

Probing Ferryl Reactivity in a Nonheme Iron Oxygenase Using an Expanded Genetic Code

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Methods

Materials

All materials were obtained from Sigma-Aldrich unless otherwise stated. H-His(3-Me)-OH (MeHis) was purchased from Bachem. Oligonucleotides were synthesized by IDT. *Escherichia coli* (*E. coli*) 5 α , *E. coli* BL21 (DE3), Q5 DNA polymerase, T4 DNA ligase and restriction enzymes were purchased from New England BioLabs. Per-*d*₇-L-Arginine was purchased from Cambridge Isotope Labs.

Construction of plasmids

The His316MeHis mutation was introduced into a pET-28c plasmid harbouring the gene encoding VioC (pET-28c_VioC) by replacing the His316 codon with a TAG stop codon using overlap assembly protocols (primers are given in Supplementary Table 10) and EcoRI and XhoI restriction sites to generate pET-28c_VioC_TAG316. A strep-II tag was introduced to replace the His₆-tag using complementary primers (Supplementary Table 10) into pET-28c_VioC and pET-28c_VioC_TAG316 using Gibson assembly, to give pET-28s_VioC and pET-28s_VioC_TAG316. Correct DNA sequences were confirmed by DNA sequencing using T7 and T7_term primers (Source BioScience).

Protein production and purification

For expression of VioC, pET-28c/s_VioC was transformed into *E. coli* BL21 (DE3) and the cells were plated onto an LB agar plate containing 50 $\mu\text{g ml}^{-1}$ kanamycin. A single colony of freshly transformed cells was used to inoculate 10 mL of LB medium containing 50 $\mu\text{g ml}^{-1}$ kanamycin and cultured at 37 °C with 180 rpm shaking for 18 h. 2 mL of the starter culture was used to inoculate 400 mL of bespoke medium (10 g L⁻¹ tryptone, 5 g L⁻¹ yeast extract, 2 mM MgSO₄, 0.5% (w/v) glucose, 8.95 g L⁻¹ Na₂HPO₄, 3.4 g L⁻¹ KH₂PO₄, 2.67 g L⁻¹ NH₄Cl, 0.71 g L⁻¹ Na₂SO₄) containing 50 $\mu\text{g ml}^{-1}$ kanamycin. The cultures were incubated for ~2 h at 37 °C with 180 rpm shaking until the OD₆₀₀ reached ~ 0.6, at which point IPTG was added to a final concentration of 200 μM . The cultures were incubated for a further ~20 h at 22 °C and the cells were subsequently harvested by centrifugation at 4000 g for 12 min.

For expression of VioC MeHis316, pET-28_VioC_TAG316 were co-transformed into *E. coli* BL21 (DE3) with pEVOL_MeHis¹⁶ and the cells plated onto an LB agar plate containing 50 $\mu\text{g ml}^{-1}$ kanamycin and 34 $\mu\text{g ml}^{-1}$ chloramphenicol. A single colony of freshly transformed cells was used to inoculate 10 mL of LB medium containing 50 $\mu\text{g ml}^{-1}$ kanamycin and 34 $\mu\text{g ml}^{-1}$

chloramphenicol and cultured at 37 °C with 180 rpm shaking for 18 h. 2 mL of the starter culture was used to inoculate 400 mL of bespoke medium (as above) containing 6 mM MeHis, 50 µg ml⁻¹ kanamycin and 34 µg ml⁻¹ chloramphenicol. The cultures were incubated for ~2 h at 37 °C with 180 rpm shaking until the OD₆₀₀ reached ~ 0.6, at which point IPTG and L-arabinose were added to final concentrations of 200 µM and 0.05% (w/v), respectively. The cultures were incubated for a further ~20 h at 22 °C and the cells were subsequently harvested by centrifugation at 4000 g for 12 min.

For purification of strep-tagged VioC and VioC MeHis316, the pelleted bacterial cells were suspended in buffer NP (see Supplementary Table 11) supplemented with lysozyme (1 mg ml⁻¹) and DNAase (0.01 U ml⁻¹) and subjected to sonication (10 mins, 50% amplitude, 1 s on/off pulse). Cell lysates were centrifuged at 10 000 g for 30 min. Supernatants were subjected to a Strep-Tactin Superflow Plus resin (Qiagen) and the purified protein was eluted using buffer NPD.

For purification of VioC MeHis316 for use in crystallography, the pelleted bacterial cells were suspended in lysis buffer (50 mM HEPES, 300 mM NaCl, 20 mM imidazole, pH 7.5) supplemented with lysozyme (1 mg ml⁻¹) and DNAase (0.01 U ml⁻¹) and subjected to sonication (10 mins, 50% amplitude, 1 s on/off pulse). Cell lysates were centrifuged at 10 000 g for 30 min. Supernatants were subjected to a nickel resin (Qiagen) and the purified protein was eluted using an elution buffer (50 mM HEPES, 300 mM NaCl, 250 mM imidazole, pH = 7.5).

After purification, proteins were desalted using 10DG desalting columns (Bio-Rad) into 100 mM Tris pH = 7.5 and stored for a maximum of 24 h at 4 °C before experimentation/crystallisation. Protein concentrations were determined by measuring the absorbance at 280 nm and assuming an extinction coefficient of 47 440 M⁻¹ cm⁻¹ for VioC and VioC MeHis316.

MS analysis

MS data for VioC and VioC MeHis were acquired on a 1200series LC (Agilent). The final protein concentrations were adjusted to 10 µM in 50 mM KPi pH 6. 5 µL of sample was injected into 1 ml min⁻¹ 5% acetonitrile (0.1% formic acid) and desalted inline. This was eluted over 1 minute by 95% acetonitrile. The resulting multiply charged spectrum was analysed by an

QTOF 6510 (Agilent) in ESI positive ion mode, and deconvoluted using Masshunter Software (Agilent). The instrument had previously been tuned and calibrated with reference solution. MS data is presented in Supplementary Table 1.

Crystallization, refinement and model building

His₆-tagged VioC MeHis316 was crystallized at 10 mg ml⁻¹ in 20 mM HEPES buffer pH 7.5 containing 400 μM ammonium iron(II) sulphate hexahydrate, 2 mM L-arginine and 2 mM succinate. Crystallization conditions were identified using the JCSG-plus screen (Molecular Dimensions). Crystals suitable for diffraction experiments were obtained by sitting drop vapour diffusion in 400 nl drops containing equal volumes of protein and reservoir solution, after 72 h incubation at 4 °C. The reservoir solution comprised of 0.02 M magnesium chloride hexahydrate, 0.1 M HEPES, pH 7.5, containing 22 % (w/v) poly(acrylic acid sodium salt) 5100 as a precipitant. Prior to data collection crystals were cryoprotected with PEG 300 and plunge cooled in liquid nitrogen. All data were collected at Diamond Light Source (Harwell, UK). Data reduction was performed with Dials and the structure solved using a model derived from VioC structure 6ALQ. Iterative rounds of model building, and refinement were performed in COOT¹ and Phenix.refine² respectively. Validation with MOLPROBITY and PDBREDO³ were incorporated into the iterative rebuild and refinement process. The resolution cut off was validated using a paired refinement in PDBREDO. Data collection and refinement statistics are shown in Supplementary Table 2.

Total turnover numbers

The total turnover numbers achieved by VioC and VioC MeHis316 were determined as follows. Reactions were performed in 1.5 mL microcentrifuge tubes (Eppendorf) containing a total volume of 100 μL in 100 mM Tris pH 7.5. A substrate mix was initiated by the addition of enzyme to give reactions with the final concentrations 1 μM enzyme, 5 mM 2-oxoglutarate (2OG), 1 mM L-arginine, 1 mM (NH₄)₂Fe(SO₄)₂(H₂O)₆, 1 mM sodium ascorbate. Reactions were incubated at 25 °C with shaking (300 rpm) for 18 h before quenching with 100 μL of 5 mM Fmoc *N*-hydroxysuccinimide ester in ACN. After a further 30 min shaking at 25 °C (300 rpm), the precipitated proteins were removed by centrifugation (14 000 g, 20 min) before high-pressure liquid chromatography (HPLC) analysis.

HPLC analysis

HPLC analysis of Fmoc-derived L-arginine and L-arginine-OH was performed on a 1290 Infinity II Agilent LC system with a Waters Acquity UPLC HSS column (2.1 x 100 mm, 1.8 μm). The column was equilibrated at 67% MPA (2 mM ammonium formate in water) and 33% MPB (90:10 v/v ACN:2 mM ammonium formate in ACN) with a flow rate of 0.2 mL min⁻¹. After injection of 2 μL of sample, it was held at 33% MPB for 6 min, followed by a one minute wash with 90% MPB. A one minute equilibration in 33% MPB was used to prepare the column for the next injection. Detection of L-arginine-Fmoc and L-arginine-Fmoc-OH was performed using absorption at 254 nm.

Stopped-flow kinetics

Stopped-flow absorbance experiments were performed inside a Belle Technology anaerobic chamber (oxygen levels < 5 ppm) using an SX20 rapid mixing stopped-flow spectrophotometer (Applied Photophysics Ltd, Leatherhead, UK) in single mixing configuration, equipped with a xenon arc lamp and a 1 cm path length in 100 mM Tris, pH 7.5 at 4 °C. Multiple wavelength data were using a photodiode array (PDA) detector and single wavelength data was obtained from a photomultiplier tube (PMT) single wavelength detector. All experiments were performed in 100 mM Tris pH 7.5 that had been degassed overnight before use. A 1 mL anaerobic substrate mix containing 18 mM 2OG, 18 mM L-arginine and 2.5 mM $(\text{NH}_4)_2\text{Fe}(\text{SO}_4)_2(\text{H}_2\text{O})_6$ was prepared in 100 mM Tris pH 7.5, and subsequently re-adjusted to pH 7.5 using 28 μL 2M NaOH. The substrate mix was added slowly to VioC or VioC MeHis316 to give a final reaction mix containing 1 mM enzyme, 6 mM 2OG, 6 mM L-arginine, 1 mM $(\text{NH}_4)_2\text{Fe}(\text{SO}_4)_2(\text{H}_2\text{O})_6$. After rapid mixing of the reactant complex with air-saturated 4 °C buffer, absorbance was monitored at 320 nm for kinetic parameter determination or across 200-800 nm for spectral characterisation of the intermediates for 100 s. Kinetic parameters were determined by fitting to a double exponential model (Equation 1) using OriginLab. The kinetic parameters are given in Supplementary Table S8 and the fits for each data set are shown in Supplementary Figure S6.

Equation 1

$$\Delta A_{320} = A_1 e^{-k_1 t} + A_2 \frac{k_1}{k_2 - k_1} (e^{-k_1 t} - e^{-k_2 t})$$

DFT methods

Two QM cluster models were used to study the mechanism of VioC. The models A and B are shown in Supplementary Figures S2 and S3, respectively. In both models a crystal water that hydrogen bonds to the N-H of His316 was omitted in the VioC MeHis316 system.

Model A was used to probe the electron affinity of the ferryl intermediates in VioC and VioC MeHis316. The cluster model, in addition to the ferryl intermediate, contained the side chains of the residues (Me)His316, His168, Glu170, Arg334, Ser158, Asp286, Thr169, Val315, Asn311, Ile309, Gly166, succinate and arginine for a total of 240 atoms.

Model B was used to study the catalytic cycle of VioC and VioC MeHis316 and determine the energy landscapes for C3-hydroxylation of L-Arg. This larger cluster model includes additional residues in proximity to the substrate L-Arginine *c.f.* that shown in Supplementary Figure S2, giving a total of 353 atoms in this larger QM cluster. This model contains the ferryl intermediate bound to succinate, which was positioned *cis* to the peptide chain His168–Thr169–Glu170 and *trans* to the peptide chain His316–Val315–Ala314. In addition, several small peptide chains were included that position the substrate, namely, Thr155–Leu156–Val157–Ser158, Asp222–Asp223–Ser224, Asp268–Gly269–Asp270–Phe271, and Ile309–Asp310–Asn311. Arg334 side chain, Leu196 and two crystal water molecules were also included.

DFT calculations were conducted using Gaussian16 at the unrestricted B3LYP level of theory. Geometry optimizations and frequency calculations used the LANL2DZ basis set (with electron core potential) on the iron and 6-31G* on all other atoms. Local minima were characterized by a frequency calculation that confirmed them with real frequencies only. Free energies (G) were calculated at 298 K and 1 bar and include relative enthalpies with zero-point (ZPE), thermal and entropic corrections.

To improve the accuracy of the energetics, we ran single-point energy calculations using LACV3P+ on iron (with core potential) and 6-311+G* for the rest of the atoms (basis set BS2). These calculations also include dispersion contributions using the (GD3 method)⁴ and solvent effects through the self-consistent reaction field approach. Chlorobenzene was selected as the solvent of choice and the conductor-like polarizable continuum model (CPCM) was used to apply a consistent perturbation to the SCF.⁵ Free energies use thermal corrections and

entropies calculated at 298 K using the analytical frequency functionality as implemented in Gaussian09.⁶

DNA sequences

His₆-VioC

ATGGGCAGCAGCCATCATCATCATCACAGCAGCGGCCTGGTGCCGCGCGGCAGCCATATGGCT
AGCATGACTGGTGGACAGCAAATGGGTCGCGGATCCGAATTCATGACCGAAAGCCCGACCACCCAT
CATGGTGCAGCACCGCCTGATAGCGTTGCAACACCGGTTTCGTCCGTGGTCAGAATTTTCGTCTGACAC
CGGCAGAAGCAGCAGCAGCCGCAGCACTGGCAGCACGTTGTGCACAGCGTTATGATGAAACCGAT
GGTCCGGAATTTCTGCTGGATGCACCGGTTATTGCACATGAACTGCCTCGTCTGCGTACCTTTAT
GGCACGTGCGCGTCTGGATGCATGGCCTCATGCACTGGTTGTTTCGTGGTAATCCGGTTGATGATGCA
GCCCTGGGTAGCACTCCGGTTCATTGGCGTACCGCACGTACACCGGGTAGCCGTCCGCTGAGCTTCC
TGCTGATGCTGTATGCAGGTCTGCTGGGTGATGTTTTTGGTTGGGCAACCCAGCAGGATGGTCGTGT
TGTTACCGATGTTCTGCCGATTAAGGTGGTGAACATACCCTGGTTAGCAGCAGCTCACGTCAAGAA
CTGGGTTGGCATAACCGAAGATGCATTTAGCCCGTATCGTGCAGATTATGTTGGTCTGCTGAGCCTGC
GTAATCCGGATGGTGTGCCACCACCTGGCAGGCGTTCCGCTGGATGATCTGGATGAACGCACCCT
GGATGTTCTGTTTCAAGAACGTTTTCTGATTCGTCCGGATGATAGCCATCTGCAGGTTAATAACAGCA
CCGCACAGCAGGGTCGTGTGGAATTTGAAGGTATTGCACAGGCAGCAGATCGTCCGGAACCGGTTG
CCATTCTGACAGGTCATCGTGCCGCACCGCATCTGCGTGTTGATGGTGAATTTTTAGCCCCCTGCCGAA
GGTATGAAGAAGCCGCAGCGGCACTGGGCACCCTGCGTAAACTGATTGATGCAAGCCTGTATGAA
CTGTTCTGGATCAGGGTGTGTGGCCTTTATTGATAATCGTCTGCGCGTT**CAT**GGTCTGCTGCATT
TCAGCCTCGCTATGATGGTCGCGATCGTTGGCTGAAACGTATTAACATTACCCGTGATCTGCATCGTA
GCCGTAAAGCATGGGCAGGCGATAGCCGTGTTCTGGGTTCAGCGTTAA

His₆-VioC MeHis

ATGGGCAGCAGCCATCATCATCATCACAGCAGCGGCCTGGTGCCGCGCGGCAGCCATATGGCT
AGCATGACTGGTGGACAGCAAATGGGTCGCGGATCCGAATTCATGACCGAAAGCCCGACCACCCAT
CATGGTGCAGCACCGCCTGATAGCGTTGCAACACCGGTTTCGTCCGTGGTCAGAATTTTCGTCTGACAC
CGGCAGAAGCAGCAGCAGCCGCAGCACTGGCAGCACGTTGTGCACAGCGTTATGATGAAACCGAT
GGTCCGGAATTTCTGCTGGATGCACCGGTTATTGCACATGAACTGCCTCGTCTGCGTACCTTTAT
GGCACGTGCGCGTCTGGATGCATGGCCTCATGCACTGGTTGTTTCGTGGTAATCCGGTTGATGATGCA
GCCCTGGGTAGCACTCCGGTTCATTGGCGTACCGCACGTACACCGGGTAGCCGTCCGCTGAGCTTCC
TGCTGATGCTGTATGCAGGTCTGCTGGGTGATGTTTTTGGTTGGGCAACCCAGCAGGATGGTCGTGT
TGTTACCGATGTTCTGCCGATTAAGGTGGTGAACATACCCTGGTTAGCAGCAGCTCACGTCAAGAA
CTGGGTTGGCATAACCGAAGATGCATTTAGCCCGTATCGTGCAGATTATGTTGGTCTGCTGAGCCTGC
GTAATCCGGATGGTGTGCCACCACCTGGCAGGCGTTCCGCTGGATGATCTGGATGAACGCACCCT
GGATGTTCTGTTTCAAGAACGTTTTCTGATTCGTCCGGATGATAGCCATCTGCAGGTTAATAACAGCA
CCGCACAGCAGGGTCGTGTGGAATTTGAAGGTATTGCACAGGCAGCAGATCGTCCGGAACCGGTTG
CCATTCTGACAGGTCATCGTGCCGCACCGCATCTGCGTGTTGATGGTGAATTTTTAGCCCCCTGCCGAA
GGTATGAAGAAGCCGCAGCGGCACTGGGCACCCTGCGTAAACTGATTGATGCAAGCCTGTATGAA
CTGTTCTGGATCAGGGTGTGTGGCCTTTATTGATAATCGTCTGCGCGTT**TAG**GGTCTGCTGCATT
TTCAGCCTCGCTATGATGGTCGCGATCGTTGGCTGAAACGTATTAACATTACCCGTGATCTGCATCGT
AGCCGTAAAGCATGGGCAGGCGATAGCCGTGTTCTGGGTTCAGCGTTAA

StreptII-VioC

ATGGGCAGCAGCTGGAGTCACCCACAGTTTGAGAAAGGCAGCCATATGGCTAGCATGACTGGTGGGA
CAGCAAATGGGTCGCGGATCCGAATTCATGACCGAAAGCCCGACCACCCATCATGGTGCAGCACCG
CCTGATAGCGTTGCAACACCGGTTTCGTCCGTGGTCAGAATTTTCGTCTGACACCGGCAGAAGCAGCA

GCAGCCGCAGCACTGGCAGCACGTTGTGCACAGCGTTATGATGAAACCGATGGTCCGGAATTTCTG
CTGGATGCACCGGTTATTGCACATGAACTGCCTCGTCGTCTGCGTACCTTTATGGCACGTGCGCGTCT
GGATGCATGGCCTCATGCACTGGTTGTTTCGTGGTAATCCGGTTGATGATGCAGCCCTGGGTAGCACT
CCGTTTCATTGGCGTACCGCACGTACACCGGGTAGCCGTCCGCTGAGCTTCCTGCTGATGCTGTATG
CAGGTCTGCTGGGTGATGTTTTTGGTTGGGCAACCCAGCAGGATGGTCGTGTTGTTACCGATGTTCT
GCCGATTAAGGTGGTGAACATACCCTGGTTAGCAGCAGCTCACGTCAAGAACTGGGTTGGCATAAC
CGAAGATGCATTTAGCCCGTATCGTGCAGATTATGTTGGTCTGCTGAGCCTGCGTAATCCGGATGGT
GTTGCCACCACCCTGGCAGGCGTTCCGCTGGATGATCTGGATGAACGCACCCTGGATGTTCTGTTTC
AAGAACGTTTTCTGATTTCGTCGGATGATAGCCATCTGCAGGTTAATAACAGCACCCGCACAGCAGGG
TCGTGTGGAATTTGAAGGTATTGCACAGGCAGCAGATCGTCCGGAACCGGTTGCCATTCTGACAGG
TCATCGTGCCGCACCGCATCTGCGTGTTGATGGTGATTTTTTCAGCCCCTGCCGAAGGTGATGAAGAA
GCCGCAGCGGCACTGGGCACCCTGCGTAAACTGATTGATGCAAGCCTGTATGAACTGGTTCTGGAT
CAGGGTGATGTGGCCTTTATTGATAATCGTCGTGCCGTT**CAT**GGTCGTGTCGATTTTCAGCCTCGCTA
TGATGGTCGCGATCGTTGGCTGAAACGTATTAACATTACCCGTGATCTGCATCGTAGCCGTAAAGCA
TGGGCAGGCGATAGCCGTGTTCTGGGTGTCAGCGTTAA

Streptococcus pneumoniae MeHis

ATGGGCAGCAGCTGGAGTCACCCACAGTTTTGAGAAAGGCAGCCATATGGCTAGCATGACTGGTGGGA
CAGCAAATGGGTCGCGGATCCGAATTCATGACCGAAAGCCCGACCACCCATCATGGTGCAGCACCG
CCTGATAGCGTTGCAACACCGGTTTCGTCGTTGTCAGAAATTCGTCGACACCGGCAGAAGCAGCA
GCAGCCGCAGCACTGGCAGCACGTTGTGCACAGCGTTATGATGAAACCGATGGTCCGGAATTTCTG
CTGGATGCACCGGTTATTGCACATGAACTGCCTCGTCGTCTGCGTACCTTTATGGCACGTGCGCGTCT
GGATGCATGGCCTCATGCACTGGTTGTTTCGTGGTAATCCGGTTGATGATGCAGCCCTGGGTAGCACT
CCGTTTCATTGGCGTACCGCACGTACACCGGGTAGCCGTCCGCTGAGCTTCCTGCTGATGCTGTATG
CAGGTCTGCTGGGTGATGTTTTTGGTTGGGCAACCCAGCAGGATGGTCGTGTTGTTACCGATGTTCT
GCCGATTAAGGTGGTGAACATACCCTGGTTAGCAGCAGCTCACGTCAAGAACTGGGTTGGCATAAC
CGAAGATGCATTTAGCCCGTATCGTGCAGATTATGTTGGTCTGCTGAGCCTGCGTAATCCGGATGGT
GTTGCCACCACCCTGGCAGGCGTTCCGCTGGATGATCTGGATGAACGCACCCTGGATGTTCTGTTTC
AAGAACGTTTTCTGATTTCGTCGGATGATAGCCATCTGCAGGTTAATAACAGCACCCGCACAGCAGGG
TCGTGTGGAATTTGAAGGTATTGCACAGGCAGCAGATCGTCCGGAACCGGTTGCCATTCTGACAGG
TCATCGTGCCGCACCGCATCTGCGTGTTGATGGTGATTTTTTCAGCCCCTGCCGAAGGTGATGAAGAA
GCCGCAGCGGCACTGGGCACCCTGCGTAAACTGATTGATGCAAGCCTGTATGAACTGGTTCTGGAT
CAGGGTGATGTGGCCTTTATTGATAATCGTCGTGCCGTT**TAG**GGTCGTGTCGATTTTCAGCCTCGCT
ATGATGGTCGCGATCGTTGGCTGAAACGTATTAACATTACCCGTGATCTGCATCGTAGCCGTAAAGC
ATGGGCAGGCGATAGCCGTGTTCTGGGTGTCAGCGTTAA

Protein sequences

His₆-VioC

MGSSHHHHHHSSGLVPRGSHMASMTGGQQMGRGSEFMTESPTTHHGAAPPDSVATPVRPWSEFRL
TPAEAAAAAALAAARCAQRYDETDGPEFLLDAPVIAHELPRRLRTFMARARLDAWPHALVVRGNPVDDA
ALGSTPVHWRTARTPGSRPLSFLLMYAGLLGDVFGWATQQDGRVVTDVLPKGGHEHTLVSSSSRQELG
WHTEDAFSPYRADYVGLLSLRNPDGVATTLAGVPLDDLERTLDVLFQERFLIRPDDSHLQVNNSTAQQ
GRVEFEGIAQAADRPEPVAILTGHRAAPHLRVDGDFSAPAEGDEEAAAALGTLRKLIDASLYELVLDQGD
VAFIDNRRRAVHGRRAFQPRYDGRDRWLKRINITRDLHRSRKAWAGDSRVLGQR-

His₆-VioC MeHis316

MGSSHHHHHHSSGLVPRGSHMASMTGGQQMGRGSEFMTESPTTHHGAAPPDSVATPVRPWSEFRL
TPAEAAAAAALAAARCAQRYDETDGPEFLLDAPVIAHELPRRLRTFMARARLDAWPHALVVRGNPVDDA
ALGSTPVHWRTARTPGSRPLSFLLMYAGLLGDVFGWATQQDGRVVTDVLPKGGHEHTLVSSSSRQELG
WHTEDAFSPYRADYVGLLSLRNPDGVATTLAGVPLDDLERTLDVLFQERFLIRPDDSHLQVNNSTAQQ
GRVEFEGIAQAADRPEPVAILTGHRAAPHLRVDGDFSAPAEGDEEAAAALGTLRKLIDASLYELVLDQGD
VAFIDNRRRAV(MeHis)GRRAFQPRYDGRDRWLKRINITRDLHRSRKAWAGDSRVLGQR-

StrepII-VioC

MGSSWSHPQFEKGSMSMASMTGGQQMGRGSEFMTESPTTHHGAAPPDSVATPVRPWSEFRLTPAEA
AAAAAALAAARCAQRYDETDGPEFLLDAPVIAHELPRRLRTFMARARLDAWPHALVVRGNPVDDAALGST
PVHWRTARTPGSRPLSFLLMYAGLLGDVFGWATQQDGRVVTDVLPKGGHEHTLVSSSSRQELGWHT
DAFSPYRADYVGLLSLRNPDGVATTLAGVPLDDLERTLDVLFQERFLIRPDDSHLQVNNSTAQQGRVE
FEGIAQAADRPEPVAILTGHRAAPHLRVDGDFSAPAEGDEEAAAALGTLRKLIDASLYELVLDQGDVAFID
NRRRAVHGRRAFQPRYDGRDRWLKRINITRDLHRSRKAWAGDSRVLGQR-

StrepII-VioC MeHis316

MGSSWSHPQFEKGSMSMASMTGGQQMGRGSEFMTESPTTHHGAAPPDSVATPVRPWSEFRLTPAEA
AAAAAALAAARCAQRYDETDGPEFLLDAPVIAHELPRRLRTFMARARLDAWPHALVVRGNPVDDAALGST
PVHWRTARTPGSRPLSFLLMYAGLLGDVFGWATQQDGRVVTDVLPKGGHEHTLVSSSSRQELGWHT
DAFSPYRADYVGLLSLRNPDGVATTLAGVPLDDLERTLDVLFQERFLIRPDDSHLQVNNSTAQQGRVE
FEGIAQAADRPEPVAILTGHRAAPHLRVDGDFSAPAEGDEEAAAALGTLRKLIDASLYELVLDQGDVAFID
NRRRAV(MeHis)GRRAFQPRYDGRDRWLKRINITRDLHRSRKAWAGDSRVLGQR-

Supplementary Tables

Supplementary Table S1. Protein mass spectrometry

Protein	Calculated (Da)	Observed (Da)
StrepII-VioC	42636.7	42636.0
StrepII-VioC MeHis316	42650.7	42649.0

Supplementary Table S2. Data collection and refinement statistics for structure determination of His₆-VioC MeHis316

	VioC MeHis316
PDB ID	9EQF
Wavelength (Å)	0.976
Resolution range	38.48 - 1.6 (1.64 - 1.6)
Space group	C 1 2 1
Unit cell dimensions	
a, b, c, (Å)	81.1 67.1 63.0
α, β, γ (°)	90 109.2 90
Total reflections	278892 (14180)
Unique reflections	41962 (2681)
Multiplicity	6.6 (5.3)
Completeness (%)	99.61 (96.09)
Mean I/sigma(I)	15.47 (1.86)
Wilson B-factor (Å ²)	17.87
R-merge	0.05875 (0.4329)
R-meas	0.06364 (0.4804)
R-pim	0.02425 (0.2041)
CC _{1/2}	0.999 (0.922)
CC*	1 (0.98)
Reflections used in refinement	41951 (2678)
Reflections used for R-free	2082 (110)
R-work	0.1573 (0.2354)
R-free	0.1865 (0.2619)
Protein residues	336
RMS(bonds)	0.003
RMS(angles)	0.74
Ramachandran favoured (%)	97.56
Ramachandran allowed (%)	1.83
Ramachandran outliers (%)	0.61
Rotamer outliers (%)	1.4
Clashscore	3.95
Average B-factor (Å ²)	26.3

Supplementary Table S3. Absolute energies, zero-point energies and free energies (in a.u.), and relative energies (in kcal mol⁻¹) of the optimized geometries for the Fe(IV) and Fe(III) complexes of as obtained in Gaussian-16 from model A. All calculations were done in the gas phase.

