

## Support information

### New insight into the proton pumping mechanism of $ba_3$

### Cytochrome c Oxidase: the functions of key residues and waters

Xiaoyue Yang <sup>a</sup>, Shaohui Liu <sup>a</sup>, Zhili Yin <sup>a</sup>, Mengguo Chen <sup>a</sup>, Jinshuai Song <sup>b</sup>, Pengfei Li <sup>c</sup> and Longhua Yang <sup>\*a</sup>

<sup>a</sup> School of Pharmaceutical Sciences & Key Laboratory of Advanced Drug Preparation Technologies, Zhengzhou University, Zhengzhou, Henan, 450001, China

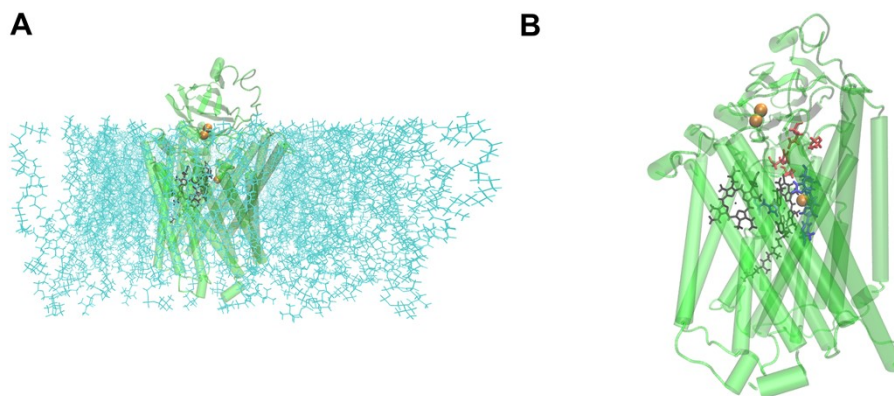
<sup>b</sup> Green Catalysis Center, and College of Chemistry, Zhengzhou University, Zhengzhou, Henan 450001, China

<sup>c</sup> Department of Chemistry and Biochemistry, Loyola University Chicago, Chicago, Illinois 60660, United States

#### Contents:

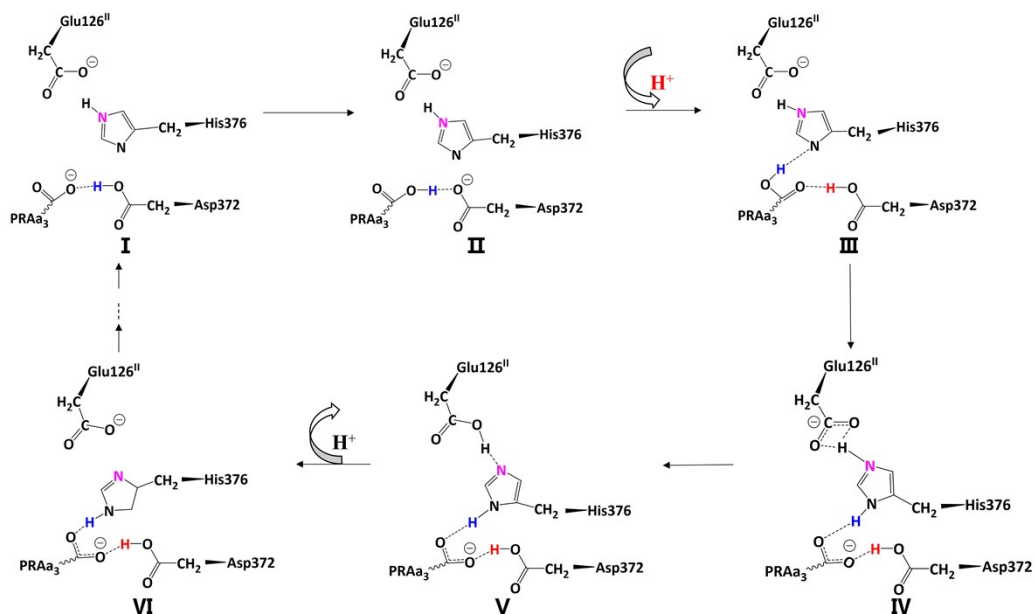
1. Schematic diagram of the protein model and the relative position of some of its structures.
2. The proposed E1 proton transfer pathway.
3. RMSD of WT and Mutants.
4. Computational active site model built from crystal structure.
5. Calculation of indirect transfer of protons from Tyr237 to  $O_{Cu}$  atom.
6. Cartesian coordinates for DFT-optimized structures.
7. The NPA charge of  $I_R$  and  $I_R'$ .

## 1 Schematic diagram of the protein model and the relative position of some of its structures.



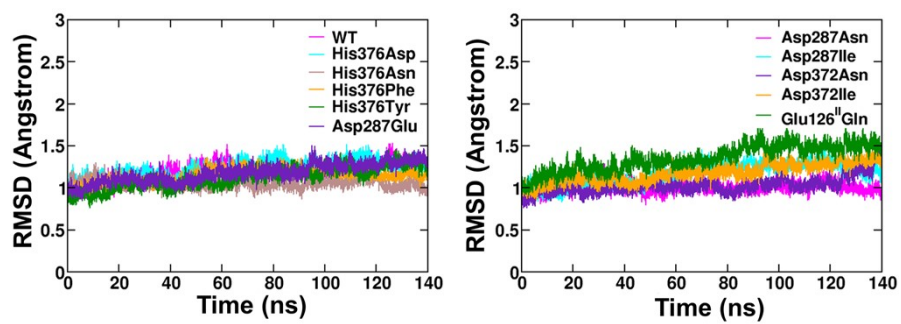
**Fig. S1** (A) The membrane added in MD simulation. The hydrophobic portion of lipids in MD simulation (in grey line representation) is retained as the low dielectric environment for MD calculations. CcO is shown as the green cartoon, Coppers are shown as orange spheres. Heme a<sub>3</sub> and heme b, are shown as black lines. (B) The residues (Asp287, Asp372, His376, Glu126<sup>II</sup>) are shown as red licorice, the residues (His233, Tyr237, His282, His283 and His384) are shown as blue licorice.

**2. The proposed E1 proton transfer pathway** (Yang, L., et al., *Biochim. Biophys. Acta - Bioenerg.*, 1857 (2016) 1594-1606.).



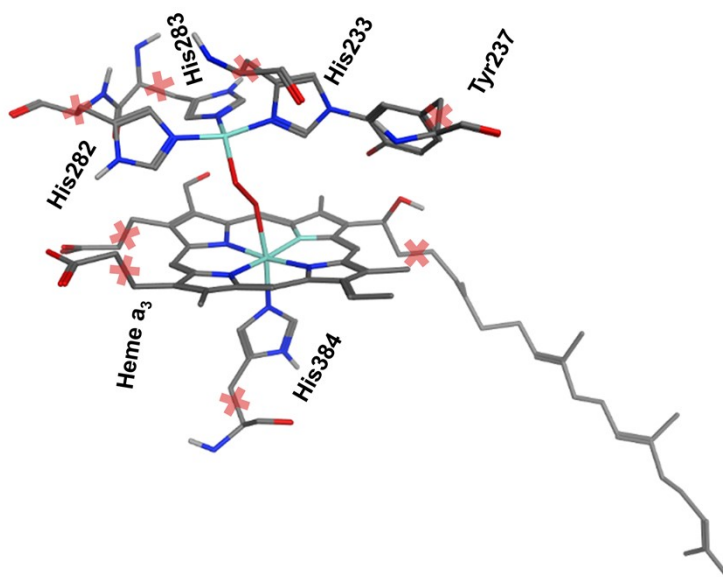
**Fig. S2** The proposed proton transfer pathway by our previous calculations. **(I)** A strong hydrogen bond exists between protonated Asp372 and PRAa<sub>3</sub>, facilitating proton transfer. **(II)** The proton is loaded on PRAa<sub>3</sub>. **(III)** Proton uptake by Asp372 results in formation of a strong hydrogen bond between protonated PRAa<sub>3</sub> and His376. **(IV)** Proton transfer from PRAa<sub>3</sub> to His376 results in a strong hydrogen bond between His376 and Glu126<sup>II</sup>. **(V)** Proton transfer from doubly protonated His376 to Glu126<sup>II</sup> and subsequent release into the water pool. **(VI)** Structure and protonation state equivalent to **(I)** with exception of the orientation of His376 and protonation site δ-nitrogen.

### 3. RMSD of WT and Mutants.



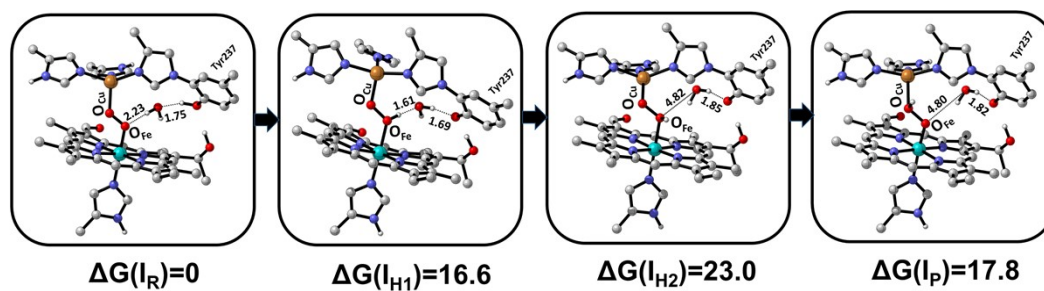
**Fig. S3** RMSD of WT and Mutants (His376Asp, His376Tyr, His376Phe, His376Asn, Asp372Asn, Asp287Asn, Asp287Ile, Asp287Glu, Asp372Ile, Glu126<sup>H</sup>Gln).

