	-2.65232900	-3.39683500	-1.97060300
C	-3.68178300	-2.51815200	-1.83269100
H	-2.53008200	-4.26793100	-2.60460200
H	-4.64740500	-2.45930900	-2.32239600
N	-1.65436000	-2.99107300	-1.08599800
N	-3.29306800	-1.59467200	-0.86667100
C	-4.03378700	-0.40887900	-0.54302000
C	-4.95869600	-0.44094100	0.51240300
C	-3.78566900	0.74965300	-1.29845100
C	-5.64379300	0.74495100	0.81537900
C	-4.50328600	1.90807200	-0.96813400
C	-5.42960600	1.92682000	0.08725700
H	-6.35754800	0.74587400	1.64494200
H	-4.33107900	2.82110700	-1.54698600
C	-0.34512500	-3.57628100	-1.05847000
C	0.56731500	-3.19832400	-2.06043300
C	-0.02832300	-4.52654300	-0.07367100

C	1.84031900	-3.78460200	-2.04344800
C	1.26105800	-5.07978600	-0.09201300
C	2.20698800	-4.72254900	-1.06616900
H	2.56523700	-3.49440400	-2.80997800
H	1.52694900	-5.81983400	0.66899200
C	3.59506900	-5.31235700	-1.04849200
H	4.02945200	-5.33790300	-2.05959000
H	4.26158900	-4.70468800	-0.41411500
H	3.58886500	-6.33469200	-0.64016400
C	-6.19275100	3.18685800	0.41461400
H	-6.53702000	3.18464900	1.45994700
H	-5.57200300	4.08155200	0.24911400
H	-7.08465500	3.28330600	-0.22882800
C	-5.16558600	-1.70431600	1.30327600
H	-5.53271000	-2.52224900	0.66109400
H	-4.20476900	-2.03442600	1.73321300
H	-5.88869100	-1.54508100	2.11606200
C	-2.76494100	0.73468500	-2.40392500
H	-1.82926900	0.28155600	-2.04093800
H	-3.11455700	0.13186000	-3.25963500
H	-2.53204100	1.75076100	-2.75123900
C	0.17976500	-2.20395700	-3.12364100
H	-0.48376800	-2.66659500	-3.87415400
H	-0.37145900	-1.35504700	-2.69057100
H	1.07129000	-1.81989500	-3.63930500
C	-1.05803900	-4.96679600	0.93307300
H	-1.54787800	-4.09766800	1.39857000
H	-1.84771300	-5.56290300	0.44388100
H	-0.59719200	-5.58422800	1.71762500
N	0.90422800	-0.95504200	0.13603000
C	1.29552200	-0.15026600	-0.87921000
C	1.82867300	-1.77904700	0.68171200
C	2.59384900	-0.15454000	-1.38528000
H	0.52857700	0.51520300	-1.27669100
C	3.13385100	-1.80057500	0.21905800
H	1.49791200	-2.43736500	1.48398600
C	3.57203100	-0.99701200	-0.83900200
C	4.98857300	-1.05435600	-1.32468200
H	5.68982600	-0.93798200	-0.48257000
H	5.19877700	-2.03435100	-1.78482800
H	5.17911400	-0.26778800	-2.06772700
N	-0.21221900	0.38236100	2.58627300
H	-0.36071500	-0.02616700	3.51396000
H	0.80910900	0.49206700	2.47491300
C	-0.83650100	1.74242900	2.58280000

H	-1.86297300	1.59962100	2.96295200
C	-0.08046100	2.74325300	3.45677700
C	-1.02134200	2.14808200	1.12200800
H	0.92186700	2.93770600	3.04747700
H	-0.63132900	3.69233100	3.55154400
H	0.02665700	2.33158500	4.47114200
O	-1.17399300	1.27330600	0.23337300
H	-2.48181800	-0.71272900	1.75379500
N	-1.07124400	3.45263500	0.79781700
H	-0.97854900	4.15673000	1.52643700
C	-1.41171900	3.86629800	-0.56599300
H	-2.22491700	3.21475100	-0.91641600
C	-1.85686300	5.32968500	-0.57885100
C	-0.25855200	3.63655900	-1.56591100
H	-1.06299400	5.99055800	-0.19520400
H	-2.09238300	5.63125300	-1.60916000
H	-2.75816900	5.45558600	0.03994700
O	-0.48479700	3.22818400	-2.70674700
N	0.99108400	3.94957000	-1.10708000
H	1.06073500	4.46037300	-0.22757000
C	2.15731200	3.94856300	-1.98618200
H	1.86728000	3.34761400	-2.86333900
C	2.52461000	5.36552200	-2.44829500
C	3.38586600	3.25474300	-1.37403500
H	2.74489800	6.00777400	-1.58054900
H	3.41566000	5.32106300	-3.08966500
H	1.68804700	5.80157300	-3.01313000
O	4.45219500	3.20309800	-1.99997000
N	3.22771400	2.73044900	-0.13345700
H	2.30260500	2.68739800	0.29343100
C	4.30636700	2.02412000	0.53549400
H	4.82372300	1.38737400	-0.20019000
C	5.33596900	2.99126300	1.15159300
C	3.69341700	1.13923000	1.60894800
H	4.85267200	3.63756700	1.89979400
H	6.14959100	2.42571700	1.62726100
H	5.74785100	3.61331000	0.34495100
O	2.53174400	1.23327200	1.98930500
O	4.59286500	0.28922800	2.11388200
C	4.13664500	-0.52287000	3.23338700
H	4.99410300	-1.14924300	3.49880200
H	3.84646900	0.12942400	4.06878700
H	3.28142100	-1.13947800	2.92519000
H	2.85384100	0.51097600	-2.21074500
F	4.01868500	-2.63115400	0.83173500