	E [a.u.]	ZPE [a.u.]	G [a.u.]	Relative to Fe(IV) [kcal mol ⁻¹]
WT Fe(IV)	-5633.509411	2.058883	-5631.651381	0.00
WT Fe(III)	-5633.642732	2.055663	-5631.786492	-85.68
MeHis Fe(IV)	-5596.379568	2.060985	-5594.518547	0.00
MeHis Fe(III)	-5596.514536	2.058215	-5594.661565	-86.43

Supplementary Table S4. Group Mulliken spin-densities for both wildtype (WT) VioC and VioC MeHis316 model optimized geometries for the Fe(IV) and Fe(III) complexes from model A, calculated at UB3LYP/6-31G* level of theory.

	Fe	O	Succinate	Arg sub	Glu ₁₇₀	(Me)His ₃₁₆	His ₁₆₈
WT Fe(IV)	3.039	0.643	0.167	0.005	0.101	-0.004	0.045
WT Fe(III)	3.845	0.832	0.113	0.011	0.088	0.037	0.068
MeHis Fe(IV)	3.036	0.643	0.167	0.005	0.103	-0.004	0.046
MeHis Fe(III)	3.873	0.840	0.115	0.006	0.075	0.027	0.061

Supplementary Table S5. Absolute energies (in a.u.) and relative energies (in kcal mol⁻¹) of single point geometries for Fe(IV) and Fe(III) models to assess the adiabatic electron affinity of VioC and VioC MeHis316 in model A. Energies were calculated for models of VioC, VioC MeHis316, and the wildtype without the ordered water molecule H-bonding to His316 N_δ were calculated in Gaussian-16. All calculations were done in the gas phase.

	E [a.u.]	Relative to Fe(IV) [kcal mol ⁻¹]
WT Fe(IV)	-5633.509411	0.00
WT Fe(III)	-5633.598648	-56.00
MeHis Fe(IV)	-5596.379568	0.00
MeHis Fe(III)	-5596.470848	-57.28
WT Fe(IV) – no H ₂ O	-5557.056319	0.00
WT Fe(III) – no H ₂ O	-5557.151635	-59.81

Supplementary Table S6. Group Mulliken spin-densities for both wildtype (WT) VioC and VioC MeHis316 optimized geometries, calculated at UB3LYP/BS1.

	Fe	O	Succ	Arg(OH)	GLU ₁₇₀	(Me)HIS ₃₁₆	HIS ₁₆₈	H ₂ O _{CRY}	Prot
⁵ Re _{WT}	3.19	0.65	0.13	0.00	0.10	-0.11	0.04	0.00	0.00
⁵ Re _{MeHis}	3.19	0.69	0.18	0.00	0.05	-0.11	0.01	-0.01	-0.01
⁵ TS _{1,WT}	4.12	-0.09	0.22	-0.36	0.07	0.03	0.01	0.00	0.00
⁵ TS _{1,MeHis}	4.12	-0.07	0.22	-0.36	0.06	0.02	0.02	0.00	-0.01
⁵ I _{WT}	4.33	0.23	0.26	-0.96	0.12	0.03	0.00	0.00	0.00
⁵ I _{MeHis}	4.34	0.26	0.25	-0.99	0.11	0.01	0.01	0.00	0.00
⁵ TS _{2,WT}	4.26	0.25	0.22	-0.85	0.09	0.03	0.01	0.00	-0.01
⁵ TS _{2,MeHis}	4.28	0.26	0.22	-0.86	0.09	0.01	0.02	0.00	-0.01
⁵ P _{WT}	3.83	-	0.09	0.00	0.03	0.02	0.02	0.00	0.00
⁵ P _{MeHis}	4.34	-	0.25	-0.73	0.11	0.01	0.01	0.00	0.00

Supplementary Table S7. Calculated Kinetic Isotope Effects (KIEs) for C-H abstraction by the ferryl intermediates in VioC and VioC MeHis316 and the imaginary frequencies for the transition states of C-H/D abstraction. Eyring primary (**KIE^a**) kinetic isotope effects for HAT as well as the KIEs in perdeuterated substrate (**KIE^b**) were calculated for both VioC and VioC MeHis316 models. Values in brackets are the KIEs including a Wigner correction using the imaginary frequencies of the transition state barriers to C-H and C-D abstraction.⁷

	VioC	VioC MeHis316
KIE ^a	6.67 (8.89)	6.48 (8.53)
KIE ^b	7.87 (10.49)	7.80 (10.27)
Frequency TS _(C-H) (cm ⁻¹)	i1182.6	i1154.0
Frequency TS _(C-D) (cm ⁻¹)	i909.5	i892.9

Supplementary Table S8. Kinetic parameters for ferryl formation and decay from stopped-flow UV-vis measurement. Values and standard errors are presented from triplicate measurements.

	VioC		VioC MeHis316	
	<i>h</i> _γ -L-Arg	<i>d</i> _γ -L-Arg	<i>h</i> _γ -L-Arg	<i>d</i> _γ -L-Arg
k _{form,obs}	41.2 ± 0.7	29.6 ± 1.0	46.8 ± 1.0	24.9 ± 0.5
k _H or k _D	11.9 ± 0.1	0.28 ± 0.01	8.3 ± 0.1	0.29 ± 0.01
ΔA ₁	0.070 ± 0.002	0.075 ± 0.002	0.030 ± 0.001	0.035 ± 0.001
ΔA ₂	0.30 ± 0.01	0.34 ± 0.01	0.20 ± 0.01	0.26 ± 0.01

Supplementary Table S9. Observed kinetic isotope effects. Kinetic isotope effects are given for the formation ($k_{\text{form,obs}}$) and decay (k) of the ferryl intermediate with errors propagated from triplicate measurements of $k_{1,\text{obs}}(\text{H})$, $k_{1,\text{obs}}(\text{D})$, $k_2(\text{H})$, and $k_2(\text{D})$.

	VioC	VioC MeHis316
$k_{\text{form,obs}}(\text{H})/k_{\text{form,obs}}(\text{D})$	1.4 ± 0.1	1.9 ± 0.1
$k_{\text{H}}/k_{\text{D}}$	43 ± 1	29 ± 1

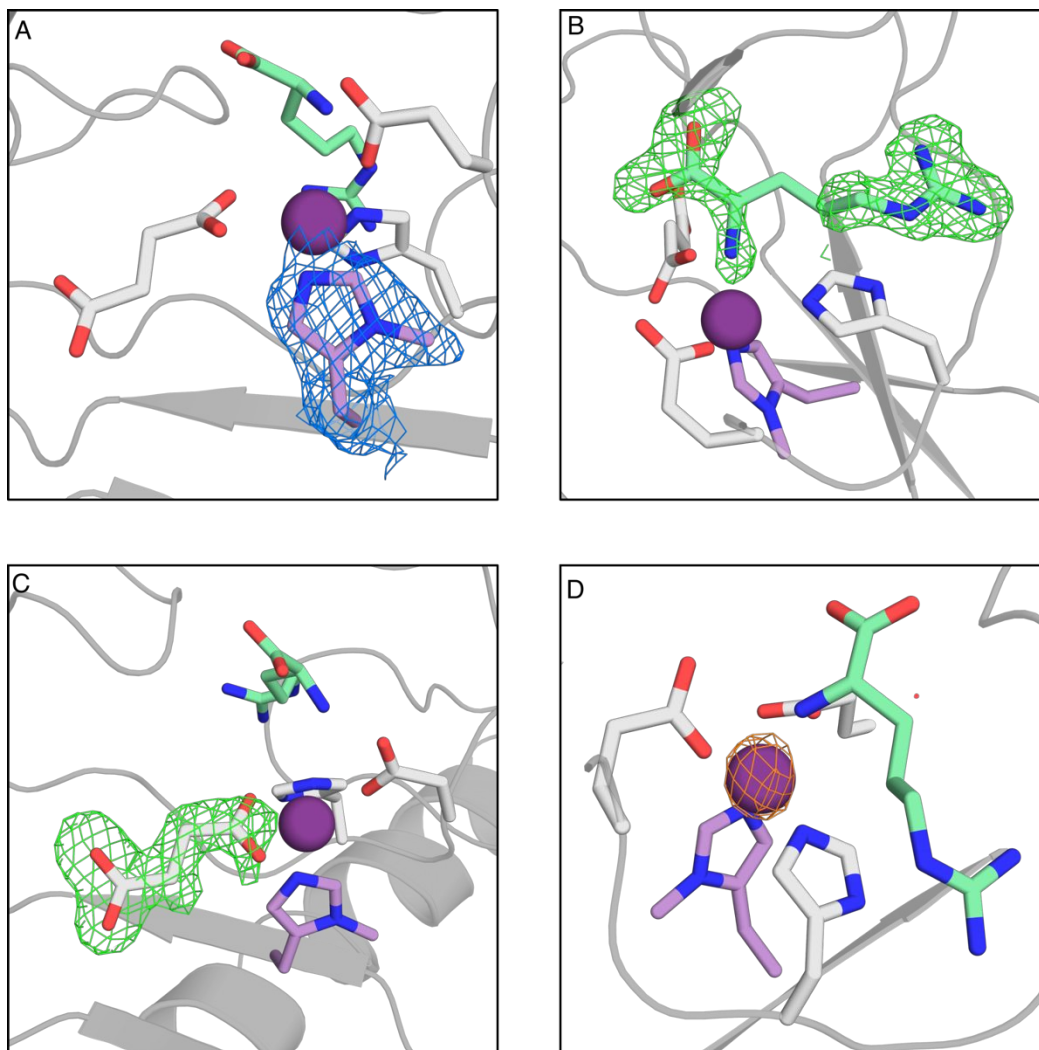
Supplementary Table S10. Primers used in this study

Primer Name	Sequence
VioC_fwd	CGCGGATCCGAATTC
VioC_rev	GTGGTGGTGCTCG
H316TAG_fwd	AATCGTCGTGCCGTTTAGGGTCGTCGTGCATTT
H316_rev	AACGGCACGACGA
VioC_fwd2	GCCAGCCATATGGCT
VioC_rev2	GCTGCTGCCCATGG
Strep_A	ACCATGGGCAGCAGCTGGAGTCACCCACAGTTTGAGAAAGGCAGC CATATGGCT
Strep_B	AGCCATATGGCTGCCTTTCTCAAAGTGTGGGTGACTCCAGCTGCT GCCCATGGT

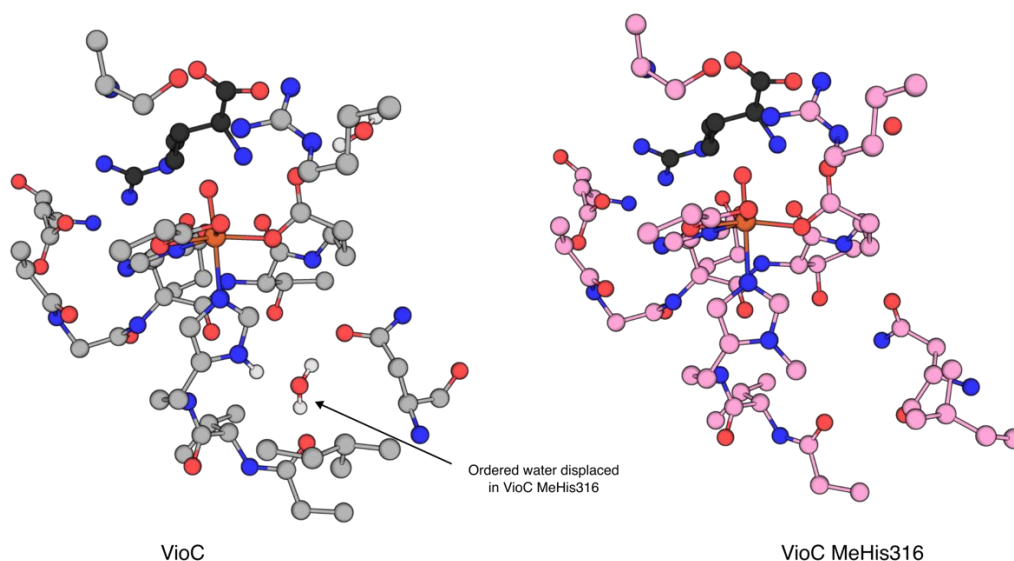
Supplementary Table S11. Buffers used in this study

Buffer	Components	pH
NP	50 mM NaH_2PO_4 , 300 mM NaCl, adjust pH with NaOH	8
NPD	50 mM NaH_2PO_4 , 300 mM NaCl, 2.5 mM desthiobiotin, adjust pH with NaOH	8
Lysis buffer	50 mM HEPES, 300 mM NaCl, 20 mM imidazole, adjust pH with HCl	7.5
Elution buffer	50 mM HEPES, 300 mM NaCl, 250 mM imidazole, adjust pH with HCl	7.5
Reaction buffer	100 mM Tris	7.5

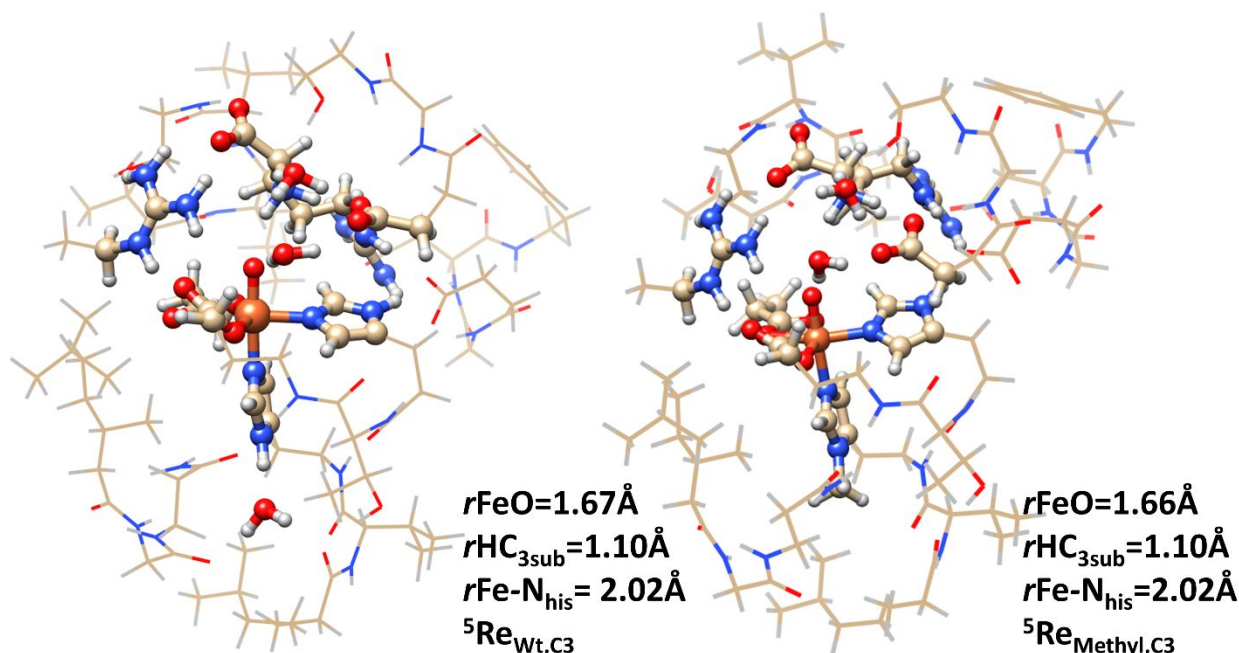
Supplementary Figures



Supplementary Figure S1. Structural characterization of VioC MeHis316. Active site residues, MeHis316 and the substrate L-Arg and are shown as atom-coloured sticks, with purple, grey, and green carbons, respectively. The iron cofactor is shown as a purple sphere. A) A $2F_o-F_c$ map is shown around the MeHis, contoured at 1σ . B) An F_o-F_c omit map is shown around the substrate L-Arg, contoured at 2.5σ . C) An F_o-F_c omit map is shown around succinate, contoured at 2.5σ . D) An anomalous map is shown around the Fe, contoured at 3σ .

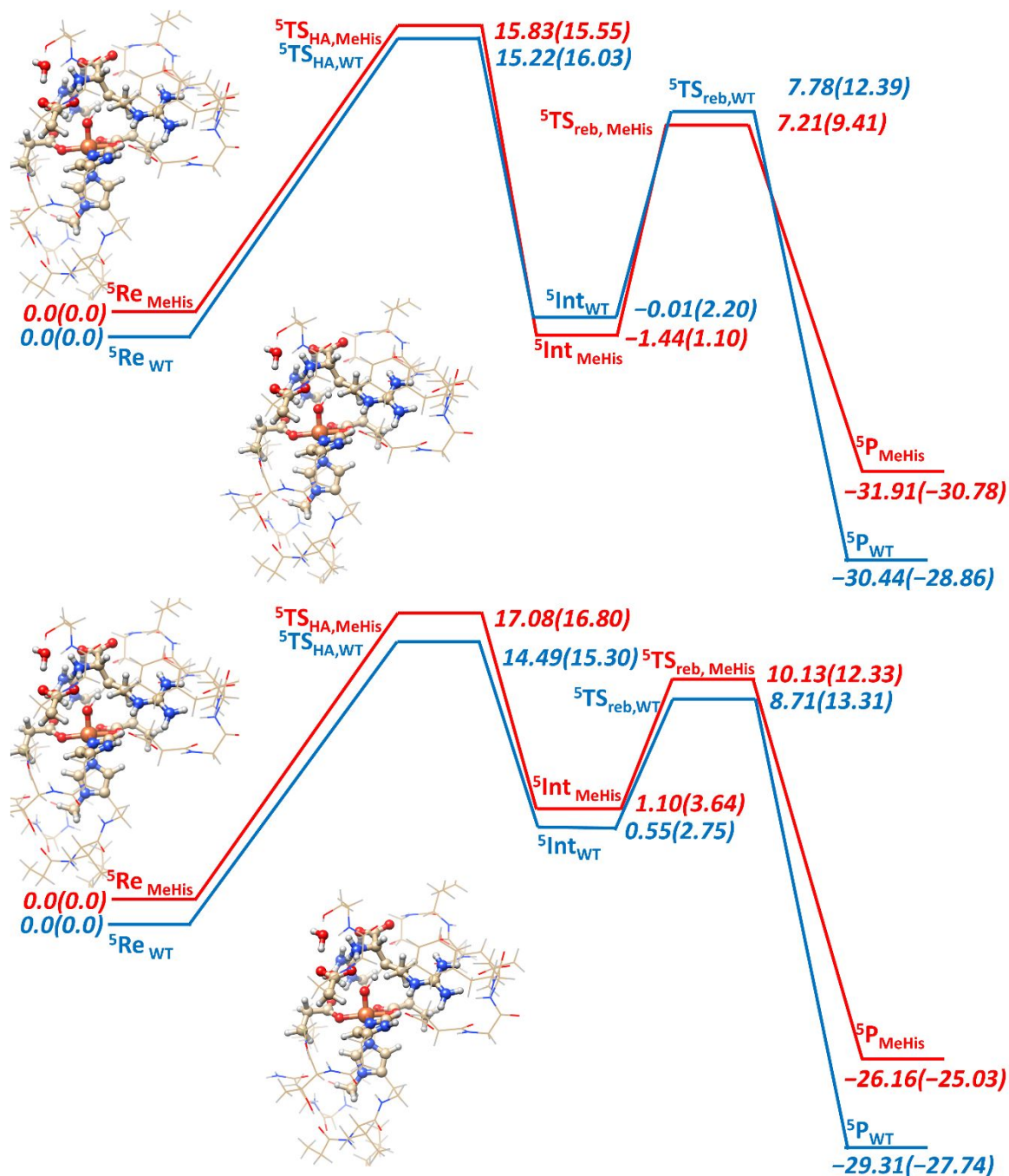


Supplementary Figure S2. QM cluster model A. A QM cluster model was generated to probe the electron affinity of the ferryl intermediates in VioC and VioC MeHis316. The cluster model, in addition to the ferryl intermediate, contained the side chains of the residues (Me)His316, His168, Glu170, Arg334, Ser158, Asp286, Thr169, Val315, Asn311, Ile309, Gly166, succinate and arginine for a total of 240 atoms.

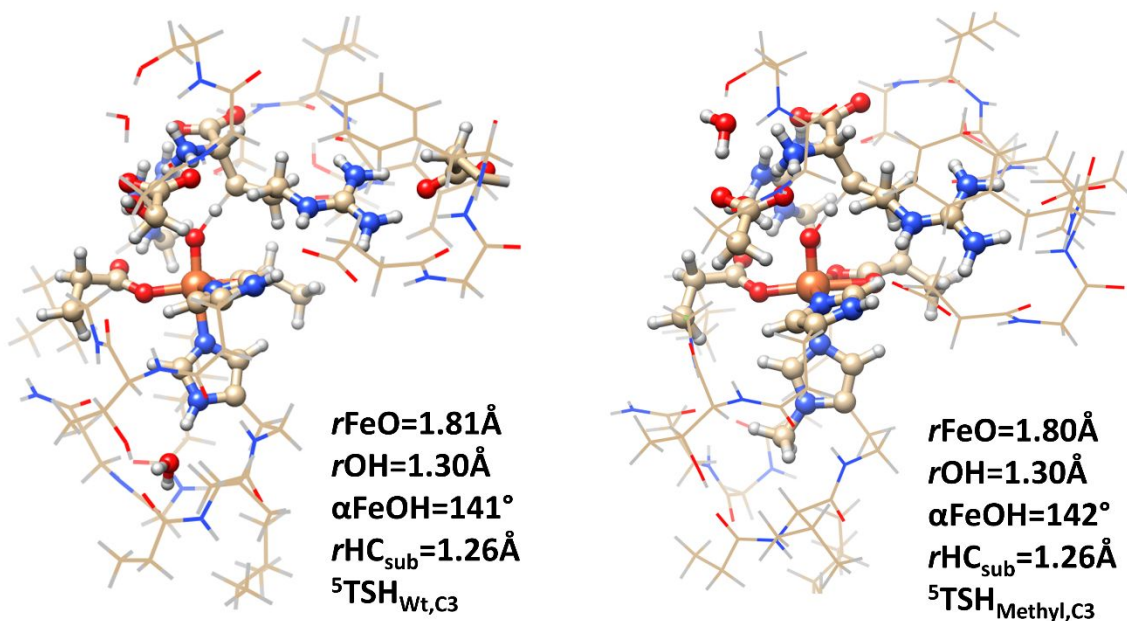


Supplementary Figure S3. QM cluster model B. A QM cluster model was generated to probe the energy landscapes for L-Arg hydroxylation. Optimised geometries of DFT models of the ferryl states in VioC and VioC MeHis316 are shown. This larger cluster model includes additional residues in proximity to the substrate L-Arginine *c.f.* that shown in Supplementary Figure S2, giving a total of 353 atoms in this larger QM cluster. This model contains the ferryl intermediate bound to succinate, which was positioned *cis* to the peptide chain His168–Thr169–Glu170 and *trans* to the peptide chain His316–Val315–Ala314. In addition, several small peptide chains were included that position the substrate, namely,

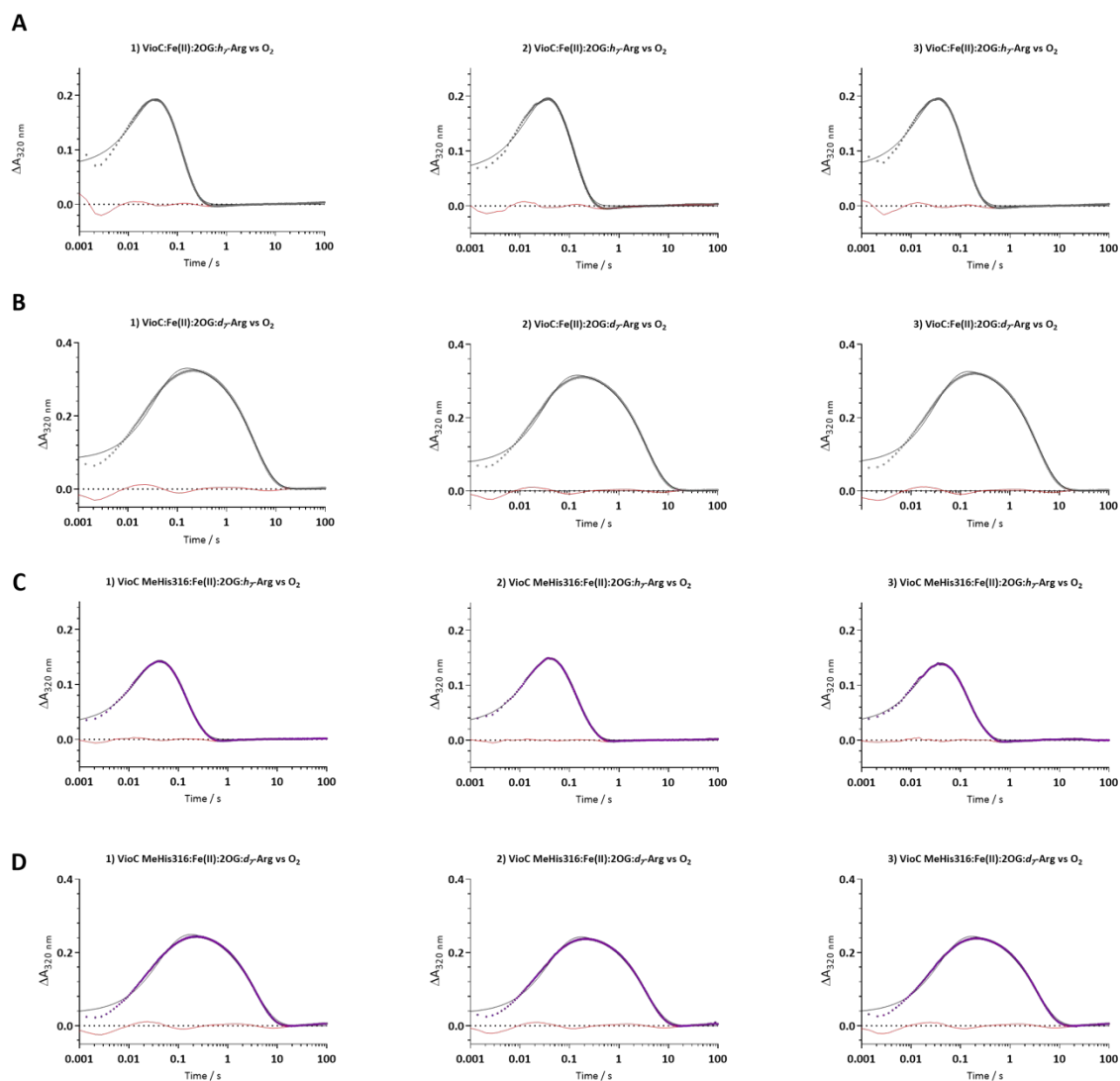
Thr155–Leu156–Val157–Ser158, Asp222–Asp223–Ser224, Asp268–Gly269–Asp270–Phe271, and Ile309–Asp310–Asn311. Arg334 side chain, Leu196 and two crystal water molecules were also included.