#### 4. Computational active site model built from crystal structure.



**Fig. S4.** Atomic coordinates were taken from the minimized structure of the crystal. The hydroxyethyl farnesyl chain was clipped at the 3-position, the heme propionates were replaced with methyl groups. For each residue included in the model, the C $\alpha$  atoms was substituted by a link H atom (H $_{link}$ ). All C atoms linked to H $_{link}$  will be fixed were then all frozen to mimic the structural constraints of the protein environment.

## 5. Calculation of indirect transfer of protons from Tyr237 to O<sub>Cu</sub> atom.



**Fig S5** The process in which H<sup>+</sup> first reaches O<sub>Fe</sub> atom from active site Tyr237 and then transfers to peroxy O<sub>Cu</sub> atom, mediated by the interstitial water molecule. Calculated ΔG values in kcal/mol, relative to I<sub>R</sub>.

## 6. Cartesian coordinates for DFT-optimized structures.

I<sub>R</sub>

Fe	0.16528300	1.86039800	0.08629200
Cu	-1.79649500	-2.16925200	-1.00076900
O	-0.04405700	0.13525400	-0.30950100
O	-1.10891000	-0.23284900	-0.96159900
C	-5.34503000	1.33527000	0.84210100
C	4.24516700	2.90790300	-3.60077700
C	-3.70614300	3.24982900	-3.72544100
N	-1.63224800	1.73629600	1.01210200
C	5.32194600	2.39460700	-4.21369100
N	1.09245000	1.23560100	1.79535600
N	-0.71763700	2.50836700	-1.58499600
C	-3.05775400	2.25669500	-0.92011800
C	-0.88661400	1.01413900	3.23523400
C	3.38588400	1.07537900	0.96145700
C	1.25725600	2.95982300	-2.94996100
C	-3.96942200	0.56764600	3.65603200
C	1.17617500	0.19476100	5.40844300
C	5.68871000	1.56179600	-1.02991800
C	-0.78985100	3.79531800	-5.11434600
O	-3.42749900	0.16649500	4.67802700
C	-2.84794200	1.82220900	0.38969400
C	0.48432400	0.97824900	3.00141900
C	3.17594800	1.61550100	-0.29900900
C	-0.11576000	2.93061300	-2.73491200
C	-3.90839400	1.42036100	1.27073500
C	1.47022200	0.50988800	3.97015900
C	4.23869400	1.85485600	-1.26034900
C	-1.11029800	3.29515200	-3.73923500
C	-3.29902300	1.09562400	2.47288900
C	2.67591900	0.45827400	3.30707600
C	3.64335300	2.42902800	-2.35857800
C	-2.33031400	3.06838500	-3.16572100
C	-1.86748200	1.29538500	2.28273400
C	2.41555900	0.93119800	1.95400900
C	2.21760900	2.51357800	-2.05334800
C	-2.07043800	2.58874700	-1.82200700
C	4.02489100	0.01691200	3.84447300
O	4.74477800	-0.78663600	2.91394700
N	1.96039900	2.02102300	-0.80130500
H	-5.70949200	2.30257400	0.47794600
H	3.76109200	3.76798100	-4.06234400
H	-4.28710000	3.97938500	-3.14899900

H	5.83696900	1.51375400	-3.84524900
H	-4.08541800	2.34027400	-1.25304400
H	-1.25044700	0.71842400	4.21119900
H	4.38017800	0.72983900	1.21188800
H	1.59989600	3.30148200	-3.91919000
H	1.98359200	-0.38346100	5.86478100
H	6.31496000	2.20225000	-1.65662900
H	-0.19525200	3.06789400	-5.67935000
H	3.84343500	-0.55690300	4.76761600
H	4.17860700	-1.51464200	2.59991000
H	-5.46759000	0.61315700	0.02655600
H	-3.67666100	3.60185800	-4.75941500
H	5.70700100	2.83796000	-5.12639500
H	-5.07718000	0.53632100	3.57813000
H	1.05864500	1.11086500	5.99968200
H	5.97286200	1.72380700	0.01385400
H	-1.69742500	3.99469300	-5.68894300
H	0.24889500	-0.37580800	5.52223400
H	5.93794500	0.52080400	-1.27191300
H	-0.21225400	4.72648900	-5.07997600
H	-4.27607700	2.31202700	-3.71986500
H	-6.00199700	1.02949300	1.65891600
C	4.95110500	1.18582500	4.19904000
H	5.90877400	0.79336700	4.55113400
H	5.13503000	1.81390300	3.32279500
H	4.51274200	1.80658200	4.98606000
C	-1.01557400	-5.41665400	-2.39373300
C	0.03661400	-4.61599100	-1.71109200
C	1.29231100	-4.99937900	-1.33104400
N	-0.10820000	-3.25955900	-1.46121500
C	1.05216800	-2.83625500	-0.98827600
N	1.93206600	-3.86026000	-0.86025800
H	1.30104600	-1.81335200	-0.75276900
H	-0.68549100	-6.44829000	-2.53873100
H	1.79873200	-5.95064600	-1.36779900
C	6.20762200	-4.64533500	-3.01032100
C	5.48371000	-4.14431700	-1.79733700
C	6.11718100	-3.67384300	-0.63690100
C	4.09855800	-4.16145500	-1.80877000
C	5.37871200	-3.24712900	0.46322200
C	3.34724200	-3.75649100	-0.70835700
C	3.97588800	-3.28560500	0.45334900
O	3.32490200	-2.88796000	1.58067100
H	7.17732700	-4.15434300	-3.14123100



H	7.20220000	-3.63366200	-0.59245400
H	3.56785800	-4.49318300	-2.69606200
H	5.87178800	-2.87143800	1.35404900
H	6.40451800	-5.72277900	-2.94216800
H	-1.95042600	-5.43839100	-1.82213500
H	2.35910200	-2.71357300	1.47478400
C	-0.84152700	7.27384400	1.36791000
C	-0.20488100	5.93200400	1.21270500
C	-0.66408500	4.75840600	0.67588200
N	1.08649200	5.64325800	1.63176300
C	1.35672600	4.34632900	1.34332700
N	0.31230500	3.78387700	0.76133300
H	2.29433200	3.85948500	1.56023700
H	-1.85220400	7.25062000	0.95529700
H	-1.62607200	4.55180600	0.23601900
H	-0.91762200	7.57127900	2.42015600
H	1.72375600	6.28763200	2.07627900
C	-5.17938700	-3.40538500	3.45214000
C	-4.02210200	-3.28391100	2.52039200
C	-3.86526000	-2.63398200	1.32445500
N	-2.79246200	-3.87373900	2.75728100
C	-1.95939400	-3.56953400	1.72943700
N	-2.58326400	-2.82021300	0.83690800
H	-0.92354700	-3.86710200	1.68869800
H	-5.42113300	-4.45197400	3.66917200
H	-4.59432500	-2.05379900	0.78172200
H	-4.98582200	-2.89819800	4.40463100
C	-7.21688900	-2.39280100	-1.94198600
C	-5.78684400	-2.06286500	-2.18586000
C	-4.64138900	-2.71536200	-1.81958600
N	-5.34466400	-0.90086400	-2.80131700
C	-3.98299000	-0.89200600	-2.77006900
N	-3.52794700	-1.97550200	-2.16847800
H	-3.37837400	-0.08850200	-3.16310200
H	-7.79485200	-2.46474500	-2.87086900
H	-4.55076600	-3.65645800	-1.29961300
H	-7.28883400	-3.35764800	-1.43553400
H	-5.92950400	-0.20285500	-3.23726100
H	-2.54563800	-4.41970800	3.56995100
H	0.47500300	-1.34163400	1.27500300
O	0.80537500	-2.01649300	1.89143600
H	0.99532900	-1.51209800	2.69897200
H	-0.28304400	8.05454900	0.83876400
H	5.62380500	-4.47862200	-3.91980400

H	-1.24493800	-4.98959900	-3.37593000
H	-7.70601300	-1.64445900	-1.30706900
H	-6.06490300	-2.94662500	3.00663800

**TS1**

Fe	0.35563300	1.88986800	0.07059000
Cu	-1.94388000	-2.11106200	-0.86444300
O	-0.09768300	0.04481100	-0.16515800
O	-1.25532500	-0.26188100	-0.81876000
C	-5.22358500	1.75503700	0.62187100
C	4.53954500	1.92803700	-3.63213700
C	-3.28645400	3.26085900	-3.98181900
N	-1.50334100	1.92360400	0.95252400
C	5.48030200	1.12959700	-4.15544000
N	1.15371400	1.28956000	1.85662700
N	-0.43125700	2.44205700	-1.67674500
C	-2.79737400	2.49323900	-1.05714300
C	-0.90586400	1.10826100	3.18494200
C	3.44456600	0.89014800	1.11667900
C	1.59122200	2.50079300	-3.03976000
C	-4.00719100	0.60279800	3.35645700
C	0.99702600	0.23445400	5.46502700
C	5.77623400	0.77119800	-0.86525000
C	-0.30846300	3.32842200	-5.32283600
O	-3.52538200	0.02209000	4.32305700
C	-2.67755700	2.08229700	0.27948000
C	0.47476600	1.06081500	3.03383900
C	3.30463800	1.28802300	-0.20175800
C	0.22141900	2.66816800	-2.84895600
C	-3.80129700	1.71136800	1.09297100
C	1.38722000	0.55656100	4.05397300
C	4.39148400	1.24980700	-1.16497800
C	-0.70916400	3.03489100	-3.91098700
C	-3.26560300	1.26744400	2.29304100
C	2.61850300	0.45062400	3.45488600
C	3.87965400	1.73570900	-2.34240700
C	-1.95329000	3.01538900	-3.34963200
C	-1.82355300	1.43131200	2.18552500
C	2.44341900	0.91100900	2.08743400
C	2.47850000	2.04954700	-2.08061800
C	-1.76922100	2.65196700	-1.95459900
C	3.91263100	-0.07730300	4.03475400
O	4.57416500	-0.96706700	3.14171400
N	2.14694800	1.76192200	-0.77547400