Ir-A₄-OMe, cycle size 8

Ir	0.27552000	-0.80079100	-1.01425400
H	-0.48627000	-1.78121900	-1.95571800
C	0.75171600	-2.32710100	0.12959300
C	1.91587500	-3.89578800	1.34212300
C	0.61581400	-4.28997600	1.32027700
H	2.79621500	-4.33823900	1.79474400
H	0.11757300	-5.15154600	1.75042000
N	1.98825600	-2.70686200	0.61793200
N	-0.08035500	-3.33613200	0.58413800
C	-1.50999900	-3.34204000	0.46245100
C	-2.26548100	-2.89186600	1.56177900
C	-2.10680200	-3.82810800	-0.71169000
C	-3.66137100	-2.90430000	1.44666900
C	-3.50874500	-3.80935300	-0.78461800
C	-4.30077700	-3.35046300	0.27886400
H	-4.26295600	-2.54478400	2.28704700
H	-3.99304100	-4.17652100	-1.69465900
C	3.20984400	-1.95789100	0.53445100
C	4.07317200	-2.16648000	-0.55526200
C	3.55689600	-1.13693600	1.62266500
C	5.30761900	-1.49790000	-0.54748400
C	4.80488100	-0.49557100	1.59218700
C	5.69203500	-0.66305600	0.51648200
H	5.99023800	-1.64333500	-1.38998300
H	5.08684600	0.15071500	2.42864500
C	7.00925400	0.06989100	0.47924600
H	7.79502100	-0.54632600	0.01583600
H	6.92154900	0.99336600	-0.11929000
H	7.33449700	0.35785700	1.49008900
C	-5.80435100	-3.31217700	0.16625000
H	-6.28185000	-3.57917300	1.12197700
H	-6.14274100	-2.29708000	-0.10027500
H	-6.16386300	-4.00141700	-0.61263900
C	-1.59171800	-2.42342000	2.82560700
H	-1.22882700	-3.27955000	3.41979000
H	-0.71642700	-1.79473700	2.60084200
H	-2.29114000	-1.84463700	3.44520900
C	-1.27661900	-4.40925500	-1.82638900
H	-0.36230300	-3.82116500	-1.99166300
H	-0.96892100	-5.43988300	-1.57668700
H	-1.85340300	-4.44589600	-2.76215700
C	3.68915300	-3.10622400	-1.66586600
H	3.63796400	-4.14431000	-1.29525500

H	2.69099100	-2.85060100	-2.05607300
H	4.42181000	-3.06516700	-2.48436800
C	2.61427200	-0.97078700	2.78460000
H	2.97137300	-0.18859800	3.46976800
H	1.60808500	-0.70665100	2.42241800
H	2.51521200	-1.91074300	3.35293100
N	-1.57885200	-0.26815000	-0.00018300
C	-2.75773100	-0.45177200	-0.63624600
C	-1.60253200	0.36881800	1.19308900
C	-3.94871500	-0.00939700	-0.08290900
H	-2.73887500	-0.97973200	-1.58900800
C	-2.77575800	0.82374500	1.78674400
H	-0.63106000	0.51981400	1.65829000
C	-4.01331800	0.63550400	1.15595500
H	-2.71393400	1.35122800	2.74001100
C	-5.31840300	1.07016400	1.75214400
H	-5.15010400	1.71977300	2.62162100
H	-5.93584000	1.60582700	1.01484300
H	-5.89903200	0.19033000	2.07778800
F	-5.09597000	-0.20565000	-0.78920400
H	1.59479900	-1.12643200	-1.85102500
N	-0.38222500	0.79483300	-2.40178400
H	-1.04704000	0.35708200	-3.04976400
H	-0.94068700	1.47181800	-1.85010600
C	0.55984700	1.60969500	-3.24062000
H	1.08499400	0.90825200	-3.90656100
C	-0.17619900	2.68207100	-4.03331400
C	1.54437400	2.19833100	-2.22853000
H	-0.68023800	3.37259600	-3.34093000
H	0.52919900	3.25465300	-4.65456500
H	-0.92645800	2.21830000	-4.69175100
O	1.32184000	3.25941100	-1.62399300
N	2.60382100	1.39310500	-1.96104500
H	2.52226700	0.44240200	-2.32973800
C	3.27501800	1.47627400	-0.66439900
H	3.78304200	0.50988300	-0.53928000
C	4.30968700	2.59975200	-0.60778000
C	2.19806800	1.50052700	0.42752000
H	3.82483300	3.58249900	-0.70387100
H	4.88379100	2.55288000	0.33121800
H	5.01721400	2.47558600	-1.43937300
O	1.21572600	0.72373900	0.40145000
N	2.32247200	2.37903500	1.44007800
H	3.08596500	3.05151000	1.42131700
C	1.35330400	2.46182900	2.52912300