Supplementary Figure S4. Calculated reaction landscapes for WT VioC and VioC MeHis316 cluster models. (upper) Energies given as both zero-point ($\Delta E+ZPE$) energies and free energies in parenthesis. All energies given in kcal mol⁻¹ as calculated at UB3LYP/BS2 level of theory. (upper) energies calculated in gas phase, (lower) solvent corrected energies.



Supplementary Figure S5. Structure and important bonding information for the hydrogen atom abstraction transition state structures of (left) VioC and (right) VioC MeHis316.



Supplementary Figure S6. Fits of stopped-flow data to kinetic models. Time dependent absorbance changes at 320 nm are shown after rapid mixing an anoxic reactant complex VioC/VioC MeHis316:h₇-Arg/d₇-Arg:2OG:Fe(II) with aerobic buffer. Data points are shown as dots and the fitted models overlaid as black lines. The residuals from fitting the model to the data are shown for each measurement as a red line. Final concentration after mixing at 5 °C with air-saturated buffer are 500 μM enzyme, 3 mM 2OG, 3 mM h₇-Arg or per-d₇-Arg, and 500 μM (NH₄)₂Fe(SO₄)₂(H₂O)₆. A1-3) The formation and decay of the ferryl intermediate of VioC in reaction with h₇-Arg. B1-3) The formation and decay of the ferryl intermediate of VioC in reaction with d₇-Arg. C1-3) The formation and decay of the ferryl intermediate of VioC MeHis316 in reaction with h₇-Arg. D1-3) The formation and decay of the ferryl intermediate of VioC MeHis316 in reaction with d₇-Arg.

Supplementary References

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Cartesian coordinates for model A

VioC MeHis316 Fe(IV) complex

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1	5.023560000	3.312719000	14.976454000	1	-1.527608000	11.056179000	18.246837000
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1	7.479851000	2.699290000	15.373149000	6	1.749828000	7.534759000	21.099854000
1	6.456270000	2.356081000	16.782269000	6	2.079621000	6.088734000	21.554413000
1	4.219470000	5.843695000	14.289724000	6	3.294995000	5.485476000	20.916754000
6	2.859494000	13.989621000	14.592507000	6	4.623397000	5.577652000	21.263350000
6	3.475352000	12.734455000	13.952464000	7	3.288328000	4.751097000	19.734021000
6	4.994167000	12.688373000	14.183008000	6	4.585523000	4.462199000	19.436871000
8	5.520221000	11.640536000	14.696908000	7	5.421872000	4.955569000	20.329869000
8	5.634022000	13.724687000	13.875956000	1	0.992564000	7.940540000	21.778434000
7	5.158606000	17.369523000	15.726879000	1	1.188349000	5.470532000	21.397180000
6	5.715729000	18.183065000	16.811760000	1	2.246441000	6.121942000	22.638646000
6	6.414810000	19.390054000	16.207881000	1	5.059785000	6.066897000	22.121863000
8	7.320737000	20.012166000	16.722499000	1	4.882363000	3.912416000	18.558221000
6	6.582174000	17.454856000	17.860107000	1	1.852224000	7.989441000	19.002086000
6	5.850214000	16.336735000	18.661239000	6	12.408525000	-1.504755000	18.970109000
8	4.698295000	16.553213000	19.088407000	6	12.020355000	-0.030863000	19.130832000
8	6.514829000	15.250025000	18.827964000	6	10.503010000	0.181864000	19.218994000
1	4.847284000	18.595975000	17.351848000	6	10.106974000	1.652660000	19.404716000
1	6.949298000	18.199141000	18.579074000	7	10.615427000	2.452249000	18.298386000
1	7.470244000	17.032582000	17.375231000	6	11.318452000	3.596647000	18.397461000
1	5.881420000	16.789538000	15.301234000	7	11.348438000	4.281952000	19.543833000
6	1.147661000	-0.595785000	18.682526000	7	12.067350000	3.969482000	17.341124000
6	0.823430000	-0.639549000	17.181950000	1	12.054247000	-2.106036000	19.817126000
6	0.237404000	-2.012343000	16.792885000	1	12.421957000	0.548307000	18.291229000
6	2.066825000	-0.276591000	16.353426000	1	12.493429000	0.377901000	20.034889000

1	10.089269000	-0.394550000	20.058265000	6	-3.519578000	3.819915000	16.957717000
1	10.023155000	-0.214218000	18.310858000	1	-3.374419000	3.955023000	15.880969000
1	10.536750000	2.047226000	20.328571000	1	-2.811601000	3.060305000	17.302680000
1	9.019712000	1.763074000	19.491656000	1	-4.535209000	3.445767000	17.128102000
1	10.488346000	2.098793000	17.354462000	1	-4.037612000	5.883777000	17.396008000
1	11.903376000	5.151380000	19.571813000	1	-3.444379000	4.986821000	18.785809000
1	10.491139000	4.287799000	20.103243000	1	-0.124575000	5.720666000	12.956075000
1	11.863898000	3.439816000	16.496089000	1	1.235723000	6.749208000	13.348076000
1	12.157516000	4.980242000	17.142782000	1	1.813908000	2.802968000	12.312544000
26	7.705603000	5.762487000	19.690451000	1	0.237372000	3.569648000	12.008322000
6	8.441354000	5.189170000	24.561353000	1	-1.205253000	2.832850000	15.437276000
6	8.961763000	4.419261000	23.347942000	1	-0.626207000	1.229160000	12.855209000
8	8.711806000	4.247881000	20.956875000	1	-0.170246000	0.683011000	14.332662000
6	8.442035000	4.924276000	22.008089000	1	2.999435000	11.826032000	14.340764000
8	7.774483000	5.991512000	21.935032000	1	3.304140000	12.756198000	12.867110000
1	7.349801000	5.128357000	24.624821000	1	3.380269000	14.879063000	14.226977000
1	8.711534000	3.352902000	23.415221000	1	1.795881000	14.078390000	14.339403000
1	10.059011000	4.462755000	23.302091000	1	2.929206000	13.955012000	15.683732000
1	8.706929000	6.248248000	24.494067000	1	4.466259000	16.730111000	16.112063000
7	9.313409000	7.293900000	16.540371000	1	5.999289000	19.684614000	15.217119000
6	10.376240000	8.354570000	16.500537000	1	5.451687000	10.390724000	20.935127000
6	11.710329000	7.599321000	16.812595000	7	3.566021000	13.652305000	20.668279000
8	11.787748000	6.468304000	16.265146000	6	2.296203000	13.101586000	20.197588000
6	10.048395000	9.475099000	17.480952000	6	2.444861000	12.454786000	18.809078000
6	8.882370000	10.382287000	17.064074000	8	2.079611000	13.029475000	17.792938000
6	9.260059000	11.451444000	16.025865000	1	3.873359000	14.551512000	20.282242000
7	8.182321000	12.394289000	15.749126000	1	1.948521000	12.375900000	20.938465000
6	7.889181000	13.434474000	16.548206000	1	1.571982000	13.912865000	20.108008000
7	8.589997000	13.713780000	17.677005000	6	6.762071000	12.762870000	22.457483000
7	6.919850000	14.273364000	16.200851000	1	6.354118000	12.234645000	23.325084000
8	12.549193000	8.162870000	17.556466000	1	7.144395000	12.009764000	21.759900000
1	9.140056000	7.027889000	17.529052000	1	7.613187000	13.366494000	22.789517000
1	10.431633000	8.717348000	15.466094000	1	11.973213000	-1.932076000	18.057791000
1	10.958017000	10.064407000	17.628635000	1	13.496214000	-1.626358000	18.907476000
1	9.829533000	9.014443000	18.449494000	6	14.167795000	8.592011000	21.638663000
1	9.699664000	6.435327000	16.122063000	1	14.264281000	7.885716000	22.474391000
1	8.494951000	10.879499000	17.961966000	1	14.753788000	8.202306000	20.800555000
1	8.041386000	9.799300000	16.670573000	1	14.603860000	9.547990000	21.957822000
1	9.534386000	10.987443000	15.072672000	1	13.142806000	10.566069000	20.321599000
1	10.138108000	12.018038000	16.359526000	1	8.428886000	7.544856000	16.078567000
1	7.400676000	12.097889000	15.142555000	1	1.173564000	2.571987000	14.748886000
1	8.122869000	14.416617000	18.270290000	6	2.130890000	4.294230000	18.978876000
1	9.039996000	12.948920000	18.158896000	1	2.485995000	3.752369000	18.099443000
1	6.433925000	14.136468000	15.292924000	1	1.514626000	3.618725000	19.582734000
1	6.520585000	14.807669000	16.975139000	1	1.513481000	5.129989000	18.646687000
8	10.285480000	2.550119000	15.373192000	WT VioC Fe(IV) complex			
1	9.717323000	3.317516000	15.668759000	6	5.699545000	13.666189000	21.817158000
1	10.554293000	2.755601000	14.465977000	6	4.452424000	12.908361000	21.379231000
8	9.086332000	6.591223000	19.056777000	8	4.280517000	11.687117000	21.589482000
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6	12.697794000	8.777300000	21.225980000	1	6.131916000	14.133166000	20.918638000
6	12.066325000	7.443471000	20.796029000	1	5.376963000	14.500649000	22.453163000
8	12.853913000	6.713123000	19.849221000	7	3.156039000	11.291744000	18.820455000
1	12.690516000	9.402295000	19.260375000	6	4.003475000	10.972977000	17.684514000
1	12.133653000	9.104760000	22.114546000	6	3.698102000	9.619081000	17.004928000
1	11.052333000	7.608794000	20.410287000	8	2.993417000	8.737426000	17.510375000
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1	12.838598000	7.197085000	18.985548000	6	5.991752000	9.891321000	18.890401000
1	1.532103000	0.387244000	18.978601000	6	6.493057000	8.683150000	18.472287000
1	0.259678000	-0.806675000	19.290529000	7	5.975679000	9.817294000	20.274990000
1	8.862045000	4.783982000	25.489348000	6	6.454164000	8.609945000	20.644901000
1	6.425762000	4.764728000	13.651842000	7	6.770395000	7.899329000	19.569688000
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1	5.670874000	12.005712000	18.596687000	1	1.462820000	2.171870000	22.469090000
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1	3.480864000	10.999139000	19.738161000	6	0.435712000	2.622882000	13.939413000
1	6.633980000	8.338996000	17.459239000	6	0.205961000	2.402836000	12.450049000
1	6.582732000	8.284878000	21.664236000	8	1.060115000	2.106265000	11.634235000
7	4.324132000	9.502693000	15.807759000	6	1.912659000	2.644733000	14.364216000
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8	2.501999000	9.382201000	13.595197000	8	-0.881748000	5.322462000	16.440059000
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1	4.534550000	9.605305000	13.217846000	6	-0.520509000	7.696650000	18.015254000
1	3.367055000	8.216070000	11.521289000	6	-0.078448000	7.531812000	19.481905000
1	4.721164000	7.317042000	12.239637000	8	-0.873186000	7.160511000	20.348690000
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1	2.550278000	10.204655000	14.107050000	6	-0.819434000	9.331329000	16.087519000
1	4.856096000	10.316131000	15.431264000	6	-1.817571000	9.885818000	18.358119000
7	5.372584000	6.233683000	14.603244000	1	0.240608000	7.245240000	17.373112000
6	6.431180000	5.237056000	14.536845000	1	0.271057000	9.673006000	17.897381000
6	6.049461000	3.957250000	15.317917000	1	-0.935551000	10.386017000	15.813192000
6	7.227904000	3.324192000	16.081064000	1	0.060496000	8.944180000	15.560335000
6	7.920627000	4.379160000	16.946573000	1	-2.430835000	7.060346000	18.559762000
8	7.185032000	4.842210000	17.904009000	1	-1.702391000	8.791892000	15.724056000
8	9.064361000	4.764203000	16.646230000	1	-2.792407000	9.487604000	18.049281000
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1	5.619183000	3.213442000	14.637435000	1	-1.818703000	10.958336000	18.136197000
1	5.264359000	4.214640000	16.033412000	7	1.223509000	7.819305000	19.735432000
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1	4.416743000	5.892210000	14.499341000	6	3.424167000	5.828000000	20.702450000
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6	3.487470000	12.659779000	14.160646000	7	3.393891000	5.360486000	19.397692000
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8	5.580747000	13.738353000	13.797309000	1	0.961917000	8.012835000	21.784768000
7	5.435459000	17.407597000	15.602527000	1	1.375127000	5.601287000	21.316087000
6	5.715740000	18.183079000	16.811768000	1	2.457981000	6.274308000	22.530162000
6	6.371592000	19.494315000	16.394621000	1	5.214019000	6.150913000	21.971410000
8	7.159109000	20.130606000	17.061280000	1	4.932913000	4.789072000	18.023716000
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6	5.802624000	16.278638000	18.651117000	6	12.376451000	-1.515263000	18.996008000
8	4.673427000	16.430518000	19.156520000	6	12.020366000	-0.030851000	19.130839000
8	6.480703000	15.182481000	18.674019000	6	10.511221000	0.230078000	19.046255000
1	4.735006000	18.475972000	17.222352000	6	10.145055000	1.709655000	19.206882000
1	6.689207000	18.245123000	18.725320000	7	10.768546000	2.505579000	18.153936000
1	7.476591000	17.173426000	17.577244000	6	11.430540000	3.663579000	18.321966000
1	6.269377000	16.919130000	15.280510000	7	11.317246000	4.356543000	19.460377000
6	1.147661000	-0.595645000	18.682515000	7	12.277624000	4.072546000	17.358690000
6	1.136402000	0.848666000	19.207248000	1	11.906731000	-2.111779000	19.787749000
6	1.204094000	0.859519000	20.747613000	1	12.536424000	0.542383000	18.351170000
6	-0.081047000	1.612255000	18.663205000	1	12.397445000	0.352491000	20.089466000
6	1.351235000	2.247904000	21.381220000	1	9.986101000	-0.337120000	19.826603000
1	0.263779000	-1.146074000	19.031680000	1	10.122115000	-0.141561000	18.086206000
1	2.039625000	1.353849000	18.830162000	1	10.512115000	2.084108000	20.166445000
1	2.051668000	0.234735000	21.063725000	1	9.057004000	1.850490000	19.201898000
1	0.302297000	0.369877000	21.145395000	1	10.723455000	2.159786000	17.199460000
1	-1.014292000	1.187901000	19.059484000	1	11.885422000	5.215752000	19.558171000
1	-0.048850000	2.673012000	18.932278000	1	10.413385000	4.343604000	19.929083000
1	-0.120549000	1.555304000	17.569121000	1	12.221961000	3.528035000	16.503075000
1	2.235389000	2.768468000	20.991806000	1	12.318678000	5.086904000	17.163633000
1	0.478413000	2.880830000	21.185259000	26	7.506990000	5.960791000	19.521939000

6	8.349782000	5.059233000	24.308882000	1	2.780556000	3.114556000	11.985725000	
6	8.789394000	4.369163000	23.017333000	1	3.510878000	4.683126000	12.209791000	
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6	8.272647000	5.023381000	21.751510000	1	2.410506000	1.736110000	14.006247000	
8	7.721710000	6.156337000	21.761198000	1	-0.863701000	2.428347000	12.150931000	
1	7.259556000	5.050966000	24.408905000	1	-0.017619000	0.622982000	14.271381000	
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1	9.885695000	4.353049000	22.939265000	1	3.114184000	11.853968000	14.804386000	
1	8.678476000	6.102137000	24.328778000	1	3.192822000	12.421553000	13.128794000	
7	9.398559000	7.565185000	16.371793000	1	3.276453000	14.805281000	13.996147000	
6	10.521629000	8.572431000	16.381341000	1	1.772041000	13.972214000	14.458736000	
6	11.777130000	7.730288000	16.799215000	1	3.050367000	14.188364000	15.651572000	
8	11.783298000	6.569587000	16.308327000	1	4.730442000	16.698045000	15.786767000	
6	10.219402000	9.741595000	17.307517000	1	6.046489000	19.841130000	15.388242000	
6	9.046597000	10.637195000	16.879373000	1	5.564363000	10.518860000	20.907423000	
6	9.417838000	11.703941000	15.833889000	7	3.554270000	13.661767000	20.701848000	
7	8.327044000	12.622931000	15.544478000	6	2.290421000	13.118461000	20.204837000	
6	7.989718000	13.642291000	16.359559000	6	2.472006000	12.490073000	18.813782000	
7	8.671711000	13.939291000	17.492739000	8	2.100316000	13.049114000	17.793348000	
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8	12.604876000	8.258946000	17.573523000	1	1.926856000	12.382674000	20.928131000	
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1	10.649012000	8.895799000	15.341630000	6	6.724989000	12.804975000	22.553427000	
1	11.139604000	10.329355000	17.384179000	1	6.281424000	12.306923000	23.421417000	
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1	10.285275000	12.285470000	16.169374000	1	14.426865000	7.948651000	22.295837000	
1	7.541700000	12.284284000	14.966179000	1	14.742658000	8.344429000	20.598640000	
1	8.140857000	14.576925000	18.112546000	1	14.612155000	9.642683000	21.806282000	
1	9.188480000	13.201842000	17.948294000	1	12.808798000	10.659407000	20.433513000	
1	6.474570000	14.260459000	15.136089000	1	8.546926000	7.816000000	15.841618000	
1	6.551198000	14.924078000	16.813763000	1	-0.046773000	3.558630000	14.250817000	
8	1.719779000	4.683407000	17.260969000					
8	10.534490000	2.858319000	15.273220000					
1	10.044607000	3.643954000	15.621012000	VioC WT Fe(III) complex	6	5.716307000	13.629552000	21.827321000
1	10.812189000	3.090221000	14.374666000	6	4.452426000	12.908362000	21.379236000	
1	2.174111000	4.858035000	16.411889000	8	4.239184000	11.697061000	21.585774000	
1	0.784236000	4.911531000	17.069893000	1	6.102575000	14.202564000	20.969403000	
8	8.948561000	6.561894000	19.047469000	1	5.418303000	14.379787000	22.573051000	
7	12.325013000	9.786468000	20.224664000	7	3.135077000	11.370158000	18.800629000	
6	12.699514000	8.774738000	21.226964000	6	3.976297000	11.043923000	17.660039000	
6	12.097486000	7.417249000	20.844131000	6	3.589842000	9.747331000	16.922423000	
8	12.823776000	6.716785000	19.831277000	8	2.859630000	8.871491000	17.398594000	
1	12.638859000	9.493714000	19.297962000	6	5.472184000	10.985478000	18.085069000	
1	12.201681000	9.066333000	22.164680000	6	5.870744000	9.777141000	18.874812000	
1	11.048660000	7.562842000	20.547823000	6	6.359408000	8.566876000	18.446204000	
1	12.119070000	6.759430000	21.721231000	7	5.826206000	9.672559000	20.258537000	
1	12.839509000	7.253652000	18.999815000	6	6.283147000	8.439180000	20.596813000	
1	1.139874000	-0.619306000	17.585933000	7	6.610272000	7.746890000	19.519816000	
1	2.034891000	-1.141628000	19.026375000	1	3.874806000	11.869272000	16.950913000	
1	8.774886000	4.546359000	25.177847000	1	5.695021000	11.910802000	18.629911000	
1	6.654314000	4.993296000	13.488795000	1	6.069293000	11.015391000	17.171297000	
1	2.584514000	8.419579000	21.184668000	1	3.449991000	11.043751000	19.710054000	
1	2.589593000	5.211262000	18.763467000	1	6.538752000	8.250717000	17.430202000	
6	-3.291529000	3.883108000	16.257070000	1	6.392186000	8.091127000	21.612274000	
1	-3.308222000	4.287609000	15.239415000	7	4.170112000	9.667363000	15.696453000	
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8	2.304542000	9.569845000	13.594559000	8	-0.985033000	5.413550000	16.323903000
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1	4.313378000	9.747813000	13.092941000	6	-0.520517000	7.696652000	18.015251000
1	3.004121000	8.366253000	11.480620000	6	-0.024142000	7.509061000	19.463558000
1	4.408743000	7.473200000	12.106960000	8	-0.807518000	7.162184000	20.355123000
1	2.766420000	7.124055000	12.725862000	6	-0.699828000	9.194316000	17.642065000
1	2.369691000	10.208585000	14.324260000	6	-0.917493000	9.358531000	16.131507000
1	4.750705000	10.458015000	15.355225000	6	-1.817296000	9.868208000	18.452288000
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6	6.400791000	5.475328000	14.446921000	1	0.251799000	9.677582000	17.895797000
6	5.987141000	4.162643000	15.137017000	1	-1.050536000	10.416765000	15.878227000
6	7.175207000	3.382846000	15.726242000	1	-0.060566000	8.983748000	15.559859000
6	7.965762000	4.288552000	16.686601000	1	-2.346427000	6.978661000	18.692267000
8	7.332463000	4.660625000	17.725388000	1	-1.813261000	8.818997000	15.799742000
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8	5.628963000	11.910179000	14.721761000	7	5.537882000	5.032434000	19.961563000
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1	4.920128000	18.704577000	17.370384000	6	10.169731000	1.742608000	19.042016000
1	7.032071000	18.270420000	18.521469000	7	10.865215000	2.510450000	18.017193000
1	7.473860000	17.029927000	17.366132000	6	11.522984000	3.672369000	18.195455000
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6	1.147663000	-0.595646000	18.682516000	7	12.346146000	4.085635000	17.207521000
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6	1.194046000	0.782758000	20.800369000	1	12.599212000	0.535471000	18.391512000
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1	2.027654000	0.135574000	21.108761000	1	9.086537000	1.895801000	18.965955000
1	0.277786000	0.289493000	21.161048000	1	10.780545000	2.205951000	17.051100000
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6	10.601678000	8.518245000	16.457966000	1	1.833776000	14.072483000	14.211680000
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8	10.604017000	2.784814000	15.090583000				
1	10.041107000	3.535001000	15.436228000				
1	10.982271000	3.110160000	14.260413000				
1	2.123300000	4.939260000	16.274095000				
1	0.723931000	4.943245000	16.908630000				
8	9.172951000	6.693362000	18.901974000				
7	12.549362000	9.817339000	20.198183000				
6	12.699513000	8.774739000	21.226963000				
6	12.098380000	7.449952000	20.733642000				
8	12.936724000	6.747755000	19.808759000				
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1	12.085240000	9.080130000	22.089718000				
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1	3.321725000	14.980157000	14.542991000				

Cartesian coordinates for model B

Wildtype

⁵Re - VioC reactant state

C 11.345235000000 4.335273000000 24.789841000000
C 11.446038000000 5.752310000000 24.244728000000
O 11.347152000000 6.006428000000 23.016545000000
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H 3.911156000000 5.668764000000 14.007840000000
H 6.620579000000 6.254344000000 13.548877000000
H 5.615836000000 3.578009000000 12.573811000000
H 5.224277000000 3.980323000000 14.239812000000
H 7.523042000000 2.727755000000 13.673511000000
H 8.093046000000 4.347028000000 13.299037000000
C 8.221656000000 -2.253926000000 14.619396000000
C 8.443777000000 -0.841243000000 15.192499000000
C 9.257712000000 0.036624000000 14.222412000000
C 7.105470000000 -0.166588000000 15.552790000000
H 7.642936000000 -2.205830000000 13.686664000000
H 9.025470000000 -0.944287000000 16.122764000000
H 10.239240000000 -0.406736000000 14.013455000000
H 8.730215000000 0.140073000000 13.261181000000
H 9.413198000000 1.040910000000 14.633085000000
H 7.274193000000 0.828361000000 15.980512000000
H 6.538832000000 -0.764762000000 16.278288000000
H 6.480746000000 -0.048229000000 14.656170000000
C -3.587275000000 6.758384000000 20.537238000000
C -3.364158000000 5.381357000000 21.186344000000
C -2.472379000000 5.417330000000 22.452351000000
C -2.585168000000 4.095791000000 23.238728000000
C -1.000118000000 5.725750000000 22.110791000000
H -2.643493000000 7.213891000000 20.218905000000
H -4.340418000000 4.949637000000 21.454998000000
H -2.907462000000 4.699800000000 20.452652000000
H -2.848193000000 6.224482000000 23.102468000000
H -1.972938000000 4.120026000000 24.148783000000
H -3.621967000000 3.890557000000 23.532718000000
H -2.240663000000 3.248230000000 22.627901000000
H -0.884936000000 6.679708000000 21.587102000000
H -0.388037000000 5.759022000000 23.021593000000
H -0.594236000000 4.944020000000 21.451879000000
C 10.442551000000 12.536834000000 14.161469000000
C 11.764957000000 13.048644000000 14.730444000000
O 12.334481000000 14.029420000000 14.193981000000
C 9.475922000000 11.775042000000 15.103349000000
C 9.961659000000 10.367860000000 15.421112000000
O 10.498041000000 10.168206000000 16.587095000000
O 9.889341000000 9.472049000000 14.500920000000
H 9.940471000000 13.419964000000 13.754959000000
H 9.306905000000 12.323056000000 16.035029000000
H 8.519569000000 11.681575000000 14.577817000000
N 12.309475000000 12.371933000000 15.792938000000