H	-5.47430800	2.74224500	0.21845100
H	4.22487400	2.79916800	-4.20637900
H	-3.85392700	4.03138900	-3.44745600
H	5.80709900	0.22206500	-3.65804800
H	-3.80296700	2.65871900	-1.42724300
H	-1.32762200	0.78948900	4.12987700
H	4.39844200	0.48635800	1.42501900
H	1.97825600	2.67804800	-4.03600000
H	1.78694300	-0.31676400	5.97998000
H	6.48575400	1.14977700	-1.60460500
H	0.16186100	2.45668100	-5.79296700
H	3.66702800	-0.60804200	4.96922900
H	3.91546700	-1.46324200	2.60650000
H	-5.39404800	1.01963300	-0.17353700
H	-3.18482800	3.58852100	-5.01867100
H	5.93656400	1.35521700	-5.11392700
H	-5.10949500	0.61600500	3.22252200
H	0.80272900	1.14711100	6.04040700
H	6.10788400	1.09576000	0.12593200
H	-1.16837900	3.60943900	-5.93475700
H	0.08358500	-0.36862000	5.50718300
H	5.82599900	-0.32525000	-0.87614400
H	0.41478000	4.15069500	-5.36998800
H	-3.90221100	2.35166800	-3.99152400
H	-5.93066300	1.54390100	1.42646900
C	4.90932900	1.04030300	4.37897000
H	5.83792900	0.59516700	4.74578000
H	5.13727300	1.63491800	3.48919200
H	4.50210300	1.70215700	5.14929400
C	-1.31791100	-5.48565600	-2.04690500
C	-0.24825100	-4.59253400	-1.52837100
C	1.01531300	-4.92182700	-1.12925700
N	-0.37051700	-3.20895000	-1.50135500
C	0.80833300	-2.72673700	-1.13813700
N	1.67553900	-3.72757200	-0.87356500
H	1.07458300	-1.68502100	-1.07178100
H	-1.02946200	-6.53522200	-1.95304600
H	1.51020300	-5.87254700	-1.01556800
C	5.96012400	-5.29544500	-2.42637100
C	5.22917600	-4.40088000	-1.47198200
C	5.83164100	-3.62177400	-0.46190400
C	3.84766400	-4.36174900	-1.56371000
C	5.07358600	-2.85710700	0.41467800
C	3.07382800	-3.62167900	-0.68265400

C	3.64451300	-2.82960800	0.36081600
O	2.94164100	-2.14183600	1.21639900
H	6.99614600	-4.97611600	-2.58058000
H	6.91461900	-3.62051600	-0.36467600
H	3.34671600	-4.91993500	-2.34926000
H	5.55122400	-2.26916600	1.19232500
H	5.99865800	-6.32706200	-2.05233800
H	-2.26010200	-5.33773000	-1.50563400
H	1.48337100	-1.91901100	1.33332500
C	-0.29718600	7.36122600	0.97721000
C	0.23789300	5.96655800	0.91950500
C	-0.29223800	4.80202300	0.42924900
N	1.48964000	5.60737300	1.40425900
C	1.67353100	4.27916500	1.19989200
N	0.60802800	3.76878900	0.60777600
H	2.55678900	3.72631400	1.47716600
H	-1.29576600	7.38905600	0.53632900
H	-1.24902800	4.63276600	-0.03578100
H	-0.37491000	7.72369600	2.00852300
H	2.15572600	6.22906700	1.83835100
C	-5.51280200	-2.81760800	3.50664600
C	-4.35440700	-2.93022100	2.57234800
C	-4.16431300	-2.50780700	1.28223400
N	-3.14649400	-3.50432300	2.93331900
C	-2.28527200	-3.40191000	1.88619200
N	-2.87838300	-2.80946300	0.86345900
H	-1.25543700	-3.72391900	1.90637600
H	-5.78086500	-3.78492200	3.94503800
H	-4.86110400	-2.00830200	0.62835700
H	-5.28169600	-2.11875000	4.31962000
C	-7.28007600	-1.98482900	-2.01213400
C	-5.83712900	-1.67211100	-2.15795400
C	-4.73072100	-2.44051500	-1.92467500
N	-5.33460300	-0.42254600	-2.49684000
C	-3.97349700	-0.48012900	-2.44252900
N	-3.58473900	-1.68988400	-2.08730400
H	-3.31681500	0.35730600	-2.62013200
H	-7.83992000	-1.82600000	-2.94133000
H	-4.68531000	-3.47152700	-1.60871000
H	-7.40024000	-3.03287700	-1.72956300
H	-5.88264800	0.37740500	-2.77735400
H	-2.92691300	-3.88746000	3.84116500
H	0.12326300	-0.71664400	0.62814900
O	0.48707700	-1.64955000	1.49853000

H	0.46436500	-1.23860400	2.37566200
H	0.33573700	8.06173500	0.42070700
H	5.46931600	-5.32329100	-3.40391700
H	-1.51260000	-5.27410600	-3.10399200
H	-7.75157700	-1.37197900	-1.23429200
H	-6.38591700	-2.43884100	2.97049500
<b>I<sub>III</sub></b>			
Fe	0.14092000	1.83545800	-0.20828700
Cu	-1.82878700	-2.62879600	-0.67515900
O	-0.28056800	-0.13844000	-0.00212900
O	-1.50407300	-0.64531800	-0.41783000
C	-5.31017000	2.06221200	0.97969000
C	4.06720400	1.45079700	-4.15590700
C	-3.86841100	1.98643900	-4.21093000
N	-1.59810900	2.08455300	0.80150700
C	5.08085300	0.70863300	-4.62418700
N	1.09638800	1.67452900	1.58755300
N	-0.82180600	1.91302400	-1.96230200
C	-3.11016600	1.95208700	-1.13185100
C	-0.77010200	2.14746400	3.10365500
C	3.30961300	1.05819000	0.76992900
C	1.10249900	1.80549300	-3.45839500
C	-3.80482100	2.27844900	3.79487100
C	1.28506600	1.66804300	5.34931600
C	5.56235500	0.87413900	-1.33158600
C	-1.02725900	1.92536800	-5.71287300
O	-3.21058100	2.32728000	4.86354800
C	-2.83961800	2.01156000	0.24912800
C	0.55601900	1.85164000	2.83836600
C	3.07975000	1.23962400	-0.59119300
C	-0.26887200	1.89880600	-3.20441300
C	-3.85344500	2.06557300	1.27167500
C	1.52507300	1.54727800	3.87324500
C	4.11536900	1.14030000	-1.60750900
C	-1.29302600	1.92447800	-4.23812700
C	-3.19009900	2.19540200	2.47352600
C	2.66306300	1.15644700	3.21734900
C	3.49935500	1.38982000	-2.81036200
C	-2.49799800	1.93976500	-3.58903400
C	-1.77877400	2.18391300	2.14907000
C	2.38469900	1.27867900	1.79438900
C	2.09063900	1.62381100	-2.50549900
C	-2.18766100	1.94238300	-2.16060400

C	3.97383300	0.76778800	3.83383400
O	4.65023600	-0.24954700	3.11617000
N	1.86138600	1.53883200	-1.15200500
H	-5.42471900	2.75985100	0.15719600
H	3.61170200	2.17412300	-4.83193400
H	-4.64038000	1.61718700	-3.52721500
H	5.55869600	-0.06283300	-4.02946200
H	-4.15715800	1.94404200	-1.41501800
H	-1.08792000	2.25179000	4.13357500
H	4.29622700	0.74087000	1.08048600
H	1.41145400	1.80565300	-4.49750600
H	2.04362600	1.12796000	5.92104000
H	6.18295700	1.22142500	-2.16131400
H	-0.40607200	1.07386100	-6.01362100
H	3.78113700	0.42833600	4.86503600
H	4.00888300	-0.89988900	2.74404900
H	-5.67409600	1.07995200	0.65670100
H	-4.15758900	3.01054200	-4.47764800
H	5.44860600	0.84278800	-5.63642500
H	-4.91501900	2.29043900	3.78515500
H	1.31757600	2.71492400	5.67445600
H	5.89618300	1.38187700	-0.42132400
H	-1.95654100	1.87342200	-6.28499100
H	0.30524300	1.27573800	5.63887300
H	5.76118800	-0.19534500	-1.18986400
H	-0.50196900	2.83513800	-6.02799100
H	-3.93198800	1.38590500	-5.13046600
H	-5.92167800	2.39927800	1.81752400
C	4.92922000	1.95706600	3.89854200
H	5.90064900	1.52814900	4.10811300
H	4.98177900	2.47812500	2.93816300
H	4.65192400	2.67117900	4.67815800
C	-0.72300100	-5.82063400	-1.04413100
C	0.29800700	-4.79556800	-0.69466300
C	1.63314600	-4.96760500	-0.45676800
N	0.02776000	-3.43500500	-0.73933000
C	1.18015200	-2.80961900	-0.53980400
N	2.18572600	-3.70181300	-0.35372700
H	1.32889400	-1.74249100	-0.54642800
H	-0.43014600	-6.81364500	-0.69502100
H	2.23363700	-5.85523900	-0.33963400
C	6.79538500	-4.62737600	-1.77562600
C	5.85296100	-3.92228100	-0.84222400
C	6.29967200	-3.08025400	0.20020700

