

Catalytic Ammonia Oxidation Mediated by High-Spin Fe(III)

Complex: Combined Experimental and DFT Study

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Materials and general method

Reagents and solvents were obtained from commercial suppliers and purified using standard methods prior to use. Unless otherwise noted, all operations were conducted under an inert He atmosphere employing standard Schlenk or glovebox techniques. Solvents were dried using conventional procedures and subsequently degassed. 2,4,6-Collidine was purified by distillation and degassing before use. The Schiff base ligand was prepared following a reported procedure.¹

Instrumentation

Elemental analyses were performed on a CE-440 analyzer (Exeter Analytical Inc.). UV–visible spectra were obtained using an Agilent Cary 4000 spectrophotometer, while IR spectra were measured as KBr pellets on a Thermo Scientific Nicolet FT-IR instrument. X-ray photoelectron spectroscopy (XPS) was conducted on a PHI VersaProbe II spectrometer (Physical Electronics) with an Al K α source (15 kV, 50 W), and the spectra were processed using the MultiPak software package (Ulvac-PHI, Inc.). Mössbauer measurements (⁵⁷Fe) were carried out with a WissEl 1200 spectrometer equipped with a proportional counter, using a ⁵⁷Co(Rh) source in constant acceleration mode. Spectral simulations were performed with WinNormos for Igor Pro, and isomer shifts (δ) are reported relative to α -iron foil at room temperature.

X-ray structure solution and refinement

Single crystal x-ray data were collected at 100 K by using the Bruker SMART APEX CCD diffractometer on graphite monochromatic MoK radiation (0.71073). The International Table for x-ray crystallography applied to the linear absorption coefficient, scattering factors for the atoms and anomalous dispersion correction.² The data integration and reduction were worked out with SAINT software.³ For the collected reflections with SADABS,⁴ empirical absorption correction was applied and the space group was defined using XPREP.⁵

The structure was solved and refined with the Olex2 1.3 package.^{6,7} Only a few H atoms could be located in the difference Fourier maps in the structure. The remaining were positioned in calculated positions using idealized geometries (riding model) and assigned fixed isotropic displacement parameters. All non-H atoms were refined anisotropically. The refinement and crystal data are presented in Table 1. The bond distance and angles are given in Tables S2-S4.

Table S1. Crystallographic data and data collection parameters for complexes.

Identification code	Fe ^{III} -complex (1)
Empirical formula	C ₂₂ H ₂₆ ClFeN ₂ O ₅
Formula weight	489.75
Temperature/K	100
Crystal system	Triclinic
Space group	P-1
a/Å	10.3050(3)
b/Å	11.2133(3)
c/Å	20.3260(6)
α/°	87.8740(10)
β/°	82.5000(10)
γ/°	68.3490(10)
Volume/Å ³	2164.19(11)
Z	4
ρ _{calc} /g/cm ³	1.503
μ/mm ⁻¹	0.857
F(000)	1020.0
Crystal size/mm ³	0.25 × 0.19 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.908 to 56.75
Index ranges	-13 ≤ h ≤ 13, -14 ≤ k ≤ 14, -27 ≤ l ≤ 27
Reflections collected	36985
Independent reflections	10797 [R _{int} = 0.0389, R _{sigma} = 0.0413]
Data/restraints/parameters	10797/9/557
Goodness-of-fit on F ²	1.137
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0609, wR ₂ = 0.1223
Final R indexes [all data]	R ₁ = 0.0715, wR ₂ = 0.1267
Largest diff. peak/hole / e Å ⁻³	1.53/-0.67
CCDC	2384217

Computational methodology

The free energies of all reaction species were computed using density functional theory (DFT) as implemented in the Gaussian 16 (revision B.01) software package.⁸ Optimized molecular structures were visualized with ChemCraft.⁹ Full geometry optimizations of the catalyst models were performed using the B3LYP¹⁰ functional with Grimme's GD3 dispersion correction. The def2-SVP basis set was applied to all non-metal atoms, while the def2-TZVP basis set was used for iron. The B3LYP functional has previously demonstrated reliable performance in modeling ammonia oxidation by various metal centers.¹¹ All relevant spin states; low, intermediate, and high were considered for each intermediate in both reactant and product forms. The spin state with the lowest free energy was used to evaluate the reaction thermodynamics (ΔG_{rxn}). Solvation effects were included via the SMD solvation model,¹² using acetonitrile (MeCN) as the continuum solvent. Reported energies are free energies in kcal/mol, including enthalpic and entropic corrections at standard conditions (298.15 K and 1 atm). All structures were confirmed to be true minima via vibrational frequency analysis using analytic Hessians; ground-state structures exhibited zero imaginary frequencies. The TD-DFT calculations were conducted at the CAM-B3LYP level with the same basis sets.¹³

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Table S2. Selected experimental FT-IR and DFT calculated spectra for complexes Fe^{III}-Complex (1) (wavenumber in cm⁻¹).

Fe ^{III} -Complex (1)		
Experimental	DFT	Assignment
480	490	Fe-O stretching
549	562	Fe-N stretching
1391, 1376	1395, 1383	ρC-H in-plane rocking
1550, 1473	1559, 1472	Ph & Im ring deformation
1617	1614	svC=N stretch (imine)
2935, 2853	2941, 2855	svC-H stretch (DACH, OCH ₃)
3062	3067	avC-H stretch (Ph), imine

sv, symmetrical stretching; av, anti-symmetrical stretching; ρ, in-plane rocking.

Table S3. Selected Bond Lengths (Å) and Geometrical Parameters for the Fe^{III}-Complex (1).

Fe ^{III} -Complex (1)		DFT	DFT	DFT
X-Ray		Sextet (HS)	Quartet (IS)	Doublet (LS)
Bond	Length/Å	Length/Å	Length/Å	Length/Å
Fe1—Cl1	2.2273(8)	2.2783	2.3350	2.2702
Fe1—O2	1.917(2)	1.9119	1.8781	1.8741
Fe1—O1	1.882(2)	1.9080	1.9009	1.8801
Fe1—N1	2.088(3)	2.1255	1.9461	1.9341
Fe1—N2	2.097(3)	2.1428	1.9779	1.9392
Δ ₁₈ ^{Fe}	0.640	0.669	0.415	0.182

Table S4. Bond Lengths (Å) for the Fe^{III}-Complex (1).

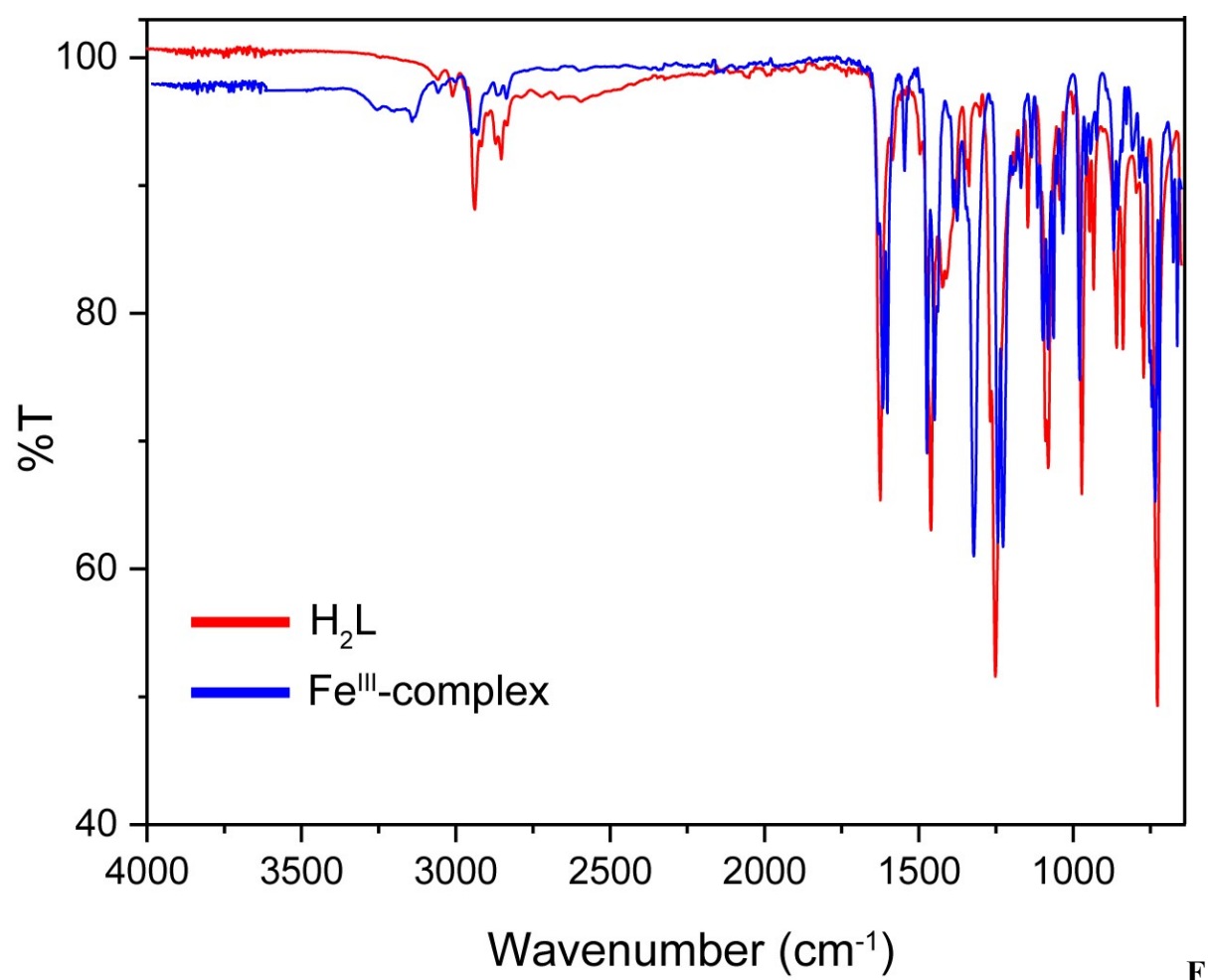
Bond	Length/Å		Bond	Length/Å
Fe1A—Cl1A	2.2426(9)		C15A—C16A	1.413(4)
Fe1A—O2A	1.892(2)		C6A—C5A	1.421(4)
Fe1A—O1A	1.902(2)		C6A—C7A	1.445(5)
Fe1A—N2A	2.102(3)		C3A—C2A	1.390(4)
Fe1A—N1A	2.083(3)		C3A—C4A	1.396(5)
Fe1—Cl1	2.2273(8)		C19A—C18A	1.384(5)
Fe1—O2	1.917(2)		C18A—C17A	1.395(5)
Fe1—O1	1.882(2)		C5A—C4A	1.365(5)
Fe1—N1	2.088(3)		C1—C2	1.3900
Fe1—N2	2.097(3)		C1—C6	1.3900
O2A—C1A	1.329(3)		C2—C3	1.3900

Bond	Length/Å		Bond	Length/Å
O1A—C20A	1.326(4)		C3—C4	1.3900
O3A—C2A	1.358(4)		C4—C5	1.3900
O3A—C22A	1.432(4)		C5—C6	1.3900
O2—C1	1.353(3)		C6—C7	1.444(5)
O1C—20	1.325(4)		C12A—C13A	1.523(5)
O4A—C19A	1.367(4)		C12A—C11A	1.527(5)
O4A—C21A	1.427(4)		C15—C20	1.400(5)
N1—C14	1.287(4)		C15—C14	1.443(5)
N1—C13	1.466(4)		C15—C16	1.420(5)
N2A—C7A	1.289(4)		C20—C19	1.423(5)
N2A—C8A	1.498(4)		C16A—C17A	1.369(5)
N1A—C14A	1.289(4)		C13—C8	1.516(5)
N1A—C13A	1.477(4)		C13—C12	1.509(5)
O4—C19	1.372(6)		C13A—C8A	1.529(5)
O4—C21	1.427(4)		C19—C18	1.382(6)
O3—C2	1.375(4)		C9A—C8A	1.532(5)
O3—C22	1.435(5)		C9A—C10A	1.538(5)
N2—C7	1.283(5)		C8—C9	1.549(5)
N2—C8	1.493(5)		C12—C11	1.509(6)
C1A—C6A	1.404(4)		C16—C17	1.380(7)
C1A—C2A	1.419(4)		C11A—C10A	1.515(6)
C20A—C15A	1.410(4)		C17—C18	1.388(7)
C20A—C19A	1.423(4)		C9—C10	1.559(7)
C15A—C14A	1.442(5)		C11—C10	1.474(8)

Table S5. Bond Angles for Fe^{III}-Complex (1).

Atom—Atom—Atom	Angle/°		Atom—Atom—Atom	Angle/°
O2A—Fe1A—C11A	103.82(7)		C18A—C19A—C20A	120.9(3)
O2A—Fe1A—O1A	92.53(9)		O3A—C2A—C1A	114.4(3)
O2A—Fe1A—N2A	87.28(10)		O3A—C2A—C3A	125.2(3)
O2A—Fe1A—N1A	153.23(10)		C3A—C2A—C1A	120.4(3)
O1A—Fe1A—C11A	114.99(8)		C19A—C18A—C17A	120.2(3)
O1A—Fe1A—N2A	143.72(10)		C4A—C5A—C6A	120.8(3)
O1A—Fe1A—N1A	87.26(10)		O2—C1—C2	117.4(2)
N2A—Fe1A—C11A	100.17(8)		O2—C1—C6	122.6(2)
N1A—Fe1A—C11A	100.47(8)		C2—C1—C6	120.0
N1A—Fe1A—N2A	77.45(10)		O3—C2—C1	114.9(2)
O2—Fe1—C11	102.57(8)		O3—C2—C3	125.1(2)
O2—Fe1—N1	157.76(11)		C1—C2—C3	120.0
O2—Fe1—N2	87.64(11)		C2—C3—C4	120.0
O1—Fe1—C11	115.93(8)		C5—C4—C3	120.0
O1—Fe1—O2	93.04(10)		C4—C5—C6	120.0

Atom—Atom—Atom	Angle/°		Atom—Atom—Atom	Angle/°
O1—Fe1—N1	87.57(11)		C1—C6—C7	123.5(2)
O1—Fe1—N2	137.35(11)		C5—C6—C1	120.0
N1—Fe1—C11	97.09(8)		C5—C6—C7	116.3(2)
N1—Fe1—N2	77.11(12)		C5A—C4A—C3A	120.6(3)
N2—Fe1—C11	105.43(8)		N2A—C7A—C6A	125.4(3)
C1A—O2A—Fe1A	128.49(19)		C13A—C12A—C11A	109.8(3)
C20A—O1A—Fe1A	133.8(2)		C20—C15—C14	122.7(3)
C2A—O3A—C22A	117.0(3)		C20—C15—C16	120.6(4)
C1—O2—Fe1	128.48(19)		C16—C15—C14	116.7(4)
C20—O1—Fe1	131.5(2)		O1—C20—C15	124.2(3)
C19A—O4A—C21A	117.3(3)		O1—C20—C19	117.3(4)
C14—N1—Fe1	126.8(2)		C15—C20—C19	118.5(3)
C14—N1—C13	121.2(3)		N1—C14—C15	124.1(3)
C13—N1—Fe1	111.9(2)		C17A—C16A—C15A	120.7(3)
C7A—N2A—Fe1A	123.5(2)		N2—C7—C6	125.8(3)
C7A—N2A—C8A	120.5(3)		C16A—C17A—C18A	120.4(3)
C8A—N2A—Fe1A	115.7(2)		N1—C13—C8	104.2(3)
C14A—N1A—Fe1A	127.2(2)		N1—C13—C12	117.3(3)
C14A—N1A—C13A	121.8(3)		C12—C13—C8	111.4(3)
C13A—N1A—Fe1A	110.7(2)		N1A—C13A—C12A	116.9(3)
C19—O4—C21	117.6(4)		N1A—C13A—C8A	105.9(3)
C2—O3—C22	118.3(4)		C12A—C13A—C8A	110.5(3)
C7—N2—Fe1	124.0(3)		O4—C19—C20	113.9(3)
C7—N2—C8	121.2(3)		O4—C19—C18	125.7(4)
C8—N2—Fe1	114.6(2)		C18—C19—C20	120.4(4)
O2A—C1A—C6A	123.3(3)		C8A—C9A—C10A	109.8(3)
O2A—C1A—C2A	117.6(3)		N2A—C8A—C13A	105.9(3)
C6A—C1A—C2A	119.0(3)		N2A—C8A—C9A	115.2(3)
O1A—C20A—C15A	123.3(3)		C13A—C8A—C9A	111.0(3)
O1A—C20A—C19A	118.8(3)		N2—C8—C13	106.8(3)
C15A—C20A—C19A	117.9(3)		N2—C8—C9	115.3(3)
C20A—C15A—C14A	122.4(3)		C13—C8—C9	111.0(3)
C20A—C15A—C16A	120.0(3)		C11—C12—C13	111.8(4)
C16A—C15A—C14A	117.6(3)		C17—C16—C15	119.0(4)
N1A—C14A—C15A	125.4(3)		C10A—C11A—C12A	112.0(3)
C1A—C6A—C5A	119.2(3)		C16—C17—C18	121.3(4)
C1A—C6A—C7A	122.4(3)		C8—C9—C10	107.8(4)
C5A—C6A—C7A	118.3(3)		C11A—C10A—C9A	111.7(3)
C2A—C3A—C4A	119.9(3)		C19—C18—C17	120.3(4)
O4A—C19A—C20A	114.4(3)		C10—C11—C12	110.0(4)
O4A—C19A—C18A	124.6(3)		C11—C10—C9	112.0(4)



F

figure S1. Experimental FTIR spectrum of Ligand LH₂ (red), and Fe^{III}-Complex (**1**) (blue).

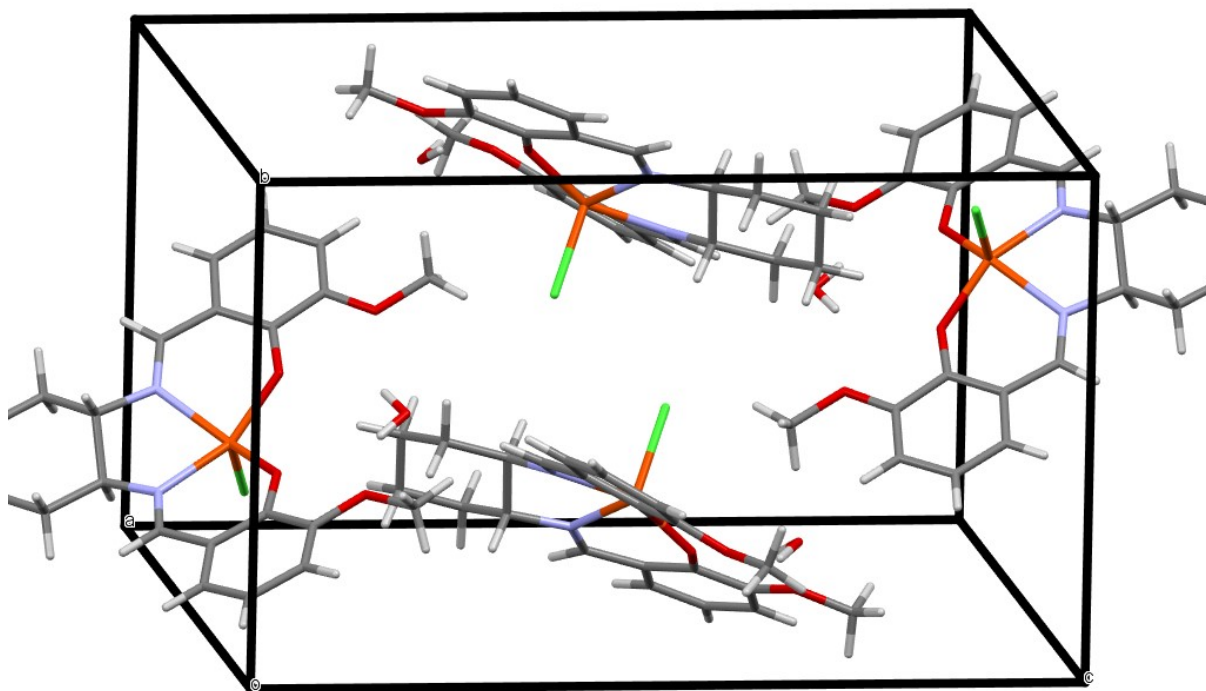


Figure S2. Diagram illustrating the packing of Fe^{III}-Complex (1) in the unit cell.

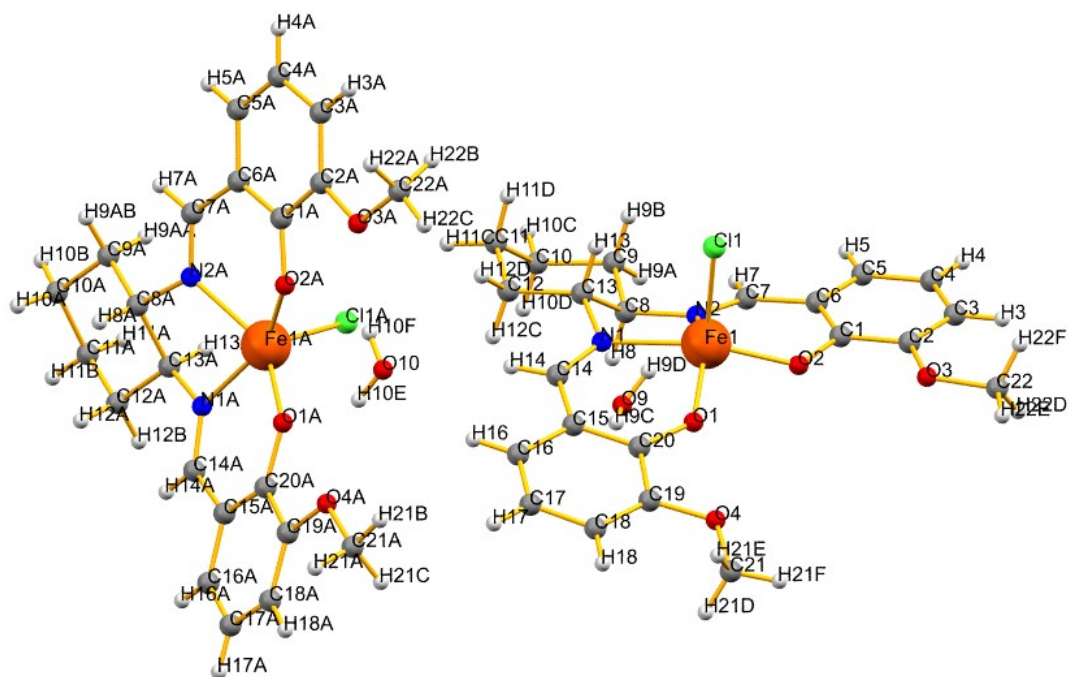


Figure S3. Diagram illustrating the atom numbering scheme of Fe^{III}-Complex (1).

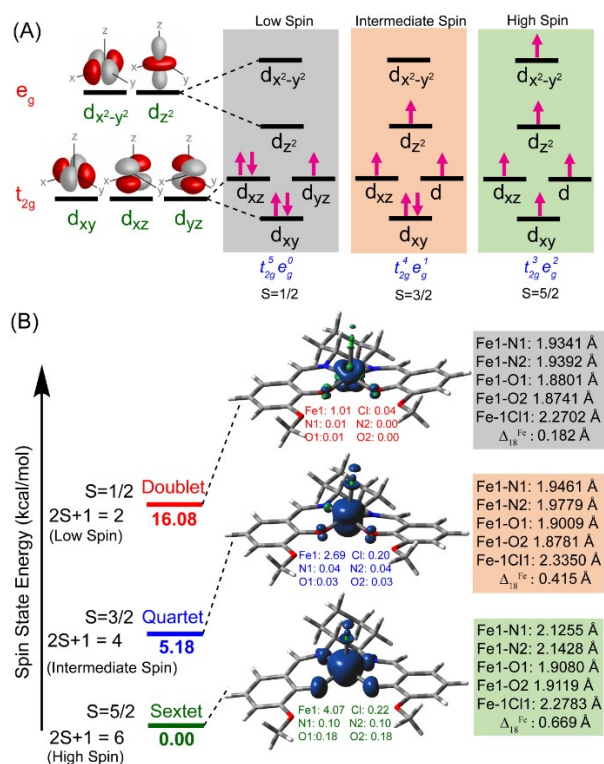
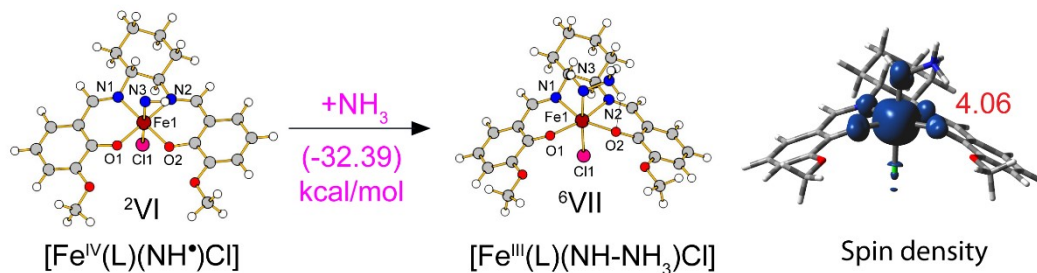


Figure S4. (A) Schematic representation of d-orbital splitting for Fe(III) in low, intermediate, and high-spin configurations. (B) DFT-optimized structures, relative spin-state energy diagram, and spin-density distribution plots for Fe(III)-Complex (1). Relative energies [$\Delta E + ZPE$] are referenced to the high-spin sextet state. Spin-density isosurfaces are shown at an isovalue of 0.01.

Nucleophilic attack by NH_3



Homocoupling or Amido Coupling

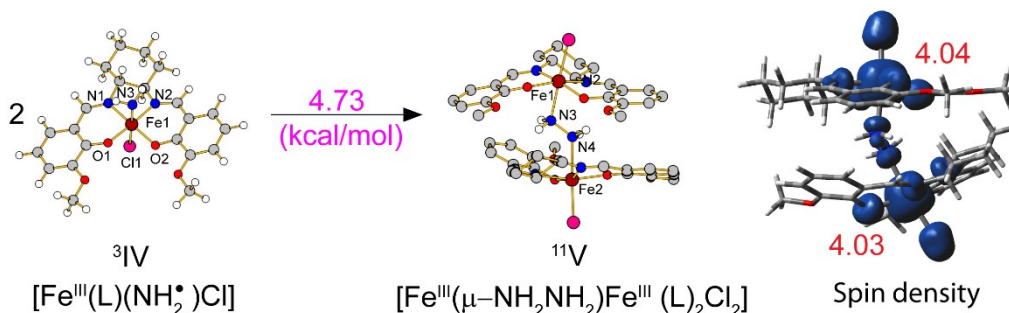


Figure S5. DFT-calculated reaction pathways and spin density plots for N–N bond formation via (top) mononuclear nucleophilic attack and (bottom) bimetallic amido coupling mechanisms.

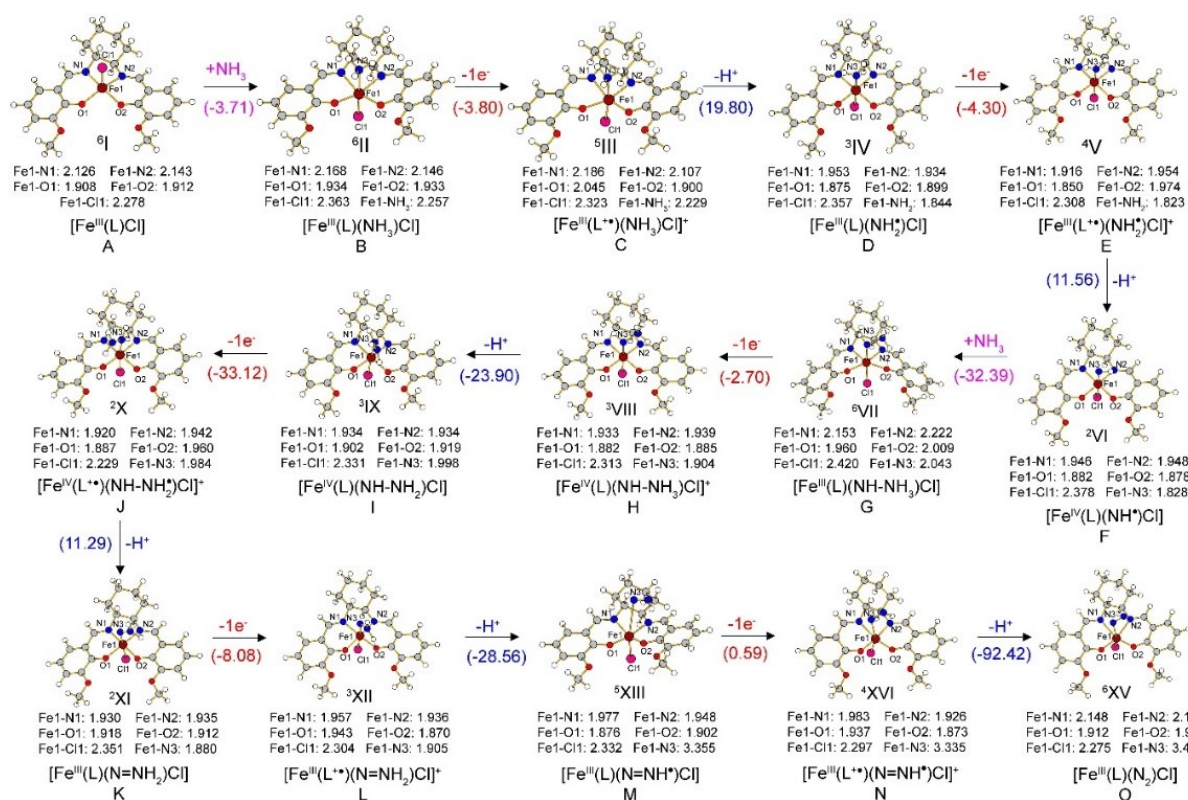


Figure S6. DFT-optimized structures of key intermediates along the Fe^{III} -complex (1)-catalyzed ammonia oxidation pathway. The computed free energy changes (ΔG , kcal/mol) are indicated for each step, highlighting the sequential electron transfer (ET) and proton transfer (PT) events that drive the catalytic cycle. Selected calculated bond distances (Å) are shown to emphasize changes in Fe–N and N–H coordination environments across intermediates. Together, these data illustrate the thermodynamic landscape and structural evolution accompanying ammonia activation and N–N bond formation.

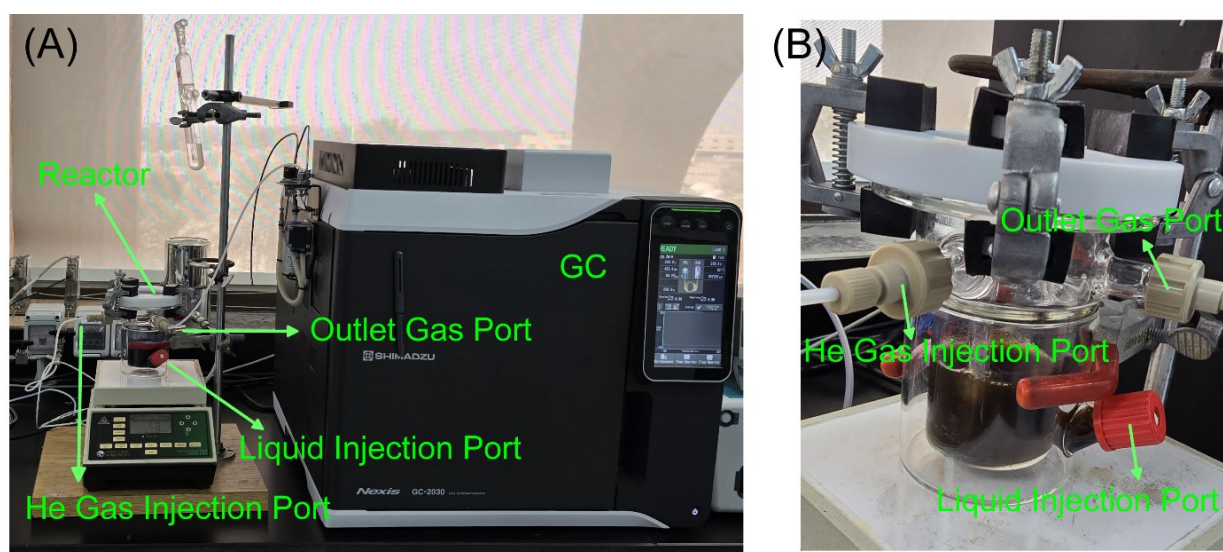


Figure S7. Experimental setup for the catalytic evaluation ammonia oxidation at room temperature.

Table S5. Total Electronic Energy (E) and Gibbs Free Energy (G^{298K}) in Hartree (E_h).

	Species	Charge	Multiplicity	E+G
1	$^1\text{NH}_3$	0	1	-56.499850
2	tris(4-bromophenyl) amine, ^1Ar	0	1	-8468.837466
3	tris(4-bromophenyl) aminium cation, $^2\text{Ar}^+$	1	2	-8468.650086
4	2,4,6-collidine, ^1col	0	1	-365.868144
5	2,4,6-collidine- H^+ , $^1\text{colH}^+$	1	1	-366.323969
6	$^1\text{N}_2$	0	1	-109.446970
Mechanistic Pathway-B				
A	$[\text{Fe}^{\text{III}}(\text{L})\text{Cl}]$, ^2I	0	2	-2985.938397
	$[\text{Fe}^{\text{III}}(\text{L})\text{Cl}]$, ^4I	0	4	-2985.957463
	$[\text{Fe}^{\text{III}}(\text{L})\text{Cl}]$, ^6I	0	6	-2985.966969
B	^2II	0	2	-3042.461028
	^4II	0	4	-3042.459935
	$[\text{Fe}^{\text{III}}(\text{L})(\text{NH}_3)\text{Cl}]$, ^6II	0	6	-3042.472738
C	^1III	1	1	-3042.262056
	^3III	1	3	-3042.282846
	$[\text{Fe}^{\text{III}}(\text{L}^+)(\text{NH}_3)\text{Cl}]^+$, ^5III	1	5	-3042.291425
D	^1IV	0	1	-3041.781657
	$[\text{Fe}^{\text{III}}(\text{L})(\text{NH}_2\bullet)\text{Cl}]$, ^3IV	0	3	-3041.804041
	^5IV	0	5	-3041.800221
E	^2V	1	2	-3041.619458
	$[\text{Fe}^{\text{III}}(\text{L}^+)(\text{NH}_2\bullet)\text{Cl}]^+$, ^4V	1	4	-3041.623518
	^6V	1	6	-3041.614880
F	$[\text{Fe}^{\text{IV}}(\text{L})(\text{NH}\bullet)\text{Cl}]$, ^2VI	0	2	-3041.149270
	^4VI	0	4	-3041.146091
	^6VI	0	6	-3041.136258
G	^2VII	0	2	-3097.687892
	^4VII	0	4	-3097.677148
	$[\text{Fe}^{\text{III}}(\text{L})(\text{NH}-\text{NH}_3)\text{Cl}]$, ^6VII	0	6	-3097.700742
H	$^1\text{VIII}$	1	1	-3097.505169
	$[\text{Fe}^{\text{IV}}(\text{L})(\text{NH}-\text{NH}_3)\text{Cl}]^+$,	1	3	-3097.517679
	$^3\text{VIII}$	1	5	-3097.506420
I	^1IX	0	1	-3097.081964
	$[\text{Fe}^{\text{IV}}(\text{L})(\text{NH}-\text{NH}_2)\text{Cl}]$, ^3IX	0	3	-3097.099947
	^5IX	0	5	-3097.095413
J	$[\text{Fe}^{\text{IV}}(\text{L}^+)(\text{NH}-\text{NH}_2\bullet)\text{Cl}]^+$,	1	2	-3096.965363
	^2X	1	4	-3096.931085
	^4X	1	6	-3096.923789
K	$[\text{Fe}^{\text{III}}(\text{L})(\text{N}=\text{NH}_2)\text{Cl}]$, ^2XI	0	2	-3096.491544
	^4XI	0	4	-3096.481659
	^6XI	0	6	-3096.455280
L	^1XII	1	1	-3096.294823
	$[\text{Fe}^{\text{III}}(\text{L}^+)(\text{N}=\text{NH}_2)\text{Cl}]^+$,	1	3	-3096.317055
	^3XII	1	5	-3096.305231
M	$^1\text{XIII}$	0	1	-3095.847075
	$^3\text{XIII}$	0	3	-3095.889482
	$[\text{Fe}^{\text{III}}(\text{L})(\text{N}=\text{NH}\bullet)\text{Cl}]$, $^5\text{XIII}$	0	5	-3095.906745
N	^2XIV	1	2	-3095.709182
	$[\text{Fe}^{\text{III}}(\text{L}^+)(\text{N}=\text{NH}\bullet)\text{Cl}]^+$,	1	4	-3095.718411
	^4XIV	1	6	-3095.716568

O	² XV	0	2	-3095.371435
	⁴ XV	0	4	-3095.399393
	[Fe ^{III} (L)(N ₂)Cl], ⁶ XV	0	6	-3095.409869
Mechanistic Pathway-A				
A	² I	0	2	-2985.938397
	⁴ I	0	4	-2985.957463
	⁶ I	0	6	-2985.966969
B	² II	1	2	-2525.669216
	⁴ II	1	4	-2525.688702
	⁶ II	1	6	-2525.684613
C	² III	1	2	-2582.197764
	⁶ III	1	6	-2582.214849
D	¹ IV	2	1	-2581.985109
	³ IV	2	3	-2582.006006
	⁵ IV	2	5	-2582.014126
E	¹ V	1	1	-2581.534433
	³ V	1	3	-2581.545834
	⁵ V	1	5	-2581.552690
F	² VI	2	2	-2581.348577
	⁴ VI	2	4	-2581.346658
	⁶ VI	2	6	-2581.338059
G	² VII	1	2	-2580.888388
	⁶ VII	1	6	-2580.871782
H	² VIII	1	2	-2637.445789
	⁶ VIII	1	6	-2637.456312
I	¹ IX	2	1	-2637.235331
	³ IX	2	3	-2637.248452
	⁵ IX	2	5	-2637.265327
J	¹ X	1	1	-2636.833483
	³ X	1	3	-2636.853083
	⁵ X	1	5	-2636.859256
K	² XI	2	2	-2636.661596
	⁴ XI	2	4	-2636.666560
	⁶ XI	2	6	-2636.664266
L	² XII	1	2	-2636.233379
	⁴ XII	1	4	-2636.236966
	⁶ XII	1	6	-2636.238876
M	¹ XIII	2	1	-2636.021319
	³ XIII	2	3	-2636.041562
	⁵ XIII	2	5	-2636.042305
N	¹ XIV	1	1	-2635.616393
	³ XIV	1	3	-2635.647069
	⁵ XIV	1	5	-2635.639666
O	² XV	2	2	-2635.428634
	⁴ XV	2	4	-2635.445994
	⁶ XV	2	6	-2635.440156
P	² XVI	1	2	-2635.111593
	⁴ XVI	1	4	-2635.130794
	⁶ XVI	1	6	-2635.124806

The DFT-optimized Cartesian coordinates (in Å) of the species involved in the catalytic ammonia oxidation (AO) cycle mediated by Fe^{III}-Complex (1) are presented below.