H	1.10602800	1.43175800	2.83091900
C	1.97208200	3.20437200	3.71615700
C	-0.00400300	3.10973100	2.16160400
H	2.26677700	4.22516000	3.42290400
H	1.22903400	3.27148200	4.52089400
H	2.85838800	2.66524500	4.08138500
O	-0.88512100	3.15496600	3.03061400
N	-0.14575000	3.61936200	0.91365600
H	0.58710700	3.50732900	0.20535200
C	-1.31714600	4.39463100	0.54214200
H	-1.80002800	4.73182700	1.47053800
C	-0.89784500	5.59735300	-0.32185100
C	-2.34624900	3.58640000	-0.25051300
H	-0.36352500	5.24154700	-1.21630100
H	-1.78274700	6.17276200	-0.63017300
H	-0.23056500	6.24912500	0.26056500
O	-2.10214900	2.70578800	-1.06104900
O	-3.58518600	4.05350600	-0.01210700
C	-4.63074300	3.52630300	-0.87446100
H	-5.55973400	3.97701200	-0.50913400
H	-4.43448300	3.81971900	-1.91587200
H	-4.66888800	2.43133300	-0.80436100

Ir-A₄-OMe, cycle size 11

Ir	0.09457600	-0.71811000	0.38016400
H	0.73150500	-2.04627800	0.87583200
C	0.36480000	-1.36413600	-1.46334900
C	-0.04569900	-2.07691200	-3.60561800
C	1.27090600	-2.30319300	-3.35042300
H	-0.65101900	-2.26004700	-4.48627000
H	2.05973300	-2.72938800	-3.95986600
N	-0.58447200	-1.51100400	-2.45395000
N	1.50818900	-1.86965500	-2.04927400
C	2.80484700	-1.90642400	-1.43581100
C	3.73577500	-0.91454300	-1.79419900
C	3.11862400	-2.94728600	-0.54506400
C	5.00481800	-0.96342500	-1.20116300
C	4.39811800	-2.94599100	0.03119700
C	5.35215100	-1.96545700	-0.28215600
H	5.73860300	-0.19517800	-1.46280500
H	4.65973100	-3.74488400	0.73179700
C	-1.95112600	-1.08440100	-2.35557300
C	-2.91833100	-1.98988400	-1.88588000
C	-2.27992700	0.20452200	-2.80561100
C	-4.24817100	-1.55202200	-1.83466300

C	-3.62176100	0.60449800	-2.71986100
C	-4.61620400	-0.25405300	-2.22690200
H	-5.01795600	-2.23995200	-1.47131600
H	-3.89414600	1.61165900	-3.04985600
C	-6.03900100	0.21711200	-2.07413400
H	-6.24320600	1.09060000	-2.71154600
H	-6.75419500	-0.58173400	-2.32592200
H	-6.21876700	0.50399300	-1.02316800
C	6.71187600	-1.97357300	0.37020100
H	7.46564300	-1.49701000	-0.27500600
H	6.68419600	-1.41453300	1.32014700
H	7.03854700	-2.99984200	0.59774700
C	3.39021600	0.14922500	-2.80414400
H	3.44635600	-0.25175100	-3.83074500
H	2.36456900	0.52219200	-2.66098700
H	4.08708300	0.99588800	-2.72792300
C	2.15039400	-4.06996200	-0.27445900
H	1.11214300	-3.71112900	-0.23877800
H	2.21349700	-4.82722800	-1.07562300
H	2.38898400	-4.56688000	0.67737500
C	-2.52108500	-3.37629600	-1.45351900
H	-2.11242200	-3.95424200	-2.29942800
H	-1.72703800	-3.32750900	-0.68914800
H	-3.38329100	-3.92409300	-1.04605400
C	-1.22118000	1.10509600	-3.38442500
H	-1.61335300	2.12035400	-3.53623100
H	-0.34774100	1.15061800	-2.71547700
H	-0.86524400	0.72018300	-4.35475300
N	1.98775600	0.31811400	0.58718200
C	2.92484400	-0.16622000	1.43609400
C	2.27020800	1.45991200	-0.08082700
C	4.13790900	0.48219900	1.61350000
H	2.70179900	-1.10022500	1.95186400
C	3.48234900	2.13039200	0.05388300
H	1.48130200	1.81981600	-0.73851200
C	4.47519600	1.64885500	0.91828000
H	3.65792200	3.03518600	-0.52987200
C	5.81460200	2.29891400	1.08586500
H	5.84864000	3.26336200	0.56154200
H	6.04438100	2.45613100	2.15125100
H	6.60721400	1.64792800	0.67950700
F	5.03200700	-0.05766000	2.47877100
H	-1.26703000	-1.52426600	0.27520300
N	-0.19427700	-0.12688200	2.47116700
H	0.73136100	0.13579300	2.83903200