C	4.47634100	-4.08425200	-0.99837900
C	5.41465500	-2.42008700	1.02908800
C	3.56766900	-3.43626100	-0.16946100
C	3.99299400	-2.55496300	0.87980800
O	3.16013500	-1.92343800	1.63785400
H	7.55485100	-3.95041400	-2.18202300
H	7.36818700	-2.94333600	0.34912500
H	4.09511900	-4.71866600	-1.79406900
H	5.77699300	-1.76987100	1.81755700
H	7.32853400	-5.44849200	-1.27997200
H	-1.70565700	-5.57725300	-0.62982900
H	-0.04589600	-0.58300700	0.88422600
C	-0.45894900	7.40901300	-0.61849000
C	0.07264600	6.03232800	-0.38662900
C	-0.48355900	4.79085600	-0.55843600
N	1.34166600	5.78036100	0.11270000
C	1.50800500	4.43959800	0.22426300
N	0.41574300	3.81181800	-0.17743400
H	2.40716000	3.96873600	0.58742000
H	-1.46929300	7.34835400	-1.02856400
H	-1.46491800	4.53863600	-0.92603400
H	-0.51354800	7.98403200	0.31318700
H	2.03130800	6.47582800	0.35677000
C	-5.39244100	-2.98499500	3.94220600
C	-4.26113300	-3.05055100	2.97104600
C	-4.18456300	-3.14709600	1.60485400
N	-2.94603800	-3.03826600	3.38414400
C	-2.13861200	-3.13106800	2.29882400
N	-2.86192700	-3.19856900	1.19393300
H	-1.06099400	-3.07259400	2.35177100
H	-5.65868600	-3.97225100	4.33757400
H	-4.99670500	-3.16872300	0.89654800
H	-5.14817200	-2.34008500	4.79288100
C	-7.26696000	-2.69551100	-1.71768600
C	-5.80721900	-2.45867000	-1.93034000
C	-4.70108300	-3.20006600	-1.60439100
N	-5.29247900	-1.26012300	-2.40267200
C	-3.93668700	-1.31140800	-2.33129000
N	-3.54640700	-2.47186400	-1.83379800
H	-3.28224800	-0.50317900	-2.61617500
H	-7.87611600	-2.31505800	-2.54402700
H	-4.66344000	-4.20027800	-1.20032300
H	-7.46552200	-3.76555100	-1.62430300
H	-5.83337600	-0.49411700	-2.77589500

H	-2.63196400	-2.97199300	4.34154600
H	1.50099600	-1.71385500	1.88669000
O	0.58316800	-1.40488000	2.12278200
H	0.72105300	-0.78634800	2.85518200
H	0.15279900	7.98116800	-1.32699000
H	6.22326600	-5.04526900	-2.60679100
H	-0.79486000	-5.84842000	-2.13539700
H	-6.27473200	-2.56542600	3.46226200
H	-7.60787300	-2.21113800	-0.78964600

**TS2**

Fe	0.28665900	1.82621900	0.32992000
Cu	-1.86342400	-1.72567300	-1.07239000
O	0.22094200	0.38076400	-1.12577000
O	-1.09401700	-0.02306900	-1.61888900
C	-5.28259600	1.69037700	0.91581300
C	4.59565800	3.55389800	-2.84089500
C	-3.33013000	4.04886100	-3.27868900
N	-1.53677900	1.40366900	1.04667900
C	5.65139100	3.12616500	-3.54826800
N	1.08960200	0.63033200	1.75694200
N	-0.48055300	2.92613300	-1.15143200
C	-2.84614500	2.54166700	-0.68425100
C	-0.95072900	0.05104100	2.99639700
C	3.44081200	0.68121600	1.06746900
C	1.57087100	3.61671200	-2.27994600
C	-4.08333900	-0.12747700	3.28478400
C	0.96519800	-1.40900700	4.93837800
C	5.86186100	1.49724700	-0.67639500
C	-0.34610000	4.93832800	-4.33195700
O	-3.61318300	-0.87087300	4.13748600
C	-2.73236300	1.82236300	0.47967600
C	0.41392700	0.04308500	2.82607300
C	3.33036300	1.53634000	-0.00618000
C	0.20152800	3.58325000	-2.15214800
C	-3.86075500	1.36433400	1.25626000
C	1.35575000	-0.63330700	3.71584700
C	4.44559600	1.94488400	-0.85019500
C	-0.74055200	4.15638300	-3.11969000
C	-3.32792900	0.62434900	2.29102300
C	2.59373300	-0.46969100	3.16238300
C	3.92340300	2.81825100	-1.77358200
C	-1.98286000	3.79206700	-2.69064400
C	-1.87138000	0.67680100	2.13286900



C	2.39514600	0.31033300	1.93913700
C	2.49021100	2.90721800	-1.47959300
C	-1.78434500	3.03364800	-1.46372000
C	3.92560800	-0.97596800	3.67907300
O	4.70626000	-1.55811000	2.64970300
N	2.15600800	2.14361500	-0.41777700
H	-5.43390900	2.77419000	0.87178500
H	4.19058100	4.53926800	-3.07025400
H	-3.97969900	4.59623700	-2.58498200
H	6.08037300	2.13976200	-3.40602100
H	-3.84859200	2.76672800	-1.02918700
H	-1.37461600	-0.48131100	3.83848200
H	4.40463700	0.23800900	1.28476500
H	1.97493400	4.16212200	-3.12510800
H	1.81738400	-1.55888500	5.60385900
H	6.55304200	2.23306400	-1.09598500
H	0.25528900	4.33029800	-5.01783400
H	3.71361400	-1.72355200	4.46040000
H	4.09758600	-2.10939100	2.10006100
H	-5.55034900	1.28087900	-0.06622700
H	-3.26521300	4.63744900	-4.19679700
H	6.10419400	3.75133900	-4.31097600
H	-5.18447500	-0.00374700	3.21372200
H	0.18231300	-0.90067800	5.50880400
H	6.11209000	1.35169100	0.37845000
H	-1.22023700	5.29271300	-4.88273700
H	0.58988100	-2.39896600	4.65260500
H	6.04596200	0.54248700	-1.18484500
H	0.25558100	5.81418100	-4.06340600
H	-3.84215600	3.11156000	-3.53288400
H	-5.98637200	1.28785500	1.64644200
C	4.78069600	0.12975500	4.29745500
H	5.74060900	-0.29135800	4.60777200
H	4.97277800	0.92058400	3.56557900
H	4.28808500	0.57294900	5.16861200
C	-1.30955000	-4.88906700	-3.05073900
C	-0.24375100	-4.30030800	-2.19250700
C	1.02517600	-4.78037600	-2.06061700
N	-0.35152500	-3.13196100	-1.43420800
C	0.82485200	-2.94075600	-0.86695400
N	1.70944600	-3.90971300	-1.22931500
H	1.09859200	-2.16141500	-0.17581300
H	-0.94069900	-5.78905300	-3.54689400
H	1.48888900	-5.66076800	-2.47292200

C	5.93612000	-4.73170500	-3.48235500
C	5.23044500	-4.21005800	-2.27324800
C	5.89578300	-3.66868700	-1.15023700
C	3.84171100	-4.26790800	-2.25141800
C	5.19223400	-3.19972100	-0.05832100
C	3.11684600	-3.83332400	-1.15462900
C	3.75869600	-3.25339000	-0.00685200
O	3.07562700	-2.79678500	0.98452400
H	5.33330700	-4.60539500	-4.38647100
H	6.98102000	-3.60897000	-1.15476900
H	3.31915400	-4.63185800	-3.12906900
H	5.70752700	-2.76507200	0.79146300
H	6.89734400	-4.23290300	-3.64318800
H	-2.19923800	-5.15661600	-2.46854800
H	0.62699000	-0.44302600	-0.82019600
C	-0.35788500	7.06135800	2.37267500
C	0.11477700	5.65382800	2.12178300
C	-0.41134100	4.61141000	1.39749600
N	1.31023000	5.15260400	2.62300000
C	1.46403900	3.87127500	2.19467100
N	0.43624500	3.51504000	1.44555000
H	2.31419200	3.24724400	2.42206200
H	-1.31664900	7.21905800	1.87448500
H	-1.33042300	4.57682100	0.83588900
H	-0.49580500	7.25820100	3.44163200
H	1.96062200	5.65388200	3.20968500
C	-5.57409500	-3.39481700	2.85598900
C	-4.37922300	-3.25511100	1.97982800
C	-4.11364100	-2.43882000	0.91392700
N	-3.20190200	-3.95263100	2.18872400
C	-2.27819700	-3.54561300	1.28352700
N	-2.80904700	-2.62697600	0.48897200
H	-1.24828200	-3.87774000	1.27189900
H	-5.86280300	-4.44220900	2.99500000
H	-4.76433400	-1.72812800	0.43217600
H	-5.37807600	-2.95432200	3.84084700
C	-7.29105900	-1.53576600	-2.40016400
C	-5.82697800	-1.26511700	-2.43940600
C	-4.75636000	-2.06561300	-2.14613100
N	-5.26738200	-0.02814400	-2.74152900
C	-3.91392500	-0.12545200	-2.61610900
N	-3.58049600	-1.34796000	-2.24303900
H	-3.21248200	0.68225500	-2.75848600
H	-7.77330900	-1.36085200	-3.36894300

H	-4.75833300	-3.09879800	-1.83539700
H	-7.46196300	-2.57962000	-2.12858300
H	-5.77397700	0.78582900	-3.05743300
H	-3.02789300	-4.60556000	2.93906700
H	1.52736600	-3.34756200	1.79212800
O	0.61830300	-3.37212700	2.15480800
H	0.41964000	-2.43983200	2.30947300
H	0.35226900	7.79780300	1.98059200
H	6.15031900	-5.80479900	-3.38331000
H	-1.62814100	-4.17470900	-3.81824400
H	-6.42408700	-2.86905100	2.41450800
H	-7.79950800	-0.90823500	-1.65836100