Coordinates of species for Mechanistic Pathway-B											
2I						4I					
Fe	6.715176000	1.899261000	10.197934000			Fe	6.778141000	2.048852000	10.278153000		
Cl	7.896156000	3.633997000	11.063972000			Cl	7.994163000	3.840449000	11.152215000		
O	6.672037000	0.819559000	11.729221000			O	6.729729000	0.969291000	11.814214000		
O	4.922091000	2.344959000	10.546128000			O	4.941677000	2.431101000	10.586201000		
N	6.655415000	2.698927000	8.437835000			N	6.688098000	2.791908000	8.481720000		
O	2.560096000	2.766971000	11.606338000			O	2.547907000	2.779512000	11.593634000		
O	6.347586000	0.090239000	14.231478000			O	6.463575000	0.274009000	14.328144000		
N	8.281596000	0.975798000	9.523841000			N	8.256613000	0.972682000	9.524327000		
C	7.688625000	0.243921000	12.303309000			C	7.704795000	0.273731000	12.328604000		
C	7.549864000	-0.178803000	13.673718000			C	7.592045000	-0.134393000	13.704346000		
C	8.609991000	-0.800759000	14.325153000			C	8.602359000	-0.886853000	14.296301000		
H	8.508286000	-1.104890000	15.367485000			H	8.517882000	-1.186400000	15.341406000		
C	9.830972000	-1.047405000	13.655389000			C	9.748349000	-1.272557000	13.564384000		
H	10.644649000	-1.540514000	14.192371000			H	10.523807000	-1.863799000	14.056689000		
C	9.985456000	-0.672615000	12.336018000			C	9.877856000	-0.904089000	12.240549000		
H	10.919850000	-0.869527000	11.803715000			H	10.754897000	-1.200942000	11.659570000		
C	8.928361000	-0.018920000	11.646141000			C	8.870118000	-0.124776000	11.609695000		
C	4.385164000	3.578419000	8.546736000			C	4.371023000	3.545346000	8.523012000		
C	4.088333000	3.050443000	9.838438000			C	4.085491000	3.057873000	9.833407000		
C	5.662978000	3.354818000	7.924802000			C	5.664850000	3.360256000	7.926353000		
H	5.783528000	3.794596000	6.927775000			H	5.771935000	3.749311000	6.906743000		
C	9.106800000	0.293866000	10.252769000			C	9.033109000	0.203400000	10.217806000		
H	10.014901000	-0.109746000	9.789438000			H	9.896461000	-0.258853000	9.723717000		
C	7.961061000	2.587882000	7.766523000			C	7.994403000	2.652737000	7.816847000		
H	8.621052000	3.293786000	8.301473000			H	8.677809000	3.312207000	8.380033000		
C	2.777540000	3.300886000	10.382932000			C	2.756990000	3.269704000	10.350226000		
C	8.475808000	1.173161000	8.075028000			C	8.448705000	1.205701000	8.079166000		
H	7.788169000	0.465666000	7.575774000			H	7.730380000	0.544919000	7.559646000		
C	8.003865000	2.890851000	6.270241000			C	8.059871000	3.007153000	6.333516000		
H	7.292887000	2.228724000	5.745252000			H	7.334824000	2.387861000	5.776738000		
H	7.688669000	3.928685000	6.081426000			H	7.778623000	4.061241000	6.183300000		
C	3.410632000	4.329484000	7.833313000			C	3.371134000	4.215894000	7.764206000		
H	3.667033000	4.720272000	6.845015000			H	3.623163000	4.574781000	6.762839000		
C	2.165654000	4.558849000	8.382610000			C	2.109941000	4.408631000	8.288053000		
H	1.415335000	5.137565000	7.838869000			H	1.339333000	4.925563000	7.711697000		
C	9.887853000	0.955392000	7.532798000			C	9.851560000	0.946907000	7.529466000		
H	10.210493000	-0.082513000	7.707372000			H	10.124901000	-0.111344000	7.660578000		
H	10.586004000	1.615008000	8.077445000			H	10.575635000	1.549735000	8.105186000		
C	1.848720000	4.042509000	9.660619000			C	1.803746000	3.932820000	9.584545000		
H	0.860017000	4.235051000	10.078670000			H	0.801139000	4.093251000	9.982570000		
C	6.121057000	-0.273997000	15.580990000			C	6.269342000	-0.068433000	15.688498000		
H	6.212689000	-1.364677000	15.733829000			H	6.232110000	-1.163051000	15.836002000		
H	5.093387000	0.033972000	15.819025000			H	5.303082000	0.363646000	15.983839000		
H	6.817047000	0.240871000	16.267918000			H	7.061282000	0.351189000	16.335164000		
C	1.300390000	2.959838000	12.223571000			C	1.270046000	2.933382000	12.183674000		
H	0.479009000	2.523882000	11.626360000			H	0.481680000	2.430823000	11.594157000		
H	1.085844000	4.030323000	12.394954000			H	0.998540000	3.997706000	12.305726000		
H	1.346447000	2.446328000	13.194060000			H	1.325907000	2.464705000	13.176084000		
C	9.422344000	2.674858000	5.727150000			C	9.474738000	2.759378000	5.795189000		
H	9.434310000	2.863204000	4.641426000			H	9.505822000	2.992831000	4.718726000		
H	10.100728000	3.415583000	6.186915000			H	10.177743000	3.450950000	6.292763000		
C	9.934243000	1.264325000	6.030511000			C	9.922526000	1.316487000	6.042009000		
H	10.965333000	1.141500000	5.661516000			H	10.950421000	1.163815000	5.675313000		
H	9.313171000	0.527040000	5.490913000			H	9.274424000	0.630653000	5.467558000		
6I						2II					
Fe	6.741890000	2.223066000	10.509999000			Fe	6.646081000	1.778337000	10.133451000		
Cl	7.940284000	4.003501000	11.274748000			Cl	7.918427000	3.460918000	11.102709000		
O	6.814006000	0.975878000	11.957371000			O	6.636386000	0.738092000	11.734182000		
O	4.867773000	2.574947000	10.577183000			O	4.989675000	2.572496000	10.670611000		

N	6.652163000	2.848276000	8.480421000	N	6.662210000	2.682315000	8.429024000
O	2.449151000	2.961261000	11.533922000	O	2.632428000	3.020649000	11.711999000
O	6.621270000	0.196541000	14.468049000	O	6.338262000	0.011301000	14.234617000
N	8.256533000	1.019138000	9.589040000	N	8.283146000	0.947901000	9.510971000
C	7.775445000	0.225283000	12.420226000	C	7.672497000	0.212590000	12.302974000
C	7.706391000	-0.229036000	13.781691000	C	7.554165000	-0.214737000	13.652814000
C	8.714357000	-1.038129000	14.300629000	C	8.631086000	-0.796408000	14.335899000
H	8.663627000	-1.378076000	15.335576000	H	8.535445000	-1.102395000	15.378497000
C	9.811117000	-1.429844000	13.502260000	C	9.864564000	-1.001306000	13.671190000
H	10.585981000	-2.067892000	13.933463000	H	10.694610000	-1.463332000	14.210916000
C	9.896564000	-1.010301000	12.188061000	C	10.004172000	-0.622931000	12.351928000
H	10.738625000	-1.313164000	11.559939000	H	10.947476000	-0.786197000	11.822941000
C	8.892878000	-0.174147000	11.630945000	C	8.927488000	-0.009156000	11.652438000
C	4.304691000	3.515110000	8.437162000	C	4.366017000	3.488899000	8.524593000
C	3.996669000	3.124170000	9.772240000	C	4.119716000	3.116378000	9.887162000
C	5.625422000	3.335058000	7.869518000	C	5.655076000	3.303688000	7.907375000
H	5.721535000	3.662898000	6.825364000	H	5.767959000	3.750540000	6.911798000
C	9.020847000	0.204262000	10.240085000	C	9.119071000	0.307708000	10.259820000
H	9.855804000	-0.280672000	9.716163000	H	10.057437000	-0.052393000	9.820229000
C	7.964175000	2.695205000	7.846888000	C	7.980658000	2.602143000	7.790392000
H	8.639347000	3.368919000	8.405751000	H	8.624965000	3.296120000	8.358686000
C	2.663086000	3.349477000	10.255947000	C	2.802561000	3.396088000	10.420876000
C	8.434906000	1.252525000	8.144099000	C	8.503814000	1.180642000	8.077081000
H	7.722687000	0.578838000	7.631423000	H	7.835458000	0.481165000	7.539793000
C	8.054852000	3.024336000	6.357018000	C	8.054245000	2.941403000	6.302923000
H	7.345804000	2.387236000	5.799339000	H	7.361316000	2.285950000	5.745993000
H	7.758004000	4.071512000	6.186873000	H	7.731578000	3.980300000	6.132242000
C	3.304588000	4.099593000	7.616978000	C	3.343090000	4.110005000	7.750888000
H	3.564154000	4.388308000	6.594894000	H	3.566675000	4.390375000	6.717651000
C	2.026544000	4.303759000	8.103767000	C	2.097833000	4.353175000	8.289214000
H	1.257327000	4.755694000	7.473266000	H	1.313266000	4.824694000	7.692730000
C	9.840964000	0.999605000	7.590715000	C	9.928135000	0.990604000	7.555873000
H	10.122430000	-0.054649000	7.734411000	H	10.258455000	-0.047661000	7.714966000
H	10.560011000	1.611649000	8.163606000	H	10.609301000	1.644362000	8.128398000
C	1.705586000	3.928912000	9.425673000	C	1.828153000	3.992545000	9.633040000
H	0.693347000	4.098978000	9.794076000	H	0.837934000	4.191260000	10.045090000
C	6.477216000	-0.180784000	15.825595000	C	6.123695000	-0.358775000	15.582339000
H	6.402279000	-1.277133000	15.942178000	H	6.253878000	-1.445543000	15.738615000
H	5.544353000	0.279446000	16.179852000	H	5.085403000	-0.087855000	15.820702000
H	7.315411000	0.186614000	16.445039000	H	6.799704000	0.180195000	16.271430000
C	1.168506000	3.159101000	12.105664000	C	1.383698000	3.255253000	12.332763000
H	0.385004000	2.598867000	11.563894000	H	0.562680000	2.713925000	11.827499000
H	0.890065000	4.228278000	12.129346000	H	1.132453000	4.331473000	12.361036000
H	1.225935000	2.783440000	13.136749000	H	1.471145000	2.884093000	13.363673000
C	9.475281000	2.786732000	5.834366000	C	9.485233000	2.750260000	5.784042000
H	9.516230000	3.010939000	4.756078000	H	9.519336000	2.966025000	4.703767000
H	10.169462000	3.486594000	6.333066000	H	10.148269000	3.483843000	6.276619000
C	9.924886000	1.348895000	6.100581000	C	10.002077000	1.336143000	6.062877000
H	10.956308000	1.192881000	5.744762000	H	11.040957000	1.229913000	5.710611000
H	9.282928000	0.655004000	5.528554000	H	9.397272000	0.608189000	5.492658000
				N	5.507706000	0.307342000	9.320813000
				H	6.057516000	-0.457659000	8.920914000
				H	4.942106000	-0.086541000	10.076787000
				H	4.865973000	0.629942000	8.591766000
⁴II				⁶II			
Fe	6.712756000	1.949337000	10.244105000	Fe	6.579659000	1.988456000	10.464640000
Cl	8.088170000	3.789890000	11.117530000	Cl	8.032890000	3.659745000	11.288416000
O	6.717250000	0.917120000	11.847621000	O	6.769245000	0.799307000	11.977458000
O	4.969695000	2.628593000	10.682796000	O	4.870381000	2.865839000	10.676256000
N	6.675798000	2.771952000	8.459858000	N	6.650979000	2.832817000	8.492808000
O	2.592962000	3.049750000	11.683515000	O	2.420197000	3.237719000	11.546404000
O	6.442509000	0.150135000	14.331957000	O	6.651635000	0.007643000	14.478195000
N	8.312240000	0.999836000	9.550534000	N	8.255030000	0.944995000	9.568253000
C	7.718011000	0.259826000	12.355704000	C	7.797188000	0.141470000	12.428089000
C	7.604795000	-0.185269000	13.722824000	C	7.773997000	-0.318518000	13.792187000
C	8.637332000	-0.898423000	14.323016000	C	8.845040000	-1.036404000	14.317185000

H	8.544213000	-1.224654000	15.359494000	H	8.819449000	-1.378907000	15.352339000
C	9.816783000	-1.210859000	13.609104000	C	9.974549000	-1.329860000	13.522820000
H	10.611741000	-1.772720000	14.104845000	H	10.803255000	-1.895793000	13.954793000
C	9.950569000	-0.808512000	12.295669000	C	10.021315000	-0.903377000	12.208504000
H	10.853195000	-1.050781000	11.728144000	H	10.890280000	-1.130547000	11.584471000
C	8.918764000	-0.069845000	11.653517000	C	8.950532000	-0.161950000	11.641629000
C	4.348671000	3.495809000	8.509508000	C	4.307702000	3.529086000	8.430519000
C	4.096070000	3.146276000	9.873995000	C	3.996150000	3.274919000	9.801683000
C	5.646106000	3.319299000	7.904149000	C	5.642680000	3.348502000	7.881613000
H	5.739739000	3.702062000	6.880203000	H	5.754341000	3.699670000	6.845881000
C	9.109415000	0.279227000	10.266166000	C	9.077663000	0.221743000	10.245346000
H	10.015571000	-0.130051000	9.801798000	H	9.978700000	-0.175283000	9.756724000
C	7.996100000	2.665394000	7.817274000	C	7.975611000	2.692156000	7.887629000
H	8.644271000	3.358208000	8.381379000	H	8.638087000	3.340316000	8.488564000
C	2.769823000	3.397231000	10.386470000	C	2.643389000	3.503573000	10.236934000
C	8.511231000	1.239783000	8.108697000	C	8.446483000	1.235253000	8.141613000
H	7.830315000	0.542981000	7.585509000	H	7.737576000	0.583222000	7.595776000
C	8.066926000	2.998258000	6.328893000	C	8.097931000	3.075388000	6.412148000
H	7.373816000	2.341376000	5.774051000	H	7.396537000	2.463502000	5.817289000
H	7.743902000	4.037142000	6.157903000	H	7.806823000	4.129225000	6.275975000
C	3.320020000	4.063941000	7.706547000	C	3.300354000	4.000652000	7.547988000
H	3.547822000	4.322994000	6.668959000	H	3.565251000	4.195929000	6.505083000
C	2.060710000	4.283648000	8.225127000	C	2.006969000	4.206912000	7.991780000
H	1.270094000	4.716746000	7.608109000	H	1.234057000	4.564900000	7.307644000
C	9.930879000	1.037675000	7.577548000	C	9.856678000	1.000909000	7.589793000
H	10.250872000	-0.004570000	7.730162000	H	10.135376000	-0.058200000	7.703988000
H	10.619812000	1.681915000	8.151583000	H	10.571752000	1.592531000	8.188653000
C	1.787201000	3.948397000	9.571734000	C	1.677764000	3.955916000	9.341011000
H	0.787532000	4.128839000	9.968881000	H	0.653672000	4.122356000	9.677290000
C	6.239410000	-0.234556000	15.678380000	C	6.536410000	-0.391041000	15.830699000
H	6.257453000	-1.332994000	15.801137000	H	6.563149000	-1.490656000	15.940875000
H	5.245648000	0.138306000	15.963673000	H	5.562926000	-0.022636000	16.183832000
H	6.994225000	0.209724000	16.352667000	H	7.333009000	0.047139000	16.459490000
C	1.327750000	3.258223000	12.281441000	C	1.119083000	3.423783000	12.070979000
H	0.532620000	2.678448000	11.777802000	H	0.376878000	2.773554000	11.572704000
H	1.042127000	4.326051000	12.280849000	H	0.785491000	4.473947000	11.984146000
H	1.412821000	2.914017000	13.321747000	H	1.169372000	3.154132000	13.135258000
C	9.496783000	2.803074000	5.809204000	C	9.524503000	2.852894000	5.901159000
H	9.530783000	3.020464000	4.729338000	H	9.583780000	3.122165000	4.833932000
H	10.163407000	3.532432000	6.303013000	H	10.214826000	3.526876000	6.439552000
C	10.004411000	1.385593000	6.085279000	C	9.961430000	1.402786000	6.114955000
H	11.042266000	1.272306000	5.732301000	H	10.996113000	1.253295000	5.765411000
H	9.393852000	0.662627000	5.514976000	H	9.321690000	0.736418000	5.508560000
N	5.452748000	0.134064000	9.255747000	N	5.362331000	0.340381000	9.518600000
H	6.005632000	-0.618471000	8.843544000	H	5.946246000	-0.426111000	9.179264000
H	4.928508000	-0.262186000	10.037123000	H	4.743427000	-0.049262000	10.233128000
H	4.775803000	0.441276000	8.555783000	H	4.772098000	0.642867000	8.740968000
¹III				³III			
Fe	6.649867000	1.726621000	10.082119000	Fe	6.649947000	1.839100000	10.117536000
Cl	7.886369000	3.398838000	11.083911000	Cl	7.958009000	3.476027000	11.069919000
O	6.643181000	0.740867000	11.672834000	O	6.675713000	0.861036000	11.817070000
O	5.010340000	2.483103000	10.613696000	O	5.025170000	2.590231000	10.654371000
N	6.655230000	2.640646000	8.413318000	N	6.668627000	2.719353000	8.420421000
O	2.715930000	2.984745000	11.752915000	O	2.660999000	2.969220000	11.702268000
O	6.246449000	-0.032217000	14.135690000	O	6.373449000	0.094701000	14.281358000
N	8.286596000	0.941117000	9.495091000	N	8.291517000	0.967022000	9.500886000
C	7.654843000	0.245312000	12.276079000	C	7.659750000	0.260622000	12.330062000
C	7.479503000	-0.202565000	13.649402000	C	7.534616000	-0.188806000	13.725879000
C	8.559243000	-0.731615000	14.348194000	C	8.599116000	-0.847463000	14.363379000
H	8.443138000	-1.049750000	15.384207000	H	8.508863000	-1.168174000	15.400913000
C	9.815848000	-0.865916000	13.723835000	C	9.772575000	-1.092071000	13.661089000
H	10.645856000	-1.289819000	14.293590000	H	10.598551000	-1.606826000	14.156010000
C	10.007957000	-0.483244000	12.402066000	C	9.915603000	-0.695558000	12.309836000
H	10.979897000	-0.619724000	11.922265000	H	10.844715000	-0.925140000	11.782544000
C	8.951474000	0.080944000	11.660853000	C	8.901260000	-0.026300000	11.636837000
C	4.372375000	3.466073000	8.516311000	C	4.369557000	3.506207000	8.516422000

C	4.140344000	3.072182000	9.886450000	C	4.131777000	3.122207000	9.872478000
C	5.647840000	3.262640000	7.884474000	C	5.659820000	3.330911000	7.893964000
H	5.757363000	3.703952000	6.887706000	H	5.769024000	3.770252000	6.895534000
C	9.155636000	0.370890000	10.266140000	C	9.106731000	0.299026000	10.232982000
H	10.118045000	0.052523000	9.850862000	H	10.036157000	-0.088913000	9.799693000
C	7.969079000	2.574445000	7.763757000	C	7.988915000	2.630447000	7.780435000
H	8.601937000	3.283188000	8.326860000	H	8.635080000	3.325816000	8.343732000
C	2.849665000	3.383891000	10.482639000	C	2.818765000	3.362773000	10.418654000
C	8.518364000	1.162170000	8.063003000	C	8.509071000	1.207558000	8.064871000
H	7.862816000	0.447591000	7.532573000	H	7.831818000	0.506671000	7.541304000
C	8.033791000	2.899868000	6.273659000	C	8.059188000	2.964779000	6.292015000
H	7.349465000	2.228937000	5.725440000	H	7.363879000	2.309093000	5.738951000
H	7.699363000	3.933175000	6.094091000	H	7.738938000	4.004239000	6.121982000
C	3.355798000	4.131613000	7.797992000	C	3.337268000	4.113725000	7.751761000
H	3.547946000	4.436103000	6.766514000	H	3.550252000	4.406779000	6.720348000
C	2.132613000	4.401520000	8.394351000	C	2.088367000	4.328112000	8.301129000
H	1.350538000	4.912383000	7.828185000	H	1.293596000	4.790680000	7.711486000
C	9.946956000	0.993830000	7.550803000	C	9.930139000	1.007169000	7.542026000
H	10.294720000	-0.036404000	7.723133000	H	10.251106000	-0.034421000	7.697643000
H	10.613970000	1.668796000	8.114715000	H	10.615835000	1.655318000	8.115238000
C	1.876195000	4.031734000	9.732058000	C	1.828627000	3.950227000	9.637739000
H	0.904990000	4.261585000	10.170480000	H	0.836202000	4.125186000	10.054549000
C	5.967047000	-0.401942000	15.481999000	C	6.108220000	-0.260301000	15.644513000
H	6.135320000	-1.480205000	15.644896000	H	6.173831000	-1.351201000	15.782244000
H	4.907569000	-0.169058000	15.650236000	H	5.086138000	0.080409000	15.849033000
H	6.585216000	0.174498000	16.191234000	H	6.813988000	0.246692000	16.321371000
C	1.494924000	3.237132000	12.438383000	C	1.407188000	3.165482000	12.331609000
H	0.646430000	2.730383000	11.947110000	H	0.599500000	2.611217000	11.820180000
H	1.285668000	4.318872000	12.500920000	H	1.132894000	4.234921000	12.375601000
H	1.621592000	2.832855000	13.451242000	H	1.509090000	2.781382000	13.356096000
C	9.468552000	2.723907000	5.758199000	C	9.489202000	2.769618000	5.772028000
H	9.497104000	2.926492000	4.675575000	H	9.520948000	2.984877000	4.691868000
H	10.118567000	3.475197000	6.240934000	H	10.154828000	3.501484000	6.263281000
C	10.010809000	1.322743000	6.053315000	C	10.001635000	1.353823000	6.049092000
H	11.051002000	1.231851000	5.701779000	H	11.039783000	1.244083000	5.696693000
H	9.418936000	0.576272000	5.493979000	H	9.393643000	0.627787000	5.480243000
N	5.545039000	0.237451000	9.252958000	N	5.576120000	0.310742000	9.341742000
H	6.117551000	-0.530292000	8.890365000	H	6.145715000	-0.479242000	9.025392000
H	4.939885000	-0.157819000	9.978056000	H	4.937093000	-0.043945000	10.058723000
H	4.937189000	0.537981000	8.485443000	H	5.001518000	0.597704000	8.543863000
⁵III				⁴IV			
Fe	6.546074000	1.982666000	10.415182000	Fe	6.621697000	1.734274000	10.064712000
Cl	8.005104000	3.485072000	11.420069000	Cl	7.985906000	3.456443000	11.021909000
O	6.749063000	0.687605000	11.984502000	O	6.641336000	0.876220000	11.771195000
O	4.870773000	2.849235000	10.646660000	O	5.075829000	2.648452000	10.674111000
N	6.649766000	2.836311000	8.492079000	N	6.670075000	2.681746000	8.392575000
O	2.418557000	3.217775000	11.525694000	O	2.765441000	3.146740000	11.781167000
O	6.675984000	-0.038401000	14.481458000	O	6.348664000	0.132471000	14.252180000
N	8.250150000	0.923868000	9.547662000	N	8.279770000	0.958634000	9.459893000
C	7.777246000	0.103148000	12.420544000	C	7.627594000	0.224366000	12.275156000
C	7.776560000	-0.340861000	13.826292000	C	7.511189000	-0.214403000	13.653483000
C	8.881011000	-1.021355000	14.363614000	C	8.534258000	-0.928653000	14.259949000
H	8.878131000	-1.349690000	15.402424000	H	8.436451000	-1.252329000	15.296755000
C	9.981918000	-1.270574000	13.555802000	C	9.717803000	-1.246424000	13.549736000
H	10.843296000	-1.799244000	13.969333000	H	10.508383000	-1.809529000	14.051181000
C	10.015061000	-0.853979000	12.200765000	C	9.863278000	-0.845930000	12.237835000
H	10.901177000	-1.077166000	11.601530000	H	10.773355000	-1.088396000	11.682169000
C	8.958284000	-0.169585000	11.619398000	C	8.839288000	-0.109915000	11.578724000
C	4.311209000	3.552342000	8.418440000	C	4.333539000	3.321378000	8.476524000
C	3.989618000	3.278336000	9.781338000	C	4.157305000	3.081298000	9.883545000
C	5.647047000	3.368598000	7.879740000	C	5.629850000	3.218991000	7.851514000
H	5.773557000	3.731142000	6.850890000	H	5.713229000	3.655238000	6.848704000
C	9.080621000	0.207629000	10.210106000	C	9.067888000	0.259296000	10.205811000
H	9.983350000	-0.188691000	9.726628000	H	10.009075000	-0.103452000	9.775155000
C	7.979448000	2.692807000	7.890836000	C	7.995581000	2.651347000	7.774258000
H	8.646814000	3.328512000	8.499594000	H	8.608807000	3.347953000	8.371014000

C	2.643800000	3.505992000	10.224534000	C	2.854953000	3.370956000	10.453441000
C	8.436109000	1.227816000	8.121254000	C	8.546419000	1.237933000	8.045496000
H	7.710227000	0.588699000	7.583832000	H	7.916350000	0.532460000	7.470045000
C	8.103841000	3.094221000	6.420447000	C	8.090656000	3.022296000	6.296765000
H	7.392833000	2.499009000	5.820651000	H	7.437993000	2.353907000	5.707791000
H	7.826761000	4.153631000	6.301711000	H	7.735500000	4.052777000	6.139077000
C	3.312607000	4.048160000	7.541521000	C	3.250992000	3.803401000	7.693083000
H	3.580597000	4.260727000	6.503271000	H	3.416466000	3.993842000	6.629388000
C	2.020143000	4.255444000	7.990379000	C	2.014213000	4.030637000	8.262664000
H	1.251535000	4.632400000	7.311851000	H	1.180527000	4.388466000	7.653969000
C	9.838347000	0.977759000	7.559357000	C	9.992885000	1.104342000	7.569651000
H	10.098258000	-0.087729000	7.656880000	H	10.350339000	0.072730000	7.711030000
H	10.566098000	1.549806000	8.161647000	H	10.632460000	1.762900000	8.182982000
C	1.684439000	3.982872000	9.332212000	C	1.816187000	3.816659000	9.647929000
H	0.660866000	4.151822000	9.668305000	H	0.832838000	4.009823000	10.078030000
C	6.527675000	-0.391622000	15.864097000	C	6.137476000	-0.235246000	15.602427000
H	6.581064000	-1.484080000	15.992321000	H	6.146871000	-1.332307000	15.736856000
H	5.536591000	-0.028216000	16.160882000	H	5.145825000	0.148751000	15.879865000
H	7.304241000	0.097886000	16.472591000	H	6.894274000	0.210607000	16.273328000
C	1.117671000	3.405474000	12.056121000	C	1.535337000	3.394934000	12.439009000
H	0.371493000	2.769781000	11.546185000	H	0.724665000	2.754868000	12.046568000
H	0.795071000	4.459901000	11.987830000	H	1.229499000	4.452847000	12.349145000
H	1.168606000	3.115989000	13.114850000	H	1.695757000	3.157612000	13.499739000
C	9.525565000	2.859340000	5.902160000	C	9.543423000	2.890433000	5.819502000
H	9.583315000	3.145029000	4.839428000	H	9.603212000	3.127315000	4.744885000
H	10.227648000	3.514361000	6.448360000	H	10.164101000	3.637385000	6.345861000
C	9.940335000	1.399581000	6.090018000	C	10.102027000	1.489814000	6.087999000
H	10.970910000	1.239087000	5.734261000	H	11.155044000	1.428991000	5.768679000
H	9.287160000	0.752437000	5.477605000	H	9.543607000	0.753536000	5.482382000
N	5.365854000	0.305094000	9.543205000	N	5.637628000	0.460129000	9.339338000
H	5.942514000	-0.484884000	9.245680000	H	4.896856000	-0.002302000	9.869945000
H	4.707037000	-0.051062000	10.240553000	H	5.695338000	0.143600000	8.370057000
H	4.810900000	0.596122000	8.734314000				
³ IV				⁵ IV			
Fe	6.603782000	1.708848000	10.096224000	Fe	6.647430000	2.178968000	10.483972000
Cl	7.955619000	3.376712000	11.069375000	Cl	8.152762000	3.853466000	11.141787000
O	6.593980000	0.683172000	11.665876000	O	6.859373000	1.074899000	12.047671000
O	5.043101000	2.621912000	10.675689000	O	4.978556000	3.100650000	10.687204000
N	6.643741000	2.677140000	8.422084000	N	6.645544000	2.883352000	8.452415000
O	2.705023000	3.051681000	11.768287000	O	2.542665000	3.376414000	11.629115000
O	6.271045000	-0.004271000	14.167441000	O	6.653978000	0.170361000	14.498405000
N	8.281800000	0.918684000	9.485299000	N	8.250445000	1.023710000	9.556933000
C	7.634004000	0.170092000	12.256873000	C	7.766661000	0.224866000	12.428563000
C	7.490827000	-0.236923000	13.631453000	C	7.694672000	-0.295055000	13.769448000
C	8.561191000	-0.814569000	14.308714000	C	8.648427000	-1.199247000	14.228181000
H	8.450534000	-1.112811000	15.351821000	H	8.591446000	-1.585653000	15.246446000
C	9.800278000	-1.023447000	13.663767000	C	9.700345000	-1.626112000	13.388840000
H	10.622670000	-1.481379000	14.218144000	H	10.437637000	-2.335762000	13.771236000
C	9.962155000	-0.653034000	12.342360000	C	9.788732000	-1.148347000	12.095022000
H	10.913604000	-0.817125000	11.829483000	H	10.597895000	-1.477784000	11.437553000
C	8.895993000	-0.047157000	11.627305000	C	8.835466000	-0.222156000	11.592027000
C	4.342287000	3.452680000	8.523862000	C	4.270875000	3.431326000	8.409255000
C	4.135871000	3.117672000	9.899950000	C	4.035691000	3.322022000	9.814993000
C	5.627447000	3.284331000	7.901257000	C	5.593723000	3.282596000	7.826840000
H	5.737284000	3.731564000	6.906007000	H	5.657076000	3.540580000	6.759933000
C	9.110380000	0.283378000	10.239552000	C	8.993507000	0.198577000	10.213181000
H	10.062463000	-0.052856000	9.811787000	H	9.846620000	-0.268794000	9.701729000
C	7.969527000	2.610198000	7.793764000	C	7.963597000	2.751632000	7.840461000
H	8.601477000	3.303102000	8.375060000	H	8.612182000	3.434676000	8.416532000
C	2.832711000	3.386877000	10.463955000	C	2.689388000	3.500828000	10.289750000
C	8.511402000	1.189976000	8.059932000	C	8.477110000	1.317299000	8.132042000
H	7.863594000	0.487505000	7.506084000	H	7.826789000	0.627654000	7.561671000
C	8.047568000	2.970692000	6.311668000	C	8.077032000	3.089328000	6.354166000
H	7.371604000	2.310282000	5.740450000	H	7.420091000	2.418668000	5.772255000
H	7.708495000	4.006243000	6.154176000	H	7.728441000	4.119826000	6.179661000