H	-0.75262200	0.73621600	2.55187500
C	-0.77588100	-1.13819100	3.43033600
H	-0.37318500	-2.11339600	3.12155600
C	-0.40615600	-0.81960700	4.87293100
C	-2.29898400	-1.08335900	3.21977900
H	-0.85353400	0.14084400	5.16933700
H	-0.78830300	-1.60305800	5.54480100
H	0.68806900	-0.76809500	4.98515500
O	-2.99385700	-0.24258800	3.80218100
N	-2.78336700	-1.94727500	2.28898700
H	-2.09174200	-2.47478900	1.75766500
C	-4.10524700	-1.75214000	1.68043000
H	-4.10933400	-2.37378300	0.77048400
C	-5.24073300	-2.19082700	2.60428500
C	-4.29713300	-0.28296500	1.20723300
H	-5.20841100	-1.60471300	3.53317500
H	-6.20681700	-2.01790500	2.11071900
H	-5.13531400	-3.25951700	2.84090800
O	-5.39752300	0.28093000	1.26414800
N	-3.17568200	0.30415000	0.72210400
H	-2.31676600	-0.25500200	0.59134800
C	-3.12810700	1.70944600	0.38706500
H	-3.94004400	1.94340500	-0.32359900
C	-3.29511600	2.59306500	1.64517600
C	-1.79649300	2.04516500	-0.27772100
H	-2.48536500	2.39286300	2.36243000
H	-3.28062500	3.66049900	1.38231800
H	-4.25666400	2.34353300	2.11232600
O	-0.75866800	1.34890100	-0.21407000
N	-1.77293600	3.23318500	-0.91862600
H	-2.60793800	3.81527600	-0.88149000
C	-0.52681400	3.87294900	-1.30856200
H	0.08822800	3.13545500	-1.84717200
C	-0.80525300	5.06778600	-2.22608400
C	0.25591700	4.30086500	-0.05270200
H	-1.42258700	5.81845000	-1.70780300
H	0.14295900	5.53544400	-2.52058700
H	-1.33556400	4.72854200	-3.12780000
O	-0.17340300	4.28269700	1.08500100
O	1.49010600	4.71909100	-0.40130500
C	2.30210900	5.21802600	0.69779000
H	3.23281300	5.56540600	0.23580000
H	1.78129600	6.04317400	1.20323200
H	2.50002500	4.40741600	1.41381800

Ir-A₄-OMe, cycle size 14

Ir	0.36788300	-0.17199900	0.08609700
H	0.91767400	-1.32271300	-0.80419200
C	0.68946600	1.04421600	-1.42972900
C	0.40166700	2.62429400	-3.06634400
C	1.67813300	2.16749300	-3.16834100
H	-0.14798500	3.36123500	-3.64088100
H	2.48232500	2.42540500	-3.84796500
N	-0.18646000	1.93668800	-2.00864200
N	1.84248500	1.20703600	-2.17417800
C	3.07536400	0.50429900	-1.96366800
C	4.15260400	1.21224600	-1.39237900
C	3.18860900	-0.83922600	-2.35943200
C	5.35457000	0.52498100	-1.18694300
C	4.41291300	-1.48661200	-2.12164700
C	5.50231000	-0.82727400	-1.53746700
H	6.19561000	1.05927900	-0.73472700
H	4.51796400	-2.53521000	-2.41679200
C	-1.58307700	2.04099300	-1.69581500
C	-2.45451300	1.12054100	-2.30380300
C	-2.03722100	3.08930600	-0.88008100
C	-3.82497300	1.25891000	-2.05108200
C	-3.41682700	3.17463100	-0.63701700
C	-4.32319100	2.26989200	-1.21201000
H	-4.51148700	0.54351200	-2.51173300
H	-3.79071800	3.97758500	0.00564500
C	-5.79941100	2.36475600	-0.91695000
H	-6.12571400	3.41451400	-0.85181300
H	-6.39327800	1.85891800	-1.69330700
H	-6.02818400	1.88884200	0.05264600
C	6.79691500	-1.55160500	-1.26681800
H	7.66485900	-0.90875000	-1.48183100
H	6.85706500	-1.84433000	-0.20554000
H	6.87615200	-2.46627900	-1.87323100
C	4.02692500	2.66926000	-1.02677000
H	4.15944000	3.31097300	-1.91472100
H	3.03454300	2.89762700	-0.60934400
H	4.79267700	2.94723200	-0.28863700
C	2.08155600	-1.57324900	-3.07418000
H	1.12596300	-1.03633900	-3.02255600
H	2.34711200	-1.71155400	-4.13629200
H	1.93953100	-2.57577300	-2.63997100
C	-1.91380500	0.04431300	-3.20624900
H	-1.37446300	0.48305500	-4.06296100
H	-1.18855400	-0.57512000	-2.65090900

H	-2.72289900	-0.60101200	-3.57076000
C	-1.08135400	4.11907500	-0.33628600
H	-1.47929000	4.57636600	0.58129400
H	-0.09947400	3.67125600	-0.12422300
H	-0.92029200	4.92606800	-1.07136500
N	2.34075400	0.07252400	0.97793700
C	3.18705400	-0.98312400	1.01084600
C	2.74085400	1.22190800	1.56929800
C	4.42609800	-0.89344300	1.62600900
H	2.87254700	-1.89790900	0.50920600
C	3.97977100	1.35673100	2.19116100
H	2.02618700	2.04152200	1.52387600
C	4.88094900	0.28355500	2.23139400
H	4.25414900	2.31302400	2.64070500
C	6.24536200	0.36722200	2.84507800
H	6.38570800	1.32924000	3.35573800
H	6.40343100	-0.45184400	3.56410900
H	7.01992500	0.26382600	2.06646900
F	5.22694300	-1.98817900	1.61565600
H	-1.07976700	-0.45433700	-0.51277900
N	0.06411600	-1.56740700	1.75196200
H	0.79740300	-1.37750700	2.44969100
C	0.15014400	-3.03187900	1.40519000
H	0.96564100	-3.12406400	0.67458700
C	0.42050800	-3.89356400	2.63130700
C	-1.19317600	-3.39328400	0.75049700
H	-0.41521500	-3.81384200	3.34183400
H	0.52895500	-4.94858700	2.33783300
H	1.35335500	-3.57036300	3.11903700
O	-2.16255900	-3.72328500	1.46055600
N	-1.23908600	-3.24963900	-0.59165500
H	-0.46413800	-2.72282800	-0.99899700
C	-2.42418600	-3.41329000	-1.44635800
H	-2.06470400	-3.28077000	-2.47629400
C	-3.04621500	-4.81282200	-1.31600900
C	-3.52566400	-2.33901300	-1.27760300
H	-3.40625500	-4.98106300	-0.29220700
H	-3.88839500	-4.89586600	-2.01832500
H	-2.29605300	-5.57798400	-1.56442200
O	-4.21304200	-2.00528500	-2.24890000
N	-3.68165000	-1.84637000	-0.01852700
H	-3.28019100	-2.41253100	0.74086100
C	-4.77057500	-0.94714100	0.33158100
H	-5.05251600	-0.41995400	-0.59325700
C	-5.98890500	-1.71772300	0.85652300