### I<sub>H2</sub>

Fe	0.24028500	1.85416200	0.31066900
Cu	-1.84536200	-1.88489200	-1.13081500
O	0.11102900	0.15935500	-0.92692000
O	-1.09552200	-0.14157700	-1.63079800
C	-5.32206000	1.53220900	0.95009700
C	4.44278800	3.54042700	-3.04192500
C	-3.52030100	3.92403300	-3.28695500
N	-1.56859500	1.47331200	1.09318600
C	5.54684800	3.16832400	-3.70637800
N	1.08966200	0.80942400	1.79421000
N	-0.58309700	2.83186500	-1.25070900
C	-2.93391200	2.44423500	-0.69691900
C	-0.90853300	0.29219200	3.12592600
C	3.41924500	0.83461300	1.02993700
C	1.42437400	3.51232700	-2.46139400
C	-4.03129900	0.06740900	3.50202300
C	1.07150800	-1.07819800	5.06797400
C	5.80473400	1.66387300	-0.77472900
C	-0.58169000	4.77778900	-4.47497900
O	-3.52925700	-0.58370700	4.40987100
C	-2.78061500	1.79581600	0.51013400
C	0.45295500	0.27469800	2.90799900
C	3.27021000	1.60212900	-0.11198100
C	0.05196200	3.46724600	-2.28851000
C	-3.88306800	1.34977300	1.32677900
C	1.42002800	-0.36734800	3.79212000
C	4.36438500	2.01904800	-0.97342500
C	-0.92356400	4.01264900	-3.23419600
C	-3.31263300	0.73703300	2.42481400
C	2.63989400	-0.23230500	3.18991500

C	3.80358600	2.81990700	-1.94352200
C	-2.15157800	3.65650800	-2.75022100
C	-1.86347400	0.82993100	2.24448700
C	2.40462600	0.49908500	1.94334000
C	2.37100200	2.85902400	-1.65831700
C	-1.90649600	2.92706900	-1.51860300
C	3.98816500	-0.70232400	3.69609800
O	4.76987800	-1.29928900	2.67365700
N	2.06853400	2.11572800	-0.55801600
H	-5.56177500	2.59110900	0.80206500
H	3.96517400	4.47374900	-3.33837900
H	-4.12770100	4.50840300	-2.58554600
H	6.06285400	2.23577900	-3.50454100
H	-3.94915700	2.62391600	-1.03177300
H	-1.30048100	-0.18629800	4.01502100
H	4.40093400	0.44102700	1.26344700
H	1.79626400	4.04013400	-3.33204500
H	1.94947500	-1.21133500	5.70306600
H	6.45385000	2.43993300	-1.18977500
H	0.00895400	4.17205000	-5.17241600
H	3.80416600	-1.43139700	4.50094000
H	4.20546300	-1.95596700	2.20257200
H	-5.55041400	1.01214500	0.01228800
H	-3.48291300	4.48384200	-4.22469500
H	5.95599700	3.78956600	-4.49655300
H	-5.13562600	0.17120200	3.45089300
H	0.32370600	-0.52934900	5.64808400
H	6.04996100	1.54339800	0.28394900
H	-1.48038900	5.10345300	-5.00387300
H	0.66630000	-2.07569900	4.85778500
H	6.06375100	0.72074400	-1.27247900
H	0.00795400	5.67314100	-4.24639000
H	-4.06789600	2.99521000	-3.49192300
H	-6.00099800	1.14920100	1.71422600
C	4.82075000	0.44208400	4.28023700
H	5.79150000	0.05424600	4.60142500
H	4.99453800	1.22131500	3.53193200
H	4.31981500	0.89396800	5.14188500
C	-1.19255400	-4.94528000	-2.93232000
C	-0.12158900	-4.34472300	-2.09147500
C	1.13668200	-4.83245900	-1.90072900
N	-0.22094200	-3.12260600	-1.42819400
C	0.94704300	-2.89629900	-0.85733600
N	1.81678200	-3.91261900	-1.11897100

H	1.22193900	-2.02045100	-0.29388300
H	-0.84684100	-5.88307200	-3.37289200
H	1.60239400	-5.74359100	-2.23873300
C	6.00962200	-4.56679400	-3.48396700
C	5.32161200	-4.16949000	-2.21900100
C	6.00804400	-3.69687000	-1.07239500
C	3.93520600	-4.23324100	-2.17272200
C	5.32460000	-3.28897400	0.05283700
C	3.22581900	-3.84789500	-1.04591400
C	3.88682300	-3.32892500	0.12384300
O	3.23063400	-2.91582600	1.14292500
H	6.67457200	-5.42714900	-3.33142100
H	7.09370500	-3.64185900	-1.08861000
H	3.39233100	-4.55518700	-3.05485200
H	5.85251400	-2.90636100	0.92057000
H	5.29316000	-4.83617500	-4.26323800
H	-2.10007800	-5.15723900	-2.35492700
H	0.74130000	0.35737400	-1.64107700
C	-0.56039600	7.09904200	2.18971200
C	-0.00877500	5.72915100	1.94634800
C	-0.49455000	4.65811700	1.24169800
N	1.21703700	5.29764300	2.43124200
C	1.42642800	4.02271000	2.01306700
N	0.40439100	3.60688700	1.28572800
H	2.30924800	3.44797500	2.24441100
H	-1.53429200	7.19424300	1.70515100
H	-1.42395600	4.57995900	0.70208300
H	-0.69776500	7.30137900	3.25809200
H	1.85306900	5.83633900	3.00042800
C	-5.41295900	-3.50889200	3.00926200
C	-4.24738200	-3.35577100	2.09395700
C	-4.06812500	-2.63491400	0.94419200
N	-3.02093800	-3.95286600	2.32132300
C	-2.15718500	-3.58147900	1.34664200
N	-2.76946900	-2.78181800	0.48431100
H	-1.10581900	-3.84374200	1.35265100
H	-5.65596800	-4.56176900	3.19119600
H	-4.78625400	-2.02197100	0.42453800
H	-5.21972500	-3.03193700	3.97731600
C	-7.27784700	-1.79893900	-2.26135800
C	-5.82434500	-1.52695100	-2.42674600
C	-4.72907100	-2.29498200	-2.13968400
N	-5.29881900	-0.30737600	-2.83302500
C	-3.94196600	-0.37914400	-2.75960900

N	-3.56812700	-1.57057900	-2.32799500
H	-3.27357800	0.43660200	-2.98884700
H	-7.83988700	-1.66161500	-3.19256800
H	-4.70742700	-3.31191800	-1.77968800
H	-7.42337000	-2.83235200	-1.93976200
H	-5.83065600	0.48244400	-3.16878500
H	-2.77659800	-4.52329600	3.11833500
H	1.61989100	-3.39310800	1.91305000
O	0.72561800	-3.35889700	2.30906200
H	0.59738400	-2.41389700	2.46462600
H	6.64082100	-3.75790700	-3.87321200
H	0.09342400	7.87860200	1.78224500
H	-1.47540400	-4.26857100	-3.74641300
H	-6.29589200	-3.03608600	2.57298100
H	-7.72925900	-1.14642700	-1.50444200

**I<sub>p</sub>**

Fe	0.28513800	1.77855300	0.30672700
Cu	-1.98533300	-1.99400700	-1.23548400
O	0.36618100	0.33062800	-0.81261900
O	-0.82083800	0.01035900	-1.55565600
C	-5.27454600	1.66153500	0.96696200
C	4.52704900	3.47267200	-3.00897100
C	-3.42026100	3.99558400	-3.27964200
N	-1.52702300	1.45400000	1.06595300
C	5.62478500	3.07498900	-3.66959700
N	1.11636700	0.78709100	1.81083000
N	-0.52463600	2.84572100	-1.22513600
C	-2.88162300	2.54779900	-0.66971700
C	-0.90261500	0.23382700	3.08995700
C	3.46239700	0.79907000	1.08120900
C	1.51583100	3.48483900	-2.41673900
C	-4.01672300	0.10219500	3.47956000
C	1.04316000	-1.20013300	5.01384500
C	5.86313700	1.58538200	-0.72948200
C	-0.44761200	4.74867100	-4.46565800
O	-3.53205700	-0.56314700	4.38618600
C	-2.73427900	1.84429900	0.51085800
C	0.46644500	0.22488900	2.89299700
C	3.33252000	1.59550800	-0.05312800
C	0.13265700	3.45153300	-2.25829600
C	-3.83875700	1.41881700	1.32485800
C	1.41520800	-0.44522300	3.77129600
C	4.43133100	1.97654700	-0.92331200

C	-0.81587600	4.01461700	-3.21253800
C	-3.28164200	0.75822000	2.40414800
C	2.64541900	-0.30205400	3.19051900
C	3.88121800	2.77961700	-1.89789600
C	-2.06176300	3.71237700	-2.72529000
C	-1.83704300	0.79918400	2.21775700
C	2.44035500	0.46613300	1.96884500
C	2.45046400	2.85198400	-1.60279100
C	-1.84888700	2.99639500	-1.48861000
C	3.98076700	-0.81250300	3.69046200
O	4.74194600	-1.42440600	2.66265800
N	2.15443300	2.14018200	-0.47625200
H	-5.47745600	2.73063100	0.83821200
H	4.06126900	4.40715400	-3.32023000
H	-4.04925700	4.53913500	-2.56530100
H	6.12901300	2.13931400	-3.45357700
H	-3.89381300	2.77940200	-0.98018400
H	-1.30680200	-0.25895300	3.96534000
H	4.43213400	0.37270200	1.30623100
H	1.89375500	3.99709900	-3.29415600
H	1.90423000	-1.33448300	5.67152400
H	6.53028800	2.34354100	-1.14925400
H	0.11699900	4.11273200	-5.15768400
H	3.77824600	-1.53925900	4.49293200
H	4.15437100	-2.05432800	2.18116500
H	-5.53449500	1.16365900	0.02545300
H	-3.36643000	4.60381300	-4.18618000
H	6.03971900	3.67769200	-4.47106700
H	-5.11784900	0.23509800	3.42914500
H	0.26598400	-0.68579800	5.58674500
H	6.11010500	1.46262500	0.32864600
H	-1.33551100	5.10105000	-4.99594600
H	0.66801800	-2.19783900	4.75466400
H	6.09622700	0.63433700	-1.22486400
H	0.17528900	5.62486500	-4.25203200
H	-3.95476500	3.07523500	-3.54876300
H	-5.95825000	1.29292700	1.73393400
C	4.84389300	0.30615100	4.27360400
H	5.80657600	-0.10680300	4.58797700
H	5.03326000	1.08504800	3.52912100
H	4.36032200	0.76674500	5.14087100
C	-1.33051600	-4.93231200	-2.91227000
C	-0.22699800	-4.31499800	-2.13000400
C	1.02009600	-4.81465300	-1.90553600