C	3.293420000	4.032867000	7.756509000	C	3.197273000	3.727835000	7.530277000
H	3.486495000	4.287263000	6.710876000	H	3.403763000	3.818925000	6.460391000
C	2.057290000	4.265088000	8.321888000	C	1.911782000	3.893111000	8.013546000
H	1.248156000	4.702634000	7.732596000	H	1.086599000	4.115448000	7.332951000
C	9.946860000	1.038215000	7.558132000	C	9.919422000	1.150320000	7.638694000
H	10.293838000	0.003771000	7.705272000	H	10.253824000	0.111866000	7.782653000
H	10.606621000	1.696665000	8.149583000	H	10.575919000	1.793501000	8.250885000
C	1.827762000	3.940734000	9.681018000	C	1.656867000	3.777834000	9.396570000
H	0.844195000	4.133242000	10.111218000	H	0.637660000	3.910857000	9.761234000
C	6.033422000	-0.364071000	15.516217000	C	6.493599000	-0.281675000	15.830526000
H	6.158347000	-1.449772000	15.680566000	H	6.340231000	-1.375213000	15.878099000
H	4.992129000	-0.088367000	15.733624000	H	5.599253000	0.220451000	16.225116000
H	6.699792000	0.179596000	16.210236000	H	7.360748000	-0.016587000	16.462235000
C	1.465755000	3.275670000	12.414806000	C	1.255115000	3.535581000	12.196270000
H	0.647448000	2.698581000	11.946993000	H	0.539831000	2.786888000	11.809964000
H	1.190144000	4.345947000	12.416141000	H	0.846526000	4.545803000	12.011912000
H	1.589804000	2.938672000	13.453417000	H	1.370947000	3.390990000	13.279501000
C	9.487537000	2.813733000	5.805685000	C	9.524668000	2.931791000	5.876964000
H	9.526741000	3.043883000	4.728732000	H	9.590243000	3.160591000	4.800790000
H	10.130352000	3.554345000	6.314003000	H	10.161009000	3.668168000	6.399623000
C	10.030175000	1.406948000	6.071127000	C	10.046709000	1.520823000	6.156431000
H	11.075244000	1.327424000	5.730824000	H	11.100005000	1.429062000	5.844842000
H	9.447513000	0.674406000	5.484342000	H	9.472679000	0.794925000	5.552728000
N	5.670988000	0.381487000	9.220693000	N	5.616756000	0.480471000	9.601480000
H	5.982185000	-0.564220000	9.455216000	H	5.966889000	-0.410228000	9.983690000
H	5.551648000	0.455997000	8.208767000	H	5.722842000	0.385584000	8.581523000
²V				⁴V			
Fe	6.610166000	1.603117000	10.018763000	Fe	6.616371000	1.584408000	10.049809000
Cl	7.648149000	3.446072000	11.033247000	Cl	7.706111000	3.360836000	11.042396000
O	6.655829000	0.684929000	11.738230000	O	6.617243000	0.592505000	11.611320000
O	4.866493000	2.275107000	10.536114000	O	4.906620000	2.393515000	10.615192000
N	6.637727000	2.588871000	8.364820000	N	6.638193000	2.609018000	8.386400000
O	2.552446000	2.775614000	11.620023000	O	2.616739000	2.942940000	11.712718000
O	6.353449000	-0.032603000	14.217824000	O	6.264183000	-0.075856000	14.116158000
N	8.331135000	0.926010000	9.474776000	N	8.315190000	0.901848000	9.483242000
C	7.678116000	0.209111000	12.298366000	C	7.670517000	0.166494000	12.248523000
C	7.555997000	-0.212059000	13.704001000	C	7.509620000	-0.224961000	13.624146000
C	8.659999000	-0.738596000	14.388241000	C	8.602881000	-0.705841000	14.343225000
H	8.571929000	-1.041983000	15.431109000	H	8.485606000	-0.993719000	15.388274000
C	9.877584000	-0.873338000	13.726481000	C	9.869048000	-0.828711000	13.736056000
H	10.735725000	-1.285059000	14.261895000	H	10.707286000	-1.212036000	14.322164000
C	10.025473000	-0.497524000	12.372047000	C	10.046628000	-0.472749000	12.409477000
H	10.991783000	-0.637939000	11.881751000	H	11.022491000	-0.577616000	11.928972000
C	8.969638000	0.041874000	11.648874000	C	8.962685000	0.036623000	11.655239000
C	4.410264000	3.559793000	8.557855000	C	4.378317000	3.506521000	8.553375000
C	4.086518000	3.011944000	9.859416000	C	4.101635000	3.052450000	9.902712000
C	5.688885000	3.327491000	7.908562000	C	5.662173000	3.290272000	7.905135000
H	5.831406000	3.867358000	6.965343000	H	5.782550000	3.791348000	6.937594000
C	9.186365000	0.358117000	10.243978000	C	9.177881000	0.345456000	10.262634000
H	10.162318000	0.056275000	9.846329000	H	10.153385000	0.060778000	9.852352000
C	7.960975000	2.528946000	7.719088000	C	7.962992000	2.538793000	7.746551000
H	8.570616000	3.270232000	8.266068000	H	8.582083000	3.260740000	8.307330000
C	2.776729000	3.321986000	10.431769000	C	2.792747000	3.387380000	10.484796000
C	8.549578000	1.143369000	8.040151000	C	8.528685000	1.137365000	8.047939000
H	7.912366000	0.393565000	7.536747000	H	7.884809000	0.406222000	7.527641000
C	8.012789000	2.826194000	6.220786000	C	8.021156000	2.861707000	6.254828000
H	7.339500000	2.127317000	5.694234000	H	7.341218000	2.181028000	5.713345000
H	7.652451000	3.846293000	6.019868000	H	7.674993000	3.890580000	6.072977000
C	3.476773000	4.364974000	7.904767000	C	3.409969000	4.229392000	7.867531000
H	3.724101000	4.781212000	6.925365000	H	3.623388000	4.581977000	6.855657000
C	2.228580000	4.649018000	8.484809000	C	2.156202000	4.525310000	8.452185000
H	1.518419000	5.282219000	7.948556000	H	1.420461000	5.091858000	7.877797000
C	9.979979000	1.003215000	7.524408000	C	9.960691000	0.992895000	7.536852000
H	10.356525000	-0.012896000	7.718791000	H	10.325273000	-0.029910000	7.717729000
H	10.630931000	1.708737000	8.069734000	H	10.615776000	1.683806000	8.095272000
C	1.876784000	4.135684000	9.735581000	C	1.848207000	4.116226000	9.743975000

H	0.901496000	4.370417000	10.161295000	H	0.878926000	4.362652000	10.176625000
C	6.087447000	-0.377994000	15.582084000	C	6.008400000	-0.422999000	15.468072000
H	6.254564000	-1.453583000	15.751908000	H	6.207255000	-1.492432000	15.659099000
H	5.031908000	-0.134147000	15.753145000	H	4.943364000	-0.219266000	15.643753000
H	6.721529000	0.211364000	16.263458000	H	6.611210000	0.184663000	16.165984000
C	1.313150000	3.010285000	12.291151000	C	1.388795000	3.192521000	12.409699000
H	0.464849000	2.634829000	11.695698000	H	0.538998000	2.741364000	11.873322000
H	1.174676000	4.084080000	12.498406000	H	1.225889000	4.275122000	12.531232000
H	1.371478000	2.457764000	13.237299000	H	1.501605000	2.720126000	13.392903000
C	9.447267000	2.676925000	5.697211000	C	9.455853000	2.702433000	5.734627000
H	9.461715000	2.856035000	4.610094000	H	9.475936000	2.898573000	4.650673000
H	10.080619000	3.456075000	6.157573000	H	10.097119000	3.466004000	6.209566000
C	10.029068000	1.298187000	6.019637000	C	10.018214000	1.311198000	6.037126000
H	11.069590000	1.227329000	5.664304000	H	11.059389000	1.233118000	5.685524000
H	9.454525000	0.523623000	5.480933000	H	9.436452000	0.552573000	5.483873000
N	5.707222000	0.189575000	9.226264000	N	5.710696000	0.269117000	9.170553000
H	4.899670000	-0.178876000	9.733316000	H	5.792821000	-0.702862000	9.474053000
H	5.510049000	0.195379000	8.223638000	H	5.322384000	0.359115000	8.229982000
⁶V				²VI			
Fe	6.690620000	2.090504000	10.480911000	Fe	6.607402000	1.681084000	10.073666000
Cl	7.809598000	4.020452000	11.075169000	Cl	7.849826000	3.487777000	10.994720000
O	6.978419000	1.104667000	12.063117000	O	6.634052000	0.769351000	11.719495000
O	4.812429000	2.918915000	10.679603000	O	4.962410000	2.415266000	10.604143000
N	6.613103000	2.794268000	8.443089000	N	6.647733000	2.667714000	8.394668000
O	2.413955000	3.366063000	11.565978000	O	2.617496000	2.845285000	11.664148000
O	6.725357000	0.162367000	14.503533000	O	6.317610000	0.060764000	14.207740000
N	8.319102000	1.034730000	9.587280000	N	8.308813000	0.933440000	9.495740000
C	7.860388000	0.224612000	12.449839000	C	7.665853000	0.217350000	12.284878000
C	7.763319000	-0.305813000	13.780200000	C	7.527881000	-0.191919000	13.660818000
C	8.706176000	-1.228438000	14.231694000	C	8.592251000	-0.792526000	14.326171000
H	8.639396000	-1.627277000	15.244332000	H	8.483862000	-1.093103000	15.368835000
C	9.755193000	-1.656056000	13.392988000	C	9.822496000	-1.022828000	13.670737000
H	10.481351000	-2.378830000	13.771584000	H	10.640391000	-1.497877000	14.217167000
C	9.860301000	-1.167658000	12.102210000	C	9.980052000	-0.652297000	12.349811000
H	10.667466000	-1.502348000	11.445791000	H	10.923737000	-0.832557000	11.828350000
C	8.921690000	-0.226036000	11.608502000	C	8.918159000	-0.026919000	11.642874000
C	4.250724000	3.418028000	8.397674000	C	4.384360000	3.546736000	8.544363000
C	3.962793000	3.259067000	9.813771000	C	4.113859000	3.065391000	9.862043000
C	5.584554000	3.242322000	7.824312000	C	5.665857000	3.352431000	7.913911000
H	5.661402000	3.548715000	6.772552000	H	5.799431000	3.848976000	6.945433000
C	9.069014000	0.203394000	10.233469000	C	9.133119000	0.298471000	10.255769000
H	9.910421000	-0.265369000	9.706091000	H	10.084763000	-0.042427000	9.830225000
C	7.943088000	2.705620000	7.835148000	C	7.971191000	2.575143000	7.756350000
H	8.553707000	3.426123000	8.407936000	H	8.608502000	3.288384000	8.306037000
C	2.585315000	3.527053000	10.270773000	C	2.810688000	3.330234000	10.418486000
C	8.512983000	1.301449000	8.148654000	C	8.514494000	1.164861000	8.060709000
H	7.883501000	0.570144000	7.608375000	H	7.850802000	0.445881000	7.544936000
C	8.044189000	3.035604000	6.346592000	C	8.025266000	2.886164000	6.261305000
H	7.403631000	2.341642000	5.773962000	H	7.333466000	2.211659000	5.726970000
H	7.669931000	4.055309000	6.164360000	H	7.691386000	3.918203000	6.074235000
C	3.227586000	3.809944000	7.545933000	C	3.394049000	4.267112000	7.823747000
H	3.442168000	3.947202000	6.483243000	H	3.633114000	4.628609000	6.820331000
C	1.910659000	4.041223000	8.015069000	C	2.154190000	4.505328000	8.382888000
H	1.138010000	4.339454000	7.303516000	H	1.391184000	5.057437000	7.829590000
C	9.956713000	1.176760000	7.647696000	C	9.938943000	0.988289000	7.537089000
H	10.325498000	0.152492000	7.806007000	H	10.283032000	-0.042262000	7.714357000
H	10.594105000	1.852485000	8.244434000	H	10.612567000	1.663173000	8.093504000
C	1.587363000	3.905553000	9.358574000	C	1.863105000	4.035595000	9.682808000
H	0.568810000	4.094616000	9.696803000	H	0.879156000	4.233189000	10.109368000
C	6.541540000	-0.308447000	15.829124000	C	6.083993000	-0.301572000	15.556775000
H	6.373457000	-1.399940000	15.854653000	H	6.190525000	-1.390166000	15.714430000
H	5.648963000	0.200351000	16.218065000	H	5.049562000	-0.008224000	15.783472000
H	7.404753000	-0.063288000	16.473021000	H	6.765510000	0.226498000	16.248037000
C	1.128877000	3.577558000	12.167358000	C	1.367590000	3.056496000	12.297314000
H	0.384619000	2.886378000	11.741594000	H	0.538466000	2.591784000	11.733809000
H	0.801515000	4.619262000	12.023129000	H	1.151104000	4.131980000	12.428744000

H	1.261421000	3.372013000	13.236287000	H	1.435960000	2.582987000	13.286449000
C	9.494482000	2.916937000	5.866317000	C	9.454643000	2.704250000	5.734502000
H	9.546198000	3.135997000	4.787665000	H	9.473700000	2.898099000	4.649929000
H	10.109350000	3.678815000	6.377652000	H	10.110136000	3.458448000	6.205259000
C	10.060544000	1.526745000	6.159258000	C	9.996063000	1.304730000	6.037114000
H	11.113902000	1.462680000	5.841946000	H	11.034211000	1.208650000	5.680424000
H	9.504308000	0.774913000	5.571147000	H	9.399174000	0.555367000	5.487190000
N	5.697128000	0.383614000	9.679779000	N	5.789542000	0.317992000	9.172088000
H	6.031872000	-0.509510000	10.071610000	H	4.924992000	0.707462000	8.747507000
H	5.728359000	0.262884000	8.656815000				
⁴VI				⁶VI			
Fe	6.603579000	1.752522000	10.095796000	Fe	6.370008000	1.430773000	10.225455000
Cl	7.985256000	3.464387000	10.975144000	Cl	7.460646000	3.326074000	11.211059000
O	6.616151000	0.786105000	11.705459000	O	6.654995000	0.379836000	11.831741000
O	5.025166000	2.621745000	10.661188000	O	4.607622000	2.338700000	10.483487000
N	6.606136000	2.647656000	8.386134000	N	6.556768000	2.612357000	8.413316000
O	2.714688000	3.112273000	11.778868000	O	2.239213000	2.917464000	11.405025000
O	6.261305000	0.010086000	14.172767000	O	6.562941000	-0.232869000	14.384497000
N	8.266218000	0.931517000	9.482708000	N	8.231479000	0.778197000	9.518727000
C	7.633379000	0.220200000	12.274249000	C	7.776008000	0.031858000	12.384213000
C	7.474891000	-0.225397000	13.638189000	C	7.773873000	-0.330091000	13.780416000
C	8.537717000	-0.831842000	14.303850000	C	8.945188000	-0.735676000	14.411946000
H	8.423053000	-1.154302000	15.339047000	H	8.933624000	-1.002785000	15.469479000
C	9.770717000	-1.040801000	13.652676000	C	10.162851000	-0.808616000	13.698481000
H	10.586681000	-1.523013000	14.195707000	H	11.069821000	-1.133002000	14.214199000
C	9.942132000	-0.647590000	12.335588000	C	10.194240000	-0.473075000	12.358251000
H	10.890016000	-0.825149000	11.821327000	H	11.130694000	-0.530879000	11.795888000
C	8.891500000	-0.011572000	11.632638000	C	9.020546000	-0.041615000	11.683425000
C	4.316395000	3.454679000	8.509590000	C	4.348083000	3.657862000	8.498077000
C	4.120813000	3.136257000	9.891604000	C	3.904457000	3.107008000	9.763711000
C	5.586409000	3.250883000	7.866659000	C	5.671238000	3.401304000	7.930506000
H	5.684423000	3.672499000	6.859263000	H	5.880022000	3.976348000	7.017731000
C	9.102922000	0.311955000	10.242548000	C	9.145163000	0.274867000	10.272138000
H	10.056902000	-0.023313000	9.819099000	H	10.130488000	0.043263000	9.843553000
C	7.926694000	2.581061000	7.746759000	C	7.898349000	2.492454000	7.828244000
H	8.547525000	3.305057000	8.301434000	H	8.530781000	3.165817000	8.434449000
C	2.831813000	3.435156000	10.471539000	C	2.565176000	3.459993000	10.240852000
C	8.502218000	1.182950000	8.052839000	C	8.415718000	1.054172000	8.095406000
H	7.880014000	0.454693000	7.501940000	H	7.730503000	0.367654000	7.564323000
C	7.991005000	2.894575000	6.253395000	C	8.010919000	2.869815000	6.347429000
H	7.331066000	2.198935000	5.705873000	H	7.296734000	2.254151000	5.772122000
H	7.625914000	3.915511000	6.063006000	H	7.723840000	3.922420000	6.202242000
C	3.269259000	4.048400000	7.752689000	C	3.493624000	4.499509000	7.792094000
H	3.451847000	4.290044000	6.702282000	H	3.827423000	4.923592000	6.841947000
C	2.046031000	4.312476000	8.334143000	C	2.208162000	4.817454000	8.275199000
H	1.238882000	4.762998000	7.751994000	H	1.564484000	5.478075000	7.690266000
C	9.942881000	1.053500000	7.560050000	C	9.830440000	0.861085000	7.543438000
H	10.315782000	0.032727000	7.735183000	H	10.149846000	-0.181540000	7.698759000
H	10.583262000	1.744958000	8.134841000	H	10.529448000	1.504211000	8.106830000
C	1.827768000	4.005108000	9.697910000	C	1.743396000	4.307405000	9.486328000
H	0.855009000	4.223544000	10.139923000	H	0.746171000	4.570380000	9.838189000
C	6.008269000	-0.378327000	15.513667000	C	6.455507000	-0.558033000	15.756177000
H	6.119801000	-1.468576000	15.650988000	H	6.728800000	-1.610863000	15.954338000
H	4.968818000	-0.094480000	15.727360000	H	5.402397000	-0.407470000	16.033180000
H	6.676728000	0.142838000	16.221775000	H	7.086438000	0.095112000	16.386852000
C	1.490180000	3.369621000	12.442019000	C	0.964527000	3.188868000	11.992628000
H	0.652424000	2.807849000	11.990608000	H	0.148018000	2.839588000	11.339839000
H	1.239827000	4.445975000	12.438851000	H	0.845594000	4.266294000	12.192478000
H	1.622442000	3.037540000	13.481121000	H	0.943302000	2.633518000	12.938540000
C	9.434898000	2.760709000	5.751283000	C	9.430786000	2.652322000	5.815841000
H	9.467576000	2.955686000	4.667229000	H	9.462912000	2.898363000	4.741893000
H	10.055869000	3.536256000	6.233965000	H	10.119943000	3.350580000	6.323901000
C	10.018850000	1.380192000	6.062566000	C	9.900139000	1.216815000	6.055612000
H	11.066826000	1.321805000	5.727101000	H	10.930647000	1.079855000	5.689340000
H	9.460580000	0.612168000	5.497911000	H	9.262102000	0.520986000	5.481563000
N	5.674523000	0.410931000	9.263843000	N	5.520793000	0.171486000	9.300434000

H	6.180694000	-0.132295000	8.545272000	H	5.164836000	0.547998000	8.405401000
²VII				⁴VII			
Fe	6.585396000	1.795894000	10.044177000	Fe	6.548126000	1.489178000	10.051764000
Cl	7.994735000	3.525937000	10.884723000	Cl	7.906405000	3.681533000	10.981584000
O	6.635567000	0.913146000	11.762815000	O	6.680278000	0.669327000	11.786559000
O	5.001386000	2.717220000	10.637281000	O	4.787960000	2.143449000	10.463513000
N	6.554171000	2.625065000	8.307093000	N	6.620345000	2.528390000	8.360686000
O	2.697965000	3.258455000	11.753630000	O	2.442003000	2.680067000	11.479267000
O	6.356801000	0.090516000	14.225786000	O	6.460041000	0.054921000	14.317416000
N	8.199286000	0.931328000	9.388434000	N	8.311025000	0.812418000	9.501655000
C	7.593633000	0.187786000	12.220405000	C	7.738874000	0.169336000	12.342031000
C	7.488733000	-0.295314000	13.584724000	C	7.661109000	-0.191159000	13.739192000
C	8.485581000	-1.080582000	14.143812000	C	8.757530000	-0.739733000	14.394103000
H	8.394149000	-1.430752000	15.172808000	H	8.687162000	-1.003374000	15.450188000
C	9.635969000	-1.439296000	13.395806000	C	9.976639000	-0.962994000	13.711503000
H	10.407712000	-2.057618000	13.860452000	H	10.822929000	-1.395712000	14.250101000
C	9.766086000	-1.006456000	12.094440000	C	10.083663000	-0.632736000	12.376335000
H	10.646944000	-1.279077000	11.505732000	H	11.019393000	-0.800262000	11.835667000
C	8.764431000	-0.195323000	11.483283000	C	8.983885000	-0.063659000	11.674897000
C	4.249414000	3.392097000	8.440986000	C	4.399651000	3.529340000	8.513334000
C	4.086764000	3.162915000	9.849995000	C	4.036518000	2.948820000	9.768689000
C	5.516420000	3.193579000	7.784545000	C	5.689686000	3.297374000	7.902898000
H	5.590184000	3.593837000	6.764912000	H	5.870677000	3.853590000	6.974194000
C	8.977609000	0.193190000	10.113838000	C	9.174277000	0.248940000	10.279973000
H	9.901812000	-0.190873000	9.663959000	H	10.153605000	-0.028891000	9.870811000
C	7.881014000	2.625302000	7.685974000	C	7.970214000	2.472841000	7.763445000
H	8.454916000	3.368716000	8.265683000	H	8.558811000	3.199219000	8.350377000
C	2.793317000	3.489701000	10.419871000	C	2.729206000	3.264100000	10.291831000
C	8.520165000	1.258340000	7.986795000	C	8.554226000	1.079367000	8.071100000
H	8.013485000	0.513156000	7.345771000	H	7.936937000	0.349084000	7.518057000
C	7.982529000	2.968319000	6.201485000	C	8.065720000	2.800176000	6.272989000
H	7.406579000	2.233532000	5.610746000	H	7.411669000	2.109674000	5.710834000
H	7.546850000	3.960433000	6.005269000	H	7.704033000	3.821674000	6.080936000
C	3.175367000	3.915386000	7.664647000	C	3.493230000	4.382320000	7.825051000
H	3.339441000	4.089938000	6.597123000	H	3.803145000	4.812971000	6.686996000
C	1.954645000	4.197436000	8.239627000	C	2.248796000	4.663511000	8.351640000
H	1.130466000	4.591215000	7.639947000	H	1.553545000	5.318992000	7.822127000
C	9.998870000	1.260381000	7.591458000	C	9.999637000	0.960644000	7.589149000
H	10.450751000	0.271916000	7.764809000	H	10.378823000	-0.056926000	7.771037000
H	10.535483000	1.984821000	8.228750000	H	10.631516000	1.656757000	8.168290000
C	1.765874000	3.982770000	9.628401000	C	1.867194000	4.101055000	9.590841000
H	0.795769000	4.212586000	10.071308000	H	0.881116000	4.331744000	9.995726000
C	6.159022000	-0.316699000	15.564545000	C	6.285334000	-0.250115000	15.687050000
H	6.116246000	-1.417549000	15.660791000	H	6.422468000	-1.327970000	15.891482000
H	5.194469000	0.104260000	15.882185000	H	5.253551000	0.030661000	15.941657000
H	6.951806000	0.064620000	16.234514000	H	6.979358000	0.322420000	16.329586000
C	1.479435000	3.542142000	12.409983000	C	1.189115000	2.937971000	12.084185000
H	0.643611000	2.937037000	12.012191000	H	0.348172000	2.596436000	11.453173000
H	1.207029000	4.611170000	12.333656000	H	1.052044000	4.012033000	12.306426000
H	1.626307000	3.288893000	13.469626000	H	1.175966000	2.375238000	13.028137000
C	9.457255000	2.959364000	5.772991000	C	9.514060000	2.671027000	5.784869000
H	9.533852000	3.166329000	4.693057000	H	9.559366000	2.875203000	4.702693000
H	9.982432000	3.780870000	6.292128000	H	10.130003000	3.442200000	6.281054000
C	10.144497000	1.631813000	6.108664000	C	10.093027000	1.288526000	6.093719000
H	11.213146000	1.676622000	5.842339000	H	11.144026000	1.229226000	5.767339000
H	9.699254000	0.827897000	5.494935000	H	9.538178000	0.523875000	5.520765000
N	5.375324000	0.401335000	9.462717000	N	5.682907000	-0.243286000	9.041646000
N	5.810044000	-0.489539000	8.424078000	N	4.612645000	0.091661000	8.144688000
H	6.709502000	-0.970209000	8.601372000	H	4.873867000	0.717357000	7.361077000
H	5.107437000	-1.219084000	8.231711000	H	4.149919000	-0.730431000	7.726431000
H	5.917665000	0.042406000	7.550783000	H	3.886834000	0.588374000	8.677405000
H	5.235379000	-0.202775000	10.277026000	H	6.349542000	-0.757252000	8.458420000
⁶VII				¹VIII			

Fe	6.279899000	1.196819000	10.136305000	Fe	6.706712000	1.689404000	9.907241000
Cl	6.929971000	3.202801000	11.323866000	Cl	7.846185000	3.421019000	10.985728000
O	6.706504000	0.107834000	11.708620000	O	6.663304000	0.688956000	11.503288000
O	4.364148000	1.779839000	9.977812000	O	5.044175000	2.437060000	10.423145000
N	6.534208000	2.430229000	8.305368000	N	6.794341000	2.680632000	8.263569000
O	2.077670000	2.511255000	11.056666000	O	2.638054000	2.697053000	11.351684000
O	6.547881000	-0.460073000	14.275492000	O	6.196288000	-0.145252000	13.927979000
N	8.303009000	0.787381000	9.525587000	N	8.396417000	0.981320000	9.391142000
C	7.826114000	0.030697000	12.360174000	C	7.672289000	0.205753000	12.135613000
C	7.793547000	-0.293303000	13.764581000	C	7.458702000	-0.267629000	13.488920000
C	8.972087000	-0.406482000	14.495675000	C	8.522193000	-0.783361000	14.218740000
H	8.936049000	-0.641382000	15.560284000	H	8.373158000	-1.124694000	15.243275000
C	10.228491000	-0.221419000	13.875630000	C	9.808651000	-0.875797000	13.642591000
H	11.140516000	-0.319549000	14.469310000	H	10.626020000	-1.289055000	14.237922000
C	10.292228000	0.075554000	12.527157000	C	10.037447000	-0.465747000	12.339527000
H	11.259681000	0.211541000	12.034947000	H	11.029534000	-0.563515000	11.892459000
C	9.108922000	0.218164000	11.754971000	C	8.988434000	0.082616000	11.566349000
C	4.520726000	3.785835000	8.658560000	C	4.523459000	3.539958000	8.337588000
C	3.881779000	2.936832000	9.609871000	C	4.210644000	3.054639000	9.649890000
C	5.799209000	3.457972000	8.053540000	C	5.830482000	3.369438000	7.751428000
H	6.157401000	4.209492000	7.330849000	H	5.993297000	3.888000000	6.799587000
C	9.257458000	0.489744000	10.337098000	C	9.239489000	0.407762000	10.188625000
H	10.288867000	0.411258000	9.962721000	H	10.223723000	0.116637000	9.805010000
C	7.864572000	2.326847000	7.688022000	C	8.131885000	2.622192000	7.663304000
H	8.496138000	3.121284000	8.128133000	H	8.747206000	3.326610000	8.250086000
C	2.625681000	3.368491000	10.159949000	C	2.868664000	3.257112000	10.148636000
C	8.492831000	0.974475000	8.089707000	C	8.666151000	1.208881000	7.970036000
H	7.867609000	0.196355000	7.614752000	H	8.011782000	0.495718000	7.433315000
C	7.865852000	2.472077000	6.158795000	C	8.240416000	2.958790000	6.177456000
H	7.200426000	1.696488000	5.738187000	H	7.562187000	2.299218000	5.608201000
H	7.447295000	3.447694000	5.868881000	H	7.921908000	3.996762000	5.996488000
C	3.911698000	5.010444000	8.275583000	C	3.546021000	4.248819000	7.598432000
H	4.420289000	5.643589000	7.542890000	H	3.809467000	4.632657000	6.609830000
C	2.703146000	5.403446000	8.820741000	C	2.277233000	4.449758000	8.115220000
H	2.239994000	6.348485000	8.527104000	H	1.527519000	4.994573000	7.537079000
C	9.915610000	0.844242000	7.542965000	C	10.104768000	1.031170000	7.490355000
H	10.338711000	-0.133538000	7.823980000	H	10.440863000	-0.001938000	7.668607000
H	10.556986000	1.619722000	7.997983000	H	10.764265000	1.699665000	8.070695000
C	2.058280000	4.578670000	9.767827000	C	1.932027000	3.946195000	9.387925000
H	1.106395000	4.901114000	10.191832000	H	0.921101000	4.098831000	9.766537000
C	6.409041000	-0.771895000	15.647433000	C	5.881246000	-0.549553000	15.254127000
H	6.897050000	-1.729957000	15.905373000	H	6.074378000	-1.625972000	15.404649000
H	5.330766000	-0.859886000	15.842149000	H	4.809908000	-0.351281000	15.390827000
H	6.824290000	0.021373000	16.296000000	H	6.455878000	0.028599000	15.998489000
C	0.849414000	2.854347000	11.668086000	C	1.343208000	2.805405000	11.927773000
H	0.034624000	2.960818000	10.928456000	H	0.576350000	2.333563000	11.288855000
H	0.924504000	3.792096000	12.248700000	H	1.067552000	3.859348000	12.105020000
H	0.600055000	2.032159000	12.353684000	H	1.387800000	2.277185000	12.889517000
C	9.279317000	2.321088000	5.586891000	C	9.685291000	2.772203000	5.695638000
H	9.246409000	2.393532000	4.487205000	H	9.741861000	2.980617000	4.615150000
H	9.902678000	3.161306000	5.942394000	H	10.330999000	3.514391000	6.198006000
C	9.921772000	0.999531000	6.017285000	C	10.206499000	1.364280000	5.996118000
H	10.955063000	0.932208000	5.639207000	H	11.253420000	1.263949000	5.667661000
H	9.363222000	0.159328000	5.566831000	H	9.619545000	0.626398000	5.420414000
N	5.652633000	-0.424739000	9.063886000	N	5.716975000	0.337693000	9.022657000
N	4.701414000	-0.117361000	8.044592000	N	4.699164000	-0.181001000	9.878075000
H	5.101670000	0.337192000	7.205783000	H	4.048741000	-0.811812000	9.388457000
H	4.144933000	-0.926071000	7.730845000	H	5.145470000	-0.700520000	10.649506000
H	4.060566000	0.571727000	8.478540000	H	5.253749000	0.599174000	8.147827000
H	6.322681000	-1.079198000	8.654837000	H	4.158790000	0.577634000	10.346783000
³ VIII				⁵ VIII			
Fe	6.595150000	1.521284000	10.005548000	Fe	6.884078000	2.434261000	10.484342000
Cl	7.674242000	3.324781000	10.972056000	Cl	8.167013000	4.199058000	11.126557000
O	6.650021000	0.593543000	11.642401000	O	6.955493000	1.246859000	11.978934000
O	4.892028000	2.172021000	10.483849000	O	5.031567000	2.872940000	10.607518000
N	6.635770000	2.534186000	8.352295000	N	6.730387000	2.947274000	8.434081000

O	2.563645000	2.651752000	11.564807000	O	2.592696000	3.103081000	11.560049000
O	6.320850000	-0.028075000	14.158584000	O	6.651778000	0.368404000	14.440715000
N	8.327497000	0.847737000	9.475009000	N	8.311047000	1.123265000	9.554690000
C	7.700960000	0.175394000	12.265768000	C	7.795692000	0.343049000	12.387849000
C	7.558412000	-0.190434000	13.656951000	C	7.669188000	-0.164012000	13.728084000
C	8.658105000	-0.658168000	14.371383000	C	8.561035000	-1.123770000	14.198247000
H	8.554287000	-0.924600000	15.423506000	H	8.470132000	-1.502275000	15.216938000
C	9.917577000	-0.794501000	13.750628000	C	9.593211000	-1.621315000	13.371524000
H	10.762228000	-1.166507000	14.334802000	H	10.278388000	-2.374519000	13.767159000
C	10.081741000	-0.465075000	12.415272000	C	9.728021000	-1.160286000	12.076457000
H	11.053564000	-0.579374000	11.928729000	H	10.518935000	-1.544962000	11.427319000
C	8.992262000	0.029082000	11.660260000	C	8.840159000	-0.175349000	11.565006000
C	4.431415000	3.547679000	8.553438000	C	4.346964000	3.455577000	8.375936000
C	4.104245000	2.954304000	9.814407000	C	4.097217000	3.211629000	9.758632000
C	5.702079000	3.316618000	7.918295000	C	5.670715000	3.325101000	7.801863000
H	5.874442000	3.874071000	6.990183000	H	5.736488000	3.572412000	6.733325000
C	9.200108000	0.317122000	10.265046000	C	9.006160000	0.233563000	10.190954000
H	10.183894000	0.047828000	9.863773000	H	9.798998000	-0.303857000	9.652954000
C	7.968946000	2.471271000	7.721518000	C	8.039918000	2.798689000	7.799211000
H	8.582097000	3.213455000	8.260894000	H	8.706828000	3.489567000	8.345783000
C	2.808821000	3.246892000	10.380727000	C	2.751140000	3.351060000	10.240776000
C	8.558157000	1.084734000	8.042393000	C	8.532482000	1.367953000	8.116135000
H	7.939421000	0.342260000	7.507730000	H	7.867033000	0.672694000	7.569517000
C	8.021828000	2.757588000	6.220357000	C	8.133385000	3.103355000	6.305427000
H	7.355478000	2.049338000	5.697107000	H	7.460617000	2.427233000	5.748604000
H	7.654343000	3.772988000	6.010557000	H	7.795264000	4.133944000	6.112560000
C	3.503424000	4.398679000	7.898034000	C	3.282985000	3.828470000	7.513808000
H	3.781990000	4.840748000	6.938185000	H	3.500262000	4.012355000	6.458233000
C	2.271962000	4.661921000	8.466665000	C	1.995073000	3.953830000	8.001244000
H	1.557354000	5.316931000	7.963458000	H	1.175248000	4.238819000	7.337931000
C	9.996513000	0.959519000	7.544563000	C	9.966601000	1.165211000	7.612455000
H	10.380547000	-0.052359000	7.745557000	H	10.286991000	0.124971000	7.773146000
H	10.634355000	1.673033000	8.094483000	H	10.638834000	1.810826000	8.204446000
C	1.924863000	4.085286000	9.708520000	C	1.728584000	3.713689000	9.365859000
H	0.948310000	4.306312000	10.140473000	H	0.706567000	3.816747000	9.732080000
C	6.079195000	-0.341095000	15.521994000	C	6.445918000	-0.067389000	15.773237000
H	6.278327000	-1.405936000	15.736164000	H	6.228889000	-1.149792000	15.821738000
H	5.016769000	-0.130144000	15.704064000	H	5.576839000	0.488107000	16.151986000
H	6.691913000	0.282456000	16.196655000	H	7.318346000	0.150512000	16.415242000
C	1.325198000	2.891733000	12.213389000	C	1.300868000	3.220160000	12.130467000
H	0.471233000	2.548754000	11.602374000	H	0.585529000	2.511658000	11.675104000
H	1.189747000	3.962072000	12.450240000	H	0.899983000	4.244976000	12.031034000
H	1.348920000	2.317730000	13.149734000	H	1.408568000	2.981156000	13.197546000
C	9.459853000	2.618455000	5.703936000	C	9.573248000	2.914739000	5.815192000
H	9.476818000	2.789648000	4.615614000	H	9.628018000	3.117352000	4.733357000
H	10.082126000	3.408194000	6.161033000	H	10.225222000	3.654799000	6.312418000
C	10.056044000	1.249109000	6.039118000	C	10.080726000	1.503461000	6.120942000
H	11.100839000	1.190192000	5.694524000	H	11.128955000	1.391856000	5.799509000
H	9.497274000	0.464268000	5.498691000	H	9.491039000	0.771735000	5.539699000
N	5.811502000	0.004114000	9.162343000	N	5.741320000	-0.529804000	9.609970000
N	4.957296000	0.169353000	8.031692000	N	5.029435000	-0.195447000	8.425693000
H	4.506062000	-0.724350000	7.779279000	H	4.629317000	-1.045651000	7.979155000
H	4.190894000	0.818890000	8.260203000	H	4.242744000	0.435953000	8.648348000
H	6.467673000	-0.742619000	8.920645000	H	6.593770000	-1.005703000	9.266030000
H	5.422677000	0.530428000	7.179138000	H	5.621381000	0.262294000	7.706030000
¹ IX				³ IX			
Fe	6.607543000	1.580687000	10.020447000	Fe	6.716442000	1.785537000	10.022969000
Cl	7.712258000	3.397902000	11.035962000	Cl	7.974440000	3.466377000	11.036405000
O	6.687400000	0.597864000	11.712523000	O	6.679245000	0.742983000	11.613881000
O	4.866292000	2.308201000	10.510952000	O	5.044394000	2.566256000	10.550393000
N	6.647550000	2.584373000	8.356511000	N	6.777303000	2.737667000	8.340863000
O	2.506883000	2.812594000	11.526411000	O	2.602582000	2.728000000	11.434652000
O	6.419204000	-0.148235000	14.207607000	O	6.335751000	-0.014935000	14.096044000
N	8.351192000	0.889498000	9.483001000	N	8.351966000	0.954239000	9.411156000
C	7.746080000	0.134532000	12.277437000	C	7.700589000	0.197185000	12.187765000
C	7.652221000	-0.300035000	13.657947000	C	7.556799000	-0.248447000	13.555444000