C	-4.32556400	0.12862400	1.33448700
H	-5.71511000	-2.31546500	1.74057300
H	-6.78544000	-1.01694100	1.14039400
H	-6.35517000	-2.39231900	0.06901500
O	-5.16349000	0.70785600	2.04071700
N	-2.99189700	0.41047300	1.41886400
H	-2.32293600	0.04896100	0.72554900
C	-2.58446100	1.41391400	2.38978200
H	-3.30933700	2.24418600	2.35170600
C	-2.59723200	0.83814300	3.82718900
C	-1.21388500	1.99614300	2.13068700
H	-1.85661000	0.02934600	3.92695700
H	-2.36974800	1.62784800	4.55649100
H	-3.60149000	0.44002200	4.02314900
O	-0.29449600	1.52696600	1.45721100
O	-1.06467200	3.11832000	2.84005600
C	0.27432000	3.68259000	2.90731600
H	0.17431700	4.57381200	3.53514700
H	0.95734700	2.95417000	3.36675100
H	0.62361200	3.95252100	1.90179300
H	-0.82051500	-1.41998200	2.25895000

Ir-A₅-OMe, cycle size 8

Ir	-0.83346000	0.69106400	-0.99682300
H	-0.36075900	1.81258300	-1.96968000
C	-2.00521300	2.00894800	-0.12695900
C	-3.83662300	3.10994800	0.72304000
C	-2.78560200	3.96817800	0.79144500
H	-4.87614000	3.21804900	1.01174100
H	-2.71122000	4.98774600	1.15267100
N	-3.35448900	1.92723800	0.16447800
N	-1.68302500	3.29454900	0.27451600
C	-0.35518700	3.83639500	0.31790400
C	0.33343500	3.79015500	1.54477600
C	0.19344800	4.42835500	-0.83066000
C	1.62577800	4.32800200	1.59136900
C	1.49617700	4.94359200	-0.73799200
C	2.22719000	4.90042200	0.45896800
H	2.18000500	4.28800000	2.53397500
H	1.94479800	5.40237300	-1.62443600
C	-4.18224100	0.75907200	0.06581600
C	-4.91021200	0.52630900	-1.11437200
C	-4.33168600	-0.04113900	1.21233700
C	-5.79578300	-0.56241500	-1.13104400
C	-5.23330300	-1.11550000	1.15245700

C	-5.97405000	-1.39017700	-0.00809200
H	-6.36680400	-0.76202200	-2.04267000
H	-5.35824900	-1.75079200	2.03431200
C	-6.91291100	-2.56880000	-0.06669600
H	-7.85464300	-2.30221400	-0.57159800
H	-6.46090900	-3.39811500	-0.63772400
H	-7.14638300	-2.94270900	0.94120700
C	3.63671200	5.43265900	0.52727300
H	3.82628100	5.93480400	1.48889000
H	4.36204600	4.60709300	0.43638400
H	3.83443500	6.14485900	-0.28797400
C	-0.30694000	3.18996800	2.76952500
H	-1.05753100	3.87567700	3.19854600
H	-0.83070200	2.25283300	2.52556200
H	0.44981400	2.98006800	3.53843200
C	-0.61012800	4.56126900	-2.09781300
H	-1.18032300	3.64401600	-2.30555200
H	-1.33544900	5.38873500	-2.00672100
H	0.04591000	4.77789100	-2.95352200
C	-4.75479800	1.44022900	-2.29938400
H	-5.11369100	2.45523900	-2.05810800
H	-3.69154900	1.52975600	-2.57534000
H	-5.32442900	1.06437200	-3.16111300
C	-3.55360000	0.26696100	2.46369000
H	-3.67057200	-0.53619800	3.20525600
H	-2.48492500	0.39026000	2.22654800
H	-3.89389900	1.21211100	2.91902700
N	0.91234600	0.99942600	0.26718300
C	2.01496400	1.57773400	-0.25865800
C	1.00028700	0.50492200	1.52297100
C	3.19217200	1.66897800	0.46644900
H	1.93641700	1.98890300	-1.26446800
C	2.15969300	0.58053300	2.28755500
H	0.10191200	0.01664000	1.89411500
C	3.31398000	1.18551600	1.77269600
H	2.16477100	0.13452800	3.28346200
C	4.59028200	1.32250200	2.54774100
H	4.57828100	0.67207500	3.43294900
H	5.46393000	1.07298400	1.92601700
H	4.72330300	2.36555400	2.88221000
F	4.27233000	2.24307900	-0.13252800
H	-2.04412700	0.41981800	-2.00246100
N	0.57019700	-0.64296900	-2.06621500
H	1.14212100	-0.04120200	-2.66965500
H	1.22355200	-1.02081700	-1.35241400