C	13.573797000000	12.787080000000	16.391012000000	H	5.582228000000	1.070059000000	21.917651000000
C	14.732842000000	11.792665000000	16.269670000000	H	7.665705000000	0.307723000000	20.712782000000
O	15.761550000000	11.960153000000	16.970943000000	H	6.737107000000	0.112612000000	19.217975000000
H	11.773761000000	11.639642000000	16.255432000000	H	6.975149000000	1.725670000000	19.909974000000
H	13.873163000000	13.716395000000	15.895304000000	H	3.252194000000	2.640021000000	19.365035000000
N	14.587599000000	10.785301000000	15.372067000000	H	5.015303000000	2.678515000000	19.289100000000
C	15.639698000000	9.815747000000	15.075336000000	H	4.199058000000	2.979632000000	20.825227000000
C	15.018981000000	8.460783000000	14.747363000000	N	0.798381000000	1.533893000000	20.734660000000
O	14.038433000000	8.665528000000	13.699299000000	C	-0.512504000000	1.708680000000	20.096700000000
H	13.761936000000	10.721727000000	14.790245000000	C	-0.428647000000	2.449874000000	18.757365000000
H	16.303564000000	9.751968000000	15.941727000000	O	-0.833148000000	3.643713000000	18.654792000000
H	14.553615000000	8.024626000000	15.640456000000	H	1.052985000000	2.163938000000	21.481120000000
H	15.808043000000	7.770832000000	14.413775000000	H	-0.959753000000	0.720313000000	19.947552000000
H	13.247267000000	8.080077000000	13.842751000000	N	0.099526000000	1.729505000000	17.739000000000
C	5.696472000000	15.380475000000	20.013973000000	C	0.312314000000	2.272632000000	16.398325000000
C	5.404633000000	15.366118000000	21.514360000000	C	1.807626000000	2.549199000000	16.120910000000
O	5.339485000000	16.440929000000	22.177009000000	C	2.056586000000	3.415571000000	14.901075000000
C	6.932354000000	14.592326000000	19.514523000000	O	2.865156000000	4.376992000000	14.936837000000
C	6.765267000000	13.081022000000	19.363137000000	N	1.382523000000	3.101879000000	13.760274000000
O	7.557992000000	12.481420000000	18.528679000000	H	0.486590000000	0.814168000000	17.986676000000
O	5.920135000000	12.444091000000	20.097066000000	H	-0.250124000000	3.204288000000	16.326273000000
H	4.803458000000	15.017271000000	19.487416000000	H	2.354425000000	1.602156000000	16.011616000000
H	7.239747000000	14.982146000000	18.538895000000	H	2.234900000000	3.085333000000	16.968199000000
H	7.787708000000	14.764233000000	20.184140000000	H	0.737662000000	2.330279000000	13.704409000000
N	5.184512000000	14.148639000000	22.078210000000	H	1.526972000000	3.668076000000	12.936653000000
C	4.647313000000	13.996083000000	23.427717000000	C	-3.084513000000	6.836311000000	16.225945000000
C	5.555164000000	14.406739000000	24.593293000000	C	-1.694785000000	7.438633000000	16.336834000000
O	5.050705000000	14.603260000000	25.722630000000	O	-0.752000000000	7.038751000000	15.570035000000
H	5.283265000000	13.339676000000	21.448865000000	C	-3.048078000000	5.313335000000	16.020208000000
H	3.739319000000	14.597072000000	23.546978000000	H	-3.678695000000	7.092855000000	17.110758000000
H	4.373954000000	12.944759000000	23.562513000000	H	-2.614038000000	4.806087000000	16.888954000000
N	6.880946000000	14.537936000000	24.320106000000	H	-4.060482000000	4.925338000000	15.867634000000
C	7.851531000000	15.013985000000	25.303049000000	H	-2.444279000000	5.070434000000	15.140852000000
C	8.024911000000	16.552202000000	25.252720000000	N	-1.515184000000	8.400693000000	17.259029000000
O	8.891806000000	17.106230000000	25.980156000000	C	-0.239070000000	9.084957000000	17.497692000000
C	9.238474000000	14.352025000000	25.126369000000	C	0.289286000000	8.652526000000	18.872797000000
C	9.310634000000	12.852423000000	25.456173000000	O	-0.506533000000	8.302618000000	19.790266000000
O	9.972226000000	12.493832000000	26.472479000000	C	-0.378830000000	10.637348000000	17.387284000000
O	8.712131000000	12.029111000000	24.625420000000	C	-0.796662000000	11.047889000000	15.962495000000
H	7.218016000000	14.265633000000	23.407468000000	C	-1.327285000000	11.235124000000	18.444976000000
H	7.451558000000	14.777731000000	26.295272000000	H	-2.232232000000	8.550880000000	17.957090000000
H	9.569570000000	14.501995000000	24.087962000000	H	0.459028000000	8.759399000000	16.725448000000
H	9.928489000000	14.881501000000	25.784038000000	H	0.632989000000	11.022603000000	17.573043000000
N	7.233726000000	17.238098000000	24.388142000000	H	-0.139716000000	10.611637000000	15.202247000000
C	7.343353000000	18.684591000000	24.210079000000	H	-0.770837000000	12.139580000000	15.861897000000
C	7.610254000000	19.073558000000	22.744309000000	H	-1.822748000000	10.721510000000	15.749992000000
C	8.895611000000	18.541664000000	22.125062000000	H	-1.060767000000	10.930400000000	19.461728000000
C	10.015705000000	18.168939000000	22.888899000000	H	-1.298480000000	12.329558000000	18.396613000000
C	8.982161000000	18.438255000000	20.723779000000	H	-2.367344000000	10.932970000000	18.261339000000
C	11.184875000000	17.714188000000	22.264661000000	N	1.630377000000	8.717098000000	19.020035000000
C	10.150172000000	17.989347000000	20.098989000000	C	2.290610000000	8.363437000000	20.275239000000
C	11.260498000000	17.625432000000	20.870687000000	C	2.623992000000	6.851123000000	20.383656000000
H	6.549996000000	16.757226000000	23.808285000000	C	3.638099000000	6.362594000000	19.394315000000
H	8.135679000000	19.030370000000	24.878304000000	N	3.305578000000	5.795378000000	18.162966000000
H	6.761509000000	18.730063000000	22.138875000000	C	5.015420000000	6.380126000000	19.436866000000
H	7.607384000000	20.174343000000	22.688548000000	C	4.451810000000	5.487616000000	17.502868000000
H	9.976004000000	18.198068000000	23.972894000000	N	5.511159000000	5.832553000000	18.253250000000
H	8.120657000000	18.713393000000	20.119498000000	H	2.201388000000	8.964357000000	18.207073000000
H	12.034137000000	17.420646000000	22.874465000000	H	1.624539000000	8.635023000000	21.099021000000
H	10.192122000000	17.917437000000	19.015895000000	H	1.689691000000	6.288061000000	20.278814000000
H	12.167338000000	17.269152000000	20.391718000000	H	2.998572000000	6.667301000000	21.398760000000
C	2.978436000000	0.450995000000	21.094952000000	H	5.677806000000	6.750094000000	20.198481000000
C	1.680268000000	0.572137000000	20.329376000000	H	4.491900000000	5.046166000000	16.525421000000
O	1.421991000000	-0.166013000000	19.336071000000	H	2.334918000000	5.664906000000	17.796873000000
C	4.213428000000	0.872758000000	20.245832000000	C	11.131545000000	0.285469000000	18.541623000000
C	5.512793000000	0.482290000000	20.989198000000	C	10.554393000000	1.657046000000	18.924339000000
C	4.166769000000	2.374989000000	19.908486000000	N	10.552727000000	2.613719000000	17.810534000000
C	6.793195000000	0.674792000000	20.159182000000	C	11.602094000000	3.378545000000	17.456898000000
H	2.949555000000	1.043296000000	22.019138000000	N	12.786254000000	3.321500000000	18.097444000000
H	4.168943000000	0.296656000000	19.309689000000	N	11.473677000000	4.233194000000	16.423091000000
H	5.437979000000	-0.571992000000	21.294285000000	H	12.176021000000	0.374642000000	18.224626000000

H 10.563164000000 -0.158816000000 17.717489000000

H 9.513025000000 1.560731000000 19.242414000000

H 11.108552000000 2.079631000000 19.771196000000

H 9.676769000000 2.810050000000 17.323023000000

H 12.896888000000 2.850522000000 18.993931000000

H 13.454275000000 4.058110000000 17.857459000000

H 10.582745000000 4.286800000000 15.945095000000

H 12.169587000000 4.972649000000 16.339909000000

Fe 7.436421000000 5.892693000000 17.635083000000

O 7.904222000000 4.271272000000 19.067379000000

O 9.017389000000 6.071277000000 17.137474000000

C 8.123084000000 5.138299000000 20.004756000000

O 7.942499000000 6.393431000000 19.715039000000

C 8.572908000000 4.723212000000 21.379765000000

C 7.824826000000 5.467077000000 22.500029000000

H 8.449788000000 3.639124000000 21.465363000000

H 9.645461000000 4.944957000000 21.472366000000

H 6.746492000000 5.271297000000 22.460383000000

H 7.982130000000 6.545270000000 22.412055000000

N 11.468022000000 17.763596000000 17.255092000000

C 12.522408000000 7.995387000000 18.306187000000

C 13.646640000000 6.934904000000 18.208940000000

O 13.486988000000 5.965230000000 17.372898000000

C 11.925175000000 7.964408000000 19.732761000000

C 10.635097000000 8.761500000000 19.993717000000

C 10.757390000000 10.292230000000 19.871891000000

N 9.539890000000 10.979955000000 20.340736000000

C 9.253786000000 11.190810000000 21.648941000000

N 10.097703000000 10.850376000000 22.630718000000

N 8.089391000000 11.775635000000 22.008110000000

O 14.621382000000 7.096962000000 19.012724000000

H 12.955896000000 8.977174000000 18.089188000000

H 11.721750000000 6.918322000000 19.998791000000

H 12.709675000000 8.305555000000 20.414012000000

H 10.315120000000 8.512518000000 21.012246000000

H 9.835766000000 8.412870000000 19.332399000000

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H 11.626723000000 10.649492000000 20.439294000000

H 8.943690000000 11.434714000000 19.648156000000

H 11.012721000000 10.422901000000 22.504516000000

H 9.778235000000 11.097270000000 23.583266000000

H 7.303414000000 11.845087000000 21.369241000000

H 8.002662000000 12.001519000000 23.014382000000

H 11.881516000000 7.467232000000 16.344358000000

H 10.968597000000 8.680131000000 17.033810000000

H 10.773510000000 7.049573000000 17.518917000000

O 0.781664000000 5.437708000000 17.297010000000

H 0.110003000000 4.938739000000 17.819044000000

H 0.367781000000 6.004785000000 16.606608000000

O 11.738503000000 7.535105000000 14.469908000000

H 11.192882000000 8.379612000000 14.441882000000

H 11.097642000000 6.835761000000 14.195500000000

O 9.135690000000 6.718723000000 14.381420000000

H 9.056468000000 6.505530000000 15.341709000000

H 9.088466000000 7.699828000000 14.280765000000

H 11.092459000000 -0.397516000000 19.398546000000

H 3.085182000000 -0.602573000000 21.379864000000

H -1.147222000000 2.297443000000 20.757651000000

H -0.101862000000 1.561625000000 15.671907000000

H 7.670753000000 -2.889905000000 15.323923000000

H 9.176369000000 -2.745300000000 14.394600000000

H -4.244838000000 6.669992000000 19.661402000000

H -4.070568000000 7.447705000000 21.242224000000

H 3.208126000000 8.953923000000 20.355952000000

H -3.574216000000 7.311441000000 15.363710000000

H 5.981254000000 5.835141000000 11.968975000000

H 4.044322000000 11.371147000000 16.936920000000

H 5.826360000000 16.434723000000 19.757076000000

H 10.677238000000 11.889303000000 13.304756000000

H 15.490776000000 4.582219000000 20.041634000000

H 10.750604000000 3.761863000000 24.072563000000

H 16.233910000000 10.159956000000 14.217076000000

H 13.450491000000 13.001337000000 17.457839000000

H 6.409851000000 19.165771000000 24.532014000000

H 8.192896000000 5.146912000000 23.480090000000

⁵TSH_{ca} – ViOC WT transition state to HAT

C 11.399845000000 4.691605000000 25.900143000000

C 11.550559000000 5.929575000000 25.029753000000

O 11.363063000000 5.915964000000 23.787192000000

C 12.732018000000 4.013577000000 26.320033000000

O 13.398122000000 3.436836000000 25.171147000000

C 12.476840000000 2.882527000000 27.317644000000

H 10.836024000000 4.951825000000 26.806834000000

H 13.386934000000 4.767226000000 26.784809000000

H 14.111329000000 4.042506000000 24.825061000000

H 13.425628000000 2.413691000000 27.594437000000

H 11.983797000000 3.249247000000 28.225632000000

H 11.841394000000 2.117384000000 26.857510000000

N 11.917751000000 7.079099000000 25.686158000000

C 11.940226000000 8.399526000000 25.032024000000

C 13.027756000000 8.466479000000 23.948928000000

O 12.879141000000 9.158708000000 22.905944000000

C 12.122057000000 9.518009000000 26.089737000000

C 11.072961000000 9.528784000000 27.233747000000

C 11.413330000000 10.651890000000 28.236466000000

C 9.637616000000 9.696788000000 26.697400000000

H 11.951064000000 7.072021000000 26.696073000000

H 10.996041000000 8.547152000000 24.498435000000

H 13.130731000000 9.435819000000 26.520911000000

H 12.065346000000 10.481880000000 25.572052000000

H 11.133116000000 8.568443000000 27.781551000000

H 9.331184000000 8.854156000000 26.063128000000

H 9.570703000000 10.623814000000 26.115104000000

H 8.926128000000 9.757718000000 27.530084000000

H 12.444772000000 10.557952000000 28.603257000000

H 11.290119000000 11.639733000000 27.772995000000

N 10.743641000000 10.599968000000 29.104418000000

H 14.157941000000 7.758509000000 24.187241000000

C 15.093815000000 7.386312000000 23.116790000000

C 15.090959000000 5.856395000000 23.119719000000

O 15.139732000000 5.230613000000 24.232773000000

C 16.511906000000 8.008754000000 23.274661000000

C 16.446550000000 9.529469000000 23.037269000000

C 17.169613000000 7.684387000000 24.629379000000

H 14.183560000000 7.155972000000 25.001399000000

H 14.659757000000 7.743835000000 22.177902000000

H 17.122881000000 7.560513000000 22.475494000000

H 17.213195000000 6.607343000000 24.815845000000

H 18.189588000000 8.085785000000 24.656798000000

H 16.608968000000 8.149549000000 25.449573000000

H 17.448057000000 9.971164000000 23.099915000000

H 15.814779000000 10.012322000000 23.791236000000

H 16.027546000000 9.763386000000 22.052870000000

N 14.982408000000 5.252795000000 21.929898000000

C 14.756845000000 3.813260000000 21.799509000000

C 13.252879000000 3.510169000000 21.903617000000

O 12.968703000000 2.156883000000 21.397930000000

H 14.773102000000 5.820604000000 21.085922000000

H 15.319660000000 3.284156000000 22.574042000000

H 12.888335000000 3.618507000000 22.927064000000

H 12.696524000000 4.186295000000 21.253766000000

H 13.096958000000 1.490952000000 22.099373000000

C 3.741591000000 11.341967000000 16.859789000000

C 3.056635000000 10.107475000000 16.294794000000

O 2.361435000000 9.331228000000 17.011263000000

C 5.293963000000 11.271297000000 16.736440000000

C 5.909357000000 10.115388000000 17.467021000000

N 6.503276000000 10.284371000000 18.713523000000

C 6.017349000000 8.767285000000 17.179808000000

C 6.951864000000 9.082644000000 19.146763000000

N 6.672543000000 8.139015000000 18.235391000000

H 3.381986000000 12.235824000000 16.332980000000

H	5.578454000000	11.231229000000	15.678121000000	C	12.487348000000	13.775814000000	15.953526000000
H	5.716149000000	12.200019000000	17.136324000000	O	13.120385000000	14.580317000000	16.684947000000
H	5.685283000000	8.217200000000	16.317786000000	H	10.320029000000	11.811829000000	15.832239000000
H	7.456795000000	8.911696000000	20.079994000000	H	10.691776000000	14.708464000000	15.242218000000
H	6.735834000000	11.220548000000	19.139581000000	N	13.083174000000	12.826073000000	15.194524000000
N	3.285200000000	9.865217000000	14.984324000000	C	14.520469000000	12.584889000000	15.159879000000
C	2.979195000000	8.611741000000	14.289843000000	C	14.765721000000	11.078627000000	15.114446000000
C	4.350437000000	8.120553000000	13.790784000000	O	14.021326000000	10.556835000000	13.988248000000
O	5.173263000000	8.952483000000	13.317557000000	H	12.528489000000	12.212948000000	14.611227000000
C	1.936162000000	8.838775000000	13.160789000000	H	14.970184000000	13.043299000000	16.044955000000
O	0.709192000000	9.349577000000	13.721065000000	H	14.429302000000	10.622551000000	16.057527000000
C	1.682881000000	7.573368000000	12.331566000000	H	15.842073000000	10.879175000000	15.003386000000
H	3.910658000000	10.470659000000	14.464944000000	H	13.667277000000	9.645035000000	14.174088000000
H	2.556223000000	7.920077000000	15.023067000000	C	6.232808000000	15.976548000000	20.684587000000
H	2.314779000000	9.636666000000	12.512716000000	C	6.415109000000	16.280574000000	22.170120000000
H	0.179588000000	8.626125000000	14.147547000000	O	6.703876000000	17.444069000000	22.571829000000
H	0.907411000000	7.781475000000	11.588623000000	C	7.221170000000	14.974613000000	20.039421000000
H	2.589586000000	7.252486000000	11.804232000000	C	6.947365000000	13.491740000000	20.278997000000
H	1.329486000000	6.758695000000	12.974832000000	O	7.405236000000	12.666060000000	19.387223000000
N	4.647951000000	6.813468000000	13.975106000000	O	6.355328000000	13.099494000000	21.350903000000
C	6.031945000000	6.322604000000	13.843902000000	H	5.205547000000	15.622915000000	20.524470000000
C	6.097024000000	4.799106000000	14.028447000000	H	7.236430000000	15.129645000000	18.956219000000
C	7.469268000000	4.312308000000	14.530523000000	H	8.246265000000	15.183901000000	20.378077000000
C	7.645383000000	4.307068000000	16.046860000000	N	6.218060000000	15.246159000000	23.031602000000
O	8.334352000000	3.390632000000	16.568177000000	C	6.139944000000	15.448381000000	24.475030000000
O	7.066955000000	5.284740000000	16.725210000000	C	7.446344000000	15.831752000000	25.182893000000
H	3.945464000000	6.175712000000	14.347525000000	O	7.408306000000	16.349162000000	26.320649000000
H	6.649442000000	6.811688000000	14.606048000000	H	6.079059000000	14.319579000000	22.606704000000
H	5.859854000000	4.302510000000	13.078271000000	H	5.434977000000	16.252751000000	24.707919000000
H	5.328588000000	4.484627000000	14.743372000000	H	5.762009000000	14.525681000000	24.926867000000
H	7.670037000000	3.292368000000	14.192415000000	N	8.592496000000	15.568795000000	24.495711000000
H	8.277399000000	4.942645000000	14.132338000000	C	9.929248000000	15.936421000000	24.963419000000
C	5.672019000000	-1.750749000000	15.872171000000	C	10.400691000000	17.291940000000	24.393056000000
C	6.349593000000	-0.409148000000	16.211504000000	O	11.593122000000	17.661616000000	24.564417000000
C	7.738117000000	-0.284598000000	15.555753000000	C	10.948503000000	14.830968000000	24.621101000000
C	5.448945000000	0.777898000000	15.817311000000	C	10.720633000000	13.555066000000	25.449525000000
H	5.518674000000	-1.842089000000	14.787673000000	O	10.938109000000	13.605055000000	26.689892000000
H	6.489378000000	-0.369271000000	17.303828000000	O	10.305087000000	12.489068000000	24.795503000000
H	8.402471000000	-1.098322000000	15.873481000000	H	8.513256000000	15.114308000000	23.595883000000
H	7.652568000000	-0.335232000000	14.461047000000	H	9.876458000000	16.038019000000	26.053286000000
H	8.211449000000	0.669936000000	15.814371000000	H	10.907521000000	14.602197000000	23.549055000000
H	5.907761000000	1.726833000000	16.117013000000	H	11.940657000000	15.230617000000	24.848742000000
H	4.464649000000	0.692703000000	16.294612000000	N	9.485703000000	18.031662000000	23.713764000000
H	5.302623000000	0.797970000000	14.727211000000	C	9.811833000000	19.326745000000	23.116884000000
C	-3.943841000000	4.990312000000	19.441037000000	C	9.478286000000	19.386891000000	21.615911000000
C	-3.607487000000	3.498859000000	19.610206000000	C	10.257218000000	18.449632000000	20.701414000000
C	-2.623172000000	3.201270000000	20.768305000000	C	11.466292000000	17.838301000000	21.076421000000
C	-2.576677000000	1.688227000000	21.061958000000	C	9.762128000000	18.202771000000	19.406287000000
C	-1.209746000000	3.741725000000	20.469590000000	C	12.155433000000	17.011982000000	20.177755000000
H	-3.048004000000	5.596008000000	19.263489000000	C	10.455164000000	17.383357000000	18.508995000000
H	-4.540248000000	2.942973000000	19.790536000000	C	11.661813000000	16.779447000000	18.888883000000
H	-3.179804000000	3.099408000000	18.678827000000	H	8.536339000000	17.693604000000	23.583102000000
H	-2.998977000000	3.707117000000	21.672803000000	H	10.871605000000	19.509564000000	23.309732000000
H	-1.872819000000	1.459188000000	21.872893000000	H	8.405055000000	19.187216000000	21.495452000000
H	-3.562316000000	1.305346000000	21.353740000000	H	9.637808000000	20.426641000000	21.286946000000
H	-2.264553000000	1.135849000000	20.163562000000	H	11.868203000000	17.982368000000	22.074210000000
H	-1.210779000000	4.825866000000	20.315399000000	H	8.825334000000	18.665243000000	19.101605000000
H	-0.523116000000	3.519101000000	21.297380000000	H	13.084007000000	16.543734000000	20.491206000000
H	-0.815225000000	3.272328000000	19.556873000000	H	10.055336000000	17.214082000000	17.512561000000
C	9.042432000000	11.443890000000	13.555160000000	H	12.199946000000	16.137602000000	18.196380000000
C	9.655381000000	12.736845000000	14.091659000000	C	2.595857000000	-0.252091000000	19.890226000000
O	9.571097000000	13.793009000000	13.419234000000	C	1.731676000000	-0.240799000000	18.644606000000
C	8.624439000000	10.359648000000	14.581452000000	O	2.193349000000	-0.504320000000	17.496845000000
C	9.801644000000	9.561432000000	15.114818000000	C	3.932266000000	0.513658000000	19.722341000000
O	10.324785000000	9.906330000000	16.243608000000	C	4.831938000000	0.284085000000	20.960642000000
O	10.259294000000	8.586207000000	14.386065000000	C	3.683435000000	2.009849000000	19.456770000000
H	8.167001000000	11.752034000000	12.975962000000	C	6.276208000000	0.783626000000	20.786901000000
H	8.098033000000	10.816551000000	15.424154000000	H	2.039741000000	0.153442000000	20.746675000000
H	7.937792000000	9.668684000000	14.082015000000	H	4.439386000000	0.083978000000	18.847178000000
N	10.321344000000	12.675114000000	15.288618000000	H	4.853509000000	-0.792828000000	21.186109000000
C	10.961134000000	13.851296000000	15.868150000000	H	4.372759000000	0.773471000000	21.833579000000

H	6.873582000000	0.553769000000	21.677152000000	H	10.754721000000	1.932406000000	20.316958000000
H	6.754679000000	0.294567000000	19.928655000000	H	9.452566000000	2.795783000000	17.823387000000
H	6.329979000000	1.865141000000	20.622909000000	H	12.633360000000	2.495096000000	19.591753000000
H	3.068980000000	2.156006000000	18.560610000000	H	13.287795000000	3.755225000000	18.564369000000
H	4.621258000000	2.551397000000	19.302587000000	H	10.582693000000	4.308649000000	16.498566000000
H	3.165248000000	2.475614000000	20.306279000000	H	12.185899000000	4.746700000000	16.977483000000
N	0.408854000000	0.047339000000	18.816875000000	Fe	7.330398000000	6.157337000000	18.492928000000
C	-0.562900000000	-0.028938000000	17.717294000000	O	7.833854000000	4.497932000000	19.862595000000
C	-0.545818000000	1.205961000000	16.808332000000	O	9.038411000000	6.637351000000	18.194095000000
O	-1.476759000000	2.049960000000	16.822310000000	C	7.857906000000	5.301414000000	20.881120000000
H	0.074102000000	0.340855000000	19.723396000000	O	7.515028000000	6.541184000000	20.678703000000
H	-0.346660000000	-0.928205000000	17.131029000000	C	8.301517000000	4.830922000000	22.240432000000
N	0.546605000000	1.311752000000	16.007666000000	C	7.517086000000	5.476702000000	23.393682000000
C	0.739956000000	2.485555000000	15.155375000000	H	8.224918000000	3.738944000000	22.262058000000
C	2.016259000000	2.341496000000	14.309027000000	H	9.367226000000	5.080624000000	22.356846000000
C	2.498397000000	3.693536000000	13.813611000000	H	6.454061000000	5.210135000000	23.353927000000
O	2.728397000000	4.635341000000	14.621819000000	H	7.595770000000	6.566166000000	23.345785000000
N	2.689830000000	3.837561000000	12.479486000000	N	11.934004000000	7.896575000000	17.157825000000
H	1.298427000000	0.635926000000	16.146555000000	C	12.295619000000	7.773946000000	18.612040000000
H	0.811263000000	3.386005000000	15.773404000000	C	13.356553000000	6.662737000000	18.816884000000
H	1.858323000000	1.641667000000	13.481277000000	O	13.458545000000	5.746081000000	17.923117000000
H	2.823523000000	1.933169000000	14.931678000000	C	11.050621000000	7.492947000000	19.495861000000
H	2.500633000000	3.094759000000	11.825967000000	C	10.560793000000	8.580025000000	20.453031000000
H	3.015646000000	4.725030000000	12.122147000000	C	10.438977000000	10.011884000000	19.874819000000
C	-2.908582000000	6.222046000000	15.371903000000	N	9.529311000000	10.882842000000	20.642673000000
C	-1.720584000000	7.114373000000	15.703420000000	C	9.770865000000	11.357479000000	21.896340000000
O	-0.813933000000	7.328694000000	14.846813000000	N	10.891510000000	11.095634000000	22.575420000000
C	-2.494430000000	4.897463000000	14.709116000000	N	8.855788000000	12.141984000000	22.499875000000
H	-3.506832000000	6.031448000000	16.270470000000	O	14.005951000000	6.752652000000	19.911579000000
H	-2.014337000000	4.222162000000	15.425287000000	H	12.751034000000	8.721943000000	18.911529000000
H	-3.374337000000	4.382270000000	14.308842000000	H	10.069916000000	7.170010000000	18.780920000000
H	-1.802811000000	5.097399000000	13.884598000000	H	11.173760000000	6.554822000000	20.046583000000
N	-1.721347000000	7.671375000000	16.939306000000	H	11.248549000000	8.577384000000	21.311992000000
C	-0.664104000000	8.539173000000	17.461248000000	H	9.586177000000	8.262585000000	20.842610000000
C	-0.248475000000	7.989021000000	18.832325000000	H	10.031287000000	9.979644000000	18.859451000000
O	-1.059907000000	7.325723000000	19.541216000000	H	11.431749000000	10.480483000000	19.807551000000
C	-1.104041000000	10.038525000000	17.568519000000	H	8.803318000000	11.379804000000	20.122925000000
C	-1.358916000000	10.637933000000	16.173501000000	H	11.613251000000	10.431732000000	22.317535000000
C	-2.323237000000	10.233520000000	18.489868000000	H	10.949488000000	11.545314000000	23.507342000000
H	-2.390025000000	7.352197000000	17.629893000000	H	7.921848000000	12.289375000000	22.122449000000
H	0.183174000000	8.491678000000	16.773414000000	H	9.110971000000	12.457463000000	23.450344000000
H	-0.243392000000	10.558918000000	18.012242000000	H	12.749439000000	7.952364000000	16.524951000000
H	-0.491447000000	10.530086000000	15.514541000000	H	11.341372000000	8.748233000000	16.934305000000
H	-1.595786000000	11.705342000000	16.260873000000	H	11.391404000000	7.078503000000	16.799534000000
H	-2.214299000000	10.149149000000	15.690586000000	O	12.854679000000	8.190910000000	14.558716000000
H	-2.165674000000	9.806606000000	19.485679000000	H	11.854984000000	8.342757000000	14.425113000000
H	-2.538601000000	11.301873000000	18.606222000000	H	13.156164000000	7.406125000000	14.067915000000
H	-3.216054000000	9.763929000000	18.057637000000	O	10.105058000000	6.235243000000	15.794597000000
N	1.012112000000	8.287099000000	19.226357000000	H	9.526365000000	6.389467000000	16.597174000000
C	1.516702000000	7.923772000000	20.551688000000	H	10.003199000000	6.965315000000	15.131778000000
C	2.005091000000	6.454362000000	20.670979000000	H	10.289936000000	-0.504654000000	19.974291000000
C	3.179749000000	6.103900000000	19.809430000000	H	2.815113000000	-1.304434000000	20.120748000000
N	3.071605000000	5.551817000000	18.524040000000	H	-1.562761000000	-0.106138000000	18.143579000000
C	4.533105000000	6.249631000000	20.030558000000	H	-0.138554000000	2.615392000000	14.513920000000
C	4.332778000000	5.388630000000	18.026670000000	H	4.692793000000	-1.829187000000	16.359843000000
N	5.239237000000	5.803350000000	18.915287000000	H	6.288323000000	-2.599955000000	16.193182000000
H	1.631285000000	8.765709000000	18.565876000000	H	-4.633270000000	5.139843000000	18.599996000000
H	0.713076000000	8.075423000000	21.279435000000	H	-4.431208000000	5.387586000000	20.341106000000
H	1.156457000000	5.794008000000	20.463004000000	H	2.338643000000	8.604407000000	20.791614000000
H	2.280807000000	6.288384000000	21.720062000000	H	-3.543714000000	6.793166000000	14.679844000000
H	5.051187000000	6.650386000000	20.884241000000	H	6.431956000000	6.623148000000	12.869583000000
H	4.548870000000	5.000046000000	17.048541000000	H	3.451246000000	11.429359000000	17.909221000000
C	10.453669000000	0.152208000000	19.111174000000	H	6.337417000000	16.939586000000	20.178862000000
C	10.130230000000	1.608532000000	19.477684000000	H	9.748625000000	11.006535000000	12.835300000000
N	10.291373000000	2.532281000000	18.349359000000	H	15.124069000000	3.494341000000	20.819522000000
C	11.410014000000	3.216633000000	18.054781000000	H	10.817502000000	3.961667000000	25.331878000000
N	12.553386000000	3.077728000000	18.760491000000	H	14.964083000000	13.051488000000	14.270060000000
N	11.416838000000	4.078680000000	17.022908000000	H	10.589835000000	14.038703000000	16.880782000000
H	11.498588000000	0.049887000000	18.797489000000	H	9.244470000000	20.115710000000	23.629603000000
H	9.817622000000	-0.192669000000	18.288751000000	H	7.916378000000	5.144150000000	24.357452000000
H	9.090077000000	1.704636000000	19.801861000000	C	1.844300000000	5.176733000000	17.819677000000