C	8.755217000	-0.817240000	14.323173000	C	8.617566000	-0.851428000	14.218971000
H	8.668496000	-1.130093000	15.364784000	H	8.504423000	-1.170147000	15.255961000
C	10.006062000	-0.948125000	13.669363000	C	9.857244000	-1.062683000	13.567431000
H	10.858719000	-1.359477000	14.214916000	H	10.674248000	-1.541869000	14.112058000
C	10.128464000	-0.559577000	12.351410000	C	10.019858000	-0.669104000	12.255346000
H	11.084303000	-0.663704000	11.829079000	H	10.968066000	-0.837805000	11.733267000
C	9.022137000	-0.014704000	11.640362000	C	8.960784000	-0.032352000	11.549361000
C	4.378928000	3.474177000	8.452815000	C	4.484319000	3.554986000	8.415724000
C	4.067519000	2.989674000	9.768396000	C	4.188295000	3.104213000	9.740808000
C	5.679159000	3.274212000	7.854414000	C	5.791948000	3.395145000	7.826872000
H	5.830069000	3.777848000	6.891250000	H	5.933258000	3.887048000	6.856203000
C	9.217326000	0.320827000	10.251164000	C	9.174128000	0.299626000	10.163948000
H	10.194640000	-0.043676000	9.835740000	H	10.116616000	-0.060105000	9.733267000
C	7.987547000	2.537393000	7.750129000	C	8.104644000	2.651883000	7.723757000
H	8.589797000	3.262510000	8.325940000	H	8.751398000	3.320185000	8.319053000
C	2.744075000	3.294552000	10.280861000	C	2.829219000	3.256630000	10.205163000
C	8.577591000	1.143981000	8.054324000	C	8.597229000	1.213627000	7.985628000
H	7.954984000	0.410637000	7.506857000	H	7.923781000	0.539537000	7.422967000
C	8.075879000	2.870853000	6.260120000	C	8.208046000	3.024176000	6.245914000
H	7.417222000	2.184741000	5.698289000	H	7.510080000	2.396410000	5.663994000
H	7.714570000	3.894160000	6.075539000	H	7.909019000	4.073204000	6.095431000
C	3.415463000	4.214657000	7.707236000	C	3.480040000	4.196968000	7.637252000
H	3.691276000	4.573568000	6.711342000	H	3.741395000	4.551607000	6.636206000
C	2.167270000	4.481350000	8.226590000	C	2.199930000	4.360122000	8.125809000
H	1.431374000	5.049991000	7.653225000	H	1.430943000	4.849927000	7.523794000
C	10.017077000	1.024328000	7.552536000	C	10.024794000	1.007707000	7.479802000
H	10.397488000	0.006346000	7.730196000	H	10.332808000	-0.040087000	7.620409000
H	10.657142000	1.718385000	8.125084000	H	10.710426000	1.635549000	8.075517000
C	1.833268000	4.016824000	9.524289000	C	1.870530000	3.876493000	9.415145000
H	0.842792000	4.236461000	9.925300000	H	0.849105000	3.990676000	9.780447000
C	6.221959000	-0.526095000	15.553986000	C	6.097553000	-0.398125000	15.436380000
H	6.414627000	-1.603158000	15.715629000	H	6.212812000	-1.488073000	15.581483000
H	5.168676000	-0.316255000	15.789325000	H	5.059231000	-0.117587000	15.663016000
H	6.862570000	0.052310000	16.245520000	H	6.770074000	0.124891000	16.140896000
C	1.253115000	3.064873000	12.127935000	C	1.296829000	2.795364000	11.976108000
H	0.420082000	2.624314000	11.549345000	H	0.560509000	2.267618000	11.342610000
H	1.063316000	4.147343000	12.249823000	H	0.962144000	3.839583000	12.113586000
H	1.281009000	2.595916000	13.121787000	H	1.339021000	2.303534000	12.958083000
C	9.519727000	2.740727000	5.759669000	C	9.642293000	2.815787000	5.743108000
H	9.556836000	2.950251000	4.678136000	H	9.696553000	3.055519000	4.668718000
H	10.142760000	3.507500000	6.254072000	H	10.312958000	3.523950000	6.261900000
C	10.096651000	1.354880000	6.057310000	C	10.126169000	1.385218000	5.996109000
H	11.143866000	1.292455000	5.719217000	H	11.167451000	1.265427000	5.655470000
H	9.532738000	0.594536000	5.487303000	H	9.514488000	0.683184000	5.401284000
N	5.806608000	0.178767000	9.277277000	N	5.609113000	0.370547000	9.171437000
N	4.784419000	0.121521000	8.500392000	N	4.484561000	-0.032461000	9.740461000
H	4.318167000	0.991139000	8.232847000	H	4.187616000	0.539569000	10.533423000
H	6.167843000	-0.764241000	9.484762000	H	5.993760000	-0.348496000	8.553471000
H	4.424674000	-0.776084000	8.169086000	H	4.245334000	-1.024137000	9.740533000
⁵ IX				² X			
Fe	6.797431000	1.959875000	10.123834000	Fe	6.676400000	1.741711000	9.999414000
Cl	8.105147000	3.801602000	11.015264000	Cl	7.826209000	3.451658000	11.019978000
O	6.780358000	0.981988000	11.749811000	O	6.607552000	0.681598000	11.546979000
O	5.032746000	2.577951000	10.532660000	O	4.970660000	2.546287000	10.531838000
N	6.799049000	2.819221000	8.365383000	N	6.724370000	2.690219000	8.305903000
O	2.568793000	2.659607000	11.360619000	O	2.651671000	3.082742000	11.568944000
O	6.448214000	0.186396000	14.214538000	O	6.186787000	-0.142828000	13.991217000
N	8.391812000	1.017911000	9.458504000	N	8.340237000	0.974088000	9.424877000
C	7.752215000	0.287093000	12.256572000	C	7.638919000	0.179897000	12.172118000
C	7.609863000	-0.172483000	13.617154000	C	7.446110000	-0.288319000	13.517465000
C	8.614848000	-0.919592000	14.221830000	C	8.510156000	-0.836096000	14.227778000
H	8.500101000	-1.255400000	15.253080000	H	8.366368000	-1.175042000	15.254294000
C	9.794639000	-1.255787000	13.518550000	C	9.786284000	-0.964274000	13.634704000
H	10.568018000	-1.844402000	14.017384000	H	10.603912000	-1.399455000	14.213947000
C	9.954888000	-0.843354000	12.211451000	C	9.989284000	-0.553123000	12.331778000
H	10.857254000	-1.104711000	11.651905000	H	10.967182000	-0.666212000	11.856403000

C	8.951026000	-0.070723000	11.564036000	C	8.928221000	0.025521000	11.584895000
C	4.487234000	3.584878000	8.398991000	C	4.409479000	3.441755000	8.371436000
C	4.178034000	3.112282000	9.710043000	C	4.141191000	3.092090000	9.759005000
C	5.801718000	3.431801000	7.822882000	C	5.721342000	3.281517000	7.762838000
H	5.930637000	3.875805000	6.827620000	H	5.831401000	3.737893000	6.772024000
C	9.167929000	0.283488000	10.182434000	C	9.169592000	0.363024000	10.203171000
H	10.075959000	-0.135058000	9.729903000	H	10.136823000	0.042534000	9.798908000
C	8.125585000	2.702431000	7.740606000	C	8.060835000	2.633059000	7.700428000
H	8.779281000	3.379376000	8.317326000	H	8.668097000	3.337601000	8.295428000
C	2.809045000	3.212975000	10.145895000	C	2.806586000	3.407532000	10.300378000
C	8.610832000	1.265423000	8.023026000	C	8.600824000	1.220137000	7.998540000
H	7.921010000	0.587369000	7.486206000	H	7.965493000	0.507234000	7.441507000
C	8.218957000	3.048866000	6.255972000	C	8.166833000	2.984428000	6.219241000
H	7.515633000	2.413781000	5.688675000	H	7.502024000	2.319297000	5.640467000
H	7.921878000	4.096407000	6.091898000	H	7.830580000	4.018924000	6.048676000
C	3.484530000	4.204305000	7.603119000	C	3.403155000	4.030914000	7.614921000
H	3.756334000	4.572016000	6.609904000	H	3.607639000	4.309722000	6.578479000
C	2.190623000	4.328982000	8.068771000	C	2.123771000	4.284586000	8.157508000
H	1.421062000	4.805551000	7.457205000	H	1.357466000	4.738197000	7.525419000
C	10.030622000	1.038293000	7.502465000	C	10.044286000	1.064909000	7.521738000
H	10.327567000	-0.011610000	7.649547000	H	10.389900000	0.032789000	7.686547000
H	10.728041000	1.663516000	8.087262000	H	10.693013000	1.731244000	8.116469000
C	1.849813000	3.820186000	9.342800000	C	1.824452000	3.983021000	9.483588000
H	0.818916000	3.902718000	9.689284000	H	0.832885000	4.200748000	9.879566000
C	6.214320000	-0.212558000	15.551675000	C	5.897509000	-0.569476000	15.310722000
H	6.202544000	-1.312810000	15.658158000	H	6.075757000	-1.652295000	15.440734000
H	5.225995000	0.181420000	15.827370000	H	4.831983000	-0.360496000	15.479534000
H	6.969454000	0.202272000	16.244154000	H	6.493759000	-0.018268000	16.060145000
C	1.248821000	2.681567000	11.872840000	C	1.403980000	3.318815000	12.233097000
H	0.542745000	2.145224000	11.213077000	H	0.595092000	2.743341000	11.755608000
H	0.883432000	3.713815000	12.020538000	H	1.156604000	4.392222000	12.225553000
H	1.283097000	2.173418000	12.846612000	H	1.544342000	2.976493000	13.265496000
C	9.648696000	2.827402000	5.746628000	C	9.616336000	2.822691000	5.742689000
H	9.696611000	3.053803000	4.669123000	H	9.675833000	3.042404000	4.664651000
H	10.326738000	3.537759000	6.252537000	H	10.249539000	3.567998000	6.256036000
C	10.123801000	1.397005000	6.013850000	C	10.152572000	1.418089000	6.032341000
H	11.161794000	1.264601000	5.667960000	H	11.203209000	1.334534000	5.711136000
H	9.502450000	0.692301000	5.432459000	H	9.579732000	0.679822000	5.443062000
N	5.616270000	0.168436000	9.221381000	N	5.608250000	0.364102000	9.051749000
N	4.405703000	-0.067610000	9.720296000	N	5.171777000	-0.708435000	9.680569000
H	4.154473000	0.537698000	10.503515000	H	5.345300000	-0.712881000	10.688614000
H	5.878249000	-0.584461000	8.578367000	H	5.611614000	0.236284000	8.036527000
H	4.019286000	-1.011937000	9.711993000	H	5.060944000	-1.590159000	9.179864000
⁴X				⁶X			
Fe	6.966920000	2.091182000	10.291883000	Fe	6.901975000	2.177530000	10.132211000
Cl	8.030351000	3.966272000	11.113972000	Cl	7.978758000	3.843226000	11.195128000
O	6.935836000	1.089205000	11.864142000	O	6.788304000	0.747595000	11.470327000
O	5.056059000	2.295572000	10.496053000	O	5.006029000	2.443933000	10.167443000
N	6.864698000	2.798625000	8.475221000	O	6.867631000	2.939285000	8.181112000
O	2.584324000	2.361929000	11.344926000	N	2.519105000	2.539162000	10.981928000
O	6.683764000	0.444921000	14.390278000	O	6.431218000	-0.286022000	13.860581000
N	8.418535000	0.985736000	9.545245000	N	8.460630000	1.072514000	9.237310000
C	7.886996000	0.353168000	12.371183000	C	7.756766000	-0.022316000	11.940199000
C	7.776443000	-0.030286000	13.752766000	C	7.599139000	-0.599456000	13.234518000
C	8.755392000	-0.831487000	14.334503000	C	8.595798000	-1.410158000	13.771870000
H	8.672493000	-1.117579000	15.383458000	H	8.474888000	-1.840976000	14.766121000
C	9.866080000	-1.284489000	13.587815000	C	9.765246000	-1.683233000	13.036990000
H	10.616939000	-1.911933000	14.073227000	H	10.534818000	-2.323915000	13.472720000
C	9.993818000	-0.935621000	12.258583000	C	9.930777000	-1.147547000	11.771453000
H	10.844450000	-1.282898000	11.666675000	H	10.831936000	-1.362061000	11.191616000
C	9.016506000	-0.111785000	11.636348000	C	8.940632000	-0.304458000	11.206155000
C	4.529089000	3.497300000	8.474335000	C	4.493887000	3.481660000	8.052977000
C	4.204846000	2.920888000	9.742784000	C	4.141545000	2.979181000	9.336617000
C	5.849931000	3.360143000	7.906491000	C	5.851415000	3.419618000	7.547741000
H	5.967278000	3.762827000	6.893557000	H	5.986299000	3.827574000	6.536980000
C	9.175833000	0.197804000	10.241411000	C	9.175349000	0.200109000	9.866132000

H	10.019543000	-0.294977000	9.743361000	H	10.051588000	-0.234032000	9.366398000
C	8.176307000	2.652517000	7.821504000	C	8.224382000	2.887645000	7.625525000
H	8.856955000	3.311002000	8.388814000	H	8.832406000	3.539472000	8.279259000
C	2.832156000	2.978369000	10.177589000	C	2.775305000	3.058757000	9.744618000
C	8.614417000	1.202598000	8.096386000	C	8.738032000	1.444204000	7.835338000
H	7.890027000	0.544495000	7.581237000	H	8.102344000	0.787962000	7.212516000
C	8.253677000	3.002786000	6.338702000	C	8.398450000	3.343322000	6.178268000
H	7.525844000	2.389474000	5.779074000	H	7.765827000	2.721720000	5.520469000
H	7.984209000	4.059448000	6.185515000	H	8.058705000	4.385661000	6.072472000
C	3.540072000	4.164075000	7.714938000	C	3.496523000	4.051919000	7.223068000
H	3.816992000	4.605249000	6.754486000	H	3.784709000	4.431935000	6.239584000
C	2.236665000	4.243195000	8.180934000	C	2.180773000	4.126786000	7.647654000
H	1.472712000	4.760449000	7.596451000	H	1.415706000	4.569282000	7.006249000
C	10.016217000	0.926329000	7.552679000	C	10.195192000	1.305395000	7.384448000
H	10.275959000	-0.134708000	7.687747000	H	10.519570000	0.256747000	7.461966000
H	10.743951000	1.522583000	8.130283000	H	10.831135000	1.898066000	8.065410000
C	1.879237000	3.642946000	9.401711000	C	1.815739000	3.626208000	8.913446000
H	0.844637000	3.700145000	9.740681000	H	0.775755000	3.687029000	9.235354000
C	6.490494000	0.120137000	15.756025000	C	6.269073000	-0.625555000	15.236006000
H	6.393221000	-0.969926000	15.908611000	H	6.240703000	-1.718392000	15.383080000
H	5.554838000	0.607908000	16.062410000	H	5.308206000	-0.193999000	15.548585000
H	7.314670000	0.497029000	16.388215000	H	7.077982000	-0.193398000	15.848645000
C	1.257784000	2.344489000	11.854458000	C	1.180267000	2.511524000	11.476345000
H	0.563268000	1.840980000	11.159481000	H	0.520463000	1.936903000	10.805342000
H	0.888857000	3.364497000	12.059148000	H	0.783844000	3.532426000	11.601175000
H	1.296986000	1.780428000	12.795895000	H	1.227030000	2.015136000	12.454635000
C	9.669269000	2.738187000	5.810833000	C	9.865537000	3.218017000	5.752246000
H	9.709347000	2.968527000	4.734168000	H	9.974041000	3.531150000	4.701367000
H	10.376430000	3.423167000	6.311293000	H	10.479912000	3.908701000	6.356931000
C	10.097938000	1.290848000	6.064450000	C	10.374727000	1.787225000	5.939846000
H	11.125803000	1.124733000	5.704057000	H	11.438247000	1.715579000	5.660281000
H	9.444891000	0.611003000	5.488521000	H	9.821377000	1.112433000	5.262416000
N	4.613796000	-0.009614000	9.416633000	N	3.641072000	-0.049626000	12.915434000
N	3.817966000	0.444550000	8.578506000	N	4.250478000	0.782217000	12.255228000
H	2.811412000	0.426679000	8.796496000	H	3.694796000	1.541482000	11.781355000
H	5.578328000	0.059809000	9.045878000	H	4.323908000	-0.740351000	13.287016000
H	4.100667000	0.837415000	7.664919000	H	5.316170000	0.745518000	12.080837000
²XI				⁴XI			
Fe	6.608217000	1.542552000	9.972739000	Fe	6.685895000	1.808630000	10.187069000
Cl	7.620877000	3.404840000	10.990292000	Cl	7.952468000	3.709123000	11.034993000
O	6.641751000	0.574988000	11.628733000	O	6.720737000	0.853690000	11.822362000
O	4.871892000	2.180536000	10.456183000	O	4.902857000	2.374909000	10.592395000
N	6.643762000	2.515822000	8.300354000	N	6.660289000	2.665493000	8.425350000
O	2.570259000	2.760527000	11.550643000	O	2.512212000	2.759814000	11.572892000
O	6.307395000	-0.169533000	14.112682000	O	6.479127000	0.175096000	14.336463000
N	8.361679000	0.918543000	9.463197000	N	8.306003000	0.909307000	9.521570000
C	7.698970000	0.157711000	12.238438000	C	7.732564000	0.228127000	12.343025000
C	7.563792000	-0.273222000	13.614401000	C	7.637762000	-0.171301000	13.726384000
C	8.662888000	-0.736710000	14.324014000	C	8.682807000	-0.853997000	14.339716000
H	8.551594000	-1.046410000	15.363995000	H	8.602473000	-1.146766000	15.387209000
C	9.940994000	-0.817667000	13.716925000	C	9.859486000	-1.177696000	13.625559000
H	10.788177000	-1.189065000	14.298392000	H	10.664348000	-1.715444000	14.131966000
C	10.101299000	-0.435139000	12.402284000	C	9.978652000	-0.814295000	12.299674000
H	11.079153000	-0.504890000	11.917386000	H	10.880290000	-1.062110000	11.732931000
C	9.000494000	0.060391000	11.646674000	C	8.933112000	-0.107509000	11.643249000
C	4.421871000	3.509558000	8.488200000	C	4.373230000	3.504481000	8.518505000
C	4.100914000	2.966358000	9.773232000	C	4.071267000	3.013777000	9.827614000
C	5.690748000	3.262182000	7.848830000	C	5.668833000	3.318497000	7.912968000
H	5.847809000	3.797585000	6.904339000	H	5.795020000	3.780786000	6.925947000
C	9.222348000	0.377730000	10.260860000	C	9.116241000	0.216579000	10.250130000
H	10.211127000	0.110567000	9.867614000	H	10.032819000	-0.179197000	9.794714000
C	7.975579000	2.475289000	7.674367000	C	7.983282000	2.564740000	7.784283000
H	8.570938000	3.237050000	8.208983000	H	8.625248000	3.268356000	8.342088000
C	2.814769000	3.311197000	10.337996000	C	2.740295000	3.252679000	10.332995000
C	8.587519000	1.108878000	8.028460000	C	8.512023000	1.147135000	8.082411000
H	7.971317000	0.340751000	7.522479000	H	7.849744000	0.436952000	7.553173000

C	8.033822000	2.742238000	6.169863000	C	8.048349000	2.886587000	6.292232000
H	7.378759000	2.018764000	5.652948000	H	7.354580000	2.221975000	5.747140000
H	7.653501000	3.749539000	5.942343000	H	7.721884000	3.922270000	6.111163000
C	3.495248000	4.353955000	7.812047000	C	3.391083000	4.205931000	7.764288000
H	3.772493000	4.756577000	6.833887000	H	3.657244000	4.571409000	6.768802000
C	2.276864000	4.662478000	8.378663000	C	2.128929000	4.420165000	8.278075000
H	1.568164000	5.311918000	7.859519000	H	1.374345000	4.958277000	7.699820000
C	10.025335000	0.988202000	7.525719000	C	9.936046000	0.959794000	7.556935000
H	10.422910000	-0.014777000	7.745262000	H	10.270499000	-0.075923000	7.722100000
H	10.657844000	1.718031000	8.060954000	H	10.615551000	1.620761000	8.123089000
C	1.936611000	4.136999000	9.648824000	C	1.804199000	3.939744000	9.567878000
H	0.969378000	4.390174000	10.084720000	H	0.802291000	4.116134000	9.961040000
C	6.071360000	-0.551697000	15.453375000	C	6.295298000	-0.162002000	15.698165000
H	6.303421000	-1.618816000	15.625927000	H	6.323592000	-1.255079000	15.860426000
H	5.001458000	-0.385929000	15.643357000	H	5.302094000	0.213394000	15.982080000
H	6.658448000	0.056754000	16.165746000	H	7.054673000	0.312194000	16.346572000
C	1.345198000	3.048350000	12.197292000	C	1.237255000	2.943873000	12.158886000
H	0.476373000	2.700771000	11.608733000	H	0.437652000	2.464170000	11.565297000
H	1.228454000	4.129391000	12.396118000	H	0.992068000	4.014297000	12.284418000
H	1.363133000	2.510537000	13.155629000	H	1.277236000	2.470067000	13.149717000
C	9.474581000	2.611697000	5.658936000	C	9.477651000	2.697444000	5.768325000
H	9.495082000	2.768307000	4.568149000	H	9.504279000	2.901508000	4.685640000
H	10.088477000	3.413280000	6.107304000	H	10.138362000	3.440494000	6.249478000
C	10.082729000	1.252699000	6.015693000	C	10.003504000	1.290043000	6.060420000
H	11.127477000	1.196316000	5.669430000	H	11.042061000	1.185862000	5.706787000
H	9.529163000	0.455296000	5.488049000	H	9.401358000	0.552171000	5.500327000
N	5.859304000	0.036415000	9.133234000	N	5.511979000	0.041854000	9.240433000
N	4.717647000	0.008368000	8.678733000	N	5.069614000	0.070410000	8.106203000
H	4.351546000	-0.848459000	8.231603000	H	4.388522000	-0.631769000	7.748458000
H	4.063583000	0.811678000	8.726036000	H	5.335209000	0.793565000	7.398953000
⁶ XI				¹ XII			
Fe	6.857318000	2.038242000	10.319435000	Fe	6.692779000	1.672736000	9.958929000
Cl	8.033977000	3.862517000	11.181755000	Cl	7.821409000	3.407868000	11.018615000
O	6.811705000	0.976821000	11.866277000	O	6.665784000	0.673035000	11.541264000
O	5.011829000	2.397283000	10.613430000	O	5.004942000	2.364946000	10.460201000
N	6.769235000	2.769912000	8.517012000	N	6.724029000	2.629217000	8.301654000
O	2.584645000	2.643063000	11.567365000	O	2.651721000	2.747934000	11.505758000
O	6.535618000	0.311246000	14.386535000	O	6.209059000	-0.155787000	13.972588000
N	8.359424000	0.984696000	9.592999000	N	8.369681000	0.956808000	9.420979000
C	7.795941000	0.308941000	12.399065000	C	7.671383000	0.207766000	12.170919000
C	7.678501000	-0.082243000	13.779250000	C	7.462464000	-0.271406000	13.531904000
C	8.698590000	-0.804841000	14.391253000	C	8.536713000	-0.766227000	14.262255000
H	8.610556000	-1.091161000	15.439807000	H	8.396785000	-1.106003000	15.288295000
C	9.859091000	-1.176576000	13.675098000	C	9.818413000	-0.838038000	13.681058000
H	10.642180000	-1.744418000	14.182676000	H	10.644031000	-1.237456000	14.274427000
C	9.993035000	-0.824421000	12.347073000	C	10.045516000	-0.427181000	12.372017000
H	10.881284000	-1.111435000	11.778254000	H	11.039454000	-0.520336000	11.928712000
C	8.975664000	-0.074975000	11.696305000	C	8.998129000	0.105613000	11.598987000
C	4.440995000	3.487133000	8.537563000	C	4.456224000	3.499014000	8.408168000
C	4.148554000	2.989666000	9.843644000	C	4.168457000	3.016046000	9.734753000
C	5.745195000	3.325733000	7.953631000	C	5.740627000	3.296942000	7.789917000
H	5.851837000	3.709547000	6.932301000	H	5.878146000	3.784661000	6.818340000
C	9.142456000	0.235961000	10.300411000	C	9.236567000	0.412422000	10.214011000
H	10.014182000	-0.222353000	9.817397000	H	10.221633000	0.130242000	9.826638000
C	8.075527000	2.628032000	7.852596000	C	8.049888000	2.574696000	7.675241000
H	8.754974000	3.307379000	8.396752000	H	8.662746000	3.297956000	8.242283000
C	2.799974000	3.144115000	10.329984000	C	2.851266000	3.273265000	10.289273000
C	8.544179000	1.190798000	8.144137000	C	8.616065000	1.173284000	7.993297000
H	7.826357000	0.512985000	7.648056000	H	7.968395000	0.445838000	7.471023000
C	8.127326000	2.944434000	6.360001000	C	8.130065000	2.889008000	6.182857000
H	7.402538000	2.302781000	5.828636000	H	7.456057000	2.207905000	5.634521000
H	7.835056000	3.991285000	6.183117000	H	7.789996000	3.917996000	5.990289000
C	3.429758000	4.114715000	7.756681000	C	3.476010000	4.229982000	7.703202000
H	3.687129000	4.479765000	6.758994000	H	3.711518000	4.603607000	6.703908000
C	2.150854000	4.254329000	8.253010000	C	2.232186000	4.472196000	8.268914000
H	1.371579000	4.736963000	7.658883000	H	1.480237000	5.037288000	7.713613000

C	9.946270000	0.932276000	7.593075000	C	10.050948000	1.015972000	7.496990000
H	10.230641000	-0.119757000	7.748505000	H	10.407946000	-0.008460000	7.684225000
H	10.668722000	1.555961000	8.148419000	H	10.706064000	1.704542000	8.058507000
C	1.836583000	3.765751000	9.543010000	C	1.914923000	3.993557000	9.556936000
H	0.819165000	3.882016000	9.918021000	H	0.925942000	4.190858000	9.970726000
C	6.332785000	-0.021111000	15.747991000	C	5.896029000	-0.544425000	15.307681000
H	6.317777000	-1.114689000	15.906731000	H	6.097008000	-1.617121000	15.468402000
H	5.353827000	0.392615000	16.027481000	H	4.824063000	-0.349324000	15.439620000
H	7.107520000	0.422515000	16.399448000	H	6.470243000	0.049097000	16.039156000
C	1.285357000	2.728791000	12.123989000	C	1.393005000	2.929670000	12.144468000
H	0.539670000	2.190153000	11.511229000	H	0.575086000	2.482317000	11.553898000
H	0.957113000	3.777255000	12.243129000	H	1.178387000	3.999153000	12.311029000
H	1.338900000	2.257938000	13.115449000	H	1.463221000	2.418330000	13.113451000
C	9.539807000	2.696071000	5.816276000	C	9.571389000	2.721934000	5.683243000
H	9.560064000	2.902259000	4.733960000	H	9.608272000	2.915003000	4.599113000
H	10.239972000	3.406999000	6.290125000	H	10.209476000	3.484015000	6.165111000
C	10.003785000	1.264481000	6.096349000	C	10.124449000	1.329161000	5.996687000
H	11.030456000	1.112547000	5.725821000	H	11.168281000	1.244629000	5.654431000
H	9.358030000	0.558023000	5.544707000	H	9.543822000	0.571376000	5.440874000
N	5.328409000	-0.267408000	8.419070000	N	5.799797000	0.234346000	9.022861000
N	4.583635000	0.304809000	7.487224000	N	4.679078000	-0.101710000	9.387850000
H	3.970774000	1.060078000	7.828074000	H	4.178899000	0.378807000	10.165056000
H	4.060161000	-0.354017000	6.893316000	H	4.191788000	-0.898087000	8.941658000
³ XII				⁵ XII			
Fe	6.625710000	1.625882000	9.945720000	Fe	6.797473000	1.973730000	10.140623000
Cl	7.664773000	3.417172000	10.955938000	Cl	7.838575000	3.820470000	11.134041000
O	6.654325000	0.660072000	11.632001000	O	6.717070000	0.856223000	11.644527000
O	4.881924000	2.155593000	10.365307000	O	4.885112000	2.601975000	10.522727000
N	6.688096000	2.618413000	8.284856000	N	6.768720000	2.818179000	8.366389000
O	2.510801000	2.550794000	11.354086000	O	2.470507000	2.991048000	11.402514000
O	6.297056000	-0.089647000	14.092632000	O	6.329145000	-0.006214000	14.074370000
N	8.378458000	0.931011000	9.421301000	N	8.374058000	1.014619000	9.437051000
C	7.676140000	0.204166000	12.220763000	C	7.721871000	0.210966000	12.198416000
C	7.519183000	-0.231346000	13.614155000	C	7.540128000	-0.271067000	13.534927000
C	8.617396000	-0.730802000	14.330820000	C	8.569965000	-0.959939000	14.173861000
H	8.503023000	-1.042899000	15.368561000	H	8.436830000	-1.314873000	15.196342000
C	9.857809000	-0.830250000	13.708850000	C	9.791182000	-1.210773000	13.513878000
H	10.709438000	-1.221385000	14.269333000	H	10.581462000	-1.752562000	14.038230000
C	10.035382000	-0.446811000	12.360392000	C	9.976759000	-0.783192000	12.212686000
H	11.017009000	-0.564266000	11.895265000	H	10.910560000	-0.988867000	11.683570000
C	8.986133000	0.070053000	11.610522000	C	8.951665000	-0.067769000	11.539549000
C	4.480355000	3.626037000	8.480019000	C	4.420172000	3.512290000	8.347274000
C	4.114201000	2.988312000	9.696424000	C	4.080515000	3.127235000	9.706270000
C	5.762977000	3.399684000	7.848822000	C	5.753461000	3.351710000	7.786391000
H	5.940009000	3.967420000	6.927483000	H	5.865260000	3.743143000	6.768573000
C	9.228208000	0.381897000	10.208871000	C	9.167681000	0.294415000	10.158356000
H	10.218704000	0.099620000	9.832323000	H	10.082866000	-0.104955000	9.704324000
C	8.022658000	2.543690000	7.660455000	C	8.098557000	2.711979000	7.736635000
H	8.638467000	3.284956000	8.199141000	H	8.745271000	3.383216000	8.328376000
C	2.803260000	3.234692000	10.223834000	C	2.700188000	3.367663000	10.160625000
C	8.603314000	1.154859000	7.988643000	C	8.582906000	1.270745000	7.999400000
H	7.963343000	0.410138000	7.480988000	H	7.887794000	0.596472000	7.466414000
C	8.086072000	2.824489000	6.158280000	C	8.191367000	3.084062000	6.259523000
H	7.413136000	2.122445000	5.635557000	H	7.492411000	2.454838000	5.681147000
H	7.729807000	3.843258000	5.945124000	H	7.891379000	4.133848000	6.115461000
C	3.575904000	4.511586000	7.839256000	C	3.443906000	4.083290000	7.539129000
H	3.884723000	4.996144000	6.909488000	H	3.699825000	4.378769000	6.518870000
C	2.326487000	4.755143000	8.380570000	C	2.125522000	4.292575000	8.006018000
H	1.631860000	5.439840000	7.888792000	H	1.388216000	4.740455000	7.336709000
C	10.036725000	1.004300000	7.484984000	C	10.000571000	1.049754000	7.472364000
H	10.406001000	-0.012530000	7.689501000	H	10.292176000	-0.003765000	7.602446000
H	10.686974000	1.709962000	8.031005000	H	10.699969000	1.663814000	8.066122000
C	1.936809000	4.111260000	9.572616000	C	1.753302000	3.942357000	9.298462000
H	0.944407000	4.304050000	9.981505000	H	0.731704000	4.115818000	9.635407000
C	6.000987000	-0.447148000	15.447784000	C	6.053961000	-0.445658000	15.394133000
H	6.189570000	-1.519041000	15.618444000	H	6.116930000	-1.545187000	15.481240000

H	4.935303000	-0.230004000	15.589200000	H	5.026738000	-0.127590000	15.619433000
H	6.600473000	0.154989000	16.148967000	H	6.740382000	0.011644000	16.128926000
C	1.238101000	2.724735000	11.953512000	C	1.170294000	3.152311000	11.985174000
H	0.420402000	2.420663000	11.275742000	H	0.419360000	2.574643000	11.422925000
H	1.072728000	3.771276000	12.266188000	H	0.885908000	4.216138000	12.009731000
H	1.222774000	2.080051000	12.843129000	H	1.250163000	2.764426000	13.007797000
C	9.522720000	2.667284000	5.643729000	C	9.622397000	2.870893000	5.750290000
H	9.543612000	2.838472000	4.555416000	H	9.670310000	3.117879000	4.677677000
H	10.155997000	3.447928000	6.101703000	H	10.300789000	3.570118000	6.270548000
C	10.098700000	1.289267000	5.978964000	C	10.091746000	1.433993000	5.990141000
H	11.141947000	1.213403000	5.632758000	H	11.129102000	1.304193000	5.642289000
H	9.526363000	0.512669000	5.440972000	H	9.467347000	0.742225000	5.397061000
N	5.915356000	0.074002000	9.100387000	N	5.405349000	0.272311000	9.120945000
N	4.742841000	-0.224833000	9.293951000	N	5.027009000	-0.499160000	9.982734000
H	4.133018000	0.377839000	9.891818000	H	5.329165000	-0.385147000	10.982280000
H	4.338540000	-1.079075000	8.873932000	H	4.393437000	-1.300240000	9.779464000
¹ XIII				³ XIII			
Fe	6.739519000	1.990496000	10.136573000	Fe	6.739144000	1.888438000	10.200528000
Cl	8.223115000	3.539177000	11.024435000	Cl	7.941641000	3.634694000	11.091002000
O	6.742533000	1.071676000	11.856128000	O	6.727523000	0.835316000	11.779191000
O	5.087660000	2.644784000	10.581640000	O	4.952732000	2.427445000	10.583941000
N	6.752098000	2.852280000	8.429079000	N	6.711449000	2.721839000	8.440373000
O	2.667401000	2.792874000	11.568465000	O	2.558613000	2.801626000	11.570848000
O	6.457738000	0.299021000	14.337894000	O	6.424000000	0.078667000	14.270697000
N	8.267417000	1.013070000	9.480124000	N	8.346814000	0.995741000	9.537146000
C	7.676740000	0.330240000	12.318622000	C	7.746075000	0.246225000	12.329430000
C	7.571635000	-0.128807000	13.694463000	C	7.619389000	-0.194889000	13.697570000
C	8.552957000	-0.929712000	14.256635000	C	8.676422000	-0.838339000	14.330752000
H	8.464189000	-1.259401000	15.292597000	H	8.578513000	-1.157976000	15.368876000
C	9.684598000	-1.334368000	13.502103000	C	9.889984000	-1.088700000	13.647472000
H	10.443166000	-1.966202000	13.970188000	H	10.702799000	-1.598790000	14.169698000
C	9.812717000	-0.932321000	12.190134000	C	10.035595000	-0.694944000	12.333177000
H	10.676172000	-1.246257000	11.596353000	H	10.964010000	-0.893278000	11.790738000
C	8.831253000	-0.101880000	11.575966000	C	8.980040000	-0.021226000	11.658095000
C	4.430546000	3.533995000	8.445615000	C	4.412795000	3.536384000	8.507424000
C	4.177056000	3.118963000	9.796565000	C	4.112812000	3.059477000	9.821185000
C	5.746575000	3.420538000	7.856046000	C	5.708631000	3.342064000	7.907037000
H	5.852371000	3.833826000	6.846681000	H	5.828984000	3.772698000	6.905923000
C	9.018650000	0.235126000	10.191124000	C	9.166591000	0.310610000	10.268769000
H	9.891960000	-0.226073000	9.713683000	H	10.082578000	-0.081153000	9.810468000
C	8.062201000	2.710433000	7.778874000	C	8.027920000	2.623241000	7.783762000
H	8.741876000	3.359842000	8.355286000	H	8.676452000	3.331962000	8.328412000
C	2.829268000	3.225399000	10.310507000	C	2.780644000	3.288241000	10.327775000
C	8.499712000	1.254859000	8.049114000	C	8.554734000	1.209063000	8.091837000
H	7.794066000	0.604354000	7.499077000	H	7.881219000	0.498180000	7.578654000
C	8.153404000	3.065158000	6.297618000	C	8.082581000	2.930704000	6.289131000
H	7.435555000	2.450441000	5.726348000	H	7.384790000	2.261550000	5.755426000
H	7.880524000	4.120837000	6.141831000	H	7.756833000	3.965216000	6.099845000
C	3.384367000	4.074768000	7.670535000	C	3.425263000	4.223924000	7.748642000
H	3.592600000	4.399262000	6.648197000	H	3.686377000	4.581267000	6.748859000
C	2.103634000	4.180148000	8.196620000	C	2.162834000	4.434405000	8.264061000
H	1.296292000	4.594908000	7.588390000	H	1.404276000	4.963100000	7.682144000
C	9.913602000	0.994598000	7.527145000	C	9.974683000	1.010081000	7.563121000
H	10.182336000	-0.064467000	7.661096000	H	10.306620000	-0.025240000	7.735705000
H	10.627723000	1.593927000	8.118702000	H	10.660192000	1.674217000	8.118151000
C	1.820067000	3.755556000	9.508544000	C	1.840082000	3.963109000	9.558252000
H	0.802983000	3.846570000	9.889697000	H	0.837436000	4.137780000	9.950143000
C	6.259307000	-0.081516000	15.684835000	C	6.205198000	-0.305874000	15.614971000
H	6.185788000	-1.178996000	15.797936000	H	6.285720000	-1.400081000	15.749126000
H	5.309987000	0.372160000	16.003104000	H	5.183092000	0.009096000	15.867895000
H	7.068636000	0.287193000	16.341830000	H	6.912549000	0.188886000	16.305298000
C	1.379505000	2.854996000	12.167287000	C	1.281594000	2.975985000	12.155763000
H	0.645717000	2.245616000	11.611672000	H	0.487195000	2.485475000	11.564102000
H	1.013656000	3.894355000	12.231535000	H	1.026039000	4.044577000	12.275719000
H	1.491744000	2.448883000	13.181347000	H	1.326030000	2.507615000	13.148969000