N	-0.30648200	-3.05506800	-1.54515400
C	0.86835300	-2.81169200	-0.98481800
N	1.71553700	-3.85760400	-1.18275900
H	1.15273400	-1.89749400	-0.48618800
H	-1.01765500	-5.89534600	-3.32260500
H	1.47279300	-5.75305100	-2.18071800
C	5.87771400	-4.74848700	-3.48302200
C	5.21584100	-4.27828200	-2.23134500
C	5.91182500	-3.84519100	-1.07966700
C	3.82587700	-4.26399600	-2.20326600
C	5.23578300	-3.40810600	0.04148400
C	3.12613200	-3.84769100	-1.08581600
C	3.79809300	-3.37902300	0.09789000
O	3.15310400	-2.95377000	1.11898100
H	6.01666200	-5.83879300	-3.47762500
H	6.99888200	-3.84535500	-1.08420900
H	3.27637900	-4.55334700	-3.09331900
H	5.77296100	-3.05802000	0.91711800
H	5.28058000	-4.50652000	-4.36709800
H	-2.22206700	-5.10266000	-2.29695900
H	-0.41799500	-0.29605100	-2.38567300
C	-0.36198500	7.10101900	2.18286800
C	0.13014200	5.70883700	1.93963400
C	-0.39490600	4.65753400	1.23344000
N	1.33653100	5.22882500	2.43054700
C	1.49784700	3.94895800	2.01527200
N	0.46204300	3.57176300	1.28452700
H	2.35634700	3.34057500	2.25123800
H	-1.33126700	7.23861200	1.69926000
H	-1.32399500	4.61611100	0.68935500
H	-0.48925400	7.30868700	3.25141100
H	1.99123700	5.74250500	3.00216200
C	-5.49542900	-3.37111000	3.03690600
C	-4.32957300	-3.25171500	2.12332200
C	-4.13751800	-2.52612200	0.97944500
N	-3.11804300	-3.88054300	2.34388100
C	-2.25005400	-3.51810800	1.36709100
N	-2.84564700	-2.69569000	0.51612000
H	-1.20565500	-3.80854600	1.36166800
H	-5.77240600	-4.41566600	3.21967100
H	-4.84493200	-1.89383500	0.46699500
H	-5.28832100	-2.90124300	4.00582200
C	-7.32742600	-1.62234700	-2.23252600
C	-5.87657500	-1.33418000	-2.38637700



C	-4.77914700	-2.11916700	-2.16435200
N	-5.35726300	-0.08803800	-2.70685100
C	-3.99952400	-0.16113100	-2.64951400
N	-3.61884600	-1.37993000	-2.30902400
H	-3.34328800	0.67663200	-2.82585600
H	-7.89425400	-1.42418400	-3.14968400
H	-4.75294100	-3.15732000	-1.87163200
H	-7.46742400	-2.67565100	-1.98084200
H	-5.89310400	0.72343300	-2.97840200
H	-2.88477400	-4.46033600	3.13722900
H	1.53726200	-3.39079800	1.84025200
O	0.64327500	-3.35806900	2.23995400
H	0.48618800	-2.40915900	2.32973900
H	6.87123200	-4.30782300	-3.61520600
H	0.32503600	7.85100300	1.77465000
H	-1.62826800	-4.28786000	-3.74736800
H	-6.36412100	-2.87108500	2.60194500
H	-7.77671800	-1.02440600	-1.43081900

**I<sub>R</sub>'**

Fe	0.01657000	1.83905400	0.19916900
Cu	-1.61771900	-2.21663600	-1.21412400
O	-0.10785100	0.30615300	-0.61436700
O	-0.58290500	-0.73735200	0.00231000
C	-5.46026800	0.96682200	0.81696600
C	4.05622100	3.54382900	-3.31118600
C	-3.89618700	3.32354000	-3.53267300
N	-1.77142700	1.52139300	1.07338200
C	5.15928000	3.16004700	-3.97030300
N	0.92902900	1.11184600	1.81586200
N	-0.88614900	2.65917800	-1.41961000
C	-3.20334100	2.14562000	-0.82581400
C	-1.02524300	0.65109100	3.23396600
C	3.24273900	1.14678600	0.99241800
C	1.06453500	3.38575000	-2.69404000
C	-4.07962300	-0.00616500	3.55540500
C	1.07861000	-0.18944400	5.34224300
C	5.54064100	1.93449700	-0.91903300
C	-1.02652500	4.29128400	-4.79928900
O	-3.52858900	-0.47871400	4.54155400
C	-2.98588400	1.61266000	0.44195900
C	0.33954400	0.71909100	2.99979200
C	3.02410200	1.80656400	-0.20872400
C	-0.30572500	3.24226800	-2.50777800

C	-4.03418500	1.07997400	1.26594400
C	1.35112300	0.24254400	3.93004600
C	4.08182500	2.20135100	-1.12335000
C	-1.31539000	3.62346200	-3.48958200
C	-3.42453300	0.66977500	2.44117900
C	2.55576200	0.31320600	3.26801100
C	3.46853400	2.88745500	-2.14576400
C	-2.51614000	3.22831700	-2.96800200
C	-2.00710200	0.95502900	2.29270400
C	2.27187100	0.87277600	1.95487100
C	2.03902800	2.87820000	-1.84621500
C	-2.23087600	2.64067300	-1.67377000
C	3.93097600	-0.03838000	3.79965100
O	4.75158100	-0.69466700	2.84166700
N	1.79885400	2.22362900	-0.66754100
H	-5.86962500	1.94523600	0.54074100
H	3.53592400	4.43215900	-3.66760900
H	-4.56351000	3.90438200	-2.88533500
H	5.71227300	2.26417000	-3.70889100
H	-4.22963200	2.19045200	-1.16960200
H	-1.37399100	0.25304600	4.17822800
H	4.24829200	0.82484400	1.22869900
H	1.39526100	3.85737800	-3.61139500
H	1.92636400	-0.73303200	5.76640100
H	6.14547800	2.68132800	-1.44041300
H	-0.37715900	3.67538100	-5.43238000
H	3.79502700	-0.68607900	4.68066900
H	4.29385700	-1.48694800	2.50478100
H	-5.54395600	0.31792000	-0.06236400
H	-3.89737000	3.80527100	-4.51359300
H	5.52858100	3.73083300	-4.81626300
H	-5.18264000	-0.08904800	3.45519700
H	0.88935400	0.67442600	5.99055200
H	5.81127200	1.95580700	0.14039700
H	-1.94444100	4.48366800	-5.35978000
H	0.19734300	-0.83535500	5.41060000
H	5.83249700	0.94924500	-1.30425600
H	-0.52111700	5.25368700	-4.65805700
H	-4.35492600	2.33510800	-3.66367800
H	-6.10606100	0.55494200	1.59505000
C	4.70654600	1.20267700	4.24254300
H	5.69493300	0.90443800	4.60280100
H	4.83830200	1.89302700	3.40471700
H	4.18198300	1.72784000	5.04630700

C	-0.58966200	-5.19614000	-2.70119200
C	0.41898500	-4.40860600	-1.95796900
C	1.67219700	-4.77751700	-1.56340900
N	0.21543600	-3.07684600	-1.63647700
C	1.34640400	-2.64560100	-1.10370700
N	2.25554000	-3.64825600	-1.00853400
H	1.55818400	-1.63709700	-0.79150100
H	-0.22747500	-6.20782500	-2.90124500
H	2.21007500	-5.70907800	-1.63706800
C	6.52960000	-4.03645600	-3.24176400
C	5.80314500	-3.69320600	-1.97739500
C	6.42507500	-3.32937400	-0.77197300
C	4.42097900	-3.75963900	-1.98856800
C	5.67750100	-3.05444000	0.37044400
C	3.66417500	-3.50418500	-0.84945700
C	4.27688100	-3.14536700	0.35606700
O	3.60376000	-2.89839400	1.51335600
H	7.43067500	-3.42875300	-3.37688900
H	7.50814000	-3.25486900	-0.72367300
H	3.89609900	-4.01502400	-2.90398200
H	6.16228300	-2.76458300	1.29709300
H	6.85342400	-5.08503600	-3.24591700
H	-1.53258600	-5.28065600	-2.14814000
C	-1.36781500	7.09239900	1.78131900
C	-0.62583200	5.81980800	1.55944000
C	-1.02130400	4.62276800	1.02631900
N	0.71304500	5.64076900	1.87262200
C	1.07288900	4.37946300	1.52395500
N	0.03974300	3.74083800	1.00665800
H	2.06485500	3.97535800	1.65082300
H	-2.40306600	6.97523600	1.45433200
H	-1.99250700	4.34365100	0.65211300
H	-1.38402700	7.38097900	2.83878200
H	1.32291600	6.32910200	2.28862500
C	-5.00459600	-3.93850000	3.13863000
C	-3.85164600	-3.69236500	2.22790000
C	-3.74619100	-3.03930300	1.02859600
N	-2.57090300	-4.14488400	2.48523700
C	-1.76282000	-3.77452100	1.46102800
N	-2.44827000	-3.10136500	0.55476300
H	-0.70215200	-3.97123200	1.44138100
H	-5.13164600	-5.00479200	3.35740600
H	-4.52362600	-2.53580500	0.47693100
H	-4.88644100	-3.40907100	4.09158600