H	2.109636000000	4.899023000000	16.798788000000	H	5.815935000000	12.100561000000	16.657072000000
H	1.354187000000	4.335154000000	18.319297000000	H	5.743199000000	8.103399000000	15.889598000000
H	1.156537000000	6.020068000000	17.786089000000	H	7.681318000000	8.813352000000	19.563640000000
⁵¹I_{C3} – ViOC WT – Intermediate							
C	11.219647000000	4.373719000000	25.283144000000	N	3.507464000000	9.519551000000	14.563291000000
C	11.393528000000	5.763818000000	24.690218000000	C	3.191841000000	8.203306000000	14.000886000000
O	11.275342000000	5.984152000000	23.458040000000	C	4.531975000000	7.702887000000	13.429508000000
C	12.523736000000	3.550499000000	25.463836000000	O	5.327757000000	8.527635000000	12.899491000000
O	13.187246000000	3.317442000000	24.192927000000	C	2.046259000000	8.289014000000	12.952405000000
C	12.226156000000	2.188343000000	26.090859000000	O	0.854061000000	8.837152000000	13.562948000000
H	10.720076000000	4.443425000000	26.258985000000	C	1.758480000000	6.939656000000	12.284598000000
H	13.212633000000	4.111844000000	26.111456000000	H	4.142044000000	10.068716000000	13.992814000000
H	13.918624000000	3.993915000000	24.058718000000	H	2.860859000000	7.564804000000	14.825594000000
H	13.156330000000	1.625747000000	26.211661000000	H	2.339987000000	9.025275000000	12.197022000000
H	11.746472000000	2.293919000000	27.070905000000	H	0.374039000000	8.162410000000	14.104450000000
H	11.561651000000	1.611927000000	25.437160000000	H	0.906353000000	7.048998000000	11.607113000000
N	11.689945000000	6.783280000000	25.559335000000	H	2.618311000000	6.583718000000	11.707106000000
C	11.703365000000	8.191437000000	25.115756000000	H	1.509094000000	6.177158000000	13.033100000000
C	12.908192000000	8.485416000000	24.206439000000	N	4.846136000000	6.400012000000	13.609850000000
O	12.840979000000	9.345169000000	23.289043000000	C	6.225212000000	5.927379000000	13.395308000000
C	11.652840000000	9.152493000000	26.328557000000	C	6.341102000000	4.410681000000	13.615142000000
C	10.468716000000	8.924870000000	27.306167000000	C	7.717450000000	3.982606000000	14.150185000000
C	10.534001000000	9.964995000000	28.445232000000	C	7.890254000000	4.094104000000	15.666465000000
C	9.103792000000	8.992924000000	26.592529000000	O	8.769770000000	3.389342000000	16.223085000000
H	11.653246000000	6.611680000000	26.554580000000	O	7.093971000000	4.941515000000	16.301988000000
H	10.827264000000	8.358483000000	24.481991000000	H	4.172018000000	5.747454000000	14.005388000000
H	12.601515000000	9.084017000000	26.881459000000	H	6.877179000000	6.451073000000	14.103007000000
H	11.576149000000	10.172077000000	25.935011000000	H	6.140639000000	3.884929000000	12.670815000000
H	10.577602000000	7.922756000000	27.764183000000	H	5.581864000000	4.089542000000	14.333568000000
H	8.982039000000	8.189914000000	25.853161000000	H	7.935186000000	2.942783000000	13.887706000000
H	9.000635000000	9.961908000000	26.088061000000	H	8.518637000000	4.583414000000	13.693716000000
H	8.290767000000	8.893570000000	27.322388000000	C	6.613989000000	-1.910829000000	15.202923000000
H	11.519766000000	9.964295000000	28.930294000000	C	7.205872000000	-0.606927000000	15.771834000000
H	10.327198000000	10.973282000000	28.062833000000	C	8.338791000000	-0.068351000000	14.876563000000
H	9.783330000000	9.735726000000	29.212182000000	C	6.112349000000	0.459856000000	15.977154000000
N	14.043566000000	7.784625000000	24.455750000000	H	6.170371000000	-1.734109000000	14.212810000000
C	15.108695000000	7.638114000000	23.449767000000	H	7.637119000000	-0.834471000000	16.759629000000
C	15.064879000000	6.156361000000	23.070539000000	H	9.147482000000	-0.802746000000	14.774030000000
O	14.920764000000	5.286278000000	24.003493000000	H	7.959592000000	0.148592000000	13.867336000000
C	16.499974000000	8.133418000000	23.935964000000	H	8.761473000000	0.856833000000	15.285060000000
C	16.483964000000	9.665205000000	24.096535000000	H	6.532555000000	1.367004000000	16.425260000000
C	16.972904000000	7.442477000000	25.229376000000	H	5.313509000000	0.088352000000	16.632403000000
H	13.993868000000	7.025948000000	25.125616000000	H	5.659092000000	0.736091000000	15.013386000000
H	14.809195000000	8.237407000000	22.584640000000	C	-3.936362000000	6.167212000000	19.880179000000
H	17.203899000000	7.877047000000	23.129044000000	C	-3.654610000000	4.735083000000	20.366442000000
H	16.968966000000	6.352567000000	25.135368000000	C	-2.822866000000	4.663571000000	21.671324000000
H	17.989645000000	7.768169000000	25.479262000000	C	-2.881960000000	3.248652000000	22.281503000000
H	16.323322000000	7.713931000000	26.070950000000	C	-1.361322000000	5.100835000000	21.444516000000
H	17.473795000000	10.031664000000	24.393209000000	H	-3.011225000000	6.717659000000	19.677979000000
H	15.765237000000	9.963613000000	24.868189000000	H	-4.612223000000	4.217422000000	20.529685000000
H	16.198450000000	10.162474000000	23.163226000000	H	-3.122885000000	4.177844000000	19.580124000000
N	15.093659000000	5.844818000000	21.773775000000	H	-3.278238000000	5.357134000000	22.397270000000
C	14.744457000000	4.492091000000	21.328326000000	H	-2.307069000000	3.193259000000	23.214412000000
C	13.207413000000	4.321691000000	21.325605000000	H	-3.914085000000	2.948211000000	22.500840000000
O	12.831483000000	2.916786000000	21.494257000000	H	-2.463627000000	2.506271000000	21.585861000000
H	15.061696000000	6.587567000000	21.037423000000	H	-1.289511000000	6.125543000000	21.066728000000
H	15.195037000000	3.758050000000	22.001931000000	H	-0.787682000000	5.039738000000	22.378822000000
H	12.750068000000	4.912078000000	22.121033000000	H	-0.882799000000	4.446471000000	20.701059000000
H	12.798596000000	4.655906000000	20.371972000000	C	8.502774000000	10.384933000000	13.303885000000
H	12.810291000000	2.742197000000	22.472071000000	C	8.349293000000	11.677090000000	14.108644000000
C	3.885817000000	11.179602000000	16.314965000000	O	7.582242000000	12.582290000000	13.686561000000
C	3.245347000000	9.885956000000	15.837923000000	C	8.747815000000	9.047370000000	14.052212000000
O	2.542506000000	9.166045000000	16.604804000000	C	10.148353000000	8.831895000000	14.600428000000
C	5.441999000000	11.158767000000	16.242109000000	O	10.493402000000	9.445298000000	15.685862000000
C	6.068204000000	10.016355000000	16.986854000000	O	10.941647000000	8.018347000000	13.972504000000
N	6.722383000000	10.190157000000	18.202023000000	H	7.575418000000	10.279097000000	12.734369000000
C	6.131066000000	8.659882000000	16.723439000000	H	8.037161000000	8.960362000000	14.880142000000
C	7.157558000000	8.983233000000	18.639804000000	H	8.545137000000	8.240026000000	13.344907000000
N	6.815397000000	8.029807000000	17.758314000000	N	9.110553000000	11.816059000000	15.233019000000
H	3.516732000000	12.018770000000	15.710860000000	C	9.211218000000	13.078385000000	15.960934000000
H	5.764276000000	11.154907000000	15.194750000000	C	10.633696000000	13.644081000000	16.018438000000

O	10.883925000000	14.659454000000	16.717878000000	H	6.849691000000	0.196493000000	19.729651000000
H	9.614547000000	10.998914000000	15.594809000000	H	6.834085000000	1.839129000000	20.389146000000
H	8.565455000000	13.803280000000	15.455865000000	H	3.264356000000	2.562142000000	19.102895000000
N	11.573332000000	12.986798000000	15.294875000000	H	4.995929000000	2.709882000000	19.404074000000
C	12.990276000000	13.327968000000	15.279393000000	H	3.853915000000	2.945877000000	20.729719000000
C	13.806873000000	12.038172000000	15.245634000000	N	0.584134000000	1.217621000000	19.996048000000
O	13.355010000000	11.279651000000	14.098965000000	C	-0.568948000000	1.338330000000	19.094525000000
H	11.318337000000	12.191665000000	14.723708000000	C	-0.296724000000	2.270452000000	17.908506000000
H	13.215444000000	13.925079000000	16.167483000000	O	-0.851096000000	3.406884000000	17.840228000000
H	13.647954000000	11.479208000000	16.180234000000	H	0.589789000000	1.773938000000	20.838511000000
H	14.878301000000	12.278269000000	15.168498000000	H	-0.829824000000	0.338433000000	18.732083000000
H	13.482421000000	10.300632000000	14.223673000000	N	0.565128000000	1.787315000000	16.989291000000
C	6.361373000000	15.783202000000	20.378447000000	C	0.999763000000	2.552009000000	15.814578000000
C	6.317688000000	16.001914000000	21.889670000000	C	2.321414000000	1.987584000000	15.274361000000
O	6.568492000000	17.131008000000	22.399385000000	C	2.947020000000	2.941705000000	14.271505000000
C	7.407999000000	14.784398000000	19.828976000000	O	3.064930000000	4.169826000000	14.522509000000
C	7.077204000000	13.301749000000	19.950788000000	N	3.389522000000	2.398623000000	13.107497000000
O	7.674725000000	12.502199000000	19.112414000000	H	1.000313000000	0.886645000000	17.204805000000
O	6.304702000000	12.869820000000	20.881069000000	H	1.141225000000	3.599620000000	16.091066000000
H	5.361058000000	15.476794000000	20.044177000000	H	2.178528000000	0.991752000000	14.838524000000
H	7.580553000000	14.992380000000	18.768472000000	H	3.032748000000	1.879490000000	16.104344000000
H	8.381483000000	14.951289000000	20.311466000000	H	3.309008000000	1.414098000000	12.909877000000
N	5.953881000000	14.930860000000	22.647338000000	H	3.855843000000	2.989127000000	12.434092000000
C	5.619997000000	15.062202000000	24.062354000000	C	-3.084549000000	6.658575000000	15.588058000000
C	6.778071000000	15.388915000000	25.013336000000	C	-1.747023000000	7.321484000000	15.867031000000
O	6.536434000000	15.859062000000	26.146850000000	O	-0.730628000000	7.061325000000	15.136660000000
H	5.858381000000	14.035559000000	22.151376000000	C	-2.934559000000	5.176806000000	15.206345000000
H	4.888098000000	15.863344000000	24.207756000000	H	-3.748450000000	6.771412000000	16.453526000000
H	5.162376000000	14.123266000000	24.390377000000	H	-2.509800000000	4.594332000000	16.031189000000
N	8.027949000000	15.126357000000	24.541039000000	H	-3.909900000000	4.749714000000	14.950580000000
C	9.256836000000	15.433120000000	25.273500000000	H	-2.271790000000	5.078568000000	14.341876000000
C	9.864453000000	16.791515000000	24.862019000000	N	-1.691338000000	8.177416000000	16.904042000000
O	11.017569000000	17.108023000000	25.259791000000	C	-0.482435000000	8.904737000000	17.306309000000
C	10.293840000000	14.307318000000	25.091265000000	C	-0.083543000000	8.445973000000	18.715719000000
C	9.876794000000	13.010917000000	25.807738000000	O	-0.956128000000	8.051481000000	19.540812000000
O	9.809402000000	13.020024000000	27.066158000000	C	-0.682282000000	10.453059000000	17.234857000000
O	9.620923000000	11.967321000000	25.043111000000	C	-0.918654000000	10.906781000000	15.781993000000
H	8.113795000000	14.720521000000	23.618522000000	C	-1.797130000000	10.958869000000	18.170995000000
H	8.994045000000	15.496133000000	26.335628000000	H	-2.461400000000	8.208503000000	17.560269000000
H	10.458227000000	14.118673000000	24.023449000000	H	0.309231000000	8.640039000000	16.604681000000
H	11.232822000000	14.665913000000	25.522880000000	H	0.273081000000	10.876257000000	17.574670000000
N	9.106900000000	17.596079000000	24.070820000000	H	-0.140504000000	10.536243000000	15.105942000000
C	9.588349000000	18.891065000000	23.591964000000	H	-0.935179000000	12.001949000000	15.726209000000
C	9.519330000000	19.014359000000	22.058773000000	H	-1.886574000000	10.544084000000	15.412774000000
C	10.323116000000	17.995571000000	21.262299000000	H	-1.655094000000	10.622589000000	19.202805000000
C	11.467708000000	17.357344000000	21.771297000000	H	-1.822133000000	12.054526000000	18.166375000000
C	9.912968000000	17.681368000000	19.952128000000	H	-2.783125000000	10.611885000000	17.833682000000
C	12.174136000000	16.432449000000	20.989159000000	N	1.234206000000	8.552535000000	18.996178000000
C	10.613594000000	16.757299000000	19.169923000000	C	1.793219000000	8.202362000000	20.299945000000
C	11.750970000000	16.127149000000	19.691423000000	C	2.212751000000	6.712290000000	20.414713000000
H	8.189175000000	17.297984000000	23.751097000000	C	3.306216000000	6.285663000000	19.482601000000
H	10.607515000000	19.007971000000	23.967763000000	N	3.065171000000	5.796769000000	18.198615000000
H	8.467470000000	18.939590000000	21.754190000000	C	4.677813000000	6.273489000000	19.633019000000
H	9.848582000000	20.032934000000	21.795765000000	C	4.258822000000	5.506236000000	17.618000000000
H	11.795993000000	17.546918000000	22.788305000000	N	5.264252000000	5.787217000000	18.463551000000
H	9.025496000000	18.164990000000	19.549062000000	H	1.868392000000	8.827856000000	18.240940000000
H	13.048421000000	15.941162000000	21.407309000000	H	1.036849000000	8.412624000000	21.061619000000
H	10.281749000000	16.494617000000	18.171428000000	H	1.320883000000	6.095332000000	20.255952000000
H	12.277232000000	15.400488000000	19.081870000000	H	2.541731000000	6.541802000000	21.447727000000
C	2.762406000000	0.341269000000	20.729747000000	H	5.282840000000	6.590500000000	20.464340000000
C	1.654546000000	0.422118000000	19.702730000000	H	4.369058000000	5.115938000000	16.622404000000
O	1.715176000000	-0.206509000000	18.607071000000	H	2.126839000000	5.718897000000	17.742612000000
C	4.123195000000	0.848545000000	20.174270000000	C	10.512712000000	0.317441000000	18.575334000000
C	5.252916000000	0.529524000000	21.181658000000	C	10.290545000000	1.764750000000	19.036556000000
C	4.056311000000	2.348197000000	19.830580000000	N	10.790374000000	2.763328000000	18.077511000000
C	6.668496000000	0.785677000000	20.637985000000	C	12.071446000000	3.142406000000	17.964302000000
H	2.500387000000	0.902197000000	21.636797000000	N	13.020952000000	2.624663000000	18.789203000000
H	4.318050000000	0.282897000000	19.250977000000	N	12.456511000000	4.033506000000	17.034162000000
H	5.169809000000	-0.526011000000	21.481238000000	H	11.579454000000	0.103175000000	18.452103000000
H	5.094977000000	1.124256000000	22.094717000000	H	10.013261000000	0.137560000000	17.617359000000
H	7.423781000000	0.495742000000	21.378085000000	H	9.225767000000	1.981888000000	19.148904000000

H	10.752309000000	1.937130000000	20.015712000000
H	10.083665000000	3.193097000000	17.471591000000
H	12.821341000000	2.363879000000	19.761289000000
H	13.972048000000	2.907001000000	18.605431000000
H	11.782500000000	4.478159000000	16.393293000000
H	13.232102000000	4.655961000000	17.279547000000
Fe	7.347833000000	5.973205000000	17.969350000000
O	7.870338000000	4.368483000000	19.389131000000
O	9.122238000000	6.466423000000	17.479969000000
C	8.018012000000	5.223639000000	20.355651000000
O	7.752686000000	6.470152000000	20.090562000000
C	8.486503000000	4.804320000000	21.720441000000
C	7.707787000000	5.491316000000	22.855946000000
H	8.415322000000	3.714041000000	21.785292000000
H	9.549282000000	5.068570000000	21.818866000000
H	6.644122000000	5.225172000000	22.830621000000
H	7.790569000000	6.578108000000	22.772100000000
N	12.479921000000	8.023856000000	16.913809000000
C	12.752550000000	8.210449000000	18.390118000000
C	13.885484000000	7.229749000000	18.842364000000
O	13.981222000000	6.111933000000	18.226182000000
C	11.500057000000	7.926904000000	19.170450000000
C	10.966690000000	8.773013000000	20.288824000000
C	10.811658000000	10.290183000000	19.953716000000
N	9.674962000000	10.934772000000	20.629634000000
C	9.640085000000	11.242248000000	21.953408000000
N	10.647809000000	10.978857000000	22.787444000000
N	8.554335000000	11.854430000000	22.474141000000
O	14.562263000000	7.636368000000	19.848928000000
H	13.108545000000	9.232077000000	18.538477000000
H	9.421237000000	7.341862000000	17.796493000000
H	11.115293000000	6.912670000000	19.078638000000
H	11.607715000000	8.661112000000	21.179442000000
H	9.984114000000	8.377598000000	20.572338000000
H	10.621548000000	10.409350000000	18.883060000000
H	11.741425000000	10.828536000000	20.181755000000
H	8.974665000000	11.392265000000	20.038563000000
H	11.479575000000	10.436066000000	22.582194000000
H	10.502227000000	11.302980000000	23.764895000000
H	7.703227000000	12.016042000000	21.940531000000
H	8.599782000000	12.040093000000	23.486113000000
H	13.301180000000	8.165068000000	16.302276000000
H	11.745358000000	8.692169000000	16.552463000000
H	12.110688000000	7.069012000000	16.696417000000
O	0.661136000000	5.572267000000	17.060571000000
H	0.003191000000	4.898043000000	17.358773000000
H	0.336302000000	6.086254000000	16.286211000000
O	13.466527000000	8.564703000000	14.384929000000
H	12.495274000000	8.325054000000	14.163259000000
H	14.086018000000	8.115348000000	13.783654000000
O	10.980637000000	5.901192000000	15.790499000000
H	10.167894000000	6.039698000000	16.390147000000
H	10.912139000000	6.414534000000	14.951625000000
H	10.105704000000	-0.382636000000	19.315195000000
H	2.864257000000	-0.713940000000	21.013912000000
H	-1.407956000000	1.750665000000	19.653257000000
H	0.224338000000	2.516897000000	15.037060000000
H	5.828985000000	-2.311773000000	15.856250000000
H	7.386242000000	-2.681364000000	15.088360000000
H	-4.539635000000	6.151878000000	18.962129000000
H	-4.501055000000	6.731300000000	20.634273000000
H	2.660888000000	8.844465000000	20.481261000000
H	-3.550136000000	7.256065000000	14.756065000000
H	6.553079000000	6.210935000000	12.389123000000
H	3.559736000000	11.336326000000	17.346002000000
H	6.568522000000	16.767153000000	19.950799000000
H	9.308109000000	10.548297000000	12.572642000000
H	15.154657000000	4.358092000000	20.324655000000
H	10.563694000000	3.819881000000	24.604914000000
H	13.230990000000	13.931594000000	14.393801000000
H	8.855372000000	12.975154000000	16.993948000000

H	8.982925000000	19.694684000000	24.033779000000
H	8.111847000000	5.191579000000	23.828074000000

⁵TS_{reb,C3} – VioC WT transition state for radical rebound

C	11.411642000000	4.295749000000	25.232809000000
C	11.534572000000	5.683609000000	24.623899000000
O	11.408698000000	5.886585000000	23.388793000000
C	12.744326000000	3.521414000000	25.423038000000
O	13.407774000000	3.282935000000	24.152833000000
C	12.496267000000	2.163036000000	26.078827000000
H	10.910340000000	4.360209000000	26.208029000000
H	13.416994000000	4.118928000000	26.055353000000
H	14.105429000000	3.986662000000	23.992041000000
H	13.445445000000	1.634217000000	26.204061000000
H	12.019655000000	2.272086000000	27.059910000000
H	11.847164000000	1.552027000000	25.441310000000
N	11.792909000000	6.724270000000	25.477339000000
C	11.750632000000	8.124782000000	25.011495000000
C	12.893080000000	8.418835000000	24.025790000000
O	12.735882000000	9.201849000000	23.052566000000
C	11.759093000000	9.096824000000	26.216148000000
C	10.616545000000	8.880898000000	27.244275000000
C	10.755636000000	9.906257000000	28.389626000000
C	9.223040000000	8.983969000000	26.592161000000
H	11.769635000000	6.567082000000	26.475318000000
H	10.834375000000	8.268728000000	24.431144000000
H	12.730927000000	9.025663000000	26.726751000000
H	11.673585000000	10.115851000000	25.822668000000
H	10.724027000000	7.871021000000	27.685509000000
H	9.049756000000	8.187378000000	25.856099000000
H	9.114170000000	9.956108000000	26.094610000000
H	8.441484000000	8.899052000000	27.357160000000
H	11.756417000000	9.866246000000	28.841365000000
H	10.573036000000	10.922854000000	28.017088000000
H	10.022930000000	9.695606000000	29.178924000000
N	14.079549000000	7.807586000000	24.274353000000
C	15.117375000000	7.667649000000	23.240320000000
C	15.131244000000	6.173335000000	22.913578000000
O	15.061584000000	5.329650000000	23.876847000000
C	16.500060000000	8.237631000000	23.668521000000
C	16.427284000000	9.773044000000	23.765592000000
C	17.030544000000	7.621213000000	24.977195000000
H	14.102005000000	7.092863000000	24.991956000000
H	14.765086000000	8.223262000000	22.366074000000
H	17.194227000000	7.973987000000	22.855515000000
H	17.067200000000	6.528979000000	24.929000000000
H	18.039180000000	7.996451000000	25.186454000000
H	16.391663000000	7.904232000000	25.823076000000
H	17.406638000000	10.188644000000	24.030326000000
H	15.709823000000	10.076652000000	24.536296000000
H	16.109646000000	10.220170000000	22.817306000000
N	15.136741000000	5.817561000000	21.625934000000
C	14.839897000000	4.433151000000	21.242437000000
C	13.312218000000	4.209652000000	21.275096000000
O	12.990428000000	2.793079000000	21.449800000000
H	15.007385000000	6.525264000000	20.873304000000
H	15.331495000000	3.750071000000	21.939847000000
H	12.853746000000	4.784945000000	22.080099000000
H	12.871741000000	4.529398000000	20.331291000000
H	13.004329000000	2.619533000000	22.426491000000
C	3.756735000000	11.248339000000	16.143962000000
C	3.155693000000	9.918045000000	15.714512000000
O	2.462526000000	9.213592000000	16.502234000000
C	5.314416000000	11.257427000000	16.099098000000
C	5.950711000000	10.178133000000	16.923349000000
N	6.538371000000	10.423654000000	18.159851000000
C	6.082042000000	8.817124000000	16.714015000000
C	7.000367000000	9.249116000000	18.658409000000
N	6.746391000000	8.253006000000	17.798117000000
H	3.377590000000	12.050277000000	15.496729000000