C	9.577058000	2.811072000	5.785363000	C	9.508866000	2.732448000	5.759845000
H	9.631125000	3.043647000	4.709491000	H	9.530287000	2.925396000	4.675036000
H	10.273031000	3.500171000	6.296361000	H	10.174359000	3.478530000	6.229700000
C	10.015710000	1.366628000	6.041949000	C	10.033024000	1.326330000	6.062811000
H	11.049933000	1.211313000	5.694211000	H	11.068943000	1.216041000	5.703397000
H	9.376774000	0.683196000	5.454206000	H	9.425196000	0.584762000	5.513953000
N	5.788773000	0.288790000	9.487314000	N	5.464034000	-0.002255000	9.062085000
N	4.986154000	0.478022000	8.626721000	N	4.882345000	0.198458000	8.065531000
H	4.440861000	-0.372987000	8.344205000	H	4.237494000	-0.547938000	7.689600000
⁵ XIII				² XIV			
Fe	6.883819000	2.095562000	10.295201000	Fe	6.665338000	1.749377000	10.048515000
Cl	8.082003000	3.902931000	11.153263000	Cl	7.857791000	3.427752000	11.042443000
O	6.829015000	1.034840000	11.842099000	O	6.690079000	0.754909000	11.732842000
O	5.037906000	2.454844000	10.582737000	O	5.011807000	2.473275000	10.589103000
N	6.795949000	2.822685000	8.490651000	N	6.699354000	2.671520000	8.376789000
O	2.597557000	2.647439000	11.512155000	O	2.648499000	2.864464000	11.627842000
O	6.543116000	0.338542000	14.351925000	O	6.363603000	-0.029086000	14.186139000
N	8.357854000	1.008927000	9.551310000	N	8.343511000	0.949163000	9.460098000
C	7.788474000	0.317710000	12.355270000	C	7.691342000	0.212317000	12.271583000
C	7.663995000	-0.092384000	13.729461000	C	7.552674000	-0.245753000	13.666057000
C	8.655910000	-0.869462000	14.320505000	C	8.636285000	-0.839837000	14.330924000
H	8.562250000	-1.171970000	15.364013000	H	8.538863000	-1.164091000	15.366629000
C	9.794749000	-1.277276000	13.589265000	C	9.840365000	-1.014356000	13.658565000
H	10.555815000	-1.887705000	14.080629000	H	10.681602000	-1.479164000	14.176759000
C	9.935166000	-0.906565000	12.267156000	C	9.997686000	-0.614087000	12.310164000
H	10.806651000	-1.220696000	11.686860000	H	10.951453000	-0.793163000	11.808200000
C	8.945866000	-0.103497000	11.636779000	C	8.965774000	-0.003737000	11.609491000
C	4.458005000	3.503712000	8.488363000	C	4.407002000	3.489787000	8.483793000
C	4.167102000	3.017234000	9.798571000	C	4.143967000	3.056791000	9.822080000
C	5.768706000	3.362771000	7.916926000	C	5.696230000	3.313387000	7.870417000
H	5.878545000	3.742945000	6.894520000	H	5.823004000	3.786332000	6.889795000
C	9.118343000	0.225101000	10.246062000	C	9.178225000	0.323745000	10.209533000
H	9.974577000	-0.251730000	9.753375000	H	10.130164000	-0.022847000	9.791083000
C	8.106910000	2.683075000	7.835546000	C	8.027173000	2.610430000	7.746791000
H	8.787175000	3.344800000	8.399509000	H	8.657570000	3.315994000	8.315243000
C	2.811085000	3.141836000	10.271989000	C	2.828953000	3.306081000	10.363320000
C	8.556788000	1.235709000	8.106262000	C	8.570277000	1.195853000	8.027274000
H	7.836950000	0.574940000	7.589422000	H	7.909004000	0.485005000	7.497601000
C	8.180071000	3.029773000	6.350910000	C	8.097513000	2.950960000	6.259470000
H	7.458314000	2.406928000	5.793829000	H	7.412570000	2.287183000	5.703414000
H	7.899017000	4.083011000	6.193868000	H	7.764740000	3.986596000	6.091318000
C	3.439953000	4.101131000	7.694066000	C	3.396951000	4.153205000	7.732959000
H	3.696343000	4.461112000	6.694315000	H	3.628904000	4.481696000	6.716560000
C	2.153949000	4.215700000	8.178731000	C	2.149105000	4.374162000	8.277441000
H	1.368790000	4.674263000	7.573399000	H	1.371537000	4.878826000	7.699562000
C	9.961575000	0.971175000	7.564387000	C	9.998091000	1.022692000	7.515096000
H	10.230901000	-0.087534000	7.699748000	H	10.337253000	-0.012721000	7.673245000
H	10.684808000	1.573352000	8.141897000	H	10.668474000	1.684382000	8.090791000
C	1.839705000	3.732482000	9.470547000	C	1.864627000	3.948136000	9.596426000
H	0.816614000	3.828468000	9.835631000	H	0.871762000	4.130807000	10.008810000
C	6.335688000	-0.007948000	15.709265000	C	6.078686000	-0.398098000	15.543075000
H	6.272664000	-1.102361000	15.849468000	H	6.201650000	-1.483528000	15.683132000
H	5.378378000	0.444268000	16.003639000	H	5.033898000	-0.114177000	15.716229000
H	7.134358000	0.389216000	16.361811000	H	6.736313000	0.148254000	16.237312000
C	1.293513000	2.713743000	12.060565000	C	1.391934000	3.064637000	12.250680000
H	0.561896000	2.153968000	11.449840000	H	0.577907000	2.551753000	11.707094000
H	0.944611000	3.756941000	12.166178000	H	1.142752000	4.137766000	12.335582000
H	1.350635000	2.255020000	13.057484000	H	1.472087000	2.636302000	13.259401000
C	9.597578000	2.778408000	5.821532000	C	9.532650000	2.778223000	5.744919000
H	9.635275000	3.007910000	4.744423000	H	9.563823000	2.994848000	4.665085000
H	10.298938000	3.470552000	6.320680000	H	10.184355000	3.520837000	6.238633000
C	10.041013000	1.335481000	6.076084000	C	10.068428000	1.371184000	6.022416000
H	11.070345000	1.179038000	5.714980000	H	11.109533000	1.280125000	5.673695000
H	9.393946000	0.649141000	5.501076000	H	9.475110000	0.634899000	5.451410000

N	5.251331000	-0.133163000	8.392381000	N	5.635746000	0.334694000	9.203280000
N	4.301768000	0.402335000	7.954430000	N	4.733010000	0.203671000	8.470184000
H	3.489774000	0.613448000	8.603074000	H	4.375034000	-0.757197000	8.241774000
⁴XIV				⁶XIV			
Fe	6.839979000	2.126571000	10.227738000	Fe	6.915450000	2.148387000	10.319369000
Cl	8.070685000	3.837888000	11.140514000	Cl	8.012112000	3.983989000	11.128667000
O	6.795935000	1.042889000	11.832991000	O	6.822916000	1.104697000	11.845882000
O	5.042865000	2.523433000	10.573352000	O	5.007419000	2.595440000	10.679212000
N	6.752565000	2.847443000	8.444022000	N	6.750025000	2.816309000	8.483458000
O	2.639318000	2.786776000	11.571364000	O	2.627200000	2.908946000	11.669685000
O	6.446738000	0.240417000	14.278847000	O	6.522840000	0.410450000	14.355324000
N	8.327525000	1.034402000	9.502665000	N	8.322582000	1.030239000	9.551327000
C	7.719791000	0.327246000	12.317131000	C	7.735350000	0.312368000	12.343830000
C	7.566000000	-0.138202000	13.703909000	C	7.594455000	-0.099637000	13.712272000
C	8.577812000	-0.902773000	14.309719000	C	8.530995000	-0.963738000	14.275272000
H	8.477044000	-1.234344000	15.342650000	H	8.427866000	-1.275242000	15.315127000
C	9.713363000	-1.236038000	13.583195000	C	9.622329000	-1.448631000	13.521209000
H	10.497069000	-1.831071000	14.056402000	H	10.338463000	-2.125150000	13.992798000
C	9.874354000	-0.831303000	12.236082000	C	9.777738000	-1.069753000	12.202686000
H	10.769362000	-1.135310000	11.688336000	H	10.615352000	-1.439689000	11.606320000
C	8.913850000	-0.059893000	11.595761000	C	8.845524000	-0.181821000	11.601227000
C	4.425290000	3.565970000	8.484260000	C	4.385473000	3.409591000	8.508423000
C	4.157270000	3.099531000	9.804266000	C	4.137247000	3.054749000	9.888888000
C	5.719980000	3.401807000	7.887533000	C	5.696517000	3.271270000	7.901119000
H	5.821795000	3.781024000	6.864271000	H	5.758600000	3.588580000	6.854005000
C	9.101287000	0.274884000	10.196123000	C	9.026316000	0.170432000	10.221349000
H	9.971906000	-0.191394000	9.720099000	H	9.838007000	-0.353961000	9.703167000
C	8.059166000	2.699500000	7.776703000	C	8.054208000	2.691218000	7.813801000
H	8.746792000	3.369195000	8.321503000	H	8.720333000	3.378779000	8.363491000
C	2.826457000	3.262149000	10.321461000	C	2.770739000	3.247973000	10.409653000
C	8.512980000	1.254993000	8.053783000	C	8.537265000	1.260169000	8.105317000
H	7.779688000	0.588224000	7.563688000	H	7.859353000	0.569764000	7.572797000
C	8.109556000	3.028289000	6.287126000	C	8.109665000	3.014785000	6.324861000
H	7.376705000	2.401448000	5.749976000	H	7.414660000	2.352343000	5.779815000
H	7.830501000	4.080787000	6.124180000	H	7.786568000	4.053161000	6.150890000
C	3.401102000	4.181964000	7.713090000	C	3.344989000	3.906452000	7.732837000
H	3.637087000	4.528609000	6.703997000	H	3.536074000	4.177659000	6.691784000
C	2.133692000	4.332441000	8.236923000	C	2.039852000	4.073276000	8.261726000
H	1.342177000	4.805148000	7.651349000	H	1.250686000	4.464658000	7.616824000
C	9.906809000	0.976584000	7.495361000	C	9.962514000	1.049633000	7.590496000
H	10.171165000	-0.082377000	7.638002000	H	10.275873000	0.006292000	7.743542000
H	10.641051000	1.582353000	8.054487000	H	10.647049000	1.691557000	8.171568000
C	1.846742000	3.870394000	9.541124000	C	1.751819000	3.751443000	9.578938000
H	0.837874000	3.995646000	9.935604000	H	0.742600000	3.889564000	9.966455000
C	6.161958000	-0.112155000	15.641549000	C	6.308969000	0.066723000	15.714437000
H	6.124612000	-1.206518000	15.756884000	H	6.155459000	-1.019773000	15.842380000
H	5.179786000	0.322098000	15.862091000	H	5.398799000	0.595590000	16.028829000
H	6.921896000	0.313777000	16.315197000	H	7.150222000	0.387480000	16.354677000
C	1.351335000	2.881941000	12.156261000	C	1.358520000	3.037859000	12.331226000
H	0.594390000	2.329473000	11.570828000	H	0.605354000	2.400177000	11.843058000
H	1.025461000	3.932217000	12.261609000	H	1.027768000	4.087912000	12.326302000
H	1.429684000	2.431003000	13.155091000	H	1.524850000	2.701265000	13.361232000
C	9.518072000	2.765928000	5.739316000	C	9.539218000	2.809712000	5.806450000
H	9.537363000	2.983032000	4.659421000	H	9.570766000	3.014112000	4.724403000
H	10.229044000	3.461856000	6.218764000	H	10.207209000	3.543603000	6.290832000
C	9.961216000	1.324575000	6.001848000	C	10.043574000	1.393446000	6.096856000
H	10.984160000	1.161211000	5.626919000	H	11.083625000	1.277887000	5.752268000
H	9.303132000	0.633407000	5.445845000	H	9.436908000	0.666797000	5.527506000
N	5.644809000	-0.877147000	9.409692000	N	5.318674000	0.004592000	8.843968000
N	5.079031000	-0.509840000	8.449505000	N	5.137669000	-0.266481000	7.717270000
H	4.954753000	0.530021000	8.287653000	H	5.399429000	0.442731000	6.970915000
²XV				⁴XV			
Fe	6.699762000	1.805349000	10.156283000	Fe	6.860288000	2.124000000	10.309853000
Cl	7.931505000	3.432310000	11.143453000	Cl	8.082988000	3.925182000	11.141819000
O	6.678924000	0.706120000	11.688952000	O	6.812886000	1.071576000	11.863732000

O	5.045228000	2.589886000	10.680416000	O	5.019272000	2.500980000	10.617160000
N	6.712041000	2.707469000	8.447232000	N	6.751757000	2.837061000	8.502733000
O	2.690175000	3.026049000	11.729026000	O	2.596471000	2.738641000	11.584297000
O	6.352644000	-0.000588000	14.194523000	O	6.536941000	0.361565000	14.370790000
N	8.339906000	0.977348000	9.523814000	N	8.307618000	1.013461000	9.550265000
C	7.722402000	0.222025000	12.293531000	C	7.761231000	0.329553000	12.361267000
C	7.583019000	-0.196722000	13.665689000	C	7.642285000	-0.087714000	13.733966000
C	8.665858000	-0.743010000	14.346297000	C	8.623547000	-0.889646000	14.309148000
H	8.560500000	-1.045028000	15.388956000	H	8.533904000	-1.197864000	15.351333000
C	9.915024000	-0.915655000	13.705542000	C	9.746182000	-1.316104000	13.563428000
H	10.747101000	-1.350650000	14.264108000	H	10.499331000	-1.945534000	14.042866000
C	10.072397000	-0.541647000	12.386118000	C	9.880298000	-0.940072000	12.242331000
H	11.029391000	-0.681176000	11.876050000	H	10.738554000	-1.269015000	11.650642000
C	8.991860000	0.037651000	11.666863000	C	8.900967000	-0.112878000	11.627278000
C	4.401278000	3.475197000	8.528493000	C	4.424069000	3.552706000	8.529251000
C	4.162246000	3.116414000	9.893846000	C	4.145543000	3.075520000	9.845339000
C	5.692520000	3.304680000	7.917313000	C	5.723144000	3.387572000	7.939798000
H	5.802176000	3.741955000	6.917584000	H	5.825147000	3.761344000	6.914105000
C	9.186126000	0.352832000	10.274843000	C	9.063296000	0.216564000	10.236005000
H	10.129667000	0.006216000	9.836738000	H	9.906128000	-0.273011000	9.732807000
C	8.032757000	2.637234000	7.810102000	C	8.054447000	2.686701000	7.834186000
H	8.674808000	3.331197000	8.380595000	H	8.744974000	3.344084000	8.390805000
C	2.848209000	3.385875000	10.433553000	C	2.800505000	3.227667000	10.340090000
C	8.557740000	1.214747000	8.089011000	C	8.496891000	1.237333000	8.102974000
H	7.888208000	0.515900000	7.552972000	H	7.771319000	0.579513000	7.589597000
C	8.104061000	2.983305000	6.324422000	C	8.117999000	3.033019000	6.349195000
H	7.412433000	2.328601000	5.765408000	H	7.389527000	2.414212000	5.796394000
H	7.779251000	4.022523000	6.160079000	H	7.841240000	4.087703000	6.194412000
C	3.369174000	4.074320000	7.749928000	C	3.405634000	4.169086000	7.749697000
H	3.585608000	4.345192000	6.712943000	H	3.653199000	4.522264000	6.745246000
C	2.123413000	4.305955000	8.291777000	C	2.130800000	4.311730000	8.255685000
H	1.329814000	4.758918000	7.693034000	H	1.345121000	4.785508000	7.662849000
C	9.981808000	1.028061000	7.567341000	C	9.897028000	0.965640000	7.551914000
H	10.312159000	-0.010787000	7.721916000	H	10.162427000	-0.094261000	7.685251000
H	10.662384000	1.680522000	8.141833000	H	10.626034000	1.564236000	8.125821000
C	1.863486000	3.959426000	9.640619000	C	1.828593000	3.836702000	9.553536000
H	0.872229000	4.150166000	10.053701000	H	0.813632000	3.953389000	9.935048000
C	6.119395000	-0.367938000	15.541509000	C	6.334079000	0.006393000	15.726618000
H	6.275779000	-1.449576000	15.706407000	H	6.248703000	-1.087754000	15.856760000
H	5.069401000	-0.123461000	15.754749000	H	5.389299000	0.476056000	16.033831000
H	6.766210000	0.194447000	16.239310000	H	7.146806000	0.379911000	16.375736000
C	1.440103000	3.249902000	12.353330000	C	1.299602000	2.819269000	12.147166000
H	0.626165000	2.688899000	11.858769000	H	0.554720000	2.270017000	11.542893000
H	1.173428000	4.322460000	12.368235000	H	0.964053000	3.866165000	12.259634000
H	1.538985000	2.893607000	13.388284000	H	1.361949000	2.357044000	13.142187000
C	9.535354000	2.796190000	5.804830000	C	9.531077000	2.775098000	5.811012000
H	9.567940000	3.017379000	4.725748000	H	9.563327000	3.004147000	4.733651000
H	10.197939000	3.527890000	6.300640000	H	10.238353000	3.464355000	6.305756000
C	10.052947000	1.380840000	6.075803000	C	9.969844000	1.330330000	6.063312000
H	11.091601000	1.276960000	5.722601000	H	10.996690000	1.169856000	5.696969000
H	9.447940000	0.655277000	5.503031000	H	9.317278000	0.646682000	5.491318000
N	5.531255000	0.333405000	9.252676000	N	5.022208000	-0.114658000	8.628674000
N	4.895773000	-0.446309000	8.808114000	N	4.118095000	0.318730000	8.174950000
⁶XV							
Fe	6.885258000	2.428292000	10.522289000				
Cl	8.173679000	4.180023000	11.191459000				
O	6.927021000	1.212188000	11.996946000				
O	5.029441000	2.861151000	10.648624000				
N	6.724774000	2.951433000	8.475884000				
O	2.593284000	3.093627000	11.609497000				
O	6.671519000	0.372587000	14.478667000				
N	8.299251000	1.115484000	9.578320000				
C	7.768984000	0.303953000	12.401254000				
C	7.662642000	-0.187129000	13.748044000				
C	8.545024000	-1.160967000	14.208821000				
H	8.467002000	-1.529428000	15.232309000				

C	9.548549000	-1.686133000	13.365142000
H	10.226098000	-2.450999000	13.751589000
C	9.665558000	-1.235629000	12.063955000
H	10.435791000	-1.639739000	11.401648000
C	8.789436000	-0.234845000	11.564874000
C	4.343011000	3.467375000	8.425598000
C	4.095398000	3.212806000	9.805791000
C	5.663913000	3.330532000	7.847829000
H	5.726054000	3.574079000	6.778232000
C	8.946043000	0.175425000	10.187298000
H	9.694132000	-0.402972000	9.627327000
C	8.029454000	2.796002000	7.832912000
H	8.706873000	3.475563000	8.381178000
C	2.751112000	3.355054000	10.291879000
C	8.503598000	1.357412000	8.136995000
H	7.814664000	0.676755000	7.602110000
C	8.118308000	3.111539000	6.340943000
H	7.433351000	2.449164000	5.782779000
H	7.793204000	4.148287000	6.158137000
C	3.279577000	3.854184000	7.569394000
H	3.495106000	4.043401000	6.514353000
C	1.993491000	3.984219000	8.060622000
H	1.173891000	4.279498000	7.401441000
C	9.929567000	1.134895000	7.618462000
H	10.235227000	0.088721000	7.769134000
H	10.617150000	1.765609000	8.209228000
C	1.728682000	3.733045000	9.423677000
H	0.708127000	3.838170000	9.793444000
C	6.493764000	-0.038577000	15.822272000
H	6.256410000	-1.115456000	15.894752000
H	5.646547000	0.539958000	16.216051000
H	7.387471000	0.171314000	16.437421000
C	1.301177000	3.200279000	12.179770000
H	0.587384000	2.496842000	11.714057000
H	0.897667000	4.225512000	12.094647000
H	1.407772000	2.946743000	13.243690000
C	9.551938000	2.905486000	5.839666000
H	9.603091000	3.117517000	4.759366000
H	10.219272000	3.630115000	6.339552000
C	10.037982000	1.483060000	6.128900000
H	11.081607000	1.356592000	5.797648000
H	9.430906000	0.766860000	5.546354000
N	5.403796000	-0.452510000	9.467318000
N	5.017271000	0.093685000	8.593826000

Coordinates of species for Mechanistic Pathway-A

² I				⁴ I			
Fe	6.715176000	1.899261000	10.197934000	Fe	6.778141000	2.048852000	10.278153000
Cl	7.896156000	3.633997000	11.063972000	Cl	7.994163000	3.840449000	11.152215000
O	6.672037000	0.819559000	11.729221000	O	6.729729000	0.969291000	11.814214000
O	4.922091000	2.344959000	10.546128000	O	4.941677000	2.431101000	10.586201000
N	6.655415000	2.698927000	8.437835000	N	6.688098000	2.791908000	8.481720000
O	2.560096000	2.766971000	11.606338000	O	2.547907000	2.779512000	11.593634000
O	6.347586000	0.090239000	14.231478000	O	6.463575000	0.274009000	14.328144000
N	8.281596000	0.975798000	9.523841000	N	8.256613000	0.972682000	9.524327000
C	7.688625000	0.243921000	12.303309000	C	7.704795000	0.273731000	12.328604000
C	7.549864000	-0.178803000	13.673718000	C	7.592045000	-0.134393000	13.704346000
C	8.609991000	-0.800799000	14.325153000	C	8.602359000	-0.886853000	14.296301000
H	8.508286000	-1.104890000	15.367485000	H	8.517882000	-1.186400000	15.341406000
C	9.830972000	-1.047405000	13.655389000	C	9.748349000	-1.272557000	13.564384000
H	10.644649000	-1.540514000	14.192371000	H	10.523807000	-1.863799000	14.056689000
C	9.985456000	-0.672615000	12.336018000	C	9.877856000	-0.904089000	12.240549000
H	10.919850000	-0.869527000	11.803715000	H	10.754897000	-1.200942000	11.659570000
C	8.928361000	-0.018920000	11.646141000	C	8.870118000	-0.124776000	11.609695000
C	4.385164000	3.578419000	8.546736000	C	4.371023000	3.545346000	8.523012000

C	4.088333000	3.050443000	9.838438000	C	4.085491000	3.057873000	9.833407000
C	5.662978000	3.354818000	7.924802000	C	5.664850000	3.360256000	7.926353000
H	5.783528000	3.794596000	6.927775000	H	5.771935000	3.749311000	6.906743000
C	9.106800000	0.293866000	10.252769000	C	9.033109000	0.203400000	10.217806000
H	10.014901000	-0.109746000	9.789438000	H	9.896461000	-0.258853000	9.723717000
C	7.961061000	2.587882000	7.766523000	C	7.994403000	2.652737000	7.816847000
H	8.621052000	3.293786000	8.301473000	H	8.677809000	3.312207000	8.380033000
C	2.777540000	3.300886000	10.382932000	C	2.756990000	3.269704000	10.350226000
C	8.475808000	1.173161000	8.075028000	C	8.448705000	1.205701000	8.079166000
H	7.788169000	0.465666000	7.575774000	H	7.730380000	0.544919000	7.559646000
C	8.003865000	2.890851000	6.270241000	C	8.059871000	3.007153000	6.333516000
H	7.292887000	2.228724000	5.745252000	H	7.334824000	2.387861000	5.776738000
H	7.688669000	3.928685000	6.081426000	H	7.778623000	4.061241000	6.183300000
C	3.410632000	4.329484000	7.833313000	C	3.371134000	4.215894000	7.764206000
H	3.667033000	4.720272000	6.845015000	H	3.623163000	4.574781000	6.762839000
C	2.165654000	4.558849000	8.382610000	C	2.109941000	4.408631000	8.288053000
H	1.415335000	5.137565000	7.838869000	H	1.339333000	4.925563000	7.711697000
C	9.887853000	0.955392000	7.532798000	C	9.851560000	0.946907000	7.529466000
H	10.210493000	-0.082513000	7.707372000	H	10.124901000	-0.111344000	7.660578000
H	10.586004000	1.615008000	8.077445000	H	10.575635000	1.549735000	8.105186000
C	1.848720000	4.042509000	9.660619000	C	1.803746000	3.932820000	9.584545000
H	0.860017000	4.235051000	10.078670000	H	0.801139000	4.093251000	9.982570000
C	6.121057000	-0.273997000	15.580990000	C	6.269342000	-0.068433000	15.688498000
H	6.212689000	-1.364677000	15.733829000	H	6.232110000	-1.163051000	15.836002000
H	5.093387000	0.033972000	15.819025000	H	5.303082000	0.363646000	15.983839000
H	6.817047000	0.240871000	16.267918000	H	7.061282000	0.351189000	16.335164000
C	1.300390000	2.959838000	12.223571000	C	1.270046000	2.933382000	12.183674000
H	0.479009000	2.523882000	11.626360000	H	0.481680000	2.430823000	11.594157000
H	1.085844000	4.030323000	12.394954000	H	0.998540000	3.997706000	12.305726000
H	1.346447000	2.446328000	13.194060000	H	1.325907000	2.464705000	13.176084000
C	9.422344000	2.674858000	5.727150000	C	9.474738000	2.759378000	5.795189000
H	9.434310000	2.863204000	4.641426000	H	9.505822000	2.992831000	4.718726000
H	10.100728000	3.415583000	6.186915000	H	10.177743000	3.450950000	6.292763000
C	9.934243000	1.264325000	6.030511000	C	9.922526000	1.316487000	6.042009000
H	10.965333000	1.141500000	5.661516000	H	10.950421000	1.163815000	5.675313000
H	9.313171000	0.527040000	5.490913000	H	9.274424000	0.630653000	5.467558000
¶I				¶II			
Fe	6.741890000	2.223066000	10.509999000	Fe	6.622439000	1.707620000	10.081936000
Cl	7.940284000	4.003501000	11.274748000	O	6.707052000	0.867738000	11.775135000
O	6.814006000	0.975878000	11.957371000	O	4.893008000	2.414460000	10.555832000
O	4.867773000	2.574947000	10.577183000	N	6.625280000	2.650371000	8.393074000
N	6.652163000	2.848276000	8.480421000	O	2.557239000	2.880093000	11.622995000
O	2.449151000	2.961261000	11.533922000	O	6.409154000	0.133430000	14.272400000
O	6.621270000	0.196541000	14.468049000	N	8.274908000	0.944388000	9.498118000
N	8.256533000	1.019138000	9.589040000	C	7.697052000	0.222774000	12.304329000
C	7.775445000	0.225283000	12.420226000	C	7.575594000	-0.203128000	13.681935000
C	7.706391000	-0.229036000	13.781691000	C	8.612200000	-0.893485000	14.297028000
C	8.714357000	-1.038129000	14.300629000	H	8.520293000	-1.207340000	15.337209000
H	8.663627000	-1.378076000	15.335576000	C	9.798544000	-1.200393000	13.589126000
C	9.811117000	-1.429844000	13.502260000	H	10.596742000	-1.745950000	14.097777000
H	10.585981000	-2.067892000	13.933463000	C	9.942906000	-0.815687000	12.271120000
C	9.896564000	-1.010301000	12.188061000	H	10.854472000	-1.054936000	11.717239000
H	10.738625000	-1.313164000	11.559939000	C	8.908325000	-0.100193000	11.608387000
C	8.892878000	-0.174147000	11.630945000	C	4.345926000	3.502490000	8.485728000
C	4.304691000	3.515110000	8.437162000	C	4.061768000	3.045521000	9.830754000
C	3.996669000	3.124170000	9.772240000	C	5.640334000	3.302367000	7.866969000
C	5.625422000	3.335058000	7.869518000	H	5.762756000	3.770127000	6.883444000
H	5.721535000	3.662898000	6.825364000	C	9.101534000	0.255202000	10.229801000
C	9.020847000	0.204262000	10.240085000	H	10.029824000	-0.110407000	9.776222000
H	9.855804000	-0.280672000	9.716163000	C	7.949580000	2.573757000	7.744518000
C	7.964175000	2.695205000	7.846888000	H	8.582348000	3.295386000	8.293178000
H	8.639347000	3.368919000	8.405751000	C	2.737520000	3.330558000	10.391087000
C	2.663086000	3.349477000	10.255947000	C	8.505052000	1.172216000	8.057183000
C	8.434906000	1.252525000	8.144099000	H	7.857017000	0.448286000	7.529887000
H	7.722687000	0.578838000	7.631423000	C	8.014131000	2.891044000	6.251956000
C	8.054852000	3.024336000	6.357018000	H	7.334560000	2.210845000	5.709130000

H	7.345804000	2.387236000	5.799339000	H	7.671367000	3.920059000	6.063406000
H	7.758004000	4.071512000	6.186873000	C	3.361453000	4.191574000	7.775340000
C	3.304588000	4.099593000	7.616978000	H	3.580620000	4.543256000	6.764410000
H	3.564154000	4.388308000	6.594894000	C	2.097890000	4.440344000	8.339425000
C	2.026544000	4.303759000	8.103767000	H	1.346523000	4.976840000	7.756032000
H	1.257327000	4.755694000	7.473266000	C	9.936187000	1.012270000	7.544919000
C	9.840964000	0.999605000	7.590715000	H	10.291072000	-0.015027000	7.718583000
H	10.122430000	-0.054649000	7.734411000	H	10.599187000	1.691136000	8.109499000
H	10.560011000	1.611649000	8.163606000	C	1.783571000	4.018336000	9.633281000
C	1.705586000	3.928912000	9.425673000	H	0.796996000	4.228383000	10.045443000
H	0.693347000	4.098978000	9.794076000	C	6.197313000	-0.222584000	15.627782000
C	6.477216000	-0.180784000	15.825595000	H	6.224970000	-1.317440000	15.773132000
H	6.402279000	-1.277133000	15.942178000	H	5.198083000	0.148264000	15.894771000
H	5.544353000	0.279446000	16.179852000	H	6.944030000	0.244706000	16.294745000
H	7.315411000	0.186614000	16.445039000	C	1.306276000	3.083687000	12.286065000
C	1.168506000	3.159101000	12.105664000	H	0.486413000	2.594690000	11.735186000
H	0.385004000	2.598867000	11.563894000	H	1.091345000	4.159040000	12.396159000
H	0.890065000	4.228278000	12.129346000	H	1.411259000	2.624360000	13.276725000
H	1.225935000	2.783440000	13.136749000	C	9.450053000	2.724875000	5.736961000
C	9.475281000	2.786732000	5.834366000	H	9.476102000	2.917840000	4.652437000
H	9.516230000	3.010939000	4.756078000	H	10.093326000	3.487130000	6.211745000
H	10.169462000	3.486594000	6.333066000	C	10.004543000	1.331973000	6.045659000
C	9.924886000	1.348895000	6.100581000	H	11.047054000	1.248039000	5.698806000
H	10.956308000	1.192881000	5.744762000	H	9.422162000	0.575970000	5.489183000
H	9.282928000	0.655004000	5.528554000				
⁴He				⁶He			
Fe	6.588226000	1.691971000	10.114748000	Fe	6.745840000	2.219328000	10.470760000
O	6.697474000	0.754155000	11.694258000	O	6.978636000	1.198205000	12.030608000
O	4.937434000	2.385890000	10.508594000	O	4.924556000	2.717439000	10.620458000
N	6.606223000	2.635854000	8.413446000	N	6.656581000	2.862452000	8.469694000
O	2.600685000	2.853748000	11.622641000	O	2.498837000	3.052655000	11.579758000
O	6.377376000	0.068126000	14.212333000	O	6.743103000	0.363044000	14.517056000
N	8.257627000	0.909698000	9.502941000	N	8.289819000	1.046375000	9.580843000
C	7.718512000	0.187824000	12.287901000	C	7.842928000	0.303183000	12.444202000
C	7.575439000	-0.209738000	13.658723000	C	7.743627000	-0.174094000	13.791604000
C	8.640855000	-0.829177000	14.307024000	C	8.652397000	-1.126581000	14.257523000
H	8.542756000	-1.128642000	15.350909000	H	8.584485000	-1.491325000	15.282719000
C	9.858189000	-1.079821000	13.634033000	C	9.662126000	-1.629558000	13.415888000
H	10.672310000	-1.569710000	14.172693000	H	10.359119000	-2.375354000	13.804542000
C	10.014909000	-0.712034000	12.312752000	C	9.767415000	-1.187961000	12.106483000
H	10.948887000	-0.906300000	11.780248000	H	10.544139000	-1.582897000	11.447042000
C	8.950502000	-0.068800000	11.625080000	C	8.866384000	-0.218681000	11.602119000
C	4.337229000	3.520555000	8.481235000	C	4.291573000	3.465902000	8.424099000
C	4.063328000	3.053552000	9.795240000	C	4.013211000	3.162977000	9.788882000
C	5.626327000	3.307916000	7.888530000	C	5.611431000	3.300812000	7.850039000
H	5.784514000	3.781497000	6.913406000	H	5.692185000	3.588021000	6.793380000
C	9.118856000	0.276753000	10.243065000	C	9.003876000	0.173333000	10.213914000
H	10.060179000	-0.045475000	9.784949000	H	9.794854000	-0.361982000	9.671540000
C	7.940933000	2.558366000	7.778994000	C	7.972678000	2.720298000	7.834758000
H	8.584206000	3.257402000	8.343505000	H	8.641358000	3.407295000	8.387149000
C	2.779768000	3.326204000	10.372432000	C	2.680479000	3.359733000	10.279495000
C	8.462906000	1.142043000	8.056113000	C	8.471375000	1.287000000	8.135038000
H	7.787361000	0.438143000	7.538085000	H	7.782249000	0.595940000	7.615182000
C	8.007093000	2.906102000	6.292706000	C	8.059422000	3.045787000	6.344436000
H	7.305068000	2.257333000	5.740622000	H	7.371927000	2.385331000	5.787278000
H	7.694514000	3.948771000	6.130733000	H	7.732750000	4.083124000	6.169187000
C	3.351311000	4.241039000	7.755701000	C	3.260033000	3.948972000	7.582271000
H	3.586979000	4.592924000	6.748574000	H	3.491326000	4.174193000	6.538133000
C	2.117979000	4.485685000	8.326560000	C	1.978975000	4.131986000	8.076471000
H	1.351849000	5.035575000	7.775530000	H	1.184067000	4.504716000	7.426594000
C	9.884046000	0.947146000	7.530603000	C	9.891747000	1.074751000	7.599627000
H	10.208403000	-0.092885000	7.687417000	H	10.202337000	0.029579000	7.746568000
H	10.570929000	1.600121000	8.096627000	H	10.583931000	1.707802000	8.182471000
C	1.832235000	4.030458000	9.632916000	C	1.687991000	3.838387000	9.422326000
H	0.852232000	4.238838000	10.063172000	H	0.673110000	3.988379000	9.791585000
C	6.144353000	-0.292726000	15.564731000	C	6.551760000	-0.067066000	15.856372000