C	-6.99681400	-2.72596500	-2.22257600
C	-5.59911600	-2.22736200	-2.37929400
C	-4.39587900	-2.81112300	-2.08654200
N	-5.26959900	-0.94329700	-2.79085000
C	-3.91697000	-0.80150600	-2.71858400
N	-3.35868000	-1.91397500	-2.27734900
H	-3.39554500	0.11039600	-2.96586900
H	-7.56126800	-2.68917400	-3.16143000
H	-4.21428700	-3.80842200	-1.71772500
H	-6.97894800	-3.76560300	-1.88918100
H	-5.91691800	-0.24675100	-3.13019600
H	-2.28067100	-4.65988000	3.30385100
H	5.89312600	-3.88822200	-4.11793700
H	-0.93210600	7.92418700	1.21560200
H	-0.81839100	-4.72108100	-3.66170000
H	-5.92761400	-3.58429600	2.67402600
H	-7.55301900	-2.14426200	-1.47815900
H	0.47736400	-1.74579200	1.33735400
O	1.00431900	-2.33686000	1.90631400
H	2.62280600	-2.82160200	1.41989200
H	1.15721800	-1.80902800	2.70600200

**TS1'**

Fe	0.14716100	1.83123300	0.16395600
Cu	-1.74437600	-1.95939600	-1.01815000
O	0.28838200	0.07626300	-0.18283800
O	-0.62765400	-0.79674200	0.36345100
C	-5.37955900	1.40240300	0.60286700
C	4.44768500	2.45347000	-3.40102500
C	-3.43952700	3.45692900	-3.74852500
N	-1.68262800	1.63631000	0.97640700
C	5.47532800	1.78135100	-3.93913400
N	0.98597300	1.19236400	1.95950100
N	-0.60569800	2.50133200	-1.49669200
C	-2.98952800	2.40345200	-0.94350600
C	-1.08509100	0.63039700	3.13343100
C	3.32028200	1.01423000	1.23455700
C	1.44354100	2.81402600	-2.82150000
C	-4.16047900	0.05586100	3.25043700
C	0.80034300	-0.44139600	5.34164800
C	5.71207900	1.19565400	-0.69128500
C	-0.44793800	3.79660800	-5.02877300
O	-3.67243100	-0.55006700	4.19743500
C	-2.86727800	1.85038800	0.32513000

C	0.29331300	0.71444100	3.04395900
C	3.19261200	1.49631900	-0.05342300
C	0.07703000	2.89124700	-2.63704400
C	-3.97350600	1.35895900	1.09122400
C	1.20737800	0.12177200	4.01244300
C	4.30152300	1.59646800	-0.98690900
C	-0.85183100	3.33071800	-3.66468500
C	-3.43146400	0.81384300	2.24132800
C	2.45826200	0.20294900	3.45349000
C	3.78040100	2.12921900	-2.14306400
C	-2.10376200	3.20092700	-3.13310200
C	-1.99617700	1.02651400	2.15329100
C	2.28905800	0.85978100	2.16585200
C	2.35825500	2.33452100	-1.88482000
C	-1.93717800	2.69559800	-1.78736400
C	3.77929600	-0.25453100	4.02472900
O	4.56893000	-0.97946100	3.09636700
N	2.02276300	1.94209500	-0.62897100
H	-5.67549400	2.42289500	0.33477300
H	4.06191800	3.31917900	-3.93898200
H	-4.03043000	4.16403500	-3.15493000
H	5.88061100	0.88461300	-3.48202700
H	-3.99107100	2.57525600	-1.31869900
H	-1.51481400	0.16451900	4.01132600
H	4.28847400	0.64194100	1.53875100
H	1.82763200	3.10666500	-3.79135400
H	1.61109700	-1.01622500	5.79452600
H	6.40884200	1.72532300	-1.34594400
H	0.07559400	3.00751400	-5.58109400
H	3.56625700	-0.88332800	4.90506200
H	3.98589600	-1.45246700	2.45533600
H	-5.50110400	0.78118300	-0.29306600
H	-3.34743800	3.87132400	-4.75486900
H	5.92679400	2.10300300	-4.87208800
H	-5.25941500	0.02771000	3.09348700
H	0.52949300	0.35626000	6.04316100
H	5.98422800	1.41197700	0.34595400
H	-1.31407400	4.09657000	-5.62255200
H	-0.07186500	-1.09864900	5.25685000
H	5.85700200	0.11886800	-0.84276000
H	0.22909000	4.65654100	-4.97247000
H	-4.03123500	2.53604100	-3.83453800
H	-6.09121400	1.04602100	1.35039200
C	4.61482700	0.94032300	4.48263900

H	5.58250800	0.58707600	4.84964000
H	4.79320900	1.62527400	3.64880600
H	4.11228500	1.49058600	5.28452500
C	-0.89014100	-5.26572800	-2.47348900
C	0.09640500	-4.33110500	-1.87418900
C	1.36113500	-4.63949100	-1.46686900
N	-0.08734900	-2.95435900	-1.76022500
C	1.07141200	-2.45975900	-1.33913900
N	1.96769900	-3.44384800	-1.12342700
H	1.28844000	-1.41988000	-1.15507400
H	-0.52715100	-6.29476300	-2.41923400
H	1.88885700	-5.57745600	-1.40868800
C	6.31738300	-4.71053600	-2.72535000
C	5.55067300	-3.91599200	-1.72102100
C	6.10956300	-3.18978400	-0.65584100
C	4.17084000	-3.93518600	-1.83355600
C	5.30509500	-2.52904700	0.26748300
C	3.36039100	-3.30058500	-0.90961100
C	3.88724600	-2.57279400	0.18659000
O	3.12667700	-1.97053000	1.07499700
H	7.37119500	-4.41616800	-2.77151100
H	7.19031200	-3.14884000	-0.54473400
H	3.70564700	-4.45707600	-2.66471600
H	5.74482000	-1.98176800	1.09530000
H	6.29746200	-5.78147200	-2.48495900
H	-1.86007600	-5.21877300	-1.96284000
C	-0.83824900	7.20692200	1.54357200
C	-0.20914300	5.85859300	1.35292500
C	-0.68824000	4.68032800	0.83805400
N	1.10718000	5.57684000	1.69805600
C	1.37673800	4.28350700	1.38825900
N	0.30562600	3.71727000	0.86304200
H	2.32443400	3.79478900	1.54965000
H	-1.87534500	7.17851700	1.20317600
H	-1.66750800	4.45864400	0.44686900
H	-0.83758900	7.50823000	2.59703500
H	1.75993500	6.22470500	2.11401600
C	-5.43284800	-3.43191000	3.11021400
C	-4.22172800	-3.29729600	2.25733100
C	-4.00021200	-2.62952100	1.08283000
N	-2.99881100	-3.86030400	2.57705800
C	-2.10120900	-3.52673000	1.61199300
N	-2.68485200	-2.78493900	0.68570000
H	-1.05571300	-3.79702500	1.62949500

H	-5.64588000	-4.47701600	3.35980900
H	-4.69819600	-2.04923300	0.50157500
H	-5.31262300	-2.87014000	4.04443300
C	-7.08495200	-2.26602100	-2.37548600
C	-5.66812500	-1.80262600	-2.40367900
C	-4.50746900	-2.42725200	-2.03442500
N	-5.27337800	-0.52228900	-2.77097800
C	-3.92458400	-0.42217100	-2.60424800
N	-3.43618000	-1.55835000	-2.14252400
H	-3.35455700	0.47177800	-2.80207000
H	-7.56009400	-2.20854500	-3.36143800
H	-4.37502600	-3.42979100	-1.65931500
H	-7.12181300	-3.30735400	-2.04894900
H	-5.87666900	0.19685600	-3.14256600
H	-2.79945000	-4.40226400	3.40510300
H	5.89865400	-4.59886200	-3.73087700
H	-0.31554500	7.98027700	0.96973500
H	-1.06751400	-5.01991300	-3.52669300
H	-6.30251500	-3.02940800	2.58555400
H	-7.68925100	-1.67293500	-1.67902800
H	0.04094900	-1.51856100	0.96748100
O	0.78503400	-2.24836500	1.67913300
H	1.81217000	-2.20237400	1.31993900
H	0.82642600	-1.82664900	2.55150300

**I<sub>P</sub>'**

Fe	0.14434300	1.85040500	0.08220600
Cu	-1.77737800	-2.16472100	-1.04818700
O	0.24729500	0.06681600	-0.24194400
O	-0.75137818	-0.86923006	0.29199373
C	-5.38321300	1.37152200	0.63717500
C	4.40670100	2.63521400	-3.48693000
C	-3.52572900	3.32264900	-3.79709400
N	-1.67744900	1.71908100	0.94315500
C	5.47107800	2.05202500	-4.05718500
N	1.00538100	1.27536700	1.87631600
N	-0.63773100	2.47363800	-1.58148400
C	-3.01307500	2.26532400	-1.02454500
C	-1.03361200	0.99053300	3.19581500
C	3.30908200	0.98183900	1.09260300
C	1.39251300	2.87546600	-2.90414400
C	-4.12743200	0.58408300	3.50123800
C	0.91095300	0.03109400	5.42645900
C	5.70520600	1.27467600	-0.83832800

C	-0.55422000	3.82736300	-5.10036700
O	-3.62623000	0.18313000	4.54397400
C	-2.87265000	1.82787800	0.28482500
C	0.34164700	0.96032600	3.03623500
C	3.17597400	1.48354000	-0.18856500
C	0.02441300	2.90331900	-2.72229600
C	-3.96991200	1.43995700	1.12321200
C	1.26978200	0.41101700	4.01970200
C	4.28167700	1.64137300	-1.12034500
C	-0.92709500	3.31086200	-3.74464700
C	-3.40945500	1.10477300	2.34323000
C	2.49060400	0.34401000	3.39410500
C	3.74960100	2.21969200	-2.24993400
C	-2.16920400	3.10445500	-3.21292800
C	-1.97098700	1.28948400	2.19793600
C	2.29415500	0.89165300	2.05903300
C	2.32316400	2.38500800	-1.98154400
C	-1.97262300	2.59438800	-1.87360800
C	3.81342500	-0.11955800	3.96369900
O	4.59216400	-0.88151300	3.06094800
N	1.99818400	1.93827300	-0.74497100
H	-5.71917200	2.33894300	0.24645200
H	3.97960800	3.50645100	-3.98305200
H	-4.10757000	4.04518200	-3.21276500
H	5.93019300	1.15636200	-3.65249300
H	-4.02047900	2.37076000	-1.40850700
H	-1.45027300	0.67388600	4.14435100
H	4.27494700	0.59734000	1.39339200
H	1.76912400	3.20318800	-3.86598100
H	1.67278500	-0.61399100	5.87091300
H	6.38515200	1.86104600	-1.46193400
H	0.02229900	3.08838400	-5.66911800
H	3.59822500	-0.71101000	4.86973100
H	4.01612800	-1.46356200	2.50587900
H	-5.48274000	0.63984000	-0.17292500
H	-3.46922600	3.70277400	-4.81997800
H	5.90169600	2.45105800	-4.96991800
H	-5.23097000	0.55514900	3.37980700
H	0.82139000	0.91720500	6.06654700
H	5.96726000	1.44896400	0.20918500
H	-1.44016500	4.07571300	-5.68920400
H	-0.04736200	-0.49540000	5.47893200
H	5.89705600	0.21417800	-1.04307900
H	0.05906400	4.73326600	-5.03175900