C	0.14537600	-1.81246300	-2.90673000
H	-0.47796800	-1.41458100	-3.72221900
C	1.34782700	-2.57468900	-3.44999600
C	-0.71689300	-2.66078200	-1.96793900
H	1.96092400	-2.94787100	-2.61621200
H	1.02091900	-3.42897600	-4.06220000
H	1.96132800	-1.90980200	-4.07816900
O	-0.23973800	-3.53797300	-1.23182100
N	-2.01947200	-2.27663300	-1.92460600
H	-2.21375300	-1.38011400	-2.37904000
C	-2.80622100	-2.50775000	-0.71310300
H	-3.63722100	-1.79043000	-0.76681000
C	-3.37009500	-3.92640600	-0.63709700
C	-1.97044100	-2.05430900	0.49095500
H	-2.55911700	-4.66498300	-0.55517700
H	-4.05865300	-4.02655000	0.21684000
H	-3.94120300	-4.13294600	-1.55295800
O	-1.32570100	-0.98023300	0.47900300
N	-1.93873000	-2.83515100	1.58764400
H	-2.41112100	-3.73603000	1.56743900
C	-1.17105500	-2.47907300	2.77774100
H	-1.32794700	-1.40519400	2.96395900
C	-1.67365100	-3.28195500	3.97996500
C	0.36208300	-2.64482100	2.64187900
H	-1.57246000	-4.36333300	3.79298300
H	-1.07190900	-3.01971100	4.85976700
H	-2.73012900	-3.04906800	4.17872300
O	1.08247200	-2.26101200	3.57388400
N	0.83174000	-3.24404700	1.52276300
H	0.21682200	-3.43957800	0.72684200
C	2.24725000	-3.52272200	1.34634700
H	2.67841800	-3.67650100	2.34837300
C	2.42546100	-4.77573300	0.47376000
C	2.98611900	-2.36295300	0.66255100
H	1.91306000	-4.62395100	-0.48865800
H	3.49283300	-4.95996000	0.28468300
H	1.98991800	-5.64869600	0.98186700
O	2.47420000	-1.65385000	-0.21357700
N	4.28942700	-2.21985200	1.01028300
H	4.70634400	-2.86871800	1.67422000
C	5.16902800	-1.37717400	0.21387100
H	4.79604400	-0.34359200	0.23769200
C	6.59885100	-1.43606600	0.75743300
C	5.14229400	-1.83367300	-1.25298800
H	6.98538600	-2.46616700	0.70724700

H	7.25197700	-0.78341700	0.16166000
H	6.61769400	-1.09615500	1.80394500
O	5.02475100	-2.98603900	-1.62791800
O	5.31615900	-0.77346000	-2.06847900
C	5.36254900	-1.08919700	-3.48518000
H	5.52731000	-0.13140400	-3.99082600
H	6.18456300	-1.78976400	-3.69131900
H	4.40905700	-1.53951600	-3.79828500

Ir-A₅-OMe, cycle size 11

Ir	0.15207400	-0.83571900	-0.58723900
H	-0.30245900	-1.86345300	-1.66250100
C	0.26606700	-2.30716000	0.72066900
C	1.08960100	-3.83773600	2.21779700
C	-0.21450600	-4.15408000	1.99309100
H	1.84230300	-4.29413300	2.85071300
H	-0.84132100	-4.94625200	2.38674100
N	1.37090600	-2.71903400	1.43873600
N	-0.70173400	-3.22122500	1.08268400
C	-2.06560000	-3.17682000	0.63963700
C	-3.01612200	-2.56322400	1.47383000
C	-2.40560300	-3.75600000	-0.59436600
C	-4.34161200	-2.50563100	1.02189400
C	-3.74376000	-3.67031600	-1.00593800
C	-4.72212300	-3.04412500	-0.21670000
H	-5.09211500	-2.01639000	1.64970900
H	-4.02802200	-4.10852800	-1.96745000
C	2.64107400	-2.04974900	1.45085000
C	3.61237200	-2.40829200	0.50021500
C	2.88907000	-1.10411100	2.45948000
C	4.84955200	-1.75237700	0.55516900
C	4.13321200	-0.45603900	2.45975000
C	5.12076400	-0.75806300	1.50979600
H	5.62310800	-2.02227000	-0.17055700
H	4.33710400	0.29560700	3.22855400
C	6.42853300	-0.00985400	1.48825200
H	6.66426500	0.41341300	2.47640200
H	7.25736300	-0.66353100	1.17460500
H	6.36658500	0.82110100	0.76412700
C	-6.14412200	-2.92159300	-0.70361800
H	-6.84790200	-2.83494400	0.13806400
H	-6.25758000	-2.02010800	-1.32892800
H	-6.43187000	-3.78818100	-1.31857000
C	-2.62048300	-1.99004600	2.80957300
H	-2.46674200	-2.79127000	3.55250900