H	6.233736000	-1.382993000	15.717364000	H	6.337293000	-1.149136000	15.909687000
H	5.116519000	0.018527000	15.795794000	H	5.685356000	0.489290000	16.239077000
H	6.839702000	0.223661000	16.250186000	H	7.430647000	0.157140000	16.486256000
C	1.355429000	3.072427000	12.267270000	C	1.210568000	3.212480000	12.152878000
H	0.522141000	2.603676000	11.714185000	H	0.460437000	2.572353000	11.655474000
H	1.143861000	4.149429000	12.390780000	H	0.871982000	4.262872000	12.109745000
H	1.433915000	2.606677000	13.259036000	H	1.299442000	2.908050000	13.204652000
C	9.433908000	2.707481000	5.764852000	C	9.490201000	2.847126000	5.832764000
H	9.455985000	2.924651000	4.685032000	H	9.530853000	3.065934000	4.753594000
H	10.104730000	3.437658000	6.251300000	H	10.159381000	3.571170000	6.331005000
C	9.944303000	1.290758000	6.036532000	C	9.982077000	1.425070000	6.109858000
H	10.980049000	1.179008000	5.678260000	H	11.022349000	1.301785000	5.767743000
H	9.331072000	0.565529000	5.472831000	H	9.370129000	0.709237000	5.532365000
²III				⁶III			
Fe	6.661772000	1.794187000	10.122343000	Fe	6.635232000	2.060896000	10.454940000
O	6.644001000	0.720062000	11.651863000	O	6.863115000	0.998466000	12.004126000
O	4.962707000	2.434396000	10.588839000	O	4.830337000	2.594964000	10.576813000
N	6.632425000	2.653562000	8.409225000	N	6.637306000	2.831072000	8.487353000
O	2.652474000	2.950338000	11.707382000	O	2.391430000	2.964537000	11.493499000
O	6.283334000	-0.024747000	14.142318000	O	6.714652000	0.216570000	14.515564000
N	8.314215000	1.003165000	9.514378000	N	8.232219000	0.970097000	9.574737000
C	7.684217000	0.231932000	12.271565000	C	7.824944000	0.228220000	12.445906000
C	7.522559000	-0.200584000	13.634916000	C	7.778044000	-0.220215000	13.807326000
C	8.601888000	-0.742162000	14.326029000	C	8.789141000	-1.042197000	14.304834000
H	8.483911000	-1.058336000	15.362958000	H	8.756281000	-1.382755000	15.340171000
C	9.861966000	-0.893266000	13.702910000	C	9.861261000	-1.444770000	13.483136000
H	10.688837000	-1.325820000	14.270803000	H	10.638967000	-2.090701000	13.896844000
C	10.040203000	-0.505901000	12.390297000	C	9.923193000	-1.027996000	12.164930000
H	11.005652000	-0.632841000	11.893959000	H	10.748154000	-1.341802000	11.520161000
C	8.963490000	0.066236000	11.659435000	C	8.915524000	-0.186412000	11.627790000
C	4.354332000	3.515714000	8.522078000	C	4.301474000	3.550932000	8.436051000
C	4.102330000	3.082304000	9.859193000	C	3.966239000	3.150123000	9.761125000
C	5.622744000	3.289951000	7.892102000	C	5.627974000	3.363051000	7.882141000
H	5.735746000	3.720595000	6.890724000	H	5.744439000	3.724328000	6.851768000
C	9.165012000	0.381134000	10.269282000	C	9.025068000	0.187180000	10.232289000
H	10.107809000	0.032648000	9.832099000	H	9.874716000	-0.272970000	9.710730000
C	7.947800000	2.586151000	7.744239000	C	7.953668000	2.672925000	7.857163000
H	8.587611000	3.323251000	8.264385000	H	8.639704000	3.329292000	8.425359000
C	2.818451000	3.388314000	10.439585000	C	2.629219000	3.371874000	10.228031000
C	8.514748000	1.194394000	8.065846000	C	8.410354000	1.219581000	8.131539000
H	7.858226000	0.457701000	7.568103000	H	7.688697000	0.561065000	7.613326000
C	7.984680000	2.876648000	6.245093000	C	8.052696000	3.028534000	6.373819000
H	7.299497000	2.183464000	5.726663000	H	7.333671000	2.412767000	5.805359000
H	7.633305000	3.900428000	6.044768000	H	7.772847000	4.083190000	6.223019000
C	3.355090000	4.225072000	7.795794000	C	3.320783000	4.155061000	7.609221000
H	3.577106000	4.548983000	6.775727000	H	3.597312000	4.454981000	6.595095000
C	2.134334000	4.497365000	8.374623000	C	2.035425000	4.360687000	8.079848000
H	1.364624000	5.039693000	7.820778000	H	1.280065000	4.826094000	7.442601000
C	9.937658000	1.026472000	7.536822000	C	9.811783000	0.959087000	7.572183000
H	10.297766000	0.003646000	7.726120000	H	10.079880000	-0.100677000	7.700437000
H	10.606586000	1.718868000	8.077440000	H	10.539738000	1.554042000	8.151928000
C	1.865774000	4.078418000	9.700332000	C	1.688656000	3.969448000	9.388289000
H	0.894409000	4.306991000	10.140224000	H	0.670618000	4.138670000	9.740347000
C	6.023379000	-0.428054000	15.476131000	C	6.580685000	-0.179383000	15.870613000
H	6.190110000	-1.511214000	15.616074000	H	6.492938000	-1.276154000	15.969648000
H	4.965798000	-0.201272000	15.669071000	H	5.657701000	0.287641000	16.240804000
H	6.647291000	0.125509000	16.200677000	H	7.430577000	0.168395000	16.484711000
C	1.421311000	3.200459000	12.362366000	C	1.094180000	3.135979000	12.039941000
H	0.573106000	2.725953000	11.836598000	H	0.331005000	2.582086000	11.464329000
H	1.220513000	4.282805000	12.458757000	H	0.805951000	4.201545000	12.083879000
H	1.507989000	2.762957000	13.366598000	H	1.132068000	2.734160000	13.061815000
C	9.412777000	2.706741000	5.709746000	C	9.469444000	2.779144000	5.846928000
H	9.419992000	2.881948000	4.621982000	H	9.512178000	3.021593000	4.772830000
H	10.061122000	3.478960000	6.160974000	H	10.174342000	3.460309000	6.356457000
C	9.978216000	1.320783000	6.031239000	C	9.897894000	1.330686000	6.087681000
H	11.014918000	1.235187000	5.668035000	H	10.926495000	1.165741000	5.728194000

H	9.389315000	0.553548000	5.497789000	H	9.245069000	0.655891000	5.505564000
N	7.607244000	3.241207000	11.066435000	N	7.661181000	3.747414000	11.248576000
H	8.594887000	3.030882000	11.244093000	H	8.660833000	3.560194000	11.375748000
H	7.576324000	4.123916000	10.545396000	H	7.583970000	4.575573000	10.650412000
H	7.158870000	3.405995000	11.973528000	H	7.291116000	4.006676000	12.168803000
¹IV				³IV			
Fe	6.694122000	1.818241000	10.097301000	Fe	6.706690000	1.884009000	10.180552000
O	6.694009000	0.826591000	11.678904000	O	6.694839000	0.815051000	11.728796000
O	4.995835000	2.451822000	10.567979000	O	4.920995000	2.372248000	10.541385000
N	6.644938000	2.669604000	8.402526000	N	6.661460000	2.716764000	8.429775000
O	2.727964000	2.979622000	11.748748000	O	2.602194000	2.871695000	11.633630000
O	6.244904000	-0.033302000	14.104622000	O	6.402189000	0.140479000	14.235509000
N	8.339730000	1.050716000	9.525612000	N	8.288823000	0.961587000	9.497504000
C	7.681031000	0.276127000	12.275988000	C	7.700061000	0.230328000	12.288469000
C	7.472261000	-0.219227000	13.631260000	C	7.566390000	-0.170222000	13.677543000
C	8.531901000	-0.805498000	14.319482000	C	8.624909000	-0.826988000	14.321453000
H	8.396500000	-1.163159000	15.339930000	H	8.530108000	-1.123284000	15.366032000
C	9.786988000	-0.943875000	13.701899000	C	9.807715000	-1.103723000	13.631194000
H	10.599976000	-1.412008000	14.261239000	H	10.621585000	-1.617140000	14.146819000
C	10.010954000	-0.512267000	12.394864000	C	9.959364000	-0.732753000	12.289513000
H	10.985732000	-0.658769000	11.924789000	H	10.885150000	-0.962551000	11.757333000
C	8.982428000	0.103060000	11.664711000	C	8.928521000	-0.062339000	11.611850000
C	4.349581000	3.468960000	8.495062000	C	4.351346000	3.494188000	8.493091000
C	4.123281000	3.065018000	9.865054000	C	4.078956000	3.034689000	9.821314000
C	5.617707000	3.251812000	7.856262000	C	5.642567000	3.298805000	7.882786000
H	5.707068000	3.646080000	6.838682000	H	5.751067000	3.710014000	6.872771000
C	9.200984000	0.440940000	10.282606000	C	9.110847000	0.271853000	10.219248000
H	10.153749000	0.108887000	9.856734000	H	10.026676000	-0.114492000	9.757578000
C	7.953497000	2.606250000	7.724539000	C	7.981416000	2.615832000	7.773181000
H	8.582412000	3.365737000	8.224290000	H	8.640229000	3.307483000	8.329658000
C	2.842192000	3.379288000	10.485964000	C	2.777224000	3.319965000	10.393103000
C	8.551000000	1.230110000	8.077075000	C	8.485693000	1.190864000	8.048464000
H	7.908361000	0.473058000	7.592599000	H	7.793587000	0.495783000	7.540009000
C	7.978536000	2.860222000	6.219585000	C	8.037009000	2.960209000	6.287395000
H	7.307299000	2.140345000	5.720217000	H	7.329535000	2.313304000	5.740273000
H	7.606912000	3.871927000	5.996621000	H	7.726181000	4.004233000	6.128919000
C	3.331917000	4.138048000	7.795332000	C	3.360595000	4.183251000	7.770331000
H	3.508127000	4.447401000	6.762862000	H	3.584032000	4.528978000	6.758453000
C	2.113505000	4.412407000	8.414585000	C	2.108268000	4.432101000	8.338491000
H	1.330231000	4.931234000	7.857569000	H	1.348167000	4.968309000	7.766973000
C	9.976444000	1.080592000	7.552250000	C	9.899597000	0.976526000	7.512315000
H	10.355486000	0.068472000	7.760078000	H	10.208431000	-0.069523000	7.659937000
H	10.631579000	1.797254000	8.077414000	H	10.598182000	1.615054000	8.080643000
C	1.864945000	4.042873000	9.748771000	C	1.817343000	4.007928000	9.639454000
H	0.901148000	4.280785000	10.198511000	H	0.837374000	4.219994000	10.066988000
C	5.923828000	-0.457425000	15.430162000	C	6.143919000	-0.202357000	15.598655000
H	6.058894000	-1.546156000	15.540172000	H	6.197818000	-1.293293000	15.747085000
H	4.868578000	-0.199532000	15.583906000	H	5.126776000	0.149421000	15.811085000
H	6.545392000	0.068635000	16.173573000	H	6.858003000	0.298955000	16.272473000
C	1.522115000	3.240610000	12.467116000	C	1.353698000	3.074650000	12.295903000
H	0.661944000	2.742090000	11.990242000	H	0.531538000	2.584605000	11.748382000
H	1.329519000	4.324251000	12.535084000	H	1.134752000	4.149685000	12.406669000
H	1.672713000	2.830056000	13.473466000	H	1.458500000	2.617022000	13.287659000
C	9.409744000	2.706998000	5.686705000	C	9.459774000	2.750588000	5.753006000
H	9.410623000	2.855146000	4.595168000	H	9.479187000	2.968854000	4.673516000
H	10.041321000	3.504194000	6.117462000	H	10.139190000	3.473770000	6.237835000
C	10.005888000	1.342066000	6.040045000	C	9.957000000	1.327794000	6.019448000
H	11.043406000	1.270821000	5.676877000	H	10.990172000	1.206934000	5.657100000
H	9.433111000	0.549188000	5.527190000	H	9.334490000	0.610957000	5.455379000
N	7.603905000	3.286399000	11.006821000	N	7.619478000	3.510345000	11.183093000
H	8.500796000	3.012829000	11.424321000	H	8.618777000	3.342781000	11.339153000
H	7.799308000	4.079213000	10.386145000	H	7.539832000	4.387667000	10.659467000
H	7.016137000	3.639970000	11.769754000	H	7.194235000	3.667841000	12.102090000
⁵IV				¹V			
Fe	6.739474000	1.883439000	10.204215000	Fe	6.846532000	2.265649000	10.281957000

O	6.723962000	0.877752000	11.744586000	O	6.865794000	1.401198000	11.987006000
O	4.886641000	2.449185000	10.607760000	O	5.063269000	2.229608000	10.361969000
N	6.688151000	2.750734000	8.457022000	N	6.794661000	3.048652000	8.491419000
O	2.523855000	2.878208000	11.598914000	O	2.648222000	2.299030000	11.360892000
O	6.449092000	0.217201000	14.267058000	O	6.708822000	0.783590000	14.532421000
N	8.282094000	0.946466000	9.499648000	N	8.079295000	1.083277000	9.517198000
C	7.728572000	0.237297000	12.297697000	C	7.677551000	0.498302000	12.408364000
C	7.601782000	-0.148463000	13.671854000	C	7.621197000	0.110699000	13.802074000
C	8.638410000	-0.848573000	14.289527000	C	8.467456000	-0.877220000	14.277770000
H	8.549157000	-1.140170000	15.336273000	H	8.429522000	-1.170505000	15.327500000
C	9.810164000	-1.188893000	13.582458000	C	9.397366000	-1.526363000	13.420230000
H	10.601983000	-1.738907000	14.095472000	H	10.046839000	-2.300651000	13.834562000
C	9.952458000	-0.830327000	12.255248000	C	9.477730000	-1.185167000	12.091882000
H	10.852495000	-1.092970000	11.694626000	H	10.189233000	-1.678001000	11.425189000
C	8.921197000	-0.107651000	11.600588000	C	8.626715000	-0.167417000	11.560102000
C	4.369529000	3.511187000	8.516384000	C	4.461671000	3.667745000	8.506249000
C	4.069806000	3.055299000	9.852879000	C	4.172075000	2.955831000	9.697580000
C	5.674444000	3.329143000	7.909433000	C	5.778825000	3.585738000	7.911404000
H	5.776307000	3.745042000	6.900446000	H	5.882024000	3.985560000	6.895788000
C	9.092938000	0.227608000	10.213820000	C	8.732545000	0.155543000	10.183522000
H	9.993120000	-0.174910000	9.735561000	H	9.452366000	-0.443040000	9.615039000
C	8.003325000	2.630322000	7.795353000	C	8.077022000	2.801857000	7.821096000
H	8.677460000	3.295879000	8.364406000	H	8.838124000	3.368029000	8.386114000
C	2.717636000	3.319040000	10.380879000	C	2.846660000	3.001813000	10.230621000
C	8.472196000	1.187120000	8.052221000	C	8.342091000	1.308191000	8.067458000
H	7.762356000	0.517222000	7.534740000	H	7.568055000	0.741245000	7.520310000
C	8.065596000	2.997700000	6.316204000	C	8.187148000	3.159960000	6.343551000
H	7.341917000	2.377985000	5.758812000	H	7.409348000	2.621683000	5.774969000
H	7.780449000	4.051880000	6.175932000	H	8.014777000	4.238750000	6.203468000
C	3.386659000	4.170544000	7.785467000	C	3.450444000	4.404064000	7.852007000
H	3.616771000	4.520461000	6.776268000	H	3.692031000	4.935482000	6.928550000
C	2.091794000	4.404061000	8.318077000	C	2.170711000	4.447741000	8.386361000
H	1.351558000	4.923111000	7.706339000	H	1.385582000	5.022499000	7.890118000
C	9.878179000	0.947166000	7.504923000	C	9.724227000	0.903090000	7.554752000
H	10.161090000	-0.108354000	7.636231000	H	9.879662000	-0.179882000	7.669634000
H	10.594666000	1.559228000	8.079969000	H	10.493715000	1.416354000	8.157189000
C	1.757415000	3.988172000	9.594627000	C	1.867954000	3.750249000	9.568069000
H	0.759821000	4.178767000	9.989295000	H	0.855382000	3.797543000	9.968976000
C	6.236888000	-0.124228000	15.628732000	C	6.569416000	0.471141000	15.908856000
H	6.245611000	-1.217938000	15.780951000	H	6.271449000	-0.581917000	16.059160000
H	5.245480000	0.266960000	15.894554000	H	5.778653000	1.126703000	16.298280000
H	6.994282000	0.336815000	16.287147000	H	7.503526000	0.662131000	16.466808000
C	1.256277000	3.049756000	12.258667000	C	1.357524000	2.289529000	11.954481000
H	0.461525000	2.536900000	11.695543000	H	0.601067000	1.859548000	11.274836000
H	1.021656000	4.120427000	12.360445000	H	1.039749000	3.303721000	12.253744000
H	1.373699000	2.592688000	13.247916000	H	1.435290000	1.658895000	12.850303000
C	9.481573000	2.759852000	5.775671000	C	9.576431000	2.765567000	5.824751000
H	9.505529000	2.995780000	4.700011000	H	9.647451000	2.994082000	4.749445000
H	10.180932000	3.455882000	6.271724000	H	10.341343000	3.378793000	6.333297000
C	9.939845000	1.319704000	6.017649000	C	9.865253000	1.281811000	6.072978000
H	10.968028000	1.176076000	5.649344000	H	10.879987000	1.025447000	5.728959000
H	9.295782000	0.629542000	5.444511000	H	9.163611000	0.670430000	5.478212000
N	7.624126000	3.553929000	11.198361000	N	7.643518000	3.637947000	10.919650000
H	8.620337000	3.392083000	11.377404000	H	7.904259000	4.471036000	10.384720000
H	7.554106000	4.427729000	10.668307000	H	7.839518000	3.699862000	11.923063000
H	7.182260000	3.714771000	12.108581000				
3V				5V			
Fe	6.702410000	1.850429000	10.158658000	Fe	7.006152000	2.540613000	10.535903000
O	6.658781000	0.762506000	11.637658000	O	7.177209000	1.480173000	12.106067000
O	4.934952000	2.268976000	10.476341000	O	4.986627000	2.860663000	10.664363000
N	6.686272000	2.692717000	8.425956000	N	6.689826000	2.881288000	8.439655000
O	2.630119000	2.790343000	11.604311000	O	2.582156000	3.097714000	11.640674000
O	6.342967000	0.163282000	14.175304000	O	6.851677000	0.607285000	14.569668000
N	8.267680000	0.907932000	9.467569000	N	8.365380000	1.172632000	9.606982000
C	7.688998000	0.230451000	12.251943000	C	7.807698000	0.384682000	12.433769000
C	7.540741000	-0.126030000	13.633461000	C	7.658298000	-0.125782000	13.768194000

C	8.607352000	-0.720594000	14.307914000	C	8.318152000	-1.292121000	14.148400000
H	8.507160000	-0.986587000	15.360460000	H	8.206014000	-1.678344000	15.162108000
C	9.824348000	-0.986358000	13.647690000	C	9.134636000	-1.992457000	13.233880000
H	10.639080000	-1.456237000	14.203024000	H	9.639659000	-2.905439000	13.557661000
C	9.985592000	-0.660890000	12.312507000	C	9.287482000	-1.524849000	11.942333000
H	10.922142000	-0.872686000	11.791321000	H	9.914346000	-2.062204000	11.225689000
C	8.928153000	-0.040400000	11.603049000	C	8.635584000	-0.334153000	11.523128000
C	4.416665000	3.573041000	8.516332000	C	4.295451000	3.303978000	8.410896000
C	4.116123000	3.033772000	9.800053000	C	4.074723000	3.128924000	9.835997000
C	5.693942000	3.350612000	7.904126000	C	5.615677000	3.176014000	7.803711000
H	5.831270000	3.802302000	6.915297000	H	5.639787000	3.360645000	6.720924000
C	9.103231000	0.248615000	10.204249000	C	8.822019000	0.092640000	10.153516000
H	10.020307000	-0.139272000	9.746357000	H	9.409923000	-0.603719000	9.535924000
C	8.002356000	2.580030000	7.765609000	C	8.000341000	2.777963000	7.793588000
H	8.676308000	3.251243000	8.327473000	H	8.619432000	3.534397000	8.308206000
C	2.838067000	3.325838000	10.385607000	C	2.696528000	3.277249000	10.342361000
C	8.473539000	1.140393000	8.023379000	C	8.590573000	1.402132000	8.167540000
H	7.765548000	0.470650000	7.502905000	H	8.015737000	0.636553000	7.614381000
C	8.061019000	2.935642000	6.282098000	C	8.081219000	3.021871000	6.288372000
H	7.333973000	2.313387000	5.731859000	H	7.476641000	2.265699000	5.757175000
H	7.778807000	3.989028000	6.132108000	H	7.661344000	4.010442000	6.042805000
C	3.458861000	4.363015000	7.826881000	C	3.217826000	3.609359000	7.593106000
H	3.712506000	4.762255000	6.842042000	H	3.382834000	3.746448000	6.521544000
C	2.231356000	4.620344000	8.405091000	C	1.906227000	3.746012000	8.112675000
H	1.489346000	5.227730000	7.882231000	H	1.087048000	3.984293000	7.431101000
C	9.881435000	0.898781000	7.484292000	C	10.059894000	1.335824000	7.727718000
H	10.169957000	-0.153715000	7.628130000	H	10.484655000	0.349245000	7.967075000
H	10.595222000	1.520720000	8.052041000	H	10.629422000	2.086166000	8.303858000
C	1.921044000	4.103843000	9.682166000	C	1.642195000	3.582393000	9.466390000
H	0.946594000	4.323735000	10.119243000	H	0.624478000	3.691273000	9.840351000
C	6.103372000	-0.161102000	15.537027000	C	6.637884000	0.179173000	15.902888000
H	6.195451000	-1.246391000	15.718562000	H	6.168577000	-0.820500000	15.942987000
H	5.073344000	0.153340000	15.752581000	H	5.957064000	0.910667000	16.359997000
H	6.793482000	0.376806000	16.210671000	H	7.578273000	0.154722000	16.482704000
C	1.387808000	3.015950000	12.252876000	C	1.304322000	3.207317000	12.284599000
H	0.543717000	2.610388000	11.667504000	H	0.604002000	2.459405000	11.880768000
H	1.213839000	4.090705000	12.438222000	H	0.891829000	4.220017000	12.153418000
H	1.441654000	2.490247000	13.215865000	H	1.487699000	3.012614000	13.347958000
C	9.475704000	2.693852000	5.739343000	C	9.543111000	2.940254000	5.827604000
H	9.496699000	2.919885000	4.661327000	H	9.597090000	3.083318000	4.736318000
H	10.174766000	3.396336000	6.226809000	H	10.110032000	3.769885000	6.286262000
C	9.940752000	1.257553000	5.993290000	C	10.187508000	1.607819000	6.223837000
H	10.969028000	1.115603000	5.624314000	H	11.251009000	1.596197000	5.934574000
H	9.298939000	0.559512000	5.427073000	H	9.697805000	0.787772000	5.668549000
N	7.555647000	3.218752000	10.988790000	N	7.921314000	4.143283000	10.906819000
H	7.241978000	4.128498000	10.629516000	H	7.804782000	5.024172000	10.401580000
H	7.350282000	3.196678000	11.994393000	H	8.603514000	4.273831000	11.656356000
²VI				⁴VI			
Fe	6.815640000	2.056231000	10.218771000	Fe	6.834280000	2.139478000	10.251511000
O	6.822673000	1.081757000	11.843910000	O	6.843534000	1.161566000	11.915902000
O	4.914162000	2.319940000	10.497892000	O	4.918406000	2.384172000	10.525186000
N	6.719423000	2.803760000	8.450067000	N	6.721147000	2.841372000	8.456048000
O	2.545462000	2.670896000	11.537556000	O	2.534961000	2.708066000	11.535964000
O	6.528862000	0.368977000	14.322633000	O	6.563252000	0.409661000	14.389118000
N	8.277320000	0.963464000	9.478823000	N	8.283457000	1.009280000	9.504506000
C	7.747609000	0.351086000	12.325151000	C	7.733086000	0.370238000	12.361432000
C	7.613428000	-0.072760000	13.722968000	C	7.606561000	-0.078576000	13.750664000
C	8.606155000	-0.871874000	14.312735000	C	8.559486000	-0.954288000	14.305443000
H	8.518710000	-1.183729000	15.353017000	H	8.465664000	-1.286075000	15.339066000
C	9.707646000	-1.266434000	13.561954000	C	9.623400000	-1.393263000	13.531266000
H	10.475599000	-1.888801000	14.025896000	H	10.361712000	-2.071246000	13.963858000
C	9.852103000	-0.890375000	12.207497000	C	9.766146000	-0.982105000	12.184782000
H	10.719500000	-1.237808000	11.641779000	H	10.606769000	-1.358283000	11.596812000
C	8.902299000	-0.094061000	11.577645000	C	8.853538000	-0.115375000	11.591344000
C	4.408708000	3.577403000	8.521254000	C	4.389230000	3.545547000	8.495906000
C	4.095485000	3.008584000	9.814440000	C	4.086341000	3.019860000	9.810081000

C	5.706863000	3.396057000	7.909623000	C	5.694814000	3.371173000	7.886665000
H	5.808921000	3.808934000	6.899746000	H	5.780165000	3.735921000	6.857180000
C	9.065429000	0.214742000	10.169641000	C	9.035968000	0.219568000	10.188518000
H	9.929368000	-0.255844000	9.686330000	H	9.883341000	-0.277101000	9.700752000
C	8.025345000	2.655649000	7.777165000	C	8.026276000	2.685380000	7.784793000
H	8.714437000	3.310114000	8.338596000	H	8.714234000	3.347925000	8.338821000
C	2.751943000	3.222354000	10.358895000	C	2.731740000	3.220725000	10.341140000
C	8.464622000	1.201682000	8.031583000	C	8.470564000	1.234892000	8.055769000
H	7.729006000	0.549440000	7.527013000	H	7.738986000	0.575694000	7.553949000
C	8.079892000	3.015309000	6.295752000	C	8.085182000	3.029979000	6.299764000
H	7.340931000	2.407708000	5.745301000	H	7.354393000	2.411073000	5.751155000
H	7.813811000	4.074346000	6.155064000	H	7.811033000	4.085519000	6.147061000
C	3.435488000	4.297805000	7.834586000	C	3.400755000	4.213578000	7.784793000
H	3.672068000	4.722442000	6.856450000	H	3.626673000	4.604751000	6.790118000
C	2.151059000	4.488224000	8.386570000	C	2.106542000	4.398455000	8.327110000
H	1.409597000	5.062034000	7.826888000	H	1.356595000	4.934445000	7.741799000
C	9.857954000	0.926064000	7.470281000	C	9.865859000	0.957859000	7.498443000
H	10.114709000	-0.136943000	7.595330000	H	10.123867000	-0.103954000	7.630908000
H	10.594974000	1.517575000	8.040767000	H	10.600350000	1.553323000	8.068304000
C	1.808236000	3.960467000	9.628444000	C	1.770503000	3.911676000	9.583742000
H	0.808789000	4.124574000	10.030399000	H	0.766704000	4.067380000	9.977908000
C	6.263609000	0.040488000	15.695054000	C	6.313872000	0.064719000	15.759633000
H	6.174369000	-1.050108000	15.819700000	H	6.152258000	-1.019881000	15.862220000
H	5.310313000	0.524373000	15.938049000	H	5.403195000	0.605900000	16.042571000
H	7.061025000	0.431667000	16.346324000	H	7.153255000	0.383255000	16.397689000
C	1.266712000	2.783218000	12.178206000	C	1.252205000	2.810162000	12.173419000
H	0.481642000	2.326962000	11.554758000	H	0.479916000	2.314672000	11.564341000
H	1.024103000	3.839069000	12.376662000	H	0.985518000	3.866061000	12.336207000
H	1.357545000	2.236938000	13.124525000	H	1.356705000	2.297572000	13.136870000
C	9.487301000	2.749648000	5.745911000	C	9.496362000	2.767152000	5.758372000
H	9.509573000	2.986352000	4.670390000	H	9.522870000	2.995179000	4.681028000
H	10.203396000	3.430620000	6.238927000	H	10.207543000	3.455006000	6.249056000
C	9.917156000	1.300022000	5.983118000	C	9.930778000	1.321028000	6.008999000
H	10.939514000	1.135312000	5.607529000	H	10.955165000	1.156771000	5.638585000
H	9.254685000	0.624535000	5.413485000	H	9.272933000	0.638972000	5.441704000
N	7.667118000	3.550575000	10.954571000	N	7.647525000	3.673534000	11.004522000
H	7.872194000	3.532712000	11.957385000	H	8.656249000	3.790700000	11.132482000
H	7.296208000	4.474086000	10.711899000	H	7.158826000	4.526360000	11.289619000
⁶VI				²VII			
Fe	6.932909000	2.422951000	10.459733000	Fe	6.766441000	2.001572000	10.185664000
O	7.085417000	1.324342000	12.047766000	O	6.738868000	0.962119000	11.826261000
O	5.000825000	2.758754000	10.601900000	O	4.964842000	2.374725000	10.540235000
N	6.717716000	2.897485000	8.424939000	N	6.680783000	2.765297000	8.428439000
O	2.607509000	3.059154000	11.591649000	O	2.596889000	2.731654000	11.604062000
O	6.868007000	0.543357000	14.530813000	O	6.400949000	0.163074000	14.282363000
N	8.304721000	1.064256000	9.537867000	N	8.305394000	1.035866000	9.524545000
C	7.811883000	0.331006000	12.400568000	C	7.697478000	0.315463000	12.336905000
C	7.714319000	-0.140560000	13.777572000	C	7.554028000	-0.148831000	13.725608000
C	8.482997000	-1.233780000	14.200281000	C	8.600868000	-0.839667000	14.351416000
H	8.418265000	-1.589500000	15.228421000	H	8.505937000	-1.168129000	15.386031000
C	9.336050000	-1.872048000	13.299468000	C	9.769004000	-1.111322000	13.642812000
H	9.929135000	-2.724185000	13.637725000	H	10.578890000	-1.653582000	14.135126000
C	9.445783000	-1.438937000	11.966973000	C	9.924254000	-0.713440000	12.297883000
H	10.118783000	-1.959296000	11.281670000	H	10.841443000	-0.970575000	11.762937000
C	8.707968000	-0.345064000	11.501067000	C	8.926001000	-0.004046000	11.635931000
C	4.333208000	3.372879000	8.383133000	C	4.394768000	3.594380000	8.540976000
C	4.092862000	3.119794000	9.784132000	C	4.112250000	3.059095000	9.834705000
C	5.653058000	3.242533000	7.789448000	C	5.671611000	3.389181000	7.909889000
H	5.700894000	3.466773000	6.715957000	H	5.773819000	3.807824000	6.902191000
C	8.864451000	0.054209000	10.113435000	C	9.105954000	0.314549000	10.234058000
H	9.528916000	-0.596808000	9.528695000	H	9.992292000	-0.128253000	9.765747000
C	8.031015000	2.752573000	7.791765000	C	7.980483000	2.642674000	7.750034000
H	8.695206000	3.440910000	8.348271000	H	8.649883000	3.355219000	8.265480000
C	2.731433000	3.291953000	10.299917000	C	2.796514000	3.273031000	10.384183000
C	8.522727000	1.319589000	8.097733000	C	8.491509000	1.227960000	8.070460000
H	7.862269000	0.624462000	7.548205000	H	7.789834000	0.520505000	7.591889000

C	8.130427000	3.070243000	6.301723000	C	8.012221000	2.921449000	6.248812000
H	7.463660000	2.393598000	5.739052000	H	7.295503000	2.253326000	5.740133000
H	7.788493000	4.100781000	6.116035000	H	7.698078000	3.957426000	6.049166000
C	3.267512000	3.755506000	7.567889000	C	3.400797000	4.319557000	7.832631000
H	3.447908000	3.945367000	6.507242000	H	3.641752000	4.716004000	6.843001000
C	1.965971000	3.898844000	8.089014000	C	2.151363000	4.517942000	8.388517000
H	1.153168000	4.195273000	7.422874000	H	1.386310000	5.078605000	7.846610000
C	9.966951000	1.136999000	7.613745000	C	9.896231000	0.988726000	7.520877000
H	10.297871000	0.101131000	7.779885000	H	10.206982000	-0.051907000	7.699691000
H	10.620658000	1.792334000	8.215441000	H	10.605592000	1.644803000	8.054949000
C	1.694109000	3.672611000	9.436264000	C	1.848303000	3.994002000	9.664979000
H	0.678363000	3.792860000	9.812124000	H	0.855796000	4.161190000	10.084438000
C	6.668707000	0.186288000	15.901856000	C	6.126712000	-0.197409000	15.642529000
H	6.286750000	-0.844067000	15.985931000	H	6.163213000	-1.290921000	15.769653000
H	5.924386000	0.891165000	16.291895000	H	5.114463000	0.169066000	15.851048000
H	7.607558000	0.283421000	16.470605000	H	6.847017000	0.283954000	16.322881000
C	1.335575000	3.198295000	12.238118000	C	1.334579000	2.892535000	12.229370000
H	0.604814000	2.494279000	11.809018000	H	0.522431000	2.438291000	11.633942000
H	0.963671000	4.230781000	12.141274000	H	1.097317000	3.957273000	12.403872000
H	1.508351000	2.960085000	13.294419000	H	1.399423000	2.377429000	13.197643000
C	9.575013000	2.890360000	5.820057000	C	9.425885000	2.692199000	5.698935000
H	9.631868000	3.095228000	4.739092000	H	9.430052000	2.866424000	4.611025000
H	10.219587000	3.634360000	6.320909000	H	10.111456000	3.435177000	6.143883000
C	10.091642000	1.481567000	6.124583000	C	9.931974000	1.282485000	6.014955000
H	11.144015000	1.381933000	5.813667000	H	10.959696000	1.149117000	5.641012000
H	9.514258000	0.746687000	5.535733000	H	9.302776000	0.542548000	5.488956000
N	7.440960000	4.154507000	11.274044000	N	7.684042000	3.301566000	10.859070000
H	8.110625000	4.833781000	10.896101000	H	8.596415000	3.005283000	11.249107000
H	7.039490000	4.514432000	12.147209000				
⁶VII				²VIII			
Fe	6.672168000	2.076320000	10.476073000	Fe	6.782627000	1.722353000	10.018461000
O	6.831420000	0.884509000	11.977260000	O	6.797726000	0.654390000	11.575484000
O	4.779320000	2.483385000	10.540486000	O	5.025011000	2.295732000	10.506350000
N	6.656023000	2.830741000	8.513875000	N	6.703662000	2.558427000	8.285542000
O	2.338869000	2.827883000	11.431517000	O	2.877691000	3.083218000	11.747922000
O	6.726804000	0.218238000	14.515777000	O	6.563295000	0.107059000	14.117146000
N	8.245958000	0.943712000	9.585320000	N	8.453692000	0.969262000	9.396412000
C	7.807748000	0.178786000	12.435514000	C	7.863949000	0.175529000	12.163147000
C	7.780079000	-0.225946000	13.826859000	C	7.762540000	-0.176459000	13.554059000
C	8.805830000	-1.023402000	14.342930000	C	8.848273000	-0.735301000	14.219908000
H	8.788032000	-1.332688000	15.387870000	H	8.766831000	-1.001674000	15.274255000
C	9.867194000	-1.426393000	13.521485000	C	10.071110000	-0.957559000	13.546609000
H	10.660469000	-2.048893000	13.940872000	H	10.907096000	-1.403381000	14.090406000
C	9.923276000	-1.038431000	12.180728000	C	10.205315000	-0.606766000	12.217923000
H	10.759727000	-1.355659000	11.553271000	H	11.148660000	-0.768283000	11.689691000
C	8.916359000	-0.233108000	11.622411000	C	9.118214000	-0.021583000	11.513304000
C	4.341734000	3.614725000	8.474562000	C	4.435266000	3.446408000	8.465231000
C	3.966281000	3.110699000	9.766893000	C	4.203055000	3.029149000	9.810472000
C	5.671668000	3.428465000	7.929565000	C	5.680885000	3.189172000	7.793193000
H	5.810280000	3.846278000	6.923788000	H	5.762288000	3.612052000	6.784790000
C	9.029964000	0.142139000	10.224832000	C	9.298804000	0.307040000	10.121399000
H	9.873050000	-0.326588000	9.700545000	H	10.224727000	-0.058568000	9.661834000
C	7.972280000	2.663429000	7.879184000	C	8.010721000	2.519242000	7.605039000
H	8.665687000	3.312927000	8.442956000	H	8.625583000	3.287125000	8.111773000
C	2.603642000	3.323771000	10.220766000	C	2.985095000	3.455913000	10.450011000
C	8.412833000	1.204011000	8.143371000	C	8.632314000	1.155309000	7.941866000
H	7.674256000	0.556716000	7.634497000	H	7.998568000	0.388459000	7.459307000
C	8.060051000	3.020528000	6.394935000	C	8.024063000	2.788391000	6.101142000
H	7.323288000	2.418480000	5.834569000	H	7.359095000	2.063410000	5.599763000
H	7.798007000	4.080146000	6.249749000	H	7.633129000	3.795248000	5.888591000
C	3.392119000	4.296568000	7.692724000	C	3.445985000	4.202405000	7.772529000
H	3.686556000	4.675398000	6.710991000	H	3.643243000	4.502478000	6.739964000
C	2.089112000	4.489028000	8.154722000	C	2.270377000	4.560765000	8.397723000
H	1.363985000	5.018638000	7.533154000	H	1.512345000	5.141020000	7.866601000
C	9.803193000	0.923772000	7.566583000	C	10.054511000	1.029367000	7.397964000
H	10.056385000	-0.140131000	7.690322000	H	10.452478000	0.022011000	7.593755000