H	5.651169000000	11.174196000000	15.058465000000	C	10.858840000000	13.673131000000	16.250962000000
H	5.664262000000	12.234004000000	16.450947000000	O	11.166726000000	14.638692000000	16.995374000000
H	5.760103000000	8.216950000000	15.882249000000	H	9.407325000000	11.155738000000	15.700659000000
H	7.493347000000	9.137468000000	19.607078000000	H	8.873687000000	14.088346000000	15.575181000000
H	6.778334000000	11.354616000000	18.579186000000	N	11.767723000000	12.936436000000	15.567507000000
N	3.442667000000	9.510732000000	14.457602000000	C	13.207365000000	13.156326000000	15.604888000000
C	3.185425000000	8.163160000000	13.941666000000	C	13.908147000000	11.805988000000	15.477427000000
C	4.558425000000	7.689318000000	13.425406000000	O	13.390710000000	11.173550000000	14.281612000000
O	5.346185000000	8.530163000000	12.905578000000	H	11.464774000000	12.201979000000	14.941408000000
C	2.067821000000	8.172492000000	12.859436000000	H	13.464522000000	13.657480000000	16.542315000000
O	0.846420000000	8.716872000000	13.411865000000	H	13.700053000000	11.197210000000	16.370653000000
C	1.833381000000	6.789066000000	12.242887000000	H	14.996219000000	11.953834000000	15.410861000000
H	4.076755000000	10.050024000000	13.877740000000	H	13.417816000000	10.181433000000	14.338560000000
H	2.854072000000	7.545829000000	14.782040000000	C	6.389505000000	15.935076000000	20.495949000000
H	2.365559000000	8.882726000000	12.080721000000	C	6.381229000000	16.105765000000	22.014069000000
H	0.367474000000	8.053447000000	13.968372000000	O	6.662175000000	17.214004000000	22.553144000000
H	0.998631000000	6.847507000000	11.537964000000	C	7.407219000000	14.937754000000	19.891468000000
H	2.718157000000	6.432199000000	11.705134000000	C	7.050845000000	13.457799000000	19.972245000000
H	1.582898000000	6.051476000000	13.015199000000	O	7.612984000000	12.672232000000	19.099223000000
N	4.904834000000	6.401263000000	13.639486000000	O	6.282576000000	13.014742000000	20.902122000000
C	6.305204000000	5.964707000000	13.484523000000	H	5.377571000000	15.654580000000	20.174264000000
C	6.450258000000	4.454262000000	13.726242000000	H	7.557291000000	15.176799000000	18.833870000000
C	7.821498000000	4.055267000000	14.305350000000	H	8.394441000000	15.072389000000	20.355774000000
C	7.925143000000	4.166238000000	15.828253000000	N	6.015399000000	15.017001000000	22.744752000000
O	8.581628000000	3.277920000000	16.445238000000	C	5.712287000000	15.105843000000	24.170610000000
O	7.328787000000	5.191061000000	16.390687000000	C	6.894429000000	15.377832000000	25.108702000000
H	4.234655000000	5.734446000000	14.018340000000	O	6.683058000000	15.798106000000	26.267848000000
H	6.913616000000	6.508441000000	14.214568000000	H	5.891532000000	14.141022000000	22.220740000000
H	6.286577000000	3.914859000000	12.782037000000	H	4.998624000000	15.914798000000	24.357477000000
H	5.674326000000	4.122371000000	14.422797000000	H	5.243146000000	14.164933000000	24.475118000000
H	8.067029000000	3.022481000000	14.044614000000	N	8.130277000000	15.127052000000	25.127020000000
H	8.619574000000	4.684663000000	13.886462000000	C	9.379517000000	15.396134000000	25.307590000000
C	6.724066000000	-1.965330000000	15.380035000000	C	9.977589000000	16.775165000000	24.950958000000
C	7.290681000000	-0.640679000000	15.926137000000	O	11.131937000000	17.078299000000	25.354772000000
C	8.434062000000	-0.108989000000	15.040008000000	C	10.412561000000	14.283666000000	25.031881000000
C	6.183965000000	0.420141000000	16.085819000000	C	10.035404000000	12.951947000000	25.702844000000
H	6.296571000000	-1.818343000000	14.378009000000	O	10.159608000000	12.864624000000	26.954990000000
H	7.705798000000	-0.839169000000	16.927396000000	O	9.608740000000	11.986411000000	24.915129000000
H	9.257738000000	-0.831339000000	14.976984000000	H	8.189903000000	14.754906000000	23.657992000000
H	8.073363000000	0.071566000000	14.016870000000	H	9.149754000000	15.407861000000	26.379008000000
H	8.825892000000	0.836305000000	15.431792000000	H	10.529119000000	14.146852000000	23.949560000000
H	6.594991000000	1.346431000000	16.501491000000	H	11.366012000000	14.626931000000	25.441854000000
H	5.382449000000	0.062455000000	16.745721000000	N	9.211888000000	17.608427000000	24.198704000000
H	5.737512000000	0.657831000000	15.108571000000	C	9.690394000000	18.918723000000	23.760686000000
C	-3.960290000000	6.054673000000	19.782571000000	C	9.642421000000	19.080083000000	22.229491000000
C	-3.645614000000	4.639519000000	20.297695000000	C	10.448010000000	18.070515000000	21.423476000000
C	-2.821677000000	4.613877000000	21.609356000000	C	11.603093000000	17.443371000000	21.922752000000
C	-2.856469000000	3.212648000000	22.252281000000	C	10.029063000000	17.750904000000	20.117615000000
C	-1.367719000000	5.075718000000	21.382775000000	C	12.310863000000	16.523799000000	21.135948000000
H	-3.047597000000	6.623603000000	19.575730000000	C	10.731817000000	16.831853000000	19.331301000000
H	-4.590512000000	4.099937000000	20.463782000000	C	11.879323000000	16.212086000000	19.842489000000
H	-3.094048000000	4.083763000000	19.524071000000	H	8.292280000000	17.321472000000	23.873767000000
H	-3.296163000000	5.314463000000	22.316031000000	H	10.703799000000	19.032219000000	24.152665000000
H	-2.289001000000	3.191514000000	23.191163000000	H	8.594083000000	19.021629000000	21.909974000000
H	-3.883846000000	2.895380000000	22.470104000000	H	9.984089000000	20.101638000000	21.995279000000
H	-2.416213000000	2.462409000000	21.578789000000	H	11.936521000000	17.634975000000	22.937607000000
H	-1.313359000000	6.091456000000	20.978925000000	H	9.133555000000	18.225590000000	19.721787000000
H	-0.800004000000	5.050058000000	22.322234000000	H	13.192901000000	16.040812000000	21.547471000000
H	-0.869245000000	4.413583000000	20.659252000000	H	10.394494000000	16.564840000000	18.335913000000
C	8.726990000000	10.817978000000	13.180586000000	H	12.403548000000	15.488504000000	19.228167000000
C	8.745353000000	12.118403000000	13.984364000000	C	2.665771000000	0.432536000000	20.817118000000
O	8.406961000000	13.193855000000	13.432106000000	C	1.587376000000	0.468065000000	19.756767000000
C	8.535720000000	9.478566000000	13.939736000000	O	1.685933000000	-0.194709000000	18.684511000000
C	9.786645000000	8.974533000000	14.634244000000	C	4.034318000000	0.939232000000	20.280137000000
O	10.010785000000	9.350173000000	15.858792000000	C	5.140359000000	0.668110000000	21.326665000000
O	10.588418000000	8.194080000000	13.982499000000	C	3.958585000000	2.425904000000	19.885250000000
H	7.912916000000	10.928330000000	12.458434000000	C	6.565513000000	0.947474000000	20.821177000000
H	7.736261000000	9.577987000000	14.677692000000	H	2.372766000000	1.019654000000	21.697662000000
H	8.224723000000	8.726893000000	13.210824000000	H	4.259340000000	0.346185000000	19.381243000000
N	9.190974000000	12.059920000000	15.278550000000	H	5.073264000000	-0.383020000000	21.644930000000
C	9.391085000000	13.266398000000	16.078735000000	H	4.941365000000	1.276806000000	22.222203000000

H	7.304834000000	0.680287000000	21.585438000000	H	9.164140000000	1.605996000000	19.528675000000
H	6.784072000000	0.355041000000	19.923345000000	H	10.771203000000	1.765310000000	20.217051000000
H	6.716323000000	2.002333000000	20.568507000000	H	9.707390000000	2.890119000000	17.738915000000
H	3.168684000000	2.610507000000	19.147603000000	H	12.747517000000	2.314287000000	19.690451000000
H	4.897126000000	2.777705000000	19.448070000000	H	13.685582000000	3.052453000000	18.454741000000
H	3.749813000000	3.053769000000	20.761809000000	H	11.145429000000	4.241199000000	16.418866000000
N	0.503461000000	1.264855000000	19.990732000000	H	12.654331000000	4.596946000000	17.153106000000
C	-0.610945000000	1.357768000000	19.039096000000	Fe	7.458843000000	6.246702000000	18.114733000000
C	-0.289469000000	2.267840000000	17.848352000000	O	8.169539000000	4.735173000000	19.485281000000
O	-0.827223000000	3.409559000000	17.746833000000	O	9.224904000000	7.036760000000	17.627891000000
H	0.477289000000	1.849658000000	20.813406000000	C	8.066337000000	5.511680000000	20.524676000000
H	-0.848959000000	0.348633000000	18.687308000000	O	7.638373000000	6.722693000000	20.336743000000
N	0.597549000000	1.761112000000	16.965901000000	C	8.461465000000	5.019938000000	21.892083000000
C	1.080359000000	2.498745000000	15.792336000000	C	7.689413000000	5.694597000000	23.034734000000
C	2.453486000000	1.965792000000	15.358935000000	H	8.333732000000	3.931699000000	21.905633000000
C	3.094884000000	2.887301000000	14.335741000000	H	9.537022000000	5.209945000000	22.026097000000
O	3.146738000000	4.131905000000	14.516324000000	H	6.614998000000	5.484617000000	22.971050000000
N	3.624837000000	2.296296000000	13.232720000000	H	7.820068000000	6.779470000000	22.998452000000
H	1.016459000000	0.860865000000	17.211306000000	N	12.075083000000	7.868410000000	16.885144000000
H	1.168092000000	3.559344000000	16.038817000000	C	12.336511000000	7.982288000000	18.363897000000
H	2.377804000000	0.941304000000	14.975721000000	C	13.528578000000	7.035135000000	18.744695000000
H	3.119797000000	1.937610000000	16.231488000000	O	13.591749000000	5.912262000000	18.131305000000
H	3.607143000000	1.298055000000	13.098422000000	C	11.116640000000	7.603033000000	19.168714000000
H	4.110914000000	2.865285000000	12.554791000000	C	10.499556000000	8.503035000000	20.193069000000
C	-3.054293000000	6.485582000000	15.443846000000	C	10.515995000000	10.023203000000	19.865753000000
C	-1.738631000000	7.186653000000	15.733401000000	N	9.469951000000	10.795487000000	20.555415000000
O	-0.709123000000	6.956006000000	15.012212000000	C	9.491731000000	11.122094000000	21.878357000000
C	-2.859125000000	5.010591000000	15.057172000000	N	10.487695000000	10.774854000000	22.695597000000
H	-3.725821000000	6.575064000000	16.306255000000	N	8.478981000000	11.836774000000	22.406602000000
H	-2.420880000000	4.439546000000	15.882746000000	O	14.286752000000	7.477193000000	19.670126000000
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H	-2.189904000000	4.934782000000	14.195424000000	H	9.161557000000	7.968546000000	17.322529000000
N	-1.717229000000	8.045975000000	16.769261000000	H	10.918271000000	6.542014000000	19.258256000000
C	-0.535197000000	8.812800000000	17.177794000000	H	11.018972000000	8.328957000000	21.154132000000
C	-0.142083000000	8.382140000000	18.597514000000	H	9.468981000000	8.168132000000	20.358452000000
O	-1.015771000000	7.972881000000	19.414736000000	H	10.330199000000	10.169202000000	18.797135000000
C	-0.779130000000	10.353373000000	17.082807000000	H	11.504015000000	10.450280000000	20.085303000000
C	-1.009445000000	10.779428000000	15.620593000000	H	8.825757000000	11.340529000000	19.975671000000
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H	-2.491739000000	8.054017000000	17.420995000000	H	10.396340000000	11.127337000000	23.667535000000
H	0.273132000000	8.562840000000	16.490341000000	H	7.628466000000	12.053435000000	21.890134000000
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H	-1.784277000000	10.518549000000	19.034292000000	O	0.734690000000	5.552585000000	16.975703000000
H	-1.977754000000	11.932825000000	17.978192000000	H	0.073066000000	4.888007000000	17.286918000000
H	-2.892077000000	10.458922000000	17.650007000000	H	0.405942000000	6.043567000000	16.188565000000
N	1.167806000000	8.526036000000	18.895544000000	O	13.153464000000	8.469440000000	14.425279000000
C	1.717588000000	8.187921000000	20.207090000000	H	12.169233000000	8.345863000000	14.183200000000
C	2.173778000000	6.708823000000	20.325312000000	H	13.730394000000	7.942933000000	13.844919000000
C	3.315940000000	6.321035000000	19.435365000000	O	10.530186000000	5.877623000000	15.668002000000
N	3.145278000000	5.832779000000	18.139765000000	H	9.899409000000	6.231633000000	16.380592000000
C	4.680022000000	6.354701000000	19.642928000000	H	10.488778000000	6.444978000000	14.864039000000
C	4.376514000000	5.590556000000	17.610162000000	H	10.314179000000	-0.635959000000	19.667365000000
N	5.334969000000	5.900193000000	18.496849000000	H	2.772693000000	-0.611468000000	21.138147000000
H	1.804032000000	8.815422000000	18.148892000000	H	-1.475900000000	1.775971000000	19.551960000000
H	0.944088000000	8.377957000000	20.956782000000	H	0.359098000000	2.406255000000	14.968689000000
H	1.305431000000	6.069543000000	20.128702000000	H	5.931590000000	-2.359160000000	16.028860000000
H	2.467551000000	6.539723000000	21.369260000000	H	7.506748000000	-2.729663000000	15.298453000000
H	5.240151000000	6.686692000000	20.499669000000	H	-4.556338000000	6.006714000000	18.860998000000
H	4.545627000000	5.216675000000	16.616944000000	H	-4.544173000000	6.618325000000	20.522263000000
H	2.228460000000	5.722347000000	17.655385000000	H	2.565843000000	8.851496000000	20.401947000000
C	10.555236000000	0.070188000000	18.863576000000	H	-3.531426000000	7.023828000000	14.611957000000
C	10.228061000000	1.505743000000	19.300338000000	H	6.663569000000	6.244772000000	12.487940000000
N	10.507464000000	2.507006000000	18.261722000000	H	3.410244000000	11.443058000000	17.161601000000
C	11.719374000000	3.013220000000	18.002771000000	H	6.602731000000	16.929313000000	20.095782000000
N	12.808307000000	2.626721000000	18.716689000000	H	9.656820000000	10.778465000000	12.594879000000
N	11.901452000000	3.917122000000	17.022513000000	H	15.242266000000	4.265962000000	20.240391000000
H	11.618624000000	-0.034256000000	18.624355000000	H	10.775320000000	3.710792000000	24.562196000000
H	9.976044000000	-0.204509000000	17.975517000000	H	13.518943000000	13.806991000000	14.776369000000

H	8.953641000000	13.145720000000	17.076917000000	H	5.736647000000	12.236763000000	16.440168000000
H	9.073013000000	19.706165000000	24.214464000000	H	5.952793000000	8.251818000000	15.772733000000
H	8.049148000000	5.335435000000	24.005269000000	H	7.549556000000	9.102029000000	19.576304000000
⁵P_{C3} – VioC WT product bound state							
C	11.472712000000	4.312122000000	25.449259000000	H	6.808567000000	11.340121000000	18.567818000000
C	11.554598000000	5.688606000000	24.810690000000	N	3.478347000000	9.516965000000	14.500824000000
O	11.419730000000	5.860027000000	23.572714000000	C	3.200469000000	8.178597000000	13.974248000000
C	12.813845000000	3.533808000000	25.550104000000	C	4.561420000000	7.691534000000	13.438198000000
O	13.392709000000	3.289181000000	24.239849000000	O	5.367814000000	8.529816000000	12.943116000000
C	12.604191000000	2.177749000000	26.223842000000	C	2.069322000000	8.214638000000	12.905621000000
H	11.045237000000	4.389818000000	26.457816000000	O	0.864398000000	8.773561000000	13.478457000000
H	13.527033000000	4.130953000000	26.136712000000	C	1.804782000000	6.841619000000	12.278030000000
H	14.079464000000	3.991398000000	24.040832000000	H	4.109874000000	10.056174000000	13.918689000000
H	13.558617000000	1.648048000000	26.293647000000	H	2.871708000000	7.555856000000	14.811696000000
H	12.186939000000	2.289939000000	27.231330000000	H	2.368954000000	8.927637000000	12.129962000000
H	11.917650000000	1.566059000000	25.627502000000	H	0.375133000000	8.110751000000	14.026820000000
N	11.789613000000	6.758836000000	25.634690000000	H	0.962057000000	6.921134000000	11.584740000000
C	11.702745000000	8.142029000000	25.124275000000	H	2.676392000000	6.476198000000	11.724727000000
C	12.834096000000	8.445040000000	24.129327000000	H	1.551965000000	6.099500000000	13.045215000000
O	12.662717000000	9.233392000000	23.164556000000	N	4.882437000000	6.390328000000	13.609441000000
C	11.668897000000	9.152355000000	26.295492000000	C	6.273187000000	5.933379000000	13.429616000000
C	10.515422000000	8.937458000000	27.311556000000	C	6.400491000000	4.427233000000	13.703171000000
C	10.615068000000	9.991744000000	28.434261000000	C	7.800763000000	4.006620000000	14.203385000000
C	9.131381000000	8.997084000000	26.634115000000	C	7.992021000000	4.176149000000	15.712590000000
H	11.771815000000	6.630941000000	26.636916000000	O	8.329808000000	3.163533000000	16.394839000000
H	10.785455000000	8.235187000000	24.534901000000	O	7.839291000000	5.391441000000	16.199371000000
H	12.634206000000	9.123517000000	26.822654000000	H	4.197670000000	5.720627000000	13.955998000000
H	11.562029000000	10.155043000000	25.867011000000	H	6.907476000000	6.485356000000	14.130957000000
H	10.635108000000	7.940273000000	27.777331000000	H	6.166330000000	3.866598000000	12.787404000000
H	8.983756000000	8.175888000000	25.920047000000	H	5.659713000000	4.125830000000	14.451424000000
H	9.015054000000	9.951279000000	26.104864000000	H	7.980705000000	2.953540000000	13.974772000000
H	8.338388000000	8.922146000000	27.388311000000	H	8.579940000000	4.592882000000	13.698154000000
H	11.609412000000	9.983717000000	28.901782000000	C	6.686351000000	-2.136340000000	15.557936000000
H	10.416659000000	10.994446000000	28.033751000000	C	7.188586000000	-0.746277000000	15.992492000000
H	9.874690000000	9.784273000000	29.217327000000	C	8.358788000000	-0.268126000000	15.111132000000
N	14.027026000000	7.835062000000	24.358453000000	C	6.046846000000	0.289391000000	15.993067000000
C	15.044257000000	7.702724000000	23.303383000000	H	6.305284000000	-2.104485000000	14.527409000000
C	15.043865000000	6.214319000000	22.953137000000	H	7.559912000000	-0.829229000000	17.026750000000
O	15.040727000000	5.355027000000	23.904340000000	H	9.201646000000	-0.969630000000	15.152980000000
C	16.438034000000	8.260005000000	23.712352000000	H	8.042335000000	-0.192826000000	14.060577000000
C	16.376399000000	9.795262000000	23.821412000000	H	8.708038000000	0.719124000000	15.432566000000
C	16.986724000000	7.632179000000	25.008013000000	H	6.415588000000	1.266663000000	16.323151000000
H	14.061887000000	7.119857000000	25.074605000000	H	5.227272300000	-0.022902000000	16.654316000000
H	14.677138000000	8.275879000000	22.446986000000	H	5.636601000000	0.406617000000	14.978462000000
H	17.117549000000	7.997758000000	22.886374000000	C	-3.877285000000	6.042776000000	19.897527000000
H	17.013803000000	6.540309000000	24.951818000000	C	-3.576187000000	4.615027000000	20.385172000000
H	18.001303000000	7.996360000000	25.202130000000	C	-2.732178000000	4.555632000000	21.682895000000
H	16.363946000000	7.914983000000	25.865888000000	C	-2.777483000000	3.144935000000	22.304253000000
H	17.361424000000	10.202900000000	24.077389000000	C	-1.275327000000	5.000450000000	21.441588000000
H	15.669790000000	10.097196000000	24.602665000000	H	-2.959433000000	6.600516000000	19.683195000000
H	16.050122000000	10.252136000000	22.880610000000	H	-4.526368000000	4.086903000000	20.557761000000
N	14.969314000000	5.876873000000	21.661672000000	H	-3.045815000000	4.064158000000	19.593336000000
C	14.671323000000	4.493417000000	21.277055000000	H	-3.185313000000	5.251330000000	22.408102000000
C	13.152086000000	4.258534000000	21.386957000000	H	-2.197159000000	3.101343000000	23.234427000000
O	12.849227000000	2.828516000000	21.463401000000	H	-3.805986000000	2.838465000000	22.531951000000
H	14.758823000000	6.575842000000	20.923715000000	H	-2.357542000000	2.398991000000	21.613157000000
H	15.204101000000	3.809047000000	21.941988000000	H	-1.212293000000	6.020298000000	21.049654000000
H	12.744652000000	4.761486000000	22.262555000000	H	-0.694811000000	4.954717000000	22.372365000000
H	12.643746000000	4.650562000000	20.506867000000	H	-0.795610000000	4.341440000000	20.702520000000
H	12.898814000000	2.583556000000	22.419931000000	C	8.815023000000	11.132600000000	13.104866000000
C	3.825764000000	11.240320000000	16.194354000000	C	8.954854000000	12.412456000000	13.929980000000
C	3.215897000000	9.913247000000	15.766892000000	O	8.723915000000	13.524625000000	13.396789000000
O	2.532939000000	9.205270000000	16.559883000000	C	8.528726000000	9.805368000000	13.855369000000
C	5.380390000000	11.261505000000	16.090408000000	C	9.758280000000	9.193552000000	14.498638000000
C	6.049117000000	10.178259000000	16.882197000000	O	10.037825000000	9.504390000000	15.729068000000
N	6.599277000000	10.405090000000	18.140152000000	O	10.497810000000	8.397365000000	13.791845000000
C	6.229706000000	8.830034000000	16.635448000000	H	8.001481000000	11.323772000000	12.398860000000
C	7.081633000000	9.230418000000	18.616878000000	H	7.772043000000	9.964626000000	14.626758000000
N	6.882618000000	8.251134000000	17.720177000000	H	8.123333000000	9.088612000000	13.136999000000
H	3.415110000000	12.049443000000	15.575679000000	N	9.379914000000	12.285565000000	15.225743000000
H	5.679362000000	11.188031000000	15.037579000000	C	9.656481000000	13.447051000000	16.067383000000
				C	11.146946000000	13.713185000000	16.304296000000

O	11.511081000000	14.612241000000	17.104129000000	H	6.720708000000	0.166461000000	19.926780000000
H	9.521284000000	11.358301000000	15.626013000000	H	6.688717000000	1.774059000000	20.670956000000
H	9.232242000000	14.325064000000	15.571287000000	H	3.180948000000	2.523576000000	19.198288000000
N	12.011457000000	12.932598000000	15.611765000000	H	4.912835000000	2.621487000000	19.506230000000
C	13.462844000000	13.024916000000	15.702663000000	H	3.772172000000	2.898105000000	20.826160000000
C	14.051243000000	11.626413000000	15.534606000000	N	0.465279000000	1.225274000000	19.961150000000
O	13.522225000000	11.093868000000	14.296114000000	C	-0.643003000000	1.359276000000	19.007643000000
H	11.667381000000	12.257128000000	14.942068000000	C	-0.298945000000	2.273956000000	17.826666000000
H	13.729418000000	13.461241000000	16.669370000000	O	-0.815755000000	3.425697000000	17.733957000000
H	13.763070000000	10.999408000000	16.392403000000	H	0.447599000000	1.794937000000	20.794706000000
H	15.149524000000	11.683596000000	15.507614000000	H	-0.906720000000	0.360955000000	18.643152000000
H	13.485217000000	10.100680000000	14.296533000000	N	0.578345000000	1.755491000000	16.940690000000
C	6.369168000000	15.985379000000	20.390722000000	C	1.065296000000	2.481523000000	15.762656000000
C	6.333665000000	16.148996000000	21.909456000000	C	2.467165000000	1.986146000000	15.373738000000
O	6.613726000000	17.252633000000	22.458229000000	C	3.067865000000	2.871440000000	14.296430000000
C	7.394216000000	14.987909000000	19.799020000000	O	3.130991000000	4.120695000000	14.437002000000
C	7.032649000000	13.508268000000	19.868886000000	N	3.537606000000	2.246686000000	13.184661000000
O	7.604020000000	12.723978000000	19.000263000000	H	0.977319000000	0.844329000000	17.179896000000
O	6.250291000000	13.064141000000	20.786093000000	H	1.112296000000	3.549396000000	15.986889000000
H	5.362404000000	15.709921000000	20.049173000000	H	2.441186000000	5.037045000000	15.056495000000
H	7.559545000000	15.230466000000	18.744396000000	H	3.124817000000	2.045788000000	16.250302000000
H	8.373996000000	15.118620000000	20.280124000000	H	3.514585000000	1.244716000000	13.082984000000
N	5.943627000000	15.060718000000	22.628015000000	H	3.977519000000	2.794914000000	12.459870000000
C	5.612376000000	15.146733000000	24.047255000000	C	-3.051942000000	6.569723000000	15.532682000000
C	6.778312000000	15.397760000000	25.012013000000	C	-1.719341000000	7.242928000000	15.809922000000
O	6.548164000000	15.813542000000	26.169119000000	O	-0.710732000000	7.016759000000	15.057928000000
H	5.828583000000	14.186407000000	22.099423000000	C	-2.888628000000	5.098643000000	15.116672000000
H	4.906546000000	15.964988000000	24.223371000000	H	-3.705899000000	6.655014000000	16.408860000000
H	5.123494000000	14.211245000000	24.337593000000	H	-2.445983000000	4.505553000000	15.924191000000
N	8.020924000000	15.135519000000	24.522512000000	H	-3.861983000000	4.665168000000	14.863821000000
C	9.260149000000	15.386523000000	25.258194000000	H	-2.235819000000	5.027245000000	14.242054000000
C	9.870945000000	16.767440000000	24.934747000000	N	-1.659529000000	8.070783000000	16.869215000000
O	11.015041000000	17.061550000000	25.373074000000	C	-0.455921000000	8.805660000000	17.273937000000
C	10.288588000000	14.271058000000	24.979006000000	C	-0.046581000000	8.330225000000	18.674656000000
C	9.897053000000	12.938198000000	25.640788000000	O	-0.913602000000	7.908976000000	19.492960000000
O	9.962214000000	12.865872000000	26.898664000000	C	-0.672649000000	10.352179000000	17.223175000000
O	9.521211000000	11.960572000000	24.843684000000	C	-0.920231000000	10.820630000000	15.776832000000
H	8.094378000000	14.768901000000	23.582893000000	C	-1.789290000000	10.833345000000	18.169943000000
H	9.015784000000	15.379888000000	26.326332000000	H	-2.417987000000	8.071359000000	17.539734000000
H	10.413463000000	14.141556000000	23.896817000000	H	0.335304000000	8.558785000000	16.565825000000
H	11.241565000000	14.604251000000	25.399004000000	H	0.279437000000	10.781264000000	17.563992000000
N	9.128966000000	17.612285000000	24.171498000000	H	-0.141266000000	10.465804000000	15.093254000000
C	9.625163000000	18.923358000000	23.756891000000	H	-0.948086000000	11.916166000000	15.733590000000
C	9.640321000000	19.088438000000	22.225085000000	H	-1.885874000000	10.452429000000	15.407164000000
C	10.475291000000	18.077434000000	21.451403000000	H	-1.637153000000	10.487553000000	19.197188000000
C	11.609140000000	17.449630000000	21.996469000000	H	-1.828547000000	11.928621000000	18.177896000000
C	10.107885000000	17.756771000000	20.130402000000	H	-2.772349000000	10.476849000000	17.834123000000
C	12.346459000000	16.528291000000	21.239576000000	N	1.269358000000	8.447551000000	18.956204000000
C	10.841621000000	16.836874000000	19.373931000000	C	1.834722000000	8.063840000000	20.249003000000
C	11.967351000000	16.215926000000	19.930033000000	C	2.270407000000	6.575382000000	20.317168000000
H	8.216670000000	17.333402000000	23.820539000000	C	3.390932000000	6.199472000000	19.395385000000
H	10.621912000000	19.035424000000	24.190009000000	N	3.191982000000	5.772717000000	18.082408000000
H	8.605635000000	19.034372000000	21.862964000000	C	4.758555000000	6.201786000000	19.582489000000
H	9.994504000000	20.109416000000	22.007273000000	C	4.411625000000	5.539414000000	17.522694000000
H	11.901082000000	17.640647000000	23.024062000000	N	5.391739000000	5.793335000000	18.404660000000
H	9.229215000000	18.231570000000	19.698474000000	H	1.897419000000	8.753914000000	18.209845000000
H	13.210410000000	16.044489000000	21.686893000000	H	1.076378000000	8.244223000000	21.016318000000
H	10.546340000000	16.572647000000	18.364569000000	H	1.388792000000	5.954640000000	20.119421000000
H	12.514344000000	15.492041000000	19.336601000000	H	2.581604000000	6.372869000000	21.349914000000
C	2.594152000000	0.314331000000	20.791321000000	H	5.340763000000	6.484031000000	20.443185000000
C	1.528441000000	0.402908000000	19.721330000000	H	4.545941000000	5.208877000000	16.508596000000
O	1.617734000000	-0.243248000000	18.638121000000	H	2.267293000000	5.691569000000	17.607893000000
C	3.983857000000	0.789691000000	20.281111000000	C	10.770714000000	0.072156000000	18.871798000000
C	5.068603000000	0.445011000000	21.328721000000	C	10.229211000000	1.466832000000	19.219057000000
C	3.961665000000	2.289664000000	19.931845000000	N	10.400524000000	2.438096000000	18.129826000000
C	6.507598000000	0.710085000000	20.856298000000	C	11.522582000000	3.140902000000	17.918070000000
H	2.309058000000	0.891086000000	21.681173000000	N	12.624515000000	2.980124000000	18.684559000000
H	4.197012000000	0.217343000000	19.366026000000	N	11.599695000000	4.031361000000	16.910650000000
H	4.970452000000	-0.617249000000	21.597935000000	H	11.845579000000	0.108317000000	18.664784000000
H	4.872779000000	1.017709000000	22.248330000000	H	10.266003000000	-0.328869000000	17.986103000000
H	7.229592000000	0.378416000000	21.611410000000	H	9.154831000000	1.420546000000	19.416045000000