H	-1.67381900	-1.43228300	2.73925000
H	-3.40003100	-1.31373600	3.18777900
C	-1.37472500	-4.47832800	-1.42159500
H	-0.45559000	-3.88062300	-1.51950500
H	-1.09342900	-5.43247100	-0.94333000
H	-1.76671900	-4.70000200	-2.42465500
C	3.31853300	-3.46297400	-0.53321400
H	3.14876000	-4.44484400	-0.06015900
H	2.39757400	-3.21087400	-1.08548300
H	4.15227700	-3.56075300	-1.24366100
C	1.86015200	-0.83253000	3.52414000
H	2.10332700	0.08624600	4.07645800
H	0.85873100	-0.73524800	3.07895600
H	1.81527100	-1.66496500	4.24644700
N	-1.90107000	-0.22246900	-0.22884400
C	-2.82776300	-0.42847000	-1.19364300
C	-2.26587900	0.51325600	0.84607900
C	-4.09913100	0.11920500	-1.09783400
H	-2.53836100	-1.04410200	-2.04504600
C	-3.53261400	1.07031600	0.98739900
H	-1.49077300	0.65735500	1.59426400
C	-4.50536800	0.89527700	-0.00748000
H	-3.74537300	1.66273200	1.87941300
C	-5.87954700	1.48735600	0.06400600
H	-5.98440300	2.11874000	0.95620400
H	-6.08835800	2.09415400	-0.83172000
H	-6.64272300	0.69224700	0.09794300
F	-4.96993000	-0.10442400	-2.11671500
H	1.63647300	-1.26140100	-0.94676300
N	0.03093400	0.70263700	-2.14214600
H	-0.96928600	0.89868200	-2.28892100
H	0.38935600	1.61403400	-1.82211100
C	0.62495700	0.41986600	-3.49795100
H	0.47678700	-0.65370200	-3.68316300
C	-0.03796600	1.26450200	-4.57893300
C	2.11924500	0.75142600	-3.36498900
H	0.15813500	2.33063800	-4.39043000
H	0.36523700	1.00478800	-5.56943300
H	-1.12484700	1.08673900	-4.58651800
O	2.53153300	1.90984800	-3.49683000
N	2.90902900	-0.28931200	-2.98889500
H	2.43271800	-1.15795500	-2.74893700
C	4.24097400	-0.05936500	-2.41723900
H	4.52776800	-1.00678100	-1.93407300
C	5.27803400	0.30497800	-3.47904200

C	4.18685300	1.00676600	-1.28738800
H	4.97253600	1.22543000	-3.99527000
H	6.25278500	0.47386500	-3.00123400
H	5.36468400	-0.51341900	-4.20845000
O	5.11587200	1.80126600	-1.09272900
N	3.05834800	0.98000000	-0.53440300
H	2.36064300	0.22847800	-0.66556800
C	2.79529200	1.99279000	0.46169300
H	3.67746100	2.08816700	1.11895800
C	2.50580900	3.36655500	-0.19122000
H	1.55440300	3.33875800	-0.74663500
H	2.45561400	4.15928800	0.57118200
H	3.32273600	3.59933900	-0.88646000
C	1.58856700	1.60504200	1.31134600
O	0.72446600	0.75896200	0.99893100
N	1.44228200	2.34742700	2.43469500
H	2.18359000	3.00037200	2.68368300
C	0.28078200	2.25723400	3.31545900
H	0.02019600	1.19317000	3.42215300
C	0.61622800	2.83756900	4.69063800
C	-1.00196800	2.91212600	2.75747700
H	0.91924900	3.89322100	4.60307400
H	-0.27521400	2.77866100	5.32874600
H	1.43211400	2.26612200	5.15712800
O	-2.07614200	2.70495000	3.33451800
N	-0.86360600	3.68366900	1.65109600
H	0.05325100	3.76588900	1.21601500
C	-1.99217600	4.26092800	0.94371200
H	-2.90022200	3.95747300	1.48527800
C	-1.91169000	5.79634500	0.88596800
C	-2.05168100	3.68255200	-0.47078200
H	-0.99501100	6.11538700	0.36571400
H	-2.78272600	6.19849600	0.34934200
H	-1.89952700	6.19834200	1.90899400
O	-1.11861200	3.13632200	-1.03997900
O	-3.25789100	3.90230400	-1.01874600
C	-3.41867600	3.47231100	-2.39883500
H	-4.36689200	3.91040100	-2.72862100
H	-2.57954300	3.83235100	-3.00990400
H	-3.46663400	2.37449100	-2.44117200

Ir-A₅-OMe, cycle size 14

Ir	-0.17650400	-0.50949500	-0.05809900
H	-0.54601800	-2.02157200	-0.05020600
C	-0.47610500	-0.50564200	1.88869200