H	10.546409000	1.507307000	8.138268000	H	10.705060000	1.750268000	7.923645000
C	1.693506000	4.006809000	9.410702000	C	2.042775000	4.195008000	9.746442000
H	0.670283000	4.168821000	9.749752000	H	1.117535000	4.507659000	10.232014000
C	6.591497000	-0.116285000	15.894507000	C	6.360271000	-0.197253000	15.486803000
H	6.511312000	-1.207526000	16.033924000	H	6.465749000	-1.278921000	15.684470000
H	5.665672000	0.364371000	16.235832000	H	5.333105000	0.111363000	15.725350000
H	7.442088000	0.266904000	16.483193000	H	7.061871000	0.354836000	16.137699000
C	1.038617000	2.990587000	11.991320000	C	1.728979000	3.473838000	12.479427000
H	0.272672000	2.496974000	11.369647000	H	0.804161000	3.053098000	12.045513000
H	0.784982000	4.057981000	12.106309000	H	1.630226000	4.573226000	12.531779000
H	1.069246000	2.514105000	12.979657000	H	1.857358000	3.078153000	13.496482000
C	9.466095000	2.750550000	5.850064000	C	9.451654000	2.663160000	5.552662000
H	9.497826000	2.995334000	4.776160000	H	9.442591000	2.822866000	4.462397000
H	10.187261000	3.419889000	6.352196000	H	10.075723000	3.464811000	5.986587000
C	9.875891000	1.295677000	6.081791000	C	10.070308000	1.303771000	5.888228000
H	10.897317000	1.116150000	5.709314000	H	11.105813000	1.249932000	5.515274000
H	9.205683000	0.631515000	5.507316000	H	9.504316000	0.508146000	5.371583000
N	7.599646000	3.622901000	11.204227000	N	7.552083000	3.170237000	10.919320000
H	8.487722000	3.902357000	10.752381000	H	8.545070000	3.025105000	11.130979000
				N	6.903595000	3.350715000	12.197459000
				H	5.883059000	3.356555000	12.021372000
				H	7.063514000	2.583585000	12.872147000
				H	7.176714000	4.241856000	12.635681000
⁶VIII				¹IX			
Fe	6.806401000	2.264943000	10.414172000	Fe	7.007234000	2.402878000	10.248420000
O	7.168795000	1.302076000	12.046194000	O	7.203962000	1.631334000	12.026744000
O	4.896111000	2.467471000	10.458574000	O	5.254972000	2.285341000	10.355363000
N	6.741289000	2.888189000	8.418513000	N	6.898518000	3.106629000	8.423597000
O	2.450382000	2.777238000	11.363985000	O	2.869024000	2.277012000	11.415118000
O	7.268698000	0.719438000	14.597215000	O	7.218854000	1.054013000	14.573291000
N	8.221923000	0.924629000	9.477207000	N	8.091307000	1.099131000	9.454645000
C	7.938454000	0.295910000	12.390741000	C	7.743745000	0.503394000	12.355889000
C	7.997144000	-0.071322000	13.773597000	C	7.755909000	0.132248000	13.747879000
C	8.771188000	-1.157583000	14.178206000	C	8.287629000	-1.090208000	14.126334000
H	8.805142000	-1.445852000	15.229387000	H	8.283015000	-1.386664000	15.175614000
C	9.520334000	-1.893835000	13.237498000	C	8.846964000	-1.976314000	13.166557000
H	10.117264000	-2.743959000	13.575487000	H	9.255311000	-2.930805000	13.505282000
C	9.507780000	-1.531328000	11.901998000	C	8.887986000	-1.633654000	11.836179000
H	10.102372000	-2.084950000	11.170497000	H	9.337271000	-2.298471000	11.094936000
C	8.730789000	-0.429299000	11.459178000	C	8.347965000	-0.383504000	11.403551000
C	4.401619000	3.583170000	8.381438000	C	4.536440000	3.587678000	8.442190000
C	4.055302000	3.088075000	9.675004000	C	4.307707000	2.923629000	9.678263000
C	5.722142000	3.406264000	7.815489000	C	5.847804000	3.547045000	7.825001000
H	5.825835000	3.748596000	6.776670000	H	5.914322000	3.879709000	6.782461000
C	8.813830000	-0.065380000	10.057288000	C	8.497233000	-0.009658000	10.044523000
H	9.471854000	-0.715666000	9.463934000	H	9.033330000	-0.728512000	9.413905000
C	8.037844000	2.662234000	7.774033000	C	8.174383000	2.829127000	7.750129000
H	8.764450000	3.272664000	8.341437000	H	8.945126000	3.386746000	8.309850000
C	2.705157000	3.275581000	10.131865000	C	2.997489000	2.922647000	10.250625000
C	8.409691000	1.182344000	8.034761000	C	8.408657000	1.331820000	8.011125000
H	7.663736000	0.567680000	7.497315000	H	7.657614000	0.765330000	7.432721000
C	8.147986000	3.018299000	6.292302000	C	8.298407000	3.162714000	6.269297000
H	7.406810000	2.433216000	5.719876000	H	7.533905000	2.609080000	5.698003000
H	7.908877000	4.083695000	6.145089000	H	8.122340000	4.238113000	6.109283000
C	3.424585000	4.237806000	7.583570000	C	3.473517000	4.225032000	7.781379000
H	3.712846000	4.602159000	6.593873000	H	3.657814000	4.721016000	6.825955000
C	2.135867000	4.411699000	8.049907000	C	2.201402000	4.221929000	8.350642000
H	1.386378000	4.918555000	7.437721000	H	1.375427000	4.724255000	7.842542000
C	9.807670000	0.867295000	7.488120000	C	9.814656000	0.930941000	7.560333000
H	10.033112000	-0.203142000	7.606740000	H	9.977877000	-0.147911000	7.697585000
H	10.549267000	1.425809000	8.086442000	H	10.553120000	1.462928000	8.184530000
C	1.775265000	3.928270000	9.326790000	C	1.960851000	3.578613000	9.570997000
H	0.752985000	4.071532000	9.678660000	H	0.955843000	3.591428000	9.992466000
C	7.285630000	0.458170000	15.991091000	C	7.188648000	0.788588000	15.968970000
H	6.880599000	-0.542624000	16.223924000	H	6.585539000	-0.107821000	16.196411000
H	6.645921000	1.219481000	16.458257000	H	6.724597000	1.664685000	16.441213000

H	8.304953000	0.538081000	16.409720000	H	8.205710000	0.651756000	16.376610000
C	1.142953000	2.899211000	11.894652000	C	1.593812000	2.215399000	12.048484000
H	0.394789000	2.382767000	11.266303000	H	0.852774000	1.706655000	11.408901000
H	0.842190000	3.956415000	12.009151000	H	1.224923000	3.222260000	12.307565000
H	1.163018000	2.425784000	12.886191000	H	1.739009000	1.634616000	12.968558000
C	9.556205000	2.714162000	5.769731000	C	9.701426000	2.764747000	5.787826000
H	9.614736000	2.957060000	4.696387000	H	9.792027000	2.966392000	4.708799000
H	10.284446000	3.365963000	6.284848000	H	10.450013000	3.398102000	6.295661000
C	9.927565000	1.249045000	6.008273000	C	10.001077000	1.289406000	6.077490000
H	10.953902000	1.048643000	5.659980000	H	11.030366000	1.042113000	5.772570000
H	9.258017000	0.602849000	5.412663000	H	9.328842000	0.656783000	5.471288000
N	7.680610000	3.862275000	11.112228000	N	7.735939000	3.884290000	10.835501000
H	7.621825000	4.815936000	10.752608000	H	7.911437000	4.726415000	12.276111000
N	8.060544000	3.922190000	12.483607000	N	8.052729000	4.126572000	12.200123000
H	7.871429000	2.990159000	12.898997000	H	7.829409000	3.258482000	12.732196000
H	9.062216000	4.133429000	12.622104000	H	9.054207000	4.354196000	12.325263000
H	7.521031000	4.611856000	13.031392000	H	7.492343000	4.903682000	12.590134000
³ IX				⁵ IX			
Fe	6.812531000	2.098610000	10.179619000	Fe	6.916627000	2.330590000	10.415358000
O	6.874205000	1.194611000	11.884403000	O	7.195925000	1.342656000	12.012886000
O	5.009140000	2.370074000	10.496159000	O	4.921631000	2.664328000	10.538025000
N	6.728385000	2.848476000	8.418624000	N	6.735926000	2.879351000	8.387283000
O	2.633135000	2.678164000	11.558698000	O	2.506896000	2.973782000	11.454244000
O	6.584776000	0.471112000	14.373509000	O	7.259653000	0.737389000	14.561379000
N	8.324674000	1.080937000	9.509423000	N	8.268938000	0.977359000	9.472072000
C	7.744043000	0.385974000	12.341674000	C	7.903439000	0.287769000	12.355016000
C	7.612187000	-0.051124000	13.732084000	C	7.935423000	-0.089758000	13.733004000
C	8.548585000	-0.941731000	14.282764000	C	8.641499000	-1.227497000	14.125706000
H	8.453022000	-1.270972000	15.317148000	H	8.659434000	-1.526809000	15.174142000
C	9.604734000	-1.404307000	13.504332000	C	9.340109000	-1.998998000	13.176709000
H	10.328086000	-2.096842000	13.939391000	H	9.882658000	-2.887944000	13.506016000
C	9.759758000	-0.996571000	12.162161000	C	9.351394000	-1.625994000	11.842434000
H	10.596752000	-1.380911000	11.574605000	H	9.910831000	-2.208563000	11.106166000
C	8.859151000	-0.112878000	11.571937000	C	8.648824000	-0.472168000	11.413582000
C	4.415777000	3.595703000	8.504130000	C	4.370437000	3.464789000	8.343793000
C	4.139427000	3.048233000	9.791897000	C	4.072534000	3.120329000	9.721289000
C	5.701142000	3.423080000	7.878094000	C	5.696985000	3.302663000	7.760725000
H	5.789339000	3.813538000	6.858218000	H	5.763345000	3.571346000	6.698236000
C	9.049330000	0.250211000	10.181336000	C	8.756951000	-0.086773000	10.020347000
H	9.876367000	-0.263363000	9.677539000	H	9.337089000	-0.784011000	9.398908000
C	8.019472000	2.695920000	7.721781000	C	8.042089000	2.691408000	7.745451000
H	8.718564000	3.405081000	8.200021000	H	8.733435000	3.344412000	8.309277000
C	2.824359000	3.229042000	10.342998000	C	2.689202000	3.310067000	10.197836000
C	8.518026000	1.279835000	8.051735000	C	8.477948000	1.236682000	8.032363000
H	7.818818000	0.573019000	7.568994000	H	7.791966000	0.573666000	7.474114000
C	8.036189000	2.953393000	6.216778000	C	8.147950000	3.025900000	6.259927000
H	7.317925000	2.275721000	5.723560000	H	7.453656000	2.384313000	5.689576000
H	7.717840000	3.985752000	6.005650000	H	7.846894000	4.071773000	6.088644000
C	3.408263000	4.296369000	7.793263000	C	3.351958000	3.950950000	7.536473000
H	3.642089000	4.701302000	6.805611000	H	3.569923000	4.207585000	6.496991000
C	2.151741000	4.459383000	8.346929000	C	2.031196000	4.121607000	8.025026000
H	1.373376000	4.999503000	7.803261000	H	1.262961000	4.507933000	7.352097000
C	9.926937000	1.041761000	7.510081000	C	9.913630000	1.010679000	7.539343000
H	10.244124000	0.005246000	7.697552000	H	10.210339000	-0.036960000	7.696918000
H	10.629652000	1.706147000	8.042744000	H	10.590566000	1.637786000	8.145795000
C	1.858415000	3.925483000	9.619425000	C	1.697503000	3.806377000	9.333778000
H	0.859627000	4.062763000	10.034451000	H	0.675308000	3.943522000	9.685457000
C	6.342023000	0.144338000	15.748773000	C	7.245891000	0.457148000	15.953329000
H	6.158127000	-0.935555000	15.863986000	H	6.774259000	-0.518204000	16.166275000
H	5.446343000	0.707540000	16.036749000	H	6.652315000	1.252669000	16.423800000
H	7.194876000	0.449661000	16.375606000	H	8.264306000	0.465797000	16.380434000
C	1.354786000	2.777800000	12.166481000	C	1.211480000	3.085959000	12.065504000
H	0.573343000	2.295255000	11.552771000	H	0.486119000	2.440033000	11.546765000
H	1.069376000	3.829093000	12.348816000	H	0.868006000	4.131830000	12.049321000
H	1.427990000	2.254692000	13.129703000	H	1.340490000	2.749038000	13.100767000
C	9.448250000	2.721046000	5.663481000	C	9.582880000	2.797830000	5.769204000

H	9.445387000	2.875765000	4.572785000	H	9.643677000	3.014839000	4.690740000
H	10.131811000	3.476052000	6.090868000	H	10.256909000	3.510340000	6.277155000
C	9.964808000	1.319961000	6.000921000	C	10.047625000	1.366926000	6.054167000
H	10.994825000	1.190693000	5.632148000	H	11.094520000	1.232207000	5.737490000
H	9.343841000	0.567894000	5.482792000	H	9.441289000	0.661624000	5.458126000
N	7.671618000	3.589778000	10.807174000	N	7.717903000	3.916139000	11.160674000
H	8.164376000	4.165541000	10.119960000	H	7.787642000	4.855160000	10.764982000
N	8.534320000	3.492685000	11.943131000	N	8.178818000	3.945671000	12.503635000
H	8.007130000	3.133081000	12.751626000	H	7.933214000	3.040168000	12.945091000
H	9.356317000	2.877458000	11.802550000	H	9.202781000	4.065362000	12.582959000
H	8.890244000	4.424858000	12.209981000	H	7.736562000	4.691305000	13.066073000
¹X				³X			
Fe	6.793664000	1.850084000	10.080997000	Fe	6.798928000	1.885258000	10.144052000
O	6.775438000	0.807989000	11.695201000	O	6.802339000	0.852416000	11.699927000
O	4.999563000	2.288489000	10.476002000	O	5.001794000	2.365840000	10.487278000
N	6.758735000	2.697504000	8.341505000	N	6.779641000	2.745508000	8.413229000
O	2.695579000	2.815092000	11.586490000	O	2.628853000	2.792253000	11.512720000
O	6.620872000	0.303067000	14.253423000	O	6.837178000	0.584715000	14.291557000
N	8.365871000	0.936279000	9.408089000	N	8.265089000	0.807765000	9.357298000
C	7.818326000	0.241066000	12.231470000	C	7.824480000	0.199030000	12.201087000
C	7.761940000	-0.085202000	13.634663000	C	7.843750000	-0.021869000	13.616295000
C	8.828533000	-0.724975000	14.253618000	C	8.856543000	-0.784059000	14.193252000
H	8.781307000	-0.964167000	15.316580000	H	8.862690000	-0.962157000	15.269080000
C	9.990440000	-1.070468000	13.522608000	C	9.890760000	-1.325914000	13.399930000
H	10.811713000	-1.578873000	14.032909000	H	10.671297000	-1.924397000	13.874846000
C	10.080105000	-0.760884000	12.181668000	C	9.923572000	-1.080735000	12.039723000
H	10.973930000	-1.019075000	11.607376000	H	10.734391000	-1.471771000	11.420060000
C	9.014248000	-0.087457000	11.520189000	C	8.909328000	-0.298449000	11.427373000
C	4.528180000	3.661173000	8.539078000	C	4.503946000	3.623290000	8.490811000
C	4.212663000	3.087626000	9.809058000	C	4.181960000	3.079836000	9.769923000
C	5.775469000	3.394281000	7.865442000	C	5.789602000	3.405675000	7.891892000
H	5.874268000	3.835769000	6.866622000	H	5.927766000	3.852656000	6.900556000
C	9.161469000	0.195688000	10.115776000	C	9.022129000	-0.006160000	10.019124000
H	10.025450000	-0.269655000	9.626172000	H	9.843664000	-0.510323000	9.496052000
C	8.040220000	2.532548000	7.628909000	C	8.073214000	2.561494000	7.727353000
H	8.747273000	3.230162000	8.117746000	H	8.809863000	3.150123000	8.304225000
C	2.927732000	3.393590000	10.385970000	C	2.867753000	3.336184000	10.298308000
C	8.527351000	1.109025000	7.947792000	C	8.439854000	1.077661000	7.916334000
H	7.810173000	0.412964000	7.474978000	H	7.669112000	0.486415000	7.389379000
C	8.043868000	2.807226000	6.126581000	C	8.142435000	2.981410000	6.261299000
H	7.299521000	2.153465000	5.639172000	H	7.368326000	2.438693000	5.691093000
H	7.747934000	3.848673000	5.927541000	H	7.930623000	4.057688000	6.165347000
C	3.588429000	4.502400000	7.880878000	C	3.545735000	4.388605000	7.767423000
H	3.853710000	4.924205000	6.907884000	H	3.821811000	4.787315000	6.787890000
C	2.368012000	4.782881000	8.460825000	C	2.294116000	4.617902000	8.298584000
H	1.648649000	5.432584000	7.957019000	H	1.554465000	5.204691000	7.749347000
C	9.918507000	0.848356000	7.371659000	C	9.812269000	0.752943000	7.327331000
H	10.220516000	-0.194288000	7.553580000	H	10.015672000	-0.325959000	7.407657000
H	10.647520000	1.498442000	7.886700000	H	10.585344000	1.280422000	7.913209000
C	2.036585000	4.225706000	9.717218000	C	1.955529000	4.089223000	9.566327000
H	1.067346000	4.456766000	10.160553000	H	0.960118000	4.279591000	9.969182000
C	6.471483000	0.043515000	15.638135000	C	6.765144000	0.430727000	15.700975000
H	6.501293000	-1.038930000	15.857427000	H	6.637541000	-0.628169000	15.986643000
H	5.487298000	0.438801000	15.925465000	H	5.885097000	0.999532000	16.030446000
H	7.250036000	0.549827000	16.237072000	H	7.663501000	0.833170000	16.201782000
C	1.456838000	3.049460000	12.231645000	C	1.354021000	2.971307000	12.104378000
H	0.604248000	2.693050000	11.625618000	H	0.549441000	2.539096000	11.482398000
H	1.308099000	4.120535000	12.459711000	H	1.130609000	4.038386000	12.284536000
H	1.484242000	2.485153000	13.174224000	H	1.381242000	2.444958000	13.068563000
C	9.439456000	2.545789000	5.544997000	C	9.529029000	2.665105000	5.686483000
H	9.421212000	2.710156000	4.455569000	H	9.557796000	2.947526000	4.621916000
H	10.148822000	3.280778000	5.965697000	H	10.285368000	3.283928000	6.201420000
C	9.929582000	1.130595000	5.863021000	C	9.881536000	1.185368000	5.856874000
H	10.947197000	0.978885000	5.468441000	H	10.890358000	0.982040000	5.463227000
H	9.278626000	0.396917000	5.354935000	H	9.178760000	0.572435000	5.264934000
N	7.522653000	3.200236000	10.908467000	N	7.703909000	3.393385000	11.171340000

H	8.172214000	3.865262000	10.461307000	H	7.936287000	4.292512000	10.735411000
N	7.244900000	3.525566000	12.124724000	N	7.481763000	3.554396000	12.453169000
H	6.651692000	2.879136000	12.653434000	H	7.129264000	2.745022000	12.969513000
H	7.697327000	4.330430000	12.564050000	H	7.471718000	4.479684000	12.883522000
⁵X				²XI			
Fe	6.697099000	2.096921000	10.394375000	Fe	6.853474000	1.943219000	10.168500000
O	6.993193000	1.089166000	11.983621000	O	6.834300000	0.964973000	11.726940000
O	4.837338000	2.514484000	10.486202000	O	4.929741000	2.317841000	10.452948000
N	6.684778000	2.831421000	8.424036000	N	6.809777000	2.796495000	8.420093000
O	2.407720000	2.917755000	11.402600000	O	2.540162000	2.684484000	11.416382000
O	6.954964000	0.429309000	14.530099000	O	6.896048000	0.730840000	14.315830000
N	8.251839000	0.936226000	9.501626000	N	8.259181000	0.828109000	9.374631000
C	7.926871000	0.267525000	12.399688000	C	7.829337000	0.255578000	12.222896000
C	7.933566000	-0.122492000	13.778963000	C	7.850911000	0.053990000	13.636701000
C	8.911239000	-0.998051000	14.251065000	C	8.822482000	-0.768118000	14.207591000
H	8.918450000	-1.297212000	15.299592000	H	8.831488000	-0.938967000	15.284560000
C	9.901464000	-1.504646000	13.385511000	C	9.806614000	-1.379473000	13.405382000
H	10.654952000	-2.191005000	13.778480000	H	10.554127000	-2.022573000	13.874780000
C	9.918452000	-1.132334000	12.052332000	C	9.838812000	-1.148547000	12.040771000
H	10.685585000	-1.518823000	11.376330000	H	10.615689000	-1.594413000	11.415204000
C	8.942082000	-0.239808000	11.541316000	C	8.867466000	-0.311235000	11.436675000
C	4.361150000	3.594264000	8.389936000	C	4.526004000	3.655831000	8.503858000
C	4.005638000	3.136848000	9.693434000	C	4.158497000	3.043610000	9.764801000
C	5.679639000	3.388712000	7.830273000	C	5.826664000	3.448091000	7.897554000
H	5.797806000	3.755360000	6.801816000	H	5.948161000	3.893790000	6.903548000
C	9.018287000	0.112176000	10.136647000	C	8.979317000	-0.026725000	10.027157000
H	9.821409000	-0.400576000	9.590741000	H	9.765569000	-0.572824000	9.492634000
C	7.985244000	2.631866000	7.771560000	C	8.093935000	2.575850000	7.723744000
H	8.701652000	3.273541000	8.317948000	H	8.843447000	3.152387000	8.294710000
C	2.667289000	3.377535000	10.157442000	C	2.796014000	3.277819000	10.273799000
C	8.404478000	1.168339000	8.052321000	C	8.421369000	1.083492000	7.927116000
H	7.652134000	0.527389000	7.555885000	H	7.630311000	0.505860000	7.416241000
C	8.063655000	2.966227000	6.281875000	C	8.157701000	2.981869000	6.254818000
H	7.315647000	2.364711000	5.735964000	H	7.363349000	2.454477000	5.698307000
H	7.810577000	4.026277000	6.122643000	H	7.974205000	4.062837000	6.153308000
C	3.400223000	4.262142000	7.583829000	C	3.595306000	4.434283000	7.827740000
H	3.693706000	4.599543000	6.586246000	H	3.869406000	4.888187000	6.872641000
C	2.119573000	4.482734000	8.053175000	C	2.296012000	4.649817000	8.350472000
H	1.381847000	4.998169000	7.433953000	H	1.595439000	5.273355000	7.791496000
C	9.785527000	0.859612000	7.466039000	C	9.778978000	0.718733000	7.327456000
H	10.024520000	-0.206459000	7.598738000	H	9.952774000	-0.364552000	7.414706000
H	10.543247000	1.437040000	8.024985000	H	10.570670000	1.230769000	7.901637000
C	1.752435000	4.040016000	9.342481000	C	1.895737000	4.081301000	9.551565000
H	0.737170000	4.222624000	9.696314000	H	0.889293000	4.257611000	9.930392000
C	6.879321000	0.105297000	15.908606000	C	6.829580000	0.597960000	15.729823000
H	6.713680000	-0.975427000	16.066058000	H	6.636982000	-0.447310000	16.027031000
H	6.021347000	0.660728000	16.311661000	H	5.991798000	1.226605000	16.059864000
H	7.791681000	0.410357000	16.451683000	H	7.757971000	0.947448000	16.214262000
C	1.115690000	3.112740000	11.950059000	C	1.253037000	2.814788000	12.042255000
H	0.334976000	2.612862000	11.348752000	H	0.465248000	2.417097000	11.384019000
H	0.865027000	4.185332000	12.038475000	H	1.049211000	3.869532000	12.283549000
H	1.132109000	2.666915000	12.954282000	H	1.308851000	2.222393000	12.962890000
C	9.461040000	2.670404000	5.728153000	C	9.529691000	2.622409000	5.670208000
H	9.488064000	2.899929000	4.650656000	H	9.553827000	2.893311000	4.602799000
H	10.196085000	3.336061000	6.215124000	H	10.307305000	3.225815000	6.171183000
C	9.852277000	1.212913000	5.976311000	C	9.842899000	1.135461000	5.852167000
H	10.867997000	1.013804000	5.597828000	H	10.841636000	0.900709000	5.450939000
H	9.168223000	0.551357000	5.415160000	H	9.117462000	0.535840000	5.274365000
N	7.675016000	3.695878000	11.096072000	N	7.609245000	3.489349000	11.149635000
H	7.756422000	4.576275000	10.574016000	H	8.000482000	4.323318000	10.696588000
N	8.346444000	3.746561000	12.208810000	N	7.654093000	3.590169000	12.448167000
H	8.283539000	2.943925000	12.836328000	H	7.264062000	2.820519000	12.999441000
H	8.866937000	4.580779000	12.485771000	H	8.077180000	4.399732000	12.905111000
⁴XI				⁶XI			

Fe	6.877219000	2.287282000	10.418238000	Fe	6.686629000	2.163593000	10.391120000
O	7.159467000	1.322658000	12.009812000	O	6.908702000	1.047825000	12.062198000
O	4.931064000	2.746053000	10.574557000	O	4.920163000	2.742867000	10.562584000
N	6.726587000	2.888537000	8.402869000	N	6.647539000	2.830382000	8.404913000
O	2.510990000	3.027452000	11.484225000	O	2.500928000	3.122799000	11.525193000
O	7.078871000	0.633310000	14.544118000	O	6.758406000	0.214011000	14.526141000
N	8.282220000	0.995167000	9.486330000	N	8.285219000	1.025009000	9.558958000
C	7.926896000	0.322993000	12.381449000	C	7.832428000	0.272426000	12.448730000
C	7.899590000	-0.086000000	13.752074000	C	7.785331000	-0.224269000	13.833270000
C	8.696086000	-1.153469000	14.171994000	C	8.783634000	-1.089908000	14.317751000
H	8.677488000	-1.474384000	15.213906000	H	8.745820000	-1.455913000	15.343321000
C	9.531011000	-1.826446000	13.260587000	C	9.816581000	-1.475778000	13.477950000
H	10.143522000	-2.659528000	13.612459000	H	10.592141000	-2.148103000	13.850075000
C	9.579886000	-1.434764000	11.931625000	C	9.883161000	-1.020468000	12.136844000
H	10.231420000	-1.952154000	11.223139000	H	10.704997000	-1.360370000	11.501909000
C	8.787536000	-0.354233000	11.473350000	C	8.927337000	-0.160581000	11.608424000
C	4.364139000	3.491139000	8.365698000	C	4.298015000	3.495899000	8.366783000
C	4.072228000	3.171396000	9.748685000	C	4.011092000	3.201069000	9.730651000
C	5.689554000	3.325017000	7.781103000	C	5.616407000	3.304173000	7.790302000
H	5.755728000	3.600525000	6.720649000	H	5.705557000	3.608841000	6.739310000
C	8.892599000	0.020217000	10.076727000	C	9.051548000	0.216144000	10.205261000
H	9.571248000	-0.613271000	9.489855000	H	9.881868000	-0.278882000	9.685397000
C	8.028634000	2.695752000	7.751170000	C	7.966110000	2.676136000	7.781884000
H	8.729414000	3.347288000	8.304955000	H	8.635779000	3.368461000	8.326964000
C	2.688046000	3.351908000	10.225230000	C	2.686592000	3.426943000	10.224710000
C	8.460828000	1.238640000	8.039124000	C	8.457490000	1.244813000	8.104801000
H	7.745137000	0.581137000	7.512422000	H	7.752048000	0.549093000	7.614304000
C	8.117021000	3.029899000	6.264396000	C	8.056809000	2.981459000	6.287175000
H	7.406468000	2.397609000	5.703974000	H	7.356731000	2.325732000	5.740541000
H	7.826182000	4.079715000	6.099745000	H	7.746627000	4.021959000	6.101819000
C	3.340279000	3.959032000	7.554045000	C	3.277765000	4.006117000	7.528249000
H	3.553706000	4.200907000	6.510073000	H	3.512718000	4.229291000	6.484519000
C	2.018740000	4.127757000	8.043190000	C	2.001079000	4.218253000	8.024459000
H	1.246582000	4.498128000	7.365851000	H	1.215217000	4.611514000	7.375713000
C	9.874156000	0.980956000	7.502089000	C	9.866924000	1.000706000	7.558685000
H	10.147281000	-0.075840000	7.639014000	H	10.159664000	-0.048020000	7.717316000
H	10.585343000	1.583947000	8.093658000	H	10.576534000	1.630234000	8.124399000
C	1.689880000	3.828513000	9.355971000	C	1.703756000	3.929635000	9.369200000
H	0.667042000	3.960655000	9.707742000	H	0.693312000	4.103467000	9.740208000
C	6.970052000	0.292109000	15.918366000	C	6.564924000	-0.191279000	15.890666000
H	6.596187000	-0.738195000	16.052732000	H	6.425623000	-1.282024000	15.949733000
H	6.248273000	0.995352000	16.355340000	H	5.656674000	0.321864000	16.227784000
H	7.936535000	0.396457000	16.441987000	H	7.423019000	0.114716000	16.508877000
C	1.214756000	3.129186000	12.097457000	C	1.218586000	3.313562000	12.102905000
H	0.497197000	2.470062000	11.584731000	H	0.451663000	2.691923000	11.607882000
H	0.859556000	4.170824000	12.072524000	H	0.905732000	4.371870000	12.061343000
H	1.350343000	2.802406000	13.135024000	H	1.303864000	3.006452000	13.154189000
C	9.539646000	2.784117000	5.749755000	C	9.481660000	2.755032000	5.772704000
H	9.587039000	3.009143000	4.672309000	H	9.521015000	2.961605000	4.691188000
H	10.234176000	3.480172000	6.252959000	H	10.164918000	3.473034000	6.260529000
C	9.979815000	1.342899000	6.016001000	C	9.949158000	1.328062000	6.063315000
H	11.016073000	1.186519000	5.675416000	H	10.983777000	1.179840000	5.714566000
H	9.344733000	0.654540000	5.430327000	H	9.318305000	0.616298000	5.501640000
N	7.786586000	3.899857000	11.116058000	N	7.695087000	3.692671000	11.175398000
H	7.852483000	4.782523000	10.591857000	H	7.195594000	4.551669000	11.444976000
N	8.398604000	3.980462000	12.251271000	N	8.958718000	3.807934000	11.387495000
H	8.358595000	3.165462000	12.868860000	H	9.569481000	3.021500000	11.150886000
H	8.877585000	4.835816000	12.544808000	H	9.361871000	4.661925000	11.785773000
² XII				⁴ XII			
Fe	6.754351000	1.937080000	10.154319000	Fe	6.781238000	1.864780000	10.111199000
O	6.711403000	0.875294000	11.697142000	O	6.828046000	0.925606000	11.725838000
O	4.978318000	2.438790000	10.559757000	O	5.018013000	2.398100000	10.498435000
N	6.670635000	2.705280000	8.384528000	N	6.736040000	2.704894000	8.373717000
O	2.646434000	2.905556000	11.649768000	O	2.667813000	2.853829000	11.565330000
O	6.398646000	0.196888000	14.214921000	O	6.750016000	0.506858000	14.294935000
N	8.322910000	1.016185000	9.494274000	N	8.291904000	0.854321000	9.391574000

C	7.715875000	0.267400000	12.269835000	C	7.811708000	0.215078000	12.225669000
C	7.577458000	-0.128224000	13.647134000	C	7.778305000	-0.068611000	13.629742000
C	8.623768000	-0.783724000	14.288282000	C	8.766486000	-0.864063000	14.204524000
H	8.526129000	-1.073856000	15.334764000	H	8.735705000	-1.088783000	15.271149000
C	9.824842000	-1.081483000	13.604416000	C	9.821262000	-1.383255000	13.422543000
H	10.625540000	-1.599800000	14.136715000	H	10.581085000	-2.007503000	13.897841000
C	9.982195000	-0.723783000	12.281403000	C	9.897108000	-1.089851000	12.074458000
H	10.903382000	-0.955413000	11.741272000	H	10.719687000	-1.469613000	11.463477000
C	8.940101000	-0.037957000	11.598571000	C	8.907314000	-0.275167000	11.462237000
C	4.390315000	3.560141000	8.503862000	C	4.456768000	3.562967000	8.461449000
C	4.126831000	3.099297000	9.830608000	C	4.171396000	3.074925000	9.770863000
C	5.654962000	3.328633000	7.866829000	C	5.737185000	3.346106000	7.848469000
H	5.753722000	3.732387000	6.852704000	H	5.861830000	3.779058000	6.849098000
C	9.119225000	0.278083000	10.205165000	C	9.051186000	0.048806000	10.067203000
H	9.999856000	-0.163608000	9.725473000	H	9.894486000	-0.430434000	9.556079000
C	7.971897000	2.595194000	7.700166000	C	8.044037000	2.560036000	7.707438000
H	8.634833000	3.325575000	8.201141000	H	8.740089000	3.203925000	8.276403000
C	2.827914000	3.372620000	10.395295000	C	2.870764000	3.342464000	10.322485000
C	8.505598000	1.193670000	8.034366000	C	8.484543000	1.105164000	7.946016000
H	7.823164000	0.467839000	7.556237000	H	7.759145000	0.457951000	7.420469000
C	7.994568000	2.860722000	6.196621000	C	8.112446000	2.939128000	6.230245000
H	7.289408000	2.173678000	5.697207000	H	7.375353000	2.339417000	5.668158000
H	7.660844000	3.888373000	5.986071000	H	7.847168000	3.999433000	6.098221000
C	3.391081000	4.266574000	7.776075000	C	3.474697000	4.286103000	7.730044000
H	3.620532000	4.607521000	6.763274000	H	3.722436000	4.645773000	6.728208000
C	2.159217000	4.513772000	8.343362000	C	2.233139000	4.525925000	8.282783000
H	1.390340000	5.056127000	7.788386000	H	1.474231000	5.080619000	7.726542000
C	9.917604000	0.980638000	7.491232000	C	9.884247000	0.840591000	7.392418000
H	10.251314000	-0.050619000	7.681282000	H	10.146141000	-0.222170000	7.508012000
H	10.610974000	1.657775000	8.019982000	H	10.614869000	1.428094000	7.975587000
C	1.877136000	4.065792000	9.655915000	C	1.931793000	4.053478000	9.580058000
H	0.896922000	4.273967000	10.086073000	H	0.945207000	4.253646000	9.999329000
C	6.175668000	-0.135008000	15.576112000	C	6.640238000	0.306495000	15.695989000
H	6.222562000	-1.225717000	15.743616000	H	6.503857000	-0.760806000	15.943982000
H	5.166026000	0.222015000	15.820918000	H	5.752424000	0.865986000	16.020523000
H	6.904292000	0.361523000	16.241583000	H	7.525714000	0.690351000	16.233134000
C	1.400368000	3.123673000	12.288288000	C	1.407277000	3.051773000	12.182764000
H	0.568661000	2.648448000	11.737525000	H	0.590103000	2.585105000	11.603866000
H	1.182047000	4.200634000	12.404267000	H	1.180993000	4.124606000	12.318739000
H	1.476418000	2.665860000	13.284261000	H	1.465305000	2.571498000	13.169277000
C	9.412210000	2.652648000	5.647866000	C	9.522470000	2.680732000	5.684080000
H	9.411311000	2.812392000	4.557733000	H	9.551151000	2.927925000	4.610798000
H	10.082512000	3.416044000	6.081457000	H	10.235328000	3.358121000	6.187051000
C	9.949104000	1.258441000	5.981992000	C	9.955078000	1.230020000	5.909915000
H	10.980044000	1.144049000	5.610509000	H	10.980540000	1.071850000	5.539265000
H	9.337651000	0.498409000	5.463856000	H	9.298629000	0.558815000	5.328028000
N	7.646333000	3.319905000	10.849166000	N	7.653939000	3.539728000	11.111530000
N	8.587067000	3.257525000	11.646739000	N	7.506505000	3.553341000	12.322097000
H	9.005248000	2.372084000	11.993068000	H	7.047058000	2.764009000	12.835370000
H	8.994492000	4.131929000	12.016021000	H	7.830765000	4.350067000	12.904746000
⁶ XII				¹ XIII			
Fe	6.902078000	2.322302000	10.376719000	Fe	6.782148000	1.847906000	10.072074000
O	7.198615000	1.343018000	12.000831000	O	6.809287000	0.887466000	11.685589000
O	5.062296000	2.776075000	10.544043000	O	5.083256000	2.542917000	10.564650000
N	6.747307000	2.880322000	8.361282000	N	6.694204000	2.641320000	8.333799000
O	2.638982000	3.058046000	11.524076000	O	2.838553000	3.124999000	11.750940000
O	7.251547000	0.740979000	14.544607000	O	6.438845000	0.116941000	14.147605000
N	8.273799000	0.981507000	9.451205000	N	8.378764000	0.970602000	9.436045000
C	7.922788000	0.306313000	12.342904000	C	7.778013000	0.246193000	12.228922000
C	7.953403000	-0.073795000	13.722414000	C	7.606207000	-0.206564000	13.603211000
C	8.673644000	-1.198498000	14.119619000	C	8.639883000	-0.894736000	14.236779000
H	8.687652000	-1.499231000	15.167796000	H	8.531179000	-1.227492000	15.268739000
C	9.392763000	-1.960365000	13.174520000	C	9.831930000	-1.165322000	13.546821000
H	9.946818000	-2.840489000	13.508477000	H	10.627168000	-1.709258000	14.061207000
C	9.405478000	-1.588229000	11.842000000	C	10.019379000	-0.762727000	12.222451000
H	9.977308000	-2.162851000	11.108786000	H	10.947603000	-1.004257000	11.700316000