H	10.700260000000	1.846527000000	20.134076000000	H	8.989602000000	19.709546000000	24.186898000000
H	9.561595000000	2.733699000000	17.614853000000	H	8.209339000000	4.936269000000	23.934940000000
H	12.599364000000	2.552998000000	19.611947000000				
H	13.375291000000	3.641943000000	18.518626000000				
H	10.839107000000	4.202543000000	16.269857000000				
H	12.313504000000	4.759983000000	16.987736000000				
Fe	7.510367000000	6.261954000000	18.099125000000				
O	8.528844000000	4.936263000000	19.385436000000				
O	9.656926000000	7.584867000000	17.978070000000				
C	8.265598000000	5.561999000000	20.504240000000				
O	7.653365000000	6.695364000000	20.456971000000				
C	8.699343000000	4.949826000000	21.814582000000				
C	7.822992000000	5.365554000000	23.003620000000				
H	8.715989000000	3.861426000000	21.686240000000				
H	9.736932000000	5.253168000000	22.014787000000				
H	6.787321000000	5.027784000000	22.875454000000				
H	7.807362000000	6.454266000000	23.103770000000				
N	11.933983000000	7.785457000000	16.677125000000				
C	12.144188000000	7.921532000000	18.152545000000				
C	13.258928000000	6.967884000000	18.645180000000				
O	13.410652000000	5.855797000000	18.014758000000				
C	10.795127000000	7.635506000000	18.913391000000				
C	10.547520000000	8.582776000000	20.103870000000				
C	10.502408000000	10.101145000000	19.758669000000				
N	9.445431000000	10.856364000000	20.454448000000				
C	9.450754000000	11.149286000000	21.785050000000				
N	10.427878000000	10.769683000000	22.610196000000				
N	8.438604000000	11.865307000000	22.314407000000				
O	13.892724000000	7.376072000000	19.674279000000				
H	12.477034000000	8.945455000000	18.336101000000				
H	9.478539000000	8.433901000000	17.514835000000				
H	10.816274000000	6.608794000000	19.283610000000				
H	11.334054000000	8.389359000000	20.843000000000				
H	9.596428000000	8.282875000000	20.554190000000				
H	10.296496000000	10.248738000000	18.692698000000				
H	11.480156000000	10.562087000000	19.954945000000				
H	8.817008000000	11.424670000000	19.879841000000				
H	11.238874000000	10.206755000000	22.382388000000				
H	10.328344000000	11.097646000000	23.588110000000				
H	7.595085000000	12.094278000000	21.792699000000				
H	8.527979000000	12.071534000000	23.322256000000				
H	12.801181000000	7.842723000000	16.122217000000				
H	11.302852000000	8.553281000000	16.319231000000				
H	11.435946000000	6.909403000000	16.394986000000				
O	0.762924000000	5.543922000000	16.939254000000				
H	0.097769000000	4.889068000000	17.264003000000				
H	0.414814000000	6.060828000000	16.177280000000				
O	13.093376000000	8.405717000000	14.238167000000				
H	12.106759000000	8.401873000000	13.991345000000				
H	13.620992000000	7.905928000000	13.591079000000				
O	10.352152000000	6.041019000000	15.252770000000				
H	9.450668000000	6.040068000000	15.663700000000				
H	10.385414000000	6.698121000000	14.513894000000				
H	10.607964000000	-0.618720000000	19.707686000000				
H	2.665362000000	-0.739106000000	21.090891000000				
H	-1.498110000000	1.793438000000	19.523677000000				
H	0.368836000000	2.344255000000	14.923716000000				
H	5.873741000000	-2.488684000000	16.205698000000				
H	7.492877000000	-2.879224000000	15.591326000000				
H	-4.489718000000	6.018312000000	18.985826000000				
H	-4.439567000000	6.603636000000	20.655816000000				
H	2.696067000000	8.708735000000	20.448607000000				
H	-3.534724000000	7.130374000000	14.719145000000				
H	6.614528000000	6.181470000000	12.418141000000				
H	3.518352000000	11.416616000000	17.227787000000				
H	6.592817000000	16.981057000000	19.999702000000				
H	9.726789000000	11.023999000000	12.500368000000				
H	15.027754000000	4.340034000000	20.255506000000				
H	10.787324000000	3.720003000000	24.835187000000				
H	13.856295000000	13.681355000000	14.914590000000				
H	9.170610000000	13.336181000000	17.044083000000				

VioC MeHis316

⁵Re_{Me} – VioC MeHis Reactant state

C	11.236822000000	5.181683000000	25.920412000000
C	11.492137000000	6.534536000000	25.277240000000
O	11.297952000000	6.740478000000	24.054515000000
C	12.430705000000	4.187780000000	25.909505000000
O	12.883186000000	3.901690000000	24.559054000000
C	12.037086000000	2.860550000000	26.556587000000
H	10.910347000000	5.313086000000	26.960731000000
H	13.268670000000	4.634332000000	26.464649000000
H	13.632027000000	4.524372000000	24.322405000000
H	12.892906000000	2.179447000000	26.555093000000
H	11.699429000000	3.002838000000	27.589688000000
H	11.227250000000	2.391931000000	25.986019000000
N	11.947828000000	7.547942000000	26.090906000000
C	12.000596000000	8.936123000000	25.598123000000
C	13.179233000000	9.171638000000	24.637417000000
O	13.157666000000	10.133740000000	23.821867000000
C	11.988599000000	9.954289000000	26.761161000000
C	10.818327000000	9.800420000000	27.769161000000
C	10.865564000000	10.966061000000	28.779163000000
C	9.433225000000	9.729237000000	27.095946000000
H	11.983434000000	7.401904000000	27.090028000000
H	11.113203000000	9.098780000000	24.976731000000
H	12.944038000000	9.899859000000	27.304626000000
H	11.937172000000	10.952244000000	26.310571000000
H	10.976954000000	8.865935000000	28.338792000000
H	9.347384000000	8.865726000000	26.424113000000
H	9.214444000000	10.643618000000	26.526612000000
H	8.654954000000	9.623670000000	27.862132000000
H	11.850725000000	11.050904000000	29.256263000000
H	10.640887000000	11.912132000000	28.273488000000
H	10.116329000000	10.826616000000	29.566722000000
N	14.211968000000	8.297923000000	24.702312000000
C	15.125294000000	8.055840000000	23.570953000000
C	14.867754000000	6.591523000000	23.203522000000
O	14.732793000000	5.747264000000	24.159736000000
C	16.615178000000	8.377568000000	23.883255000000
C	16.801350000000	9.898294000000	24.043853000000
C	17.152767000000	7.617868000000	25.110381000000
H	14.114750000000	7.504118000000	25.325803000000
H	14.798659000000	8.704482000000	22.753039000000
H	17.181518000000	8.050761000000	22.997234000000
H	17.020953000000	6.536545000000	25.012549000000
H	18.220225000000	7.829343000000	25.243603000000
H	16.633619000000	7.942622000000	26.020452000000
H	17.856634000000	10.138580000000	24.217976000000
H	16.221727000000	10.270455000000	24.896141000000
H	16.467823000000	10.440712000000	23.152549000000
N	14.720434000000	6.257664000000	21.919972000000
C	14.200143000000	4.933973000000	21.558348000000
C	12.660231000000	4.919650000000	21.690474000000
O	12.173972000000	3.547205000000	21.859815000000
H	14.715842000000	6.935299000000	21.137435000000
H	14.634075000000	4.181127000000	22.221465000000
H	12.334897000000	5.525779000000	22.537464000000
H	12.194537000000	5.313423000000	20.787302000000
H	12.256718000000	3.337451000000	22.825497000000
C	3.662112000000	11.039466000000	17.518431000000
C	2.961333000000	9.892579000000	16.812742000000
O	2.277079000000	9.029203000000	17.436723000000
C	5.212559000000	11.008150000000	17.368022000000
C	5.862947000000	9.776567000000	17.932930000000
N	6.726393000000	9.844249000000	19.024796000000
C	5.770255000000	8.433826000000	17.615250000000
C	7.120429000000	8.591090000000	19.351991000000
N	6.541106000000	7.709261000000	18.521710000000
H	3.296011000000	11.994905000000	17.120301000000
H	5.481674000000	11.120878000000	16.309451000000
H	5.598520000000	11.889901000000	17.893085000000

H	5.200472000000	7.941869000000	16.847518000000
H	7.787476000000	8.331883000000	20.154398000000
H	7.125195000000	10.740910000000	19.417441000000
N	3.160399000000	9.815500000000	15.476657000000
C	2.833882000000	8.654681000000	14.640869000000
C	4.194965000000	8.222168000000	14.071184000000
O	4.957399000000	9.088996000000	13.563575000000
C	1.788190000000	9.013829000000	13.551922000000
O	0.562660000000	9.458258000000	14.169581000000
C	1.532874000000	7.849923000000	12.586014000000
H	3.761144000000	10.492688000000	15.020890000000
H	2.412309000000	7.885757000000	15.293687000000
H	2.166463000000	9.878572000000	12.996787000000
H	0.040407000000	8.691422000000	14.522464000000
H	0.762392000000	8.142243000000	11.866685000000
H	2.440396000000	7.585309000000	12.029545000000
H	1.169831000000	6.971226000000	13.133118000000
N	4.544284000000	6.923746000000	14.235956000000
C	5.934298000000	6.469054000000	14.056810000000
C	6.010413000000	4.935129000000	13.986188000000
C	7.340665000000	4.377816000000	14.511753000000
C	7.440555000000	4.220519000000	16.029507000000
O	8.340976000000	3.464999000000	16.484026000000
O	6.583307000000	4.901585000000	16.774436000000
H	3.883220000000	6.273175000000	14.659028000000
H	6.531789000000	6.831006000000	14.902590000000
H	5.857284000000	4.604685000000	12.950610000000
H	5.199724000000	4.504589000000	14.582526000000
H	7.553037000000	3.393719000000	14.081352000000
H	8.181732000000	5.025504000000	14.221554000000
C	6.237856000000	-1.975038000000	15.069163000000
C	6.534284000000	-0.571144000000	15.631505000000
C	7.846682000000	-0.002285000000	15.058723000000
C	5.352562000000	0.385501000000	15.373952000000
H	6.111549000000	-1.935283000000	13.978336000000
H	6.655957000000	-0.663383000000	16.722899000000
H	8.690896000000	-0.672656000000	15.263678000000
H	7.772377000000	0.111861000000	13.967833000000
H	8.080735000000	0.978315000000	15.489357000000
H	5.551836000000	1.373865000000	15.806642000000
H	4.424557000000	-0.004759000000	15.810839000000
H	5.195534000000	0.513684000000	14.293052000000
C	-4.079581000000	4.587411000000	19.625016000000
C	-3.735110000000	3.091891000000	19.731103000000
C	-2.803286000000	2.742156000000	20.917758000000
C	-2.748776000000	1.216751000000	21.135512000000
C	-1.384907000000	3.313888000000	20.718885000000
H	-3.183385000000	5.207080000000	19.508510000000
H	-4.668859000000	2.518894000000	19.837898000000
H	-3.261055000000	2.750002000000	18.799215000000
H	-3.229458000000	3.194732000000	21.828178000000
H	-2.097857000000	0.955639000000	21.979823000000
H	-3.745023000000	0.804498000000	21.336989000000
H	-2.362217000000	0.713944000000	20.236466000000
H	-1.393019000000	4.404385000000	20.620756000000
H	-0.736429000000	3.054514000000	21.566483000000
H	-0.939218000000	2.899708000000	19.802862000000
C	8.586310000000	11.607403000000	13.391310000000
C	9.294625000000	12.898297000000	13.804560000000
O	9.184277000000	13.926828000000	13.093555000000
C	8.221127000000	10.581790000000	14.498033000000
C	9.407808000000	9.758288000000	14.971239000000
O	10.115520000000	10.205877000000	15.952452000000
O	9.685080000000	8.655297000000	14.338942000000
H	7.671567000000	11.924433000000	12.881916000000
H	7.791340000000	11.102806000000	15.359912000000
H	7.465937000000	9.901281000000	14.093875000000
N	10.072245000000	12.858468000000	14.932042000000
C	10.828184000000	14.018770000000	15.386215000000
C	12.345068000000	13.817249000000	15.405077000000
O	13.075071000000	14.552130000000	16.119347000000

H	10.107180000000	12.006316000000	15.497718000000	H	6.461067000000	1.266784000000	20.189911000000
H	10.587942000000	14.848096000000	14.711969000000	H	3.183501000000	1.794108000000	18.217317000000
N	12.824287000000	12.838954000000	14.600109000000	H	4.792594000000	2.057710000000	18.895882000000
C	14.232185000000	12.475710000000	14.495815000000	H	3.382030000000	2.074805000000	19.962535000000
C	14.353993000000	10.953414000000	14.491223000000	N	0.359661000000	-0.131154000000	18.604707000000
O	13.507679000000	10.457324000000	13.428201000000	C	-0.677944000000	-0.110985000000	17.564348000000
H	12.190740000000	12.268221000000	14.055098000000	C	-0.654707000000	1.160088000000	16.707605000000
H	14.767088000000	12.922994000000	15.338072000000	O	-1.553875000000	2.033489000000	16.796728000000
H	14.037294000000	10.558274000000	15.468524000000	H	0.089169000000	0.114839000000	19.546054000000
H	15.403730000000	10.664196000000	14.331160000000	H	-0.543968000000	-0.992057000000	16.927539000000
H	13.116796000000	9.570448000000	13.658515000000	N	0.406337000000	1.265103000000	15.865851000000
C	7.997737000000	15.783767000000	19.172758000000	C	0.605780000000	2.467106000000	15.055290000000
C	7.444543000000	16.419392000000	20.440562000000	C	1.996451000000	2.450914000000	14.392195000000
O	7.854866000000	17.536826000000	20.857828000000	C	2.442233000000	3.855909000000	14.027851000000
C	8.582148000000	14.369378000000	19.364091000000	O	2.654707000000	4.718045000000	14.926113000000
C	7.545900000000	13.250048000000	19.468890000000	N	2.607063000000	4.140690000000	12.713700000000
O	8.012357000000	12.057640000000	19.752901000000	H	1.126833000000	0.544666000000	15.922795000000
O	6.309606000000	13.492167000000	19.283042000000	H	0.507879000000	3.349021000000	15.695328000000
H	7.201109000000	15.735036000000	18.420079000000	H	2.005749000000	1.785572000000	13.521987000000
H	9.223191000000	14.126886000000	18.505227000000	H	2.733982000000	2.066779000000	15.107396000000
H	9.242161000000	14.327357000000	20.239129000000	H	2.440964000000	3.459441000000	11.990545000000
N	6.492641000000	15.708057000000	21.114055000000	H	2.902113000000	5.069620000000	12.444611000000
C	5.812894000000	16.254707000000	22.288486000000	C	-3.018180000000	6.149448000000	15.530124000000
C	6.695051000000	16.549639000000	23.511832000000	C	-1.830866000000	7.010650000000	15.938170000000
O	6.289143000000	17.365047000000	24.368736000000	O	-0.934453000000	7.315099000000	15.098356000000
H	6.122147000000	14.880543000000	20.646490000000	C	-2.601476000000	4.887102000000	14.756549000000
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C	8.861574000000	16.114114000000	24.659757000000	H	-1.905129000000	5.157089000000	13.956395000000
C	9.860994000000	17.242159000000	24.329891000000	N	-1.820466000000	7.439724000000	17.223814000000
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O	9.047360000000	12.502781000000	25.304911000000	C	-1.490425000000	10.461325000000	16.709663000000
H	8.109808000000	15.212645000000	22.872315000000	C	-2.427201000000	9.860704000000	18.993834000000
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H	10.467342000000	15.104295000000	25.630522000000	H	-0.355240000000	10.239783000000	18.524121000000
N	9.665086000000	17.940882000000	23.183042000000	H	-0.626355000000	10.425832000000	16.038832000000
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C	11.037959000000	18.781039000000	21.278296000000	H	-2.341829000000	10.002081000000	16.192095000000
C	11.814332000000	17.507840000000	20.966673000000	H	-2.255188000000	9.359008000000	19.951731000000
C	12.446233000000	16.732594000000	21.954077000000	H	-2.650259000000	10.914586000000	19.195572000000
C	11.927947000000	17.096972000000	19.623659000000	H	-3.320766000000	9.417705000000	18.535977000000
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C	12.653893000000	15.956014000000	19.264023000000	C	1.373942000000	7.479521000000	20.892082000000
C	13.278935000000	15.195269000000	20.262097000000	C	1.849227000000	6.001998000000	20.961725000000
H	8.875480000000	17.736863000000	22.576216000000	C	2.974451000000	5.669915000000	20.031820000000
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H 0.721264000000 5.351936000000 18.453081000000
⁵TSH_{Me} – ViOC MeHis Transition state for HAT
C 11.399845000000 4.691605000000 25.900143000000
C 11.550559000000 5.929575000000 25.029753000000
O 11.363063000000 5.915964000000 23.787192000000
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C	4.350437000000	8.120553000000	13.790784000000	O	14.021326000000	10.556835000000	13.988248000000
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O	0.709192000000	9.349577000000	13.721065000000	H	14.429302000000	10.622551000000	16.057527000000
C	1.682881000000	7.573368000000	12.331566000000	H	15.842073000000	10.879175000000	15.003386000000
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H	1.329486000000	6.758695000000	12.974832000000	O	7.405236000000	12.666060000000	19.387223000000
N	4.647951000000	6.813468000000	13.975106000000	O	6.355328000000	13.099494000000	21.350903000000
C	6.031945000000	6.322604000000	13.843902000000	H	5.205547000000	15.622915000000	20.524470000000
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H	5.907761000000	1.726833000000	16.117013000000	H	11.940657000000	15.230617000000	24.848742000000
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H	5.302623000000	0.797970000000	14.727211000000	C	9.811833000000	19.326745000000	23.116884000000
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H	-4.540248000000	2.942973000000	19.790536000000	C	11.661813000000	16.779447000000	18.888883000000
H	-3.179804000000	3.099408000000	18.678827000000	H	8.536339000000	17.693604000000	23.583102000000
H	-2.998977000000	3.707117000000	21.672803000000	H	10.871605000000	19.509564000000	23.309732000000
H	-1.872819000000	1.459188000000	21.872893000000	H	8.405055000000	19.187216000000	21.495452000000
H	-3.562316000000	1.305346000000	21.353740000000	H	9.637808000000	20.426641000000	21.286946000000
H	-2.264553000000	1.135849000000	20.163562000000	H	11.868203000000	17.982368000000	22.074210000000
H	-1.210779000000	4.825866000000	20.315399000000	H	8.825334000000	18.665243000000	19.101605000000
H	-0.523116000000	3.519101000000	21.297380000000	H	13.084007000000	16.543734000000	20.491206000000
H	-0.815225000000	3.272328000000	19.556873000000	H	10.055336000000	17.214082000000	17.512561000000
C	9.042432000000	11.443890000000	13.555160000000	H	12.199946000000	16.137602000000	18.196380000000
C	9.655381000000	12.736845000000	14.091659000000	C	2.595857000000	-0.252091000000	19.890226000000
O	9.571097000000	13.793009000000	13.419234000000	C	1.731676000000	-0.240799000000	18.644606000000
C	8.624439000000	10.359648000000	14.581452000000	O	2.193349000000	-0.504328000000	17.496845000000
C	9.801644000000	9.561432000000	15.114818000000	C	3.932266000000	0.513658000000	19.722341000000
O	10.324785000000	9.906330000000	16.243608000000	C	4.831938000000	0.284085000000	20.960642000000
O	10.259294000000	8.586207000000	14.386065000000	C	3.683435000000	2.009849000000	19.456770000000
H	8.167001000000	11.752034000000	12.975962000000	C	6.276208000000	0.783626000000	20.786901000000
H	8.098033000000	10.816551000000	15.424154000000	H	2.039741000000	0.153442000000	20.746675000000
H	7.937792000000	9.668684000000	14.082015000000	H	4.439386000000	0.083978000000	18.847178000000
N	10.321344000000	12.675114000000	15.288618000000	H	4.853509000000	-0.792828000000	21.186109000000
C	10.961134000000	13.851296000000	15.868150000000	H	4.372759000000	0.773471000000	21.833579000000
C	12.487348000000	13.775814000000	15.953526000000	H	6.873582000000	0.553769000000	21.677152000000
O	13.120385000000	14.580317000000	16.684947000000	H	6.754679000000	0.294567000000	19.928655000000
H	10.320029000000	11.811829000000	15.832239000000	H	6.329979000000	1.865141000000	20.622909000000

H	3.068980000000	2.156006000000	18.560610000000	H	13.287795000000	3.755225000000	18.564369000000
H	4.621258000000	2.551397000000	19.302587000000	H	10.582693000000	4.308649000000	16.498566000000
H	3.165248000000	2.475614000000	20.306279000000	H	12.185899000000	4.746700000000	16.977483000000
N	0.408854000000	0.047339000000	18.816875000000	Fe	7.330398000000	6.157337000000	18.492928000000
C	-0.562900000000	-0.028938000000	17.717294000000	O	7.833854000000	4.497932000000	19.862595000000
C	-0.545818000000	1.205961000000	16.808332000000	O	9.038411000000	6.637351000000	18.194095000000
O	-1.476759000000	2.049960000000	16.822310000000	C	7.857906000000	5.301414000000	20.881120000000
H	0.074102000000	0.340855000000	19.723396000000	O	7.515028000000	6.541184000000	20.678703000000
H	-0.346660000000	-0.928205000000	17.131029000000	C	8.301517000000	4.830922000000	22.240432000000
N	0.546605000000	1.311752000000	16.007666000000	C	7.517086000000	5.476702000000	23.393682000000
C	0.739956000000	2.485555000000	15.155375000000	H	8.224918000000	3.738944000000	22.262058000000
C	2.016259000000	2.341496000000	14.309027000000	H	9.367226000000	5.080624000000	22.356846000000
C	2.498397000000	3.693536000000	13.813611000000	H	6.454061000000	5.210135000000	23.353927000000
O	2.728397000000	4.635341000000	14.621819000000	H	7.595770000000	6.566166000000	23.345785000000
N	2.689830000000	3.837561000000	12.479486000000	N	11.934004000000	7.896575000000	17.151825000000
H	1.298427000000	0.635926000000	16.146555000000	C	12.295619000000	7.773946000000	18.612040000000
H	0.811263000000	3.386005000000	15.773404000000	C	13.356553000000	6.662737000000	18.816884000000
H	1.858323000000	1.641667000000	13.481277000000	O	13.458545000000	5.746081000000	17.923117000000
H	2.823523000000	1.933169000000	14.931678000000	C	11.050621000000	7.492947000000	19.495861000000
H	2.500633000000	3.094759000000	11.825967000000	C	10.560793000000	8.580025000000	20.453031000000
H	3.015646000000	4.725030000000	12.122147000000	C	10.438977000000	10.011884000000	19.874819000000
C	-2.908582000000	6.222046000000	15.371903000000	N	9.529311000000	10.882842000000	20.642673000000
C	-1.720584000000	7.114373000000	15.703420000000	C	9.770865000000	11.357479000000	21.896310000000
O	-0.813933000000	7.328694000000	14.846813000000	N	10.891510000000	11.095634000000	22.575420000000
C	-2.494430000000	4.897463000000	14.709116000000	N	8.855788000000	12.141984000000	22.499875000000
H	-3.506832000000	6.031448000000	16.270470000000	O	14.005951000000	6.752652000000	19.911579000000
H	-2.014337000000	4.222162000000	15.425287000000	H	12.751034000000	8.721943000000	18.911529000000
H	-3.374337000000	4.382270000000	14.308842000000	H	10.069916000000	7.170010000000	18.780920000000
H	-1.802811000000	5.097399000000	13.884598000000	H	11.173760000000	6.554822000000	20.046583000000
N	-1.721347000000	7.671375000000	16.939306000000	H	11.248549000000	8.577384000000	21.311992000000
C	-0.664104000000	8.539173000000	17.461248000000	H	9.586177000000	8.262585000000	20.842610000000
C	-0.248475000000	7.989021000000	18.832325000000	H	10.031287000000	9.979644000000	18.859451000000
O	-1.059907000000	7.325723000000	19.541216000000	H	11.431749000000	10.480483000000	19.807551000000
C	-1.104041000000	10.038525000000	17.568519000000	H	8.803318000000	11.379804000000	20.122925000000
C	-1.358916000000	10.637933000000	16.173501000000	H	11.613251000000	10.431732000000	22.317535000000
C	-2.323237000000	10.233520000000	18.489868000000	H	10.949488000000	11.545314000000	23.507342000000
H	-2.390025000000	7.352197000000	17.629893000000	H	7.921848000000	12.289375000000	22.122449000000
H	0.183174000000	8.491678000000	16.773414000000	H	9.110971000000	12.457463000000	23.450344000000
H	-0.243392000000	10.558918000000	18.012242000000	H	12.749439000000	7.952364000000	16.524951000000
H	-0.491447000000	10.530086000000	15.514541000000	H	11.341372000000	8.748233000000	16.934305000000
H	-1.595786000000	11.705342000000	16.260873000000	H	11.391404000000	7.078503000000	16.799534000000
H	-2.124299000000	10.149149000000	15.690586000000	O	12.854679000000	8.190916000000	14.558716000000
H	-2.165674000000	9.806606000000	19.485679000000	H	11.854984000000	8.342757000000	14.425113000000
H	-2.538601000000	11.301873000000	18.606222000000	H	13.156164000000	7.406125000000	14.067915000000
H	-3.216054000000	9.763929000000	18.057637000000	O	10.105058000000	6.235243000000	15.794597000000
N	1.012112000000	8.287099000000	19.226357000000	H	9.526365000000	6.389467000000	16.597174000000
C	1.516702000000	7.923772000000	20.551688000000	H	10.003199000000	6.965315000000	15.131778000000
C	2.005091000000	6.454362000000	20.670979000000	H	10.289936000000	-0.504654000000	19.974291000000
C	3.179749000000	6.103900000000	19.809430000000	H	2.815113000000	-1.304434000000	20.120748000000
N	3.071605000000	5.551817000000	18.524040000000	H	-1.562761000000	-0.106138000000	18.143579000000
C	4.533105000000	6.249631000000	20.030558000000	H	-0.138554000000	2.615392000000	14.513920000000
C	4.332778000000	5.388630000000	18.026670000000	H	4.692793000000	-1.829187000000	16.359843000000
N	5.239237000000	5.803350000000	18.915287000000	H	6.288323000000	-2.599955000000	16.193182000000
H	1.631285000000	8.765709000000	18.565876000000	H	-4.633270000000	5.139843000000	18.599996000000
H	0.713076000000	8.075423000000	21.279435000000	H	-4.431208000000	5.387586000000	20.341106000000
H	1.156457000000	5.794008000000	20.463004000000	H	2.338643000000	8.604407000000	20.791614000000
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H	5.051187000000	6.650386000000	20.884241000000	H	6.431956000000	6.623148000000	12.869583000000
H	4.548870000000	5.000046000000	17.048541000000	H	3.451246000000	11.429359000000	17.909221000000
C	10.453669000000	0.152208000000	19.111174000000	H	6.337417000000	16.939586000000	20.178862000000
C	10.130230000000	1.608532000000	19.477684000000	H	9.748625000000	11.006535000000	12.835300000000
N	10.291373000000	2.532281000000	18.349359000000	H	15.124069000000	3.494341000000	20.819522000000
C	11.410014000000	3.216633000000	18.054781000000	H	10.817502000000	3.961667000000	25.331878000000
N	12.553386000000	3.077728000000	18.760491000000	H	14.964083000000	13.051488000000	14.270060000000
N	11.416838000000	4.078680000000	17.022908000000	H	10.589835000000	14.038703000000	16.880782000000
H	11.498588000000	0.049887000000	18.797489000000	H	9.244470000000	20.115710000000	23.629603000000
H	9.817622000000	-0.192669000000	18.288751000000	H	7.916378000000	5.144150000000	24.357452000000
H	9.090077000000	1.704636000000	19.801861000000	C	1.844300000000	5.176733000000	17.819677000000
H	10.754721000000	1.932406000000	20.316958000000	H	2.109636000000	4.899023000000	16.798788000000
H	9.452566000000	2.795783000000	17.823387000000	H	1.354187000000	4.335154000000	18.319297000000
H	12.633360000000	2.495096000000	19.591753000000	H	1.156537000000	6.020068000000	17.786089000000