C	-0.20440200	-0.19443300	4.14506200
C	-1.39767400	-0.82132400	3.96690200
H	0.31256800	0.12915000	5.04137400
H	-2.14761800	-1.15454800	4.67509800
N	0.34181200	-0.00688400	2.87879800
N	-1.55374500	-1.00898200	2.59615900
C	-2.71064300	-1.62802700	2.01667100
C	-3.92714900	-0.91446800	2.03807200
C	-2.61397500	-2.92198700	1.47673600
C	-5.04778400	-1.50865600	1.44601800
C	-3.76451800	-3.46801600	0.88309900
C	-4.98357400	-2.77874800	0.84967800
H	-5.99415000	-0.95918600	1.44370600
H	-3.70451400	-4.47028200	0.44762900
C	1.67126500	0.48631300	2.66431600
C	2.70698400	-0.45864700	2.57822000
C	1.89982800	1.87055600	2.62262500
C	4.01166800	0.02228200	2.40734400
C	3.21838600	2.30517100	2.42176200
C	4.28369300	1.39682100	2.30690200
H	4.82620600	-0.70376200	2.33513700
H	3.41733000	3.37994300	2.36843600
C	5.68873900	1.88561600	2.05637700
H	5.89200800	2.81639500	2.60877300
H	6.43176900	1.13023500	2.35419300
H	5.83515400	2.10157300	0.98349700
C	-6.19564000	-3.36998400	0.17495000
H	-7.10811900	-3.18630500	0.76381800
H	-6.34422600	-2.90928500	-0.81577100
H	-6.08203700	-4.45468000	0.02971900
C	-4.03596700	0.43784700	2.69576800
H	-4.17349900	0.33349500	3.78578700
H	-3.12839900	1.04014100	2.54081300
H	-4.89824600	0.99032200	2.29595200
C	-1.36016200	-3.75526400	1.57426600
H	-0.49504000	-3.16794000	1.90669500
H	-1.51699000	-4.58352500	2.28635200
H	-1.11745200	-4.20501500	0.59822700
C	2.40238600	-1.92866200	2.68518700
H	1.91765200	-2.16091200	3.64872100
H	1.69480600	-2.21862000	1.88905700
H	3.31618700	-2.52582900	2.57671500
C	0.77001500	2.84210600	2.83946900
H	1.04665000	3.84696400	2.49131900
H	-0.13338800	2.50990400	2.30660400

H	0.51189900	2.90717400	3.91022300
N	-2.23124300	-0.00377300	-0.54463300
C	-2.99246800	-0.86697400	-1.25633500
C	-2.78534600	1.17471700	-0.17983400
C	-4.30059500	-0.55917300	-1.59813800
H	-2.55136200	-1.82710500	-1.52322200
C	-4.09782000	1.51759000	-0.49111300
H	-2.13252300	1.83677800	0.38626600
C	-4.91308200	0.64099700	-1.21983500
H	-4.49297000	2.47602400	-0.15161900
C	-6.34337700	0.93009300	-1.55881300
H	-6.60479600	1.96366500	-1.29488700
H	-6.53309400	0.76989400	-2.63161900
H	-7.01082200	0.24512000	-1.00884100
F	-5.01082500	-1.47360300	-2.30476000
H	1.33796700	-0.92034000	0.21869000
N	0.09846800	-0.58582600	-2.22972100
H	-0.71259200	-0.11762900	-2.65916500
C	0.18850800	-1.96278700	-2.83600800
H	-0.54444200	-2.57972600	-2.29739600
C	-0.10534600	-1.94493000	-4.33023500
C	1.61363600	-2.46754300	-2.55243300
H	0.65898600	-1.35651500	-4.85872100
H	-0.09640000	-2.96905800	-4.73264800
H	-1.09919400	-1.50732800	-4.51177900
O	2.53851600	-2.19622100	-3.34241300
N	1.76952900	-3.13578800	-1.38896300
H	0.99465300	-3.04089300	-0.72857000
C	3.03874300	-3.61817500	-0.82353800
H	2.76525800	-4.16100600	0.09181200
C	3.76825200	-4.58248800	-1.77210800
C	4.01738900	-2.51831600	-0.34393800
H	4.04486500	-4.07138800	-2.70398300
H	4.67646200	-4.95380700	-1.27523600
H	3.11600000	-5.43589100	-2.00938800
O	4.74138200	-2.71944700	0.63750500
N	4.02869600	-1.37916000	-1.08626000
H	3.61704100	-1.44286000	-2.02702400
C	4.96873800	-0.29679300	-0.83953300
H	5.23870800	-0.35381400	0.22661300
C	6.23977400	-0.44495400	-1.68375700
C	4.30970900	1.07427000	-1.06013500
H	5.99161700	-0.45837100	-2.75685100
H	6.92031000	0.39589800	-1.49365900
H	6.73867500	-1.38885600	-1.41992400

O	4.99520600	2.05771800	-1.37696700
N	2.95777700	1.15764700	-0.89262800
H	2.40884600	0.37237700	-0.51738800
C	2.32453700	2.44002100	-1.15086300
H	3.01518700	3.22065200	-0.78894400
C	2.12041300	2.66413500	-2.66752600
C	0.99079100	2.62807300	-0.44687100
H	1.43407000	1.91265900	-3.08613500
H	1.69409800	3.65790800	-2.86408300
H	3.09883300	2.57885900	-3.15991800
O	0.18688800	1.72710300	-0.12730100
H	0.91364200	-0.04827600	-2.55734300
N	0.66351500	3.92610700	-0.25098900
H	1.31674500	4.63709100	-0.57495200
C	-0.69785800	4.35773000	0.01843200
H	-1.11808200	3.71055200	0.80354100
C	-0.70880400	5.81142700	0.50208500
C	-1.56099200	4.17025100	-1.24456400
H	-0.27670900	6.47654700	-0.26237200
H	-1.74078100	6.12783500	0.69985100
H	-0.12038100	5.89984100	1.42676800
O	-1.14794700	3.80887500	-2.33053800
O	-2.84606100	4.47663800	-0.97619600
C	-3.74773400	4.40043700	-2.11528200
H	-4.73022600	4.68930400	-1.72581600
H	-3.41577700	5.09402500	-2.90045000
H	-3.76824700	3.37407300	-2.50870100