C	8.685267000	-0.444945000	11.406193000	C	9.017894000	-0.052104000	11.546269000
C	4.380233000	3.452367000	8.336565000	C	4.397292000	3.434085000	8.441044000
C	4.130781000	3.174293000	9.713636000	C	4.200343000	3.109087000	9.841838000
C	5.692520000	3.289806000	7.741959000	C	5.654503000	3.196074000	7.784060000
H	5.753407000	3.541245000	6.674258000	H	5.719638000	3.548183000	6.749147000
C	8.791634000	-0.063429000	10.013855000	C	9.209484000	0.282362000	10.156621000
H	9.399370000	-0.745819000	9.402412000	H	10.117927000	-0.118897000	9.694667000
C	8.052078000	2.694049000	7.725629000	C	7.997354000	2.560057000	7.651115000
H	8.745859000	3.345872000	8.290921000	H	8.631476000	3.299027000	8.174820000
C	2.797197000	3.344596000	10.215212000	C	2.923627000	3.452431000	10.467972000
C	8.490618000	1.239386000	8.011570000	C	8.576187000	1.167849000	7.983714000
H	7.806139000	0.576969000	7.450474000	H	7.919188000	0.426461000	7.494118000
C	8.167191000	3.032181000	6.240927000	C	8.029943000	2.843064000	6.152591000
H	7.476822000	2.391183000	5.665060000	H	7.355790000	2.139715000	5.633941000
H	7.863286000	4.077496000	6.071150000	H	7.667255000	3.862549000	5.950494000
C	3.324990000	3.889216000	7.499378000	C	3.359567000	4.051723000	7.728071000
H	3.536300000	4.095618000	6.447024000	H	3.511145000	4.304366000	6.676475000
C	2.045503000	4.048492000	8.006012000	C	2.147720000	4.349647000	8.353834000
H	1.232236000	4.384531000	7.358786000	H	1.349858000	4.826477000	7.780281000
C	9.927579000	1.013088000	7.522987000	C	9.998577000	1.006678000	7.452065000
H	10.224056000	-0.035436000	7.675508000	H	10.360312000	-0.016821000	7.632756000
H	10.603592000	1.636333000	8.134671000	H	10.664751000	1.698005000	7.996782000
C	1.780385000	3.775644000	9.361707000	C	1.924788000	4.057827000	9.710526000
H	0.766278000	3.904478000	9.740953000	H	0.964938000	4.309462000	10.160985000
C	7.226208000	0.456676000	15.934691000	C	6.154101000	-0.257513000	15.496952000
H	6.771210000	-0.528498000	16.139526000	H	6.181570000	-1.353130000	15.615733000
H	6.611412000	1.238664000	16.400757000	H	5.142245000	0.111162000	15.706194000
H	8.238804000	0.483307000	16.375217000	H	6.870111000	0.208392000	16.193851000
C	1.350033000	3.177229000	12.104493000	C	1.637634000	3.396438000	12.476052000
H	0.621184000	2.501804000	11.622121000	H	0.783728000	2.852918000	12.039192000
H	0.970513000	4.213025000	12.048793000	H	1.421198000	4.477406000	12.488794000
H	1.457316000	2.892044000	13.160004000	H	1.814999000	3.043340000	13.499490000
C	9.604698000	2.807666000	5.756911000	C	9.462252000	2.686617000	5.624100000
H	9.672761000	3.028171000	4.679422000	H	9.472427000	2.861763000	4.536611000
H	10.275580000	3.518827000	6.271145000	H	10.100922000	3.464356000	6.079226000
C	10.068905000	1.376004000	6.039753000	C	10.036904000	1.305114000	5.946947000
H	11.117506000	1.242646000	5.727723000	H	11.074997000	1.227123000	5.586654000
H	9.466016000	0.672754000	5.437688000	H	9.454822000	0.533553000	5.412428000
N	7.508427000	4.075074000	11.359236000	N	7.769051000	3.258701000	10.727548000
N	7.606698000	3.996406000	12.573549000	N	7.814194000	3.513526000	11.934033000
H	7.472402000	3.084876000	13.076364000	H	7.319977000	2.961329000	12.660459000
H	7.824790000	4.828246000	13.155884000	H	8.355154000	4.330849000	12.261807000
³ XIII				⁵ XIII			
Fe	6.909304000	1.963487000	10.170740000	Fe	6.975976000	2.330512000	10.362629000
O	6.946874000	1.053191000	11.770337000	O	7.236406000	1.375562000	11.970717000
O	4.969961000	2.300569000	10.433452000	O	5.044933000	2.775040000	10.557732000
N	6.837660000	2.794342000	8.411807000	N	6.762051000	2.874888000	8.350095000
O	2.597517000	2.697952000	11.434387000	O	2.657849000	3.088707000	11.537880000
O	6.952330000	0.687444000	14.341834000	O	7.194327000	0.738000000	14.510500000
N	8.297825000	0.839848000	9.380180000	N	8.316086000	0.996086000	9.444343000
C	7.894017000	0.264339000	12.241151000	C	7.920164000	0.312607000	12.326325000
C	7.892965000	0.009178000	13.646126000	C	7.902018000	-0.076517000	13.701135000
C	8.827847000	-0.870865000	14.190012000	C	8.595771000	-1.219192000	14.103852000
H	8.824325000	-1.080328000	15.260194000	H	8.579845000	-1.530533000	15.148677000
C	9.789944000	-1.494782000	13.369841000	C	9.322081000	-1.981144000	13.169332000
H	10.509275000	-2.181983000	13.820256000	H	9.854458000	-2.872726000	13.507675000
C	9.833337000	-1.226996000	12.013247000	C	9.372460000	-1.601656000	11.836455000
H	10.588995000	-1.689300000	11.373974000	H	9.949632000	-2.182900000	11.113303000
C	8.897597000	-0.331952000	11.433597000	C	8.684196000	-0.445534000	11.395648000
C	4.547543000	3.633720000	8.487804000	C	4.390739000	3.409198000	8.336697000
C	4.191837000	3.031061000	9.754842000	C	4.150805000	3.151252000	9.740426000
C	5.847300000	3.426924000	7.880204000	C	5.706612000	3.258576000	7.727208000
H	5.963672000	3.858671000	6.879532000	H	5.750165000	3.499092000	6.657066000
C	9.009812000	-0.026926000	10.030746000	C	8.813381000	-0.059622000	10.006052000
H	9.788356000	-0.576153000	9.488485000	H	9.411777000	-0.748758000	9.393736000
C	8.126278000	2.582504000	7.722577000	C	8.070243000	2.700905000	7.710027000

H	8.866308000	3.168612000	8.297322000	H	8.750467000	3.369085000	8.271931000
C	2.838887000	3.276038000	10.282058000	C	2.782235000	3.334097000	10.257215000
C	8.464489000	1.094089000	7.931334000	C	8.529859000	1.254442000	8.004016000
H	7.680272000	0.507970000	7.419812000	H	7.858711000	0.576787000	7.445962000
C	8.193644000	2.984665000	6.252752000	C	8.173231000	3.029112000	6.223231000
H	7.406608000	2.448653000	5.694147000	H	7.491908000	2.371128000	5.655975000
H	8.000959000	4.063650000	6.147598000	H	7.852537000	4.068066000	6.046552000
C	3.610821000	4.407055000	7.814596000	C	3.330149000	3.806850000	7.535991000
H	3.875173000	4.854228000	6.853666000	H	3.505002000	4.002143000	6.475176000
C	2.317287000	4.628555000	8.351028000	C	2.018692000	3.963204000	8.059512000
H	1.611324000	5.248311000	7.794627000	H	1.214773000	4.272685000	7.388654000
C	9.827688000	0.737389000	7.339556000	C	9.972343000	1.052658000	7.521759000
H	10.008464000	-0.344414000	7.429768000	H	10.286979000	0.011270000	7.685853000
H	10.612791000	1.256451000	7.916352000	H	10.633964000	1.695423000	8.128447000
C	1.930785000	4.074198000	9.562366000	C	1.741205000	3.732655000	9.396045000
H	0.930298000	4.257764000	9.953228000	H	0.726921000	3.857318000	9.773982000
C	6.880918000	0.521908000	15.752439000	C	7.133037000	0.447721000	15.901031000
H	6.658154000	-0.524265000	16.023809000	H	6.659021000	-0.531305000	16.088410000
H	6.061378000	1.166234000	16.097420000	H	6.519387000	1.237526000	16.354461000
H	7.819078000	0.832517000	16.244421000	H	8.136399000	0.458626000	16.361386000
C	1.319184000	2.840325000	12.077242000	C	1.385287000	3.216243000	12.197590000
H	0.521425000	2.437891000	11.434317000	H	0.657321000	2.517559000	11.757468000
H	1.123480000	3.898762000	12.308467000	H	1.017440000	4.250585000	12.117884000
H	1.386495000	2.258469000	13.003710000	H	1.568611000	2.959433000	13.247241000
C	9.571164000	2.634488000	5.675662000	C	9.613952000	2.824212000	5.738893000
H	9.597746000	2.902214000	4.607532000	H	9.673862000	3.034387000	4.659119000
H	10.341692000	3.245464000	6.178255000	H	10.272418000	3.553333000	6.243513000
C	9.894799000	1.150536000	5.863392000	C	10.105590000	1.404317000	6.035036000
H	10.897140000	0.922070000	5.467651000	H	11.156577000	1.289139000	5.724628000
H	9.176642000	0.543531000	5.284217000	H	9.516726000	0.683376000	5.440331000
N	7.185558000	3.735487000	11.268746000	N	7.538408000	4.113498000	11.322955000
N	7.020813000	3.651842000	12.472190000	N	7.659848000	4.057697000	12.533898000
H	6.819547000	2.732447000	12.940363000	H	7.537436000	3.159983000	13.062888000
H	7.076679000	4.490160000	13.084033000	H	7.889996000	4.902142000	13.094862000
¹ XIV				³ XIV			
Fe	6.849920000	2.021715000	10.182884000	Fe	6.668962000	1.611256000	10.074158000
O	6.793000000	0.994780000	11.786237000	O	6.753878000	0.579574000	11.593693000
O	5.042922000	2.269938000	10.444500000	O	4.955455000	2.171500000	10.403158000
N	6.769476000	2.795743000	8.405088000	N	6.690461000	2.570639000	8.377007000
O	2.694528000	2.637990000	11.544041000	O	2.688984000	2.755169000	11.602137000
O	6.561939000	0.340643000	14.314904000	O	6.452830000	-0.049724000	14.129687000
N	8.269468000	0.948754000	9.454835000	N	8.338046000	0.831926000	9.439318000
C	7.765782000	0.304261000	12.293557000	C	7.809389000	0.121545000	12.220296000
C	7.672123000	-0.091015000	13.678980000	C	7.677311000	-0.248953000	13.599674000
C	8.681991000	-0.850711000	14.255095000	C	8.776751000	-0.767418000	14.279701000
H	8.616293000	-1.140323000	15.304269000	H	8.686387000	-1.044774000	15.330398000
C	9.809490000	-1.260288000	13.501677000	C	10.018539000	-0.943134000	13.629058000
H	10.584522000	-1.858312000	13.986278000	H	10.859852000	-1.354719000	14.191075000
C	9.920683000	-0.912418000	12.173027000	C	10.165137000	-0.602760000	12.298639000
H	10.781076000	-1.230665000	11.579142000	H	11.117815000	-0.743600000	11.782409000
C	8.910955000	-0.124601000	11.550541000	C	9.067375000	-0.058498000	11.580830000
C	4.498446000	3.642642000	8.533163000	C	4.499040000	3.626611000	8.554289000
C	4.204367000	3.037515000	9.786730000	C	4.169560000	3.026003000	9.799006000
C	5.769971000	3.428139000	7.886499000	C	5.753497000	3.343229000	7.917508000
H	5.867987000	3.837133000	6.874255000	H	5.926364000	3.857769000	6.965863000
C	9.037604000	0.164997000	10.154429000	C	9.220890000	0.241510000	10.183428000
H	9.861679000	-0.341136000	9.639032000	H	10.164264000	-0.077559000	9.726616000
C	8.054352000	2.601953000	7.711932000	C	8.001078000	2.450134000	7.699843000
H	8.779235000	3.252099000	8.235122000	H	8.677122000	3.147340000	8.228166000
C	2.906264000	3.249136000	10.361250000	C	2.920653000	3.360543000	10.419127000
C	8.458043000	1.147810000	7.998325000	C	8.505530000	1.030471000	7.986367000
H	7.712665000	0.501881000	7.500103000	H	7.801803000	0.329975000	7.502138000
C	8.097790000	2.920036000	6.220285000	C	8.023430000	2.765126000	6.204340000
H	7.339180000	2.313574000	5.695752000	H	7.287053000	2.121226000	5.692875000
H	7.850818000	3.979716000	6.051935000	H	7.728057000	3.810470000	6.029648000
C	3.527433000	4.436337000	7.874606000	C	3.597144000	4.531805000	7.933639000

H	3.776475000	4.887262000	6.911047000	H	3.872364000	4.980849000	6.976416000
C	2.285503000	4.635190000	8.451855000	C	2.397104000	4.836724000	8.544891000
H	1.534846000	5.250671000	7.950997000	H	1.698702000	5.534209000	8.077182000
C	9.846022000	0.832176000	7.441471000	C	9.905388000	0.799593000	7.421916000
H	10.087668000	-0.230932000	7.591028000	H	10.218995000	-0.240772000	7.597047000
H	10.596057000	1.425388000	7.993094000	H	10.620217000	1.456074000	7.947950000
C	1.973665000	4.041367000	9.691326000	C	2.058677000	4.253098000	9.786486000
H	0.988245000	4.208727000	10.126913000	H	1.107255000	4.512967000	10.251731000
C	6.372827000	-0.005351000	15.676575000	C	6.224310000	-0.400682000	15.485176000
H	6.321579000	-1.100054000	15.816847000	H	6.393100000	-1.477920000	15.661491000
H	5.415188000	0.439291000	15.980467000	H	5.172013000	-0.163959000	15.693527000
H	7.176340000	0.399725000	16.317800000	H	6.866483000	0.179824000	16.171226000
C	1.430663000	2.774439000	12.174360000	C	1.477813000	3.029178000	12.288304000
H	0.615669000	2.376522000	11.544026000	H	0.595676000	2.732495000	11.693419000
H	1.209648000	3.827385000	12.424075000	H	1.390514000	4.098685000	12.550368000
H	1.483053000	2.190058000	13.103065000	H	1.503167000	2.434961000	13.211901000
C	9.493967000	2.612183000	5.663540000	C	9.426392000	2.525775000	5.631539000
H	9.510380000	2.813116000	4.580456000	H	9.414573000	2.717912000	4.546775000
H	10.226858000	3.296765000	6.126416000	H	10.127209000	3.254086000	6.076914000
C	9.903863000	1.164058000	5.943887000	C	9.921609000	1.106503000	5.918759000
H	10.921686000	0.972952000	5.567821000	H	10.942518000	0.968683000	5.528353000
H	9.228800000	0.481919000	5.397251000	H	9.277312000	0.379604000	5.393225000
N	7.706555000	3.273195000	10.831753000	N	7.620284000	3.273668000	11.033005000
N	8.361562000	4.108838000	11.312184000	N	7.186629000	4.359957000	10.956626000
H	7.942742000	4.990150000	11.686311000	H	7.678898000	5.138167000	11.464717000
⁵ XIV				² XV			
Fe	6.666787000	1.748854000	10.118515000	Fe	6.742911000	1.832636000	10.054264000
O	6.760270000	0.756480000	11.665729000	O	6.784631000	0.880128000	11.704428000
O	5.005293000	2.429838000	10.503069000	O	5.004234000	2.268052000	10.421163000
N	6.665776000	2.661006000	8.397996000	N	6.670925000	2.614414000	8.294351000
O	2.666167000	2.885837000	11.617564000	O	2.754540000	2.847941000	11.635036000
O	6.493924000	0.110956000	14.202183000	O	6.476605000	0.169678000	14.184286000
N	8.273464000	0.870437000	9.437959000	N	8.348635000	0.942385000	9.412961000
C	7.778283000	0.164522000	12.235893000	C	7.764330000	0.270620000	12.236157000
C	7.663828000	-0.215517000	13.614672000	C	7.626067000	-0.146903000	13.639089000
C	8.725135000	-0.867376000	14.236818000	C	8.682575000	-0.816561000	14.283453000
H	8.647996000	-1.153443000	15.286189000	H	8.588976000	-1.119950000	15.325828000
C	9.911822000	-1.167201000	13.529875000	C	9.848021000	-1.091042000	13.582663000
H	10.724480000	-1.680636000	14.048512000	H	10.665342000	-1.612832000	14.084278000
C	10.040732000	-0.816289000	12.200970000	C	10.001244000	-0.716896000	12.225046000
H	10.951119000	-1.047231000	11.642716000	H	10.924898000	-0.969384000	11.699380000
C	8.980578000	-0.139810000	11.539607000	C	8.994056000	-0.040644000	11.545640000
C	4.396319000	3.546010000	8.470862000	C	4.429319000	3.546198000	8.464108000
C	4.127056000	3.086615000	9.788682000	C	4.169266000	3.038400000	9.771842000
C	5.679875000	3.320597000	7.869928000	C	5.678926000	3.285540000	7.799958000
H	5.824977000	3.769619000	6.881338000	H	5.786669000	3.721340000	6.800577000
C	9.120112000	0.189815000	10.149515000	C	9.177154000	0.273485000	10.142999000
H	10.026907000	-0.185458000	9.663061000	H	10.094298000	-0.121492000	9.691946000
C	7.984707000	2.548354000	7.741173000	C	7.981833000	2.519408000	7.625276000
H	8.660748000	3.215489000	8.305943000	H	8.623091000	3.259896000	8.140657000
C	2.841667000	3.355598000	10.365390000	C	2.918739000	3.353248000	10.402340000
C	8.459318000	1.109505000	7.990335000	C	8.539311000	1.128372000	7.956417000
H	7.749539000	0.438369000	7.474613000	H	7.868874000	0.389084000	7.482232000
C	8.044312000	2.919414000	6.260751000	C	8.012491000	2.797025000	6.123647000
H	7.317763000	2.302628000	5.703948000	H	7.317417000	2.105724000	5.616612000
H	7.761839000	3.974072000	6.121703000	H	7.670519000	3.822892000	5.919705000
C	3.405649000	4.257871000	7.743066000	C	3.457027000	4.329096000	7.800661000
H	3.637079000	4.603032000	6.732557000	H	3.670292000	4.704003000	6.797230000
C	2.172735000	4.502009000	8.314883000	C	2.252904000	4.615725000	8.425357000
H	1.403615000	5.045953000	7.762069000	H	1.500781000	5.222598000	7.916682000
C	9.864465000	0.873063000	7.438629000	C	9.956387000	0.938320000	7.421103000
H	10.153406000	-0.180793000	7.570344000	H	10.302786000	-0.088812000	7.611327000
H	10.581858000	1.489177000	8.008239000	H	10.636308000	1.625409000	7.954236000
C	1.890319000	4.052004000	9.624263000	C	1.983533000	4.133808000	9.719912000
H	0.909842000	4.258127000	10.054590000	H	1.030611000	4.377602000	10.189981000
C	6.293701000	-0.223909000	15.566173000	C	6.188371000	-0.164288000	15.553002000

H	6.347140000	-1.314831000	15.730788000	H	6.230559000	-1.254767000	15.697382000
H	5.286725000	0.128864000	15.827659000	H	5.172334000	0.202111000	15.739303000
H	7.030938000	0.274086000	16.220882000	H	6.901414000	0.336096000	16.226155000
C	1.417119000	3.091413000	12.258648000	C	1.542551000	3.101958000	12.334519000
H	0.590359000	2.613568000	11.703431000	H	0.670308000	2.697664000	11.792193000
H	1.193225000	4.166051000	12.381239000	H	1.394641000	4.182070000	12.506507000
H	1.497638000	2.626933000	13.250879000	H	1.633861000	2.591657000	13.302517000
C	9.458178000	2.684180000	5.714113000	C	9.436382000	2.609718000	5.583740000
H	9.477864000	2.923371000	4.638905000	H	9.438118000	2.775670000	4.494791000
H	10.158797000	3.379773000	6.209235000	H	10.093781000	3.379466000	6.025396000
C	9.919640000	1.244690000	5.951156000	C	9.989010000	1.220956000	5.912847000
H	10.946485000	1.102676000	5.578129000	H	11.023019000	1.121493000	5.546433000
H	9.273813000	0.554268000	5.380216000	H	9.389537000	0.455061000	5.389833000
N	7.885016000	3.415761000	11.061968000	N	7.604536000	3.361537000	10.855662000
N	8.745560000	3.983588000	11.617377000	N	7.974789000	3.454719000	11.957294000
H	8.607902000	5.000380000	11.878094000	H	8.480124000	4.322595000	12.262638000
4XV				6XV			
Fe	6.636828000	1.809023000	10.085775000	Fe	6.929607000	2.230517000	10.412040000
O	6.773060000	0.878292000	11.736254000	O	7.185039000	1.214758000	12.045046000
O	5.022898000	2.503552000	10.479045000	O	5.004687000	2.728510000	10.609327000
N	6.657556000	2.711101000	8.372474000	N	6.762541000	2.852564000	8.404958000
O	2.665792000	2.895917000	11.585691000	O	2.617543000	3.088101000	11.568217000
O	6.550033000	0.266975000	14.262841000	O	6.969424000	0.353913000	14.507972000
N	8.253171000	0.904242000	9.421120000	N	8.341741000	0.938351000	9.478896000
C	7.754533000	0.262519000	12.260646000	C	7.963990000	0.257898000	12.390364000
C	7.662167000	-0.105426000	13.676948000	C	7.880209000	-0.244686000	13.751857000
C	8.722652000	-0.799707000	14.293546000	C	8.732649000	-1.277095000	14.174310000
H	8.662274000	-1.070609000	15.347234000	H	8.680329000	-1.652355000	15.196122000
C	9.843917000	-1.139804000	13.553025000	C	9.650377000	-1.828813000	13.282488000
H	10.661447000	-1.680878000	14.033137000	H	10.307980000	-2.632915000	13.619229000
C	9.952654000	-0.801431000	12.181321000	C	9.736484000	-1.373597000	11.954305000
H	10.846173000	-1.091609000	11.624191000	H	10.450946000	-1.837459000	11.270362000
C	8.940520000	-0.101807000	11.532400000	C	8.914818000	-0.343870000	11.489991000
C	4.369000000	3.545678000	8.424327000	C	4.408781000	3.471604000	8.403010000
C	4.109951000	3.110730000	9.749825000	C	4.139858000	3.169988000	9.795082000
C	5.661685000	3.337235000	7.829233000	C	5.722374000	3.286009000	7.791023000
H	5.801396000	3.766555000	6.831270000	H	5.770779000	3.551420000	6.726884000
C	9.082369000	0.209885000	10.125971000	C	9.029580000	0.034349000	10.086615000
H	9.978886000	-0.197435000	9.646385000	H	9.772762000	-0.549649000	9.527243000
C	7.985209000	2.594498000	7.731856000	C	8.061927000	2.654243000	7.752750000
H	8.657174000	3.256092000	8.307508000	H	8.763474000	3.303639000	8.309393000
C	2.824072000	3.344878000	10.327622000	C	2.772080000	3.389713000	10.300622000
C	8.445788000	1.149679000	7.972230000	C	8.499357000	1.192309000	8.031483000
H	7.727665000	0.485502000	7.459692000	H	7.767184000	0.539681000	7.521503000
C	8.058278000	2.975950000	6.254992000	C	8.145521000	2.993257000	6.265930000
H	7.333753000	2.366362000	5.688347000	H	7.426416000	2.367994000	5.708522000
H	7.782128000	4.033264000	6.125209000	H	7.858032000	4.045223000	6.109599000
C	3.361892000	4.212454000	7.685287000	C	3.375985000	3.949583000	7.609872000
H	3.580832000	4.545859000	6.668515000	H	3.570977000	4.177460000	6.559135000
C	2.119722000	4.429719000	8.257035000	C	2.068412000	4.150827000	8.125682000
H	1.335487000	4.939330000	7.693183000	H	1.289344000	4.529050000	7.460616000
C	9.850996000	0.901156000	7.428992000	C	9.898591000	0.922692000	7.466696000
H	10.124422000	-0.157943000	7.550920000	H	10.159894000	-0.138536000	7.592892000
H	10.570214000	1.503000000	8.011412000	H	10.627993000	1.512522000	8.049346000
C	1.849692000	3.998862000	9.570867000	C	1.763057000	3.876329000	9.448620000
H	0.863223000	4.182378000	9.997383000	H	0.751828000	4.035632000	9.821963000
C	6.309655000	-0.023138000	15.651461000	C	6.787429000	-0.045164000	15.868802000
H	6.317643000	-1.110747000	15.820693000	H	6.490097000	-1.104614000	15.932569000
H	5.317220000	0.386449000	15.871826000	H	5.982654000	0.587251000	16.263811000
H	7.070036000	0.465823000	16.279755000	H	7.707527000	0.118915000	16.452813000
C	1.414749000	3.084821000	12.233713000	C	1.340924000	3.234412000	12.212584000
H	0.598335000	2.571643000	11.696123000	H	0.593125000	2.586138000	11.730305000
H	1.166803000	4.156136000	12.331321000	H	1.012425000	4.284517000	12.178122000
H	1.517256000	2.646285000	13.235315000	H	1.495156000	2.922000000	13.251979000
C	9.475758000	2.734530000	5.720687000	C	9.560123000	2.741086000	5.734801000

H	9.506176000	2.984465000	4.648424000	H	9.598964000	2.976908000	4.659298000
H	10.177690000	3.418594000	6.229406000	H	10.266803000	3.424639000	6.238298000
C	9.920400000	1.288089000	5.945907000	C	9.986575000	1.292893000	5.981877000
H	10.948988000	1.139185000	5.581204000	H	11.015855000	1.125941000	5.625681000
H	9.272501000	0.609958000	5.363151000	H	9.334446000	0.617032000	5.400449000
N	7.855378000	3.358262000	11.049441000	N	7.508921000	4.091956000	11.334366000
N	8.802801000	3.115753000	11.685385000	N	7.806458000	4.946964000	12.077823000
H	9.348962000	3.882217000	12.155516000	H	7.839811000	5.942328000	11.719499000
²XVI				⁴XVI			
Fe	6.720809000	1.584149000	9.946932000	Fe	6.667427000	1.570206000	9.922545000
O	6.832738000	0.778683000	11.654275000	O	6.787760000	0.613826000	11.486935000
O	5.003359000	2.288789000	10.440316000	O	5.029773000	2.275322000	10.339164000
N	6.717408000	2.533342000	8.263779000	N	6.686979000	2.538794000	8.231434000
O	2.781928000	2.953485000	11.628270000	O	2.788458000	2.900747000	11.559439000
O	6.587943000	0.128256000	14.179169000	O	6.529871000	0.097303000	14.047484000
N	8.368186000	0.819350000	9.355600000	N	8.339581000	0.801687000	9.303941000
C	7.834941000	0.154874000	12.183580000	C	7.849561000	0.162096000	12.109197000
C	7.740457000	-0.229682000	13.575800000	C	7.740638000	-0.144803000	13.504674000
C	8.787432000	-0.906036000	14.189278000	C	8.849328000	-0.640710000	14.186359000
H	8.715455000	-1.191061000	15.239243000	H	8.777958000	-0.865797000	15.250979000
C	9.958257000	-1.235263000	13.466557000	C	10.074531000	-0.862549000	13.518554000
H	10.764811000	-1.769783000	13.973711000	H	10.922704000	-1.258432000	14.081447000
C	10.079072000	-0.885059000	12.135941000	C	10.198773000	-0.581073000	12.172031000
H	10.980347000	-1.140204000	11.572512000	H	11.140738000	-0.750580000	11.644955000
C	9.034389000	-0.185149000	11.474189000	C	9.092942000	-0.053849000	11.453685000
C	4.487470000	3.499912000	8.432547000	C	4.486301000	3.576513000	8.399394000
C	4.208300000	3.018259000	9.769062000	C	4.204686000	3.062126000	9.693417000
C	5.749972000	3.238943000	7.773689000	C	5.739211000	3.292446000	7.760398000
H	5.871426000	3.720103000	6.796555000	H	5.902028000	3.788491000	6.797205000
C	9.205055000	0.140685000	10.085031000	C	9.232181000	0.226296000	10.052071000
H	10.124349000	-0.236931000	9.623024000	H	10.175437000	-0.088501000	9.592307000
C	8.025883000	2.426250000	7.585781000	C	7.996168000	2.409384000	7.550222000
H	8.681077000	3.148682000	8.106503000	H	8.676546000	3.109677000	8.067730000
C	2.942216000	3.407003000	10.394122000	C	2.969140000	3.417396000	10.327173000
C	8.571084000	1.023242000	7.907364000	C	8.499677000	0.990393000	7.847329000
H	7.902776000	0.299550000	7.405650000	H	7.792427000	0.286787000	7.373110000
C	8.058089000	2.717145000	6.086498000	C	8.010980000	2.709287000	6.051554000
H	7.355362000	2.037338000	5.573518000	H	7.270805000	2.061524000	5.550491000
H	7.724498000	3.747139000	5.887999000	H	7.716093000	3.753388000	5.868594000
C	3.535209000	4.282579000	7.775524000	C	3.547373000	4.415915000	7.742393000
H	3.746422000	4.644209000	6.766431000	H	3.784729000	4.799807000	6.747419000
C	2.319039000	4.617266000	8.394552000	C	2.357033000	4.736711000	8.364831000
H	1.592915000	5.228942000	7.854766000	H	1.628425000	5.380812000	7.867582000
C	9.988093000	0.837050000	7.366243000	C	9.896040000	0.751646000	7.277814000
H	10.334833000	-0.191221000	7.550654000	H	10.207817000	-0.287918000	7.460775000
H	10.671975000	1.517952000	7.902750000	H	10.615432000	1.411479000	7.793190000
C	2.022431000	4.193126000	9.692858000	C	2.068520000	4.241354000	9.656108000
H	1.076657000	4.479463000	10.152229000	H	1.124865000	4.514449000	10.129378000
C	6.401783000	-0.187249000	15.548613000	C	6.356139000	-0.062081000	15.446251000
H	6.426653000	-1.277624000	15.724373000	H	6.509766000	-1.109659000	15.760192000
H	5.410242000	0.197213000	15.824623000	H	5.319871000	0.229233000	15.664637000
H	7.164591000	0.294856000	16.186043000	H	7.042243000	0.589004000	16.016339000
C	1.595774000	3.270748000	12.360783000	C	1.595722000	3.206149000	12.264973000
H	0.701919000	2.872913000	11.853220000	H	0.700338000	2.846661000	11.727492000
H	1.495586000	4.360616000	12.490824000	H	1.495437000	4.291248000	12.445031000
H	1.708276000	2.790580000	13.340692000	H	1.666148000	2.687666000	13.230819000
C	9.478535000	2.522803000	5.539501000	C	9.410427000	2.461799000	5.473585000
H	9.480156000	2.695709000	4.451282000	H	9.392777000	2.643398000	4.387115000
H	10.142620000	3.285339000	5.984219000	H	10.115037000	3.193051000	5.907915000
C	10.024176000	1.128973000	5.860137000	C	9.904321000	1.044351000	5.771677000
H	11.056919000	1.026401000	5.489884000	H	10.922897000	0.900740000	5.377385000
H	9.419819000	0.370103000	5.331743000	H	9.255846000	0.313702000	5.256645000
N	6.828622000	4.290735000	11.883527000	N	7.000763000	3.216473000	12.935714000
N	5.836735000	4.716625000	12.095189000	N	6.208400000	3.040728000	13.678076000

⁶ XVI				
Fe	6.904692000	2.238908000	10.306688000	
O	7.119548000	1.214479000	11.866897000	
O	5.083051000	2.743792000	10.478707000	
N	6.778435000	2.839695000	8.299703000	
O	2.679885000	3.126031000	11.474716000	
O	7.020223000	0.570960000	14.407659000	
N	8.309177000	0.925210000	9.378175000	
C	7.975364000	0.315023000	12.283401000	
C	7.946352000	-0.065970000	13.663787000	
C	8.844085000	-1.024437000	14.136025000	
H	8.829985000	-1.317634000	15.186330000	
C	9.774219000	-1.626028000	13.265863000	
H	10.464436000	-2.375843000	13.658905000	
C	9.814471000	-1.272325000	11.926494000	
H	10.534202000	-1.738728000	11.249267000	
C	8.924026000	-0.295714000	11.416114000	
C	4.434397000	3.517724000	8.295133000	
C	4.171183000	3.215896000	9.663201000	
C	5.734608000	3.303204000	7.695720000	
H	5.800061000	3.564922000	6.631434000	
C	9.006217000	0.034794000	10.007701000	
H	9.743633000	-0.557652000	9.449499000	
C	8.062399000	2.603988000	7.628781000	
H	8.795592000	3.241335000	8.157807000	
C	2.849726000	3.438152000	10.173763000	
C	8.460949000	1.137653000	7.924491000	
H	7.705242000	0.498182000	7.432214000	
C	8.130414000	2.916278000	6.135024000	
H	7.384007000	2.303888000	5.599625000	
H	7.872912000	3.973641000	5.963257000	
C	3.401428000	4.028596000	7.470688000	
H	3.621848000	4.251136000	6.423642000	
C	2.133076000	4.238432000	7.985043000	
H	1.336707000	4.631630000	7.349159000	
C	9.844479000	0.816928000	7.348409000	
H	10.078664000	-0.248671000	7.490350000	
H	10.599551000	1.395954000	7.909042000	
C	1.855887000	3.943038000	9.333951000	
H	0.849687000	4.111733000	9.718603000	
C	6.959281000	0.327631000	15.803597000	
H	6.707592000	-0.724741000	16.024030000	
H	6.164608000	0.976490000	16.195673000	
H	7.911238000	0.581995000	16.302429000	
C	1.400594000	3.298791000	12.063446000	
H	0.636005000	2.673990000	11.568411000	
H	1.076162000	4.354130000	12.033721000	
H	1.496424000	2.983315000	13.111349000	
C	9.528981000	2.612657000	5.587225000	
H	9.557901000	2.826576000	4.506710000	
H	10.262701000	3.285506000	6.066034000	
C	9.920072000	1.158069000	5.855756000	
H	10.938780000	0.956769000	5.486730000	
H	9.241160000	0.489611000	5.296736000	
N	6.941490000	3.869061000	13.210889000	
N	6.657265000	3.566067000	14.229150000	

(END)