H	-4.11080500	2.39489100	-3.83263300
H	-6.07946300	1.08519000	1.42822400
C	4.67405400	1.07366700	4.36773000
H	5.63729100	0.71621800	4.74313100
H	4.86305900	1.72236300	3.50744700
H	4.19280100	1.66792900	5.15116700
C	-0.89907000	-5.34749700	-2.33433000
C	0.12465500	-4.46230000	-1.73574700
C	1.38155500	-4.80352400	-1.33405700
N	-0.04260000	-3.09308300	-1.57642100
C	1.10972400	-2.62644000	-1.11795600
N	1.99551700	-3.63021400	-0.93351000
H	1.33766700	-1.59205800	-0.91341000
H	-0.53397000	-6.37593200	-2.39221000
H	1.89439700	-5.75095900	-1.29984800
C	6.29978500	-4.75460300	-2.71568500
C	5.56287900	-4.05776900	-1.62647800
C	6.14847000	-3.38661100	-0.53546100
C	4.17938900	-4.09403100	-1.70254500
C	5.36738700	-2.77558300	0.43486500
C	3.38922900	-3.50481600	-0.73909800
C	3.93837300	-2.80421300	0.37678400
O	3.18825900	-2.23008100	1.26495300
H	7.33975400	-4.42140800	-2.79690800
H	7.23174000	-3.34406800	-0.45297000
H	3.70119000	-4.57943600	-2.54790000
H	5.82471200	-2.25762800	1.27204700
H	6.32983000	-5.84024700	-2.55036100
H	-1.82995200	-5.35507100	-1.75418900
C	-0.86601600	7.22681000	1.35256900
C	-0.20363600	5.90088200	1.18491400
C	-0.67113800	4.70817500	0.70216900
N	1.12047900	5.65102600	1.51409100
C	1.40340500	4.35634400	1.22542500
N	0.33404300	3.76058000	0.72901200
H	2.36497100	3.89547800	1.38581900
H	-1.90549500	7.16177300	1.02469400
H	-1.65694700	4.47354300	0.33577800
H	-0.86668200	7.55509900	2.39832700
H	1.77046900	6.31644100	1.90630200
C	-5.36501500	-3.39525100	3.27111900
C	-4.17537000	-3.30020500	2.38713200
C	-4.00065200	-2.74019400	1.15125500
N	-2.93693300	-3.82250500	2.71060700

C	-2.08220000	-3.57824800	1.68456700
N	-2.70119800	-2.92172900	0.71802300
H	-1.03260100	-3.82984500	1.70663200
H	-5.59859700	-4.43303000	3.53581100
H	-4.73113000	-2.22392900	0.54942100
H	-5.22556200	-2.83515200	4.20360600
C	-7.11119200	-2.38456300	-2.21627000
C	-5.68500800	-1.99439900	-2.38430500
C	-4.53609100	-2.62561300	-1.99471300
N	-5.25695500	-0.78409900	-2.91087600
C	-3.89985000	-0.72766700	-2.80580200
N	-3.43561400	-1.82444400	-2.23601000
H	-3.30700500	0.11248000	-3.13344200
H	-7.65622100	-2.40455200	-3.16725300
H	-4.43542500	-3.59217000	-1.52663900
H	-7.16780200	-3.38588000	-1.78437500
H	-5.84500300	-0.08703600	-3.34414200
H	-2.70287300	-4.30405900	3.56668900
H	5.82262700	-4.59349700	-3.68748800
H	-0.37641100	8.00652300	0.75782000
H	-1.15392200	-5.02136800	-3.34922400
H	-6.23889300	-2.98040000	2.76360600
H	-7.64343800	-1.69972300	-1.54546100
H	-0.15715155	-1.38874949	0.92274953
O	0.69093900	-2.24512800	1.90323000
H	1.64108600	-2.33832800	1.57364300
H	0.77737500	-1.73131100	2.71966400

## 7. The NPA charge of $I_R$ and $I_R'$

$I_R$

Fe	0.34339
Cu	0.65884
O	-0.03857
O	-0.23584
C	-0.71429
C	-0.24941
C	-0.70258
N	-0.42872
C	-0.40080
N	-0.46282
N	-0.42714
C	-0.25388
C	-0.23984
C	-0.25644
C	-0.25130
C	0.38229
C	-0.70965
C	-0.71401
C	-0.71105
O	-0.55530
C	0.17573
C	0.16305
C	0.17891
C	0.20346
C	0.01390
C	-0.06123
C	-0.00654
C	-0.02667
C	-0.17635
C	-0.08313
C	-0.07908
C	-0.04841
C	0.20130
C	0.17813
C	0.21486
C	0.18485
C	0.08432
O	-0.78639
N	-0.43629
H	0.25464
H	0.23484
H	0.25171

H	0.21903
H	0.23989
H	0.27279
H	0.27133
H	0.24804
H	0.24860
H	0.25722
H	0.25361
H	0.21807
H	0.50200
H	0.24780
H	0.25340
H	0.22886
H	0.14742
H	0.25928
H	0.24836
H	0.24784
H	0.25117
H	0.25619
H	0.25332
H	0.22688
H	0.25056
C	-0.68911
H	0.25078
H	0.23027
H	0.23599
C	-0.71138
C	0.13591
C	-0.08473
N	-0.58597
C	0.23469
N	-0.37919
H	0.24555
H	0.25194
H	0.25582
C	-0.69834
C	-0.04620
C	-0.21152
C	-0.22232
C	-0.27058
C	0.06314
C	0.32771
O	-0.74194
H	0.24680

H	0.24755
H	0.24698
H	0.26167
H	0.25189
H	0.24673
H	0.52655
C	-0.72436
C	0.12500
C	-0.05642
N	-0.55355
C	0.24009
N	-0.42613
H	0.24832
H	0.26423
H	0.25091
H	0.25527
H	0.45134
C	-0.72650
C	0.12497
C	-0.08193
N	-0.55588
C	0.22544
N	-0.57858
H	0.25152
H	0.25355
H	0.23934
H	0.26367
C	-0.72500
C	0.11710
C	-0.08245
N	-0.56485
C	0.21905
N	-0.57351
H	0.24545
H	0.25685
H	0.24776
H	0.26496
H	0.44829
H	0.45054
H	0.51656
O	-0.97881
H	0.51054
H	0.25480
H	0.24394

H	0.25933
H	0.25149
H	0.25882

**I<sub>R</sub>'**

Fe	0.35803
Cu	0.65739
O	0.02993
O	-0.28388
C	-0.71446
C	-0.25016
C	-0.70331
N	-0.42476
C	-0.39941
N	-0.43840
N	-0.44156
C	-0.26923
C	-0.23986
C	-0.26353
C	-0.25161
C	0.38368
C	-0.71067
C	-0.71392
C	-0.71070
O	-0.55677
C	0.16400
C	0.17582
C	0.18237
C	0.20662
C	0.02175
C	-0.06339
C	-0.00720
C	-0.02904
C	-0.18019
C	-0.07532
C	-0.07732
C	-0.04759
C	0.21723
C	0.18239
C	0.21583
C	0.17746
C	0.08312
O	-0.78690
N	-0.44469

H	0.25472
H	0.23492
H	0.25081
H	0.21924
H	0.24008
H	0.27286
H	0.27354
H	0.24855
H	0.24925
H	0.25710
H	0.25382
H	0.21869
H	0.50299
H	0.24727
H	0.25469
H	0.22917
H	0.14788
H	0.26052
H	0.24922
H	0.24811
H	0.25184
H	0.25644
H	0.25286
H	0.22696
H	0.25128
C	-0.68875
H	0.25094
H	0.23103
H	0.23603
C	-0.71134
C	0.13387
C	-0.08404
N	-0.59095
C	0.23834
N	-0.38208
H	0.24609
H	0.25246
H	0.25586
C	-0.69781
C	-0.04684
C	-0.21086
C	-0.22134
C	-0.27072
C	0.06223

C	0.32788
O	-0.74120
H	0.24702
H	0.24772
H	0.24716
H	0.26075
H	0.25203
H	0.24592
C	-0.72423
C	0.12431
C	-0.05675
N	-0.55426
C	0.23346
N	-0.43506
H	0.24723
H	0.26387
H	0.25024
H	0.25479
H	0.45112
C	-0.72648
C	0.12428
C	-0.08452
N	-0.55478
C	0.21697
N	-0.58170
H	0.25014
H	0.25301
H	0.23536
H	0.26346
C	-0.72509
C	0.11956
C	-0.08194
N	-0.56561
C	0.22037
N	-0.58031
H	0.24424
H	0.25727
H	0.25092
H	0.26622
H	0.44915
H	0.44901
H	0.24299
H	0.25460
H	0.25829



H	0.25735
H	0.25257
H	0.51607
O	-0.98641
H	0.52911
H	0.50721