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C	11.099784000000	4.647261000000	25.503961000000	H	7.126702000000	11.384871000000	18.587923000000
C	11.262877000000	6.041496000000	24.920300000000	N	3.384698000000	9.710411000000	14.725938000000
O	11.155528000000	6.266790000000	23.688799000000	C	2.996637000000	8.432236000000	14.119964000000
C	12.400171000000	3.804108000000	25.608641000000	C	4.301565000000	7.844525000000	13.560319000000
O	13.012376000000	3.599234000000	24.308421000000	O	5.118191000000	8.592582000000	12.956929000000
C	12.109334000000	2.428513000000	26.208404000000	C	1.887806000000	8.639615000000	13.048500000000
H	10.648232000000	4.707177000000	26.503236000000	O	0.713134000000	9.207675000000	13.664808000000
H	13.119727000000	4.339248000000	26.245095000000	C	1.546862000000	7.348334000000	12.293848000000
H	13.725623000000	4.291333000000	24.155424000000	H	4.007489000000	10.274094000000	14.157891000000
H	13.036535000000	1.852736000000	26.279738000000	H	2.592224000000	7.800669000000	14.915419000000
H	11.666702000000	2.512016000000	27.207846000000	H	2.244380000000	9.398113000000	12.343524000000
H	11.414800000000	1.877976000000	25.563686000000	H	0.181605000000	8.514420000000	14.136282000000
N	11.535394000000	7.065093000000	25.794557000000	H	0.725746000000	7.546433000000	11.598736000000
C	11.507455000000	8.470930000000	25.346063000000	H	2.406099000000	6.982488000000	11.718542000000
C	12.717830000000	8.812733000000	24.459133000000	H	1.219073000000	6.571452000000	12.994889000000
O	12.654506000000	9.738990000000	23.608464000000	N	4.547304000000	6.536401000000	13.815622000000
C	11.375532000000	9.442786000000	26.543486000000	C	5.884586000000	5.955814000000	13.597011000000
C	10.195781000000	9.152980000000	27.511323000000	C	5.902834000000	4.450821000000	13.909751000000
C	10.140394000000	10.244814000000	28.601991000000	C	7.296758000000	3.942265000000	14.308314000000
C	8.839955000000	9.051465000000	26.784213000000	C	7.713363000000	4.208382000000	15.759855000000
H	11.494103000000	6.892083000000	26.789214000000	O	8.715225000000	3.599135000000	16.212890000000
H	10.641627000000	8.594874000000	24.687433000000	O	6.977625000000	5.069806000000	16.444318000000
H	12.317608000000	9.449051000000	27.111676000000	H	3.855422000000	5.973445000000	14.308827000000
H	11.241620000000	10.447240000000	26.126913000000	H	6.594987000000	6.473753000000	14.250001000000
H	10.394576000000	8.190563000000	28.020998000000	H	5.542377000000	3.887045000000	13.038876000000
H	8.816431000000	8.217705000000	26.069921000000	H	5.211654000000	4.242099000000	14.732435000000
H	8.628245000000	9.986455000000	26.248826000000	H	7.373288000000	2.860345000000	14.154671000000
H	8.036151000000	8.883286000000	27.511852000000	H	8.072405000000	4.388242000000	13.668117000000
H	11.118407000000	10.383396000000	29.082014000000	C	6.151624000000	-2.026403000000	15.618056000000
H	9.813951000000	11.203195000000	28.179940000000	C	6.512448000000	-0.592970000000	16.053959000000
H	9.419953000000	9.966749000000	29.381085000000	C	7.785135000000	-0.095370000000	-15.341829000000
N	13.841412000000	8.074941000000	24.643911000000	C	5.329146000000	0.367493000000	15.818997000000
C	14.886080000000	7.954549000000	23.612071000000	H	5.944972000000	-2.061425000000	14.539409000000
C	14.822496000000	6.485889000000	23.184672000000	H	6.717589000000	-0.610954000000	17.136448000000
O	14.702974000000	5.592211000000	24.098903000000	H	8.629533000000	-0.772184000000	15.523032000000
C	16.291932000000	8.419879000000	24.087817000000	H	7.625690000000	-0.051089000000	14.254997000000
C	16.294653000000	9.945998000000	24.297045000000	H	8.076153000000	0.905204000000	15.683318000000
C	16.780574000000	7.684393000000	25.350196000000	H	5.575627000000	1.381042000000	16.159335000000
H	13.786118000000	7.283069000000	25.273783000000	H	4.432946000000	0.030555000000	16.355063000000
H	14.579742000000	8.588371000000	22.775264000000	H	5.089508000000	0.419482000000	14.746812000000
H	16.978606000000	8.182342000000	23.260478000000	C	-3.705312000000	5.271250000000	20.029966000000
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H	17.803346000000	7.995694000000	25.593648000000	C	-2.302929000000	3.540326000000	21.351491000000
H	16.145757000000	7.932867000000	26.209836000000	C	-2.257318000000	2.049553000000	21.742687000000
H	17.292521000000	10.292302000000	24.590814000000	C	-0.913775000000	4.023282000000	20.886061000000
H	15.589828000000	10.227258000000	25.087665000000	H	-2.817336000000	5.838119000000	19.729357000000
H	16.001450000000	10.476275000000	23.384482000000	H	-4.308992000000	3.269454000000	20.576480000000
N	14.816915000000	6.204860000000	21.881290000000	H	-3.056551000000	3.313875000000	19.334666000000
C	14.481053000000	4.856107000000	21.410776000000	H	-2.581686000000	4.114284000000	22.250354000000
C	12.947495000000	4.647717000000	21.429524000000	H	-1.491250000000	1.859387000000	22.505814000000
O	12.608581000000	3.234635000000	21.615739000000	H	-3.220851000000	1.708731000000	22.140995000000
H	14.800319000000	6.949366000000	21.147337000000	H	-2.030594000000	1.430782000000	20.861871000000
H	14.958849000000	4.115355000000	22.058047000000	H	-0.905784000000	5.095599000000	20.664520000000
H	12.488172000000	5.233354000000	22.227919000000	H	-0.155458000000	3.831726000000	21.657412000000
H	12.517387000000	4.961390000000	20.477567000000	H	-0.620318000000	3.489691000000	19.970809000000
H	12.606001000000	3.061831000000	22.594383000000	C	8.275310000000	10.306773000000	13.157119000000
C	3.736458000000	11.361875000000	16.496338000000	C	8.137888000000	11.596239000000	13.967175000000
C	3.116085000000	10.064947000000	16.002871000000	O	7.373740000000	12.507797000000	13.555197000000
O	2.411912000000	9.337137000000	16.761317000000	C	8.472476000000	8.961960000000	13.907063000000
C	5.287256000000	11.400817000000	16.389134000000	C	9.847509000000	8.751759000000	14.514745000000
C	5.980760000000	10.265122000000	17.085928000000	O	10.061350000000	9.211495000000	15.711854000000
N	6.810074000000	10.462381000000	18.185809000000	O	10.744802000000	8.125006000000	13.827160000000
C	5.994055000000	8.901591000000	16.852665000000	H	7.354381000000	10.226557000000	12.574205000000
C	7.300454000000	9.264058000000	18.583475000000	H	7.719966000000	8.874399000000	14.695294000000
N	6.822498000000	8.290881000000	17.790556000000	H	8.303427000000	8.163546000000	13.180402000000
H	3.322061000000	12.202482000000	15.924135000000	N	8.910890000000	11.735086000000	15.087500000000
H	5.588805000000	11.444368000000	15.335112000000	C	8.960909000000	12.983658000000	15.846470000000
H	5.630039000000	12.344379000000	16.826656000000	C	10.349056000000	13.619284000000	15.920835000000
H	5.482070000000	8.327028000000	16.102194000000	O	10.551007000000	14.593782000000	16.693839000000
H	7.966212000000	9.114298000000	19.414872000000	H	9.360243000000	10.907711000000	15.487756000000
				H	8.275857000000	13.689000000000	15.366155000000

N	11.305669000000	13.069340000000	15.135336000000	H	4.919047000000	2.511624000000	19.154615000000
C	12.707062000000	13.468543000000	15.120707000000	H	3.573572000000	2.636369000000	20.296954000000
C	13.575989000000	12.212748000000	15.076612000000	N	0.515259000000	0.243651000000	19.315901000000
O	13.139846000000	11.435461000000	13.935885000000	C	-0.562314000000	0.125393000000	18.323770000000
H	11.072086000000	12.297702000000	14.523352000000	C	-0.594760000000	1.290382000000	17.327106000000
H	12.910042000000	14.067630000000	16.012415000000	O	-1.498237000000	2.163183000000	17.356542000000
H	13.452255000000	11.648238000000	16.013395000000	H	0.279508000000	0.609054000000	20.227516000000
H	14.635652000000	12.494508000000	14.984428000000	H	-0.432688000000	-0.820844000000	17.787796000000
H	13.270433000000	10.459559000000	14.077010000000	N	0.427420000000	1.303178000000	16.432393000000
C	7.495235000000	16.287152000000	19.889852000000	C	0.584999000000	2.409851000000	15.488411000000
C	7.283473000000	16.630569000000	21.362188000000	C	1.860733000000	2.226998000000	14.647030000000
O	7.788250000000	17.670279000000	21.875624000000	C	2.311956000000	3.549199000000	14.052742000000
C	8.285872000000	14.995806000000	19.572216000000	O	2.597442000000	4.526815000000	14.797792000000
C	7.520089000000	13.684965000000	19.687712000000	N	2.405780000000	3.629302000000	12.702778000000
O	7.998920000000	15.780674000000	19.009949000000	H	1.165095000000	0.607850000000	16.550629000000
O	6.513080000000	13.560729000000	20.469813000000	H	0.638552000000	3.355421000000	16.037337000000
H	6.514818000000	16.240694000000	19.397503000000	H	1.712364000000	1.465406000000	13.873739000000
H	8.702041000000	15.054625000000	18.560735000000	H	2.677055000000	1.881694000000	15.294862000000
H	9.164860000000	14.923332000000	20.229672000000	H	2.172126000000	2.856316000000	12.100746000000
N	6.496990000000	15.780674000000	22.078032000000	H	2.701849000000	4.499054000000	12.281276000000
C	6.005997000000	16.118246000000	23.410900000000	C	-2.904611000000	6.186972000000	15.615159000000
C	7.051671000000	16.185567000000	24.531059000000	C	-1.693119000000	7.083277000000	15.832935000000
O	6.803498000000	16.828342000000	25.574687000000	O	-0.851220000000	7.265644000000	14.905758000000
H	6.219937000000	14.910874000000	21.606085000000	C	-2.535982000000	4.821263000000	15.011361000000
H	5.525499000000	17.101824000000	23.402297000000	H	-3.459130000000	6.055224000000	16.551573000000
H	5.250970000000	15.375948000000	23.689805000000	H	-2.044183000000	4.178436000000	15.749055000000
N	8.211725000000	15.509090000000	24.304156000000	H	-3.437157000000	4.301217000000	14.668645000000
C	9.348247000000	15.511408000000	25.226215000000	H	-1.869591000000	4.964967000000	14.154857000000
C	10.379049000000	16.609845000000	24.890357000000	N	-1.604198000000	7.678588000000	17.047273000000
O	11.484661000000	16.636456000000	25.496003000000	C	-0.520644000000	8.572474000000	17.456077000000
C	10.037703000000	14.135061000000	25.235952000000	C	-0.017041000000	8.102833000000	18.827040000000
C	9.169755000000	13.040260000000	25.885376000000	O	-0.771934000000	7.460030000000	19.614479000000
O	8.762719000000	13.217162000000	27.063807000000	C	-0.960332000000	10.075790000000	17.510564000000
O	8.942943000000	11.963165000000	25.157038000000	C	-1.307598000000	10.600008000000	16.105370000000
H	8.301116000000	14.991378000000	23.439703000000	C	-2.117363000000	10.318094000000	18.498503000000
H	8.956058000000	15.710554000000	26.229543000000	H	-2.220865000000	7.384295000000	17.794899000000
H	10.321386000000	13.849527000000	24.215910000000	H	0.283886000000	8.489478000000	16.722275000000
H	10.958564000000	14.245029000000	25.818163000000	H	-0.075375000000	10.620360000000	17.868345000000
N	10.043972000000	17.501495000000	23.921294000000	H	-0.479320000000	10.465907000000	15.402463000000
C	10.964330000000	18.542716000000	23.469238000000	H	-1.550443000000	11.668647000000	16.152770000000
C	11.233182000000	18.468342000000	21.953901000000	H	-2.185150000000	10.079945000000	15.701540000000
C	11.843838000000	17.171410000000	21.440301000000	H	-1.891198000000	9.947727000000	19.503816000000
C	12.663082000000	16.348422000000	22.233777000000	H	-2.331342000000	11.390657000000	18.570260000000
C	11.595752000000	16.779220000000	20.111460000000	H	-3.033921000000	9.822523000000	18.153908000000
C	13.220200000000	15.177041000000	21.704124000000	N	1.253549000000	8.451947000000	19.133296000000
C	12.145363000000	15.607690000000	19.577121000000	C	1.837592000000	8.211141000000	20.453699000000
C	12.967227000000	14.804457000000	20.378754000000	C	2.364973000000	6.767323000000	20.675613000000
H	9.145246000000	17.445721000000	23.449136000000	C	3.448324000000	6.341519000000	19.732542000000
H	11.880013000000	18.432200000000	24.055034000000	N	3.214070000000	5.611598000000	18.556326000000
H	10.284971000000	18.640623000000	21.428751000000	C	4.808193000000	6.567827000000	19.756946000000
H	11.891657000000	19.313095000000	21.693258000000	C	4.411829000000	5.424936000000	17.928089000000
H	12.840190000000	16.592279000000	23.276257000000	N	5.395714000000	5.993071000000	18.631361000000
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H	13.397738000000	13.891280000000	19.976936000000	H	2.750299000000	6.717756000000	21.701850000000
C	2.785275000000	-0.070488000000	20.196150000000	H	5.404106000000	7.101397000000	20.476825000000
C	1.805070000000	-0.106481000000	19.039285000000	H	4.533225000000	4.906528000000	16.994906000000
O	2.144922000000	-0.465256000000	17.875305000000	C	10.401006000000	0.518368000000	18.651881000000
C	4.145357000000	0.576422000000	19.836127000000	C	10.170767000000	1.977337000000	19.069997000000
C	5.141440000000	0.389924000000	21.005429000000	N	10.720742000000	2.946457000000	18.108500000000
C	3.969454000000	2.056911000000	19.451581000000	C	12.008005000000	3.312525000000	18.046936000000
C	6.583285000000	0.813719000000	20.678764000000	N	12.910150000000	2.824208000000	18.631697000000
H	2.342121000000	0.447684000000	21.057850000000	N	12.449188000000	4.158342000000	17.098369000000
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H	6.661934000000	1.884793000000	20.464199000000	H	12.666399000000	2.622580000000	19.917670000000
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H 13.201098000000 4.797121000000 17.366479000000
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O 8.156410000000 4.731683000000 19.340486000000
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C 8.670870000000 5.136890000000 21.701433000000
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H 2.026615000000 4.859753000000 17.020434000000
H 1.663146000000 4.175473000000 18.632010000000
H 1.145154000000 5.823773000000 18.222934000000

⁵TS_{me,reb} – VioC MeHis Transition state for radical rebound

C 11.514792000000 4.624485000000 25.492739000000
C 11.684571000000 5.976661000000 24.818189000000
O 11.518730000000 6.134115000000 23.581099000000
C 12.812526000000 3.789999000000 25.667922000000
O 13.413210000000 3.463388000000 24.385949000000
C 12.521085000000 2.475797000000 26.392292000000
H 11.056585000000 4.757603000000 26.482144000000
H 13.539069000000 4.377627000000 26.247656000000
H 14.139595000000 4.122020000000 24.170011000000
H 13.446387000000 1.904246000000 26.508066000000
H 12.087024000000 2.651880000000 27.383345000000
H 11.818862000000 1.872435000000 25.805839000000
N 12.032075000000 7.036467000000 25.614506000000
C 12.042126000000 8.417465000000 25.091998000000
C 13.155814000000 8.609243000000 24.049476000000
O 12.999176000000 9.355149000000 23.047248000000
C 12.155470000000 9.435692000000 26.252644000000
C 11.065179000000 9.310685000000 27.350302000000
C 11.302096000000 10.382939000000 28.434920000000
C 9.642005000000 9.433787000000 26.769753000000
H 12.042410000000 6.921241000000 26.618429000000
H 11.109338000000 8.588097000000 24.546054000000
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H 10.611654000000 10.231648000000 29.274290000000
N 14.319268000000 7.949617000000 24.282205000000
C 15.309033000000 7.710878000000 23.219799000000
C 15.234148000000 6.204974000000 22.960585000000
O 15.151167000000 5.409185000000 23.962756000000
C 16.735053000000 8.223187000000 23.572459000000
C 16.750184000000 9.763128000000 23.596475000000
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H 14.332275000000 7.265684000000 25.029543000000
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H 17.383699000000 7.883454000000 22.750092000000
H 17.252216000000 6.546156000000 24.895005000000
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H 17.760294000000 10.134449000000 23.805903000000
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N 15.178635000000 5.794785000000 21.690635000000
C 14.792879000000 4.414741000000 21.377068000000
C 13.257702000000 4.276934000000 21.474254000000
O 12.868164000000 2.888399000000 21.721932000000
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H	6.900611000000	11.523370000000	18.795671000000	N	11.716476000000	12.920704000000	15.455750000000
N	3.431834000000	9.729888000000	14.735499000000	C	13.156455000000	13.140535000000	15.428350000000
C	3.102336000000	8.433731000000	14.134485000000	C	13.855750000000	11.785968000000	15.348159000000
C	4.453370000000	7.880974000000	13.649174000000	O	13.302657000000	11.092924000000	14.203023000000
O	5.278403000000	8.658002000000	13.093578000000	H	11.387549000000	12.164173000000	14.870423000000
C	2.043726000000	8.599976000000	13.007138000000	H	13.445224000000	13.691049000000	16.328042000000
O	0.830238000000	9.156138000000	13.554195000000	H	13.676713000000	11.223556000000	16.277267000000
C	1.766662000000	7.289677000000	12.260322000000	H	14.940974000000	11.931113000000	15.240141000000
H	4.066417000000	10.291174000000	14.178937000000	H	13.341221000000	10.105186000000	14.307741000000
H	2.678656000000	7.802034000000	14.919677000000	C	6.708302000000	16.180873000000	20.526524000000
H	2.420619000000	9.353208000000	12.306828000000	C	6.771849000000	16.416030000000	22.034742000000
H	0.288604000000	8.460989000000	14.011343000000	O	7.099754000000	17.539575000000	22.511921000000
H	0.975179000000	7.457357000000	11.524002000000	C	7.675540000000	15.134678000000	19.921279000000
H	2.659905000000	6.935500000000	11.731476000000	C	7.288618000000	13.669170000000	20.079971000000
H	1.425569000000	6.515085000000	12.957126000000	O	7.784863000000	12.834546000000	19.211774000000
N	4.730918000000	6.584385000000	13.924646000000	O	6.560018000000	13.282235000000	21.064756000000
C	6.107299000000	6.061433000000	13.819743000000	H	5.676867000000	15.912281000000	20.261502000000
C	6.160697000000	4.554389000000	14.113527000000	H	7.785292000000	15.326404000000	18.849291000000
C	7.539104000000	4.090436000000	14.626054000000	H	8.684914000000	15.263721000000	20.337084000000
C	7.753429000000	4.252036000000	16.132941000000	N	6.416884000000	15.368126000000	22.828060000000
O	8.397529000000	3.353322000000	16.744120000000	C	6.188295000000	15.523690000000	24.261445000000
O	7.251556000000	5.331312000000	16.690672000000	C	7.422160000000	15.809307000000	25.126522000000
H	4.025791000000	5.991125000000	14.360360000000	O	7.278735000000	16.284986000000	26.274495000000
H	6.733180000000	6.592045000000	14.544712000000	H	6.249927000000	14.473518000000	22.349951000000
H	5.899834000000	3.992270000000	13.206684000000	H	5.500804000000	16.354784000000	24.449548000000
H	5.403805000000	4.299845000000	14.864127000000	H	5.717617000000	14.606599000000	24.630089000000
H	7.704233000000	3.034954000000	14.394546000000	N	8.625037000000	15.505926000000	24.566023000000
H	8.344141000000	4.651147000000	14.128742000000	C	9.914056000000	15.771682000000	25.204153000000
C	5.629899000000	-1.697573000000	16.130423000000	C	10.522994000000	17.122122000000	24.766750000000
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C	7.729678000000	-0.274778000000	15.837459000000	C	10.905560000000	14.624272000000	24.921667000000
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H	5.483138000000	-1.769111000000	15.043376000000	O	10.678089000000	13.303733000000	26.917136000000
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H	7.641707000000	-0.316878000000	14.742384000000	H	9.738855000000	15.827459000000	26.284475000000
H	8.219593000000	0.669888000000	16.101145000000	H	10.964704000000	14.440765000000	23.841681000000
H	5.950881000000	1.769969000000	16.429386000000	H	11.886611000000	14.959150000000	25.269246000000
H	4.481738000000	0.770605000000	16.593861000000	N	9.736534000000	17.946007000000	24.025500000000
H	5.321609000000	0.876616000000	15.027864000000	C	10.217743000000	19.230177000000	23.519070000000
C	-3.946239000000	5.592278000000	20.076174000000	C	10.096109000000	19.341656000000	21.987409000000
C	-3.796947000000	4.101405000000	19.726975000000	C	10.833938000000	18.284214000000	21.177881000000
C	-2.626424000000	3.390224000000	20.449887000000	C	12.006269000000	17.655998000000	21.633610000000
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H	-1.927537000000	1.347422000000	20.815405000000	H	9.300978000000	19.300978000000	21.722383000000
H	-3.688728000000	1.479348000000	20.661214000000	H	10.451102000000	20.345293000000	21.701253000000
H	-2.666375000000	1.601881000000	19.209935000000	H	12.402877000000	17.882560000000	22.618077000000
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C	9.747695000000	8.912060000000	14.779773000000	C	3.593069000000	0.395026000000	19.939297000000
O	10.038464000000	9.346977000000	15.971695000000	C	4.468710000000	0.167996000000	16.17946030000000
O	10.524202000000	8.118080000000	14.116406000000	C	3.146988000000	1.862426000000	19.794696000000
H	7.636728000000	10.727115000000	12.695807000000	C	5.808470000000	0.922435000000	21.173186000000
H	7.679670000000	9.432175000000	14.929829000000	H	1.717344000000	-0.302219000000	20.814743000000
H	8.122843000000	8.569499000000	13.453830000000	H	4.186386000000	0.123383000000	19.055104000000
N	9.140056000000	12.008994000000	15.344907000000	H	4.668391000000	-0.909621000000	21.290766000000
C	9.367157000000	13.250117000000	16.082930000000	H	3.896219000000	0.457624000000	22.089615000000
C	10.838143000000	13.669952000000	16.165889000000	H	6.412733000000	0.663394000000	22.050133000000
O	11.177212000000	14.657118000000	16.867169000000	H	6.389194000000	0.665816000000	20.278289000000

H	5.670620000000	2.008746000000	21.178063000000	H	12.561498000000	2.336961000000	19.995287000000
H	2.523748000000	2.001700000000	18.903418000000	H	13.525451000000	2.939184000000	18.707512000000
H	4.005970000000	2.533381000000	19.700085000000	H	11.033235000000	4.218265000000	16.662909000000
H	2.564704000000	2.181878000000	20.675042000000	H	12.570814000000	4.506573000000	17.357422000000
N	0.248776000000	-0.313537000000	18.748022000000	Fe	7.502017000000	6.418777000000	18.383794000000
C	-0.626225000000	-0.359090000000	17.568101000000	O	8.268978000000	4.965639000000	19.764321000000
C	-0.574313000000	0.929920000000	16.737440000000	O	9.240605000000	7.163023000000	17.807425000000
O	-1.531033000000	1.745074000000	16.724560000000	C	8.141239000000	5.744942000000	20.799871000000
H	-0.163045000000	-0.049486000000	19.631440000000	O	7.689273000000	6.945085000000	20.601332000000
H	-0.325387000000	-1.214173000000	16.954120000000	C	8.536343000000	5.264709000000	22.170573000000
N	0.581732000000	1.113244000000	16.046657000000	C	7.772643000000	5.954847000000	23.309094000000
C	0.832598000000	2.344847000000	15.298013000000	H	8.400725000000	4.177422000000	22.193819000000
C	2.051543000000	2.180481000000	14.376629000000	H	9.614032000000	5.447106000000	22.298515000000
C	2.562018000000	3.525912000000	13.892248000000	H	6.696598000000	5.752439000000	23.250013000000
O	2.785979000000	4.468808000000	14.700482000000	H	7.911498000000	7.038397000000	23.263767000000
N	2.792354000000	3.658876000000	12.562635000000	N	12.105228000000	7.850313000000	16.982248000000
H	1.337073000000	0.447579000000	16.215137000000	C	12.412431000000	7.999742000000	18.450072000000
H	1.009203000000	3.179595000000	15.984658000000	C	13.570923000000	7.010169000000	18.827708000000
H	1.816015000000	1.515456000000	13.538549000000	O	13.557747000000	5.864012000000	18.257313000000
H	2.874520000000	1.717538000000	14.939004000000	C	11.201413000000	7.696365000000	19.297720000000
H	2.605823000000	2.916496000000	11.907958000000	C	10.646580000000	8.647781000000	20.311248000000
H	3.150129000000	4.536425000000	12.211376000000	C	10.684264000000	10.154830000000	19.928526000000
C	-2.816401000000	6.112438000000	15.386140000000	N	9.688550000000	10.975131000000	20.637222000000
C	-1.626036000000	7.026704000000	15.645879000000	C	9.788192000000	11.359061000000	21.941381000000
O	-0.744803000000	7.209621000000	14.756422000000	N	10.820842000000	11.027356000000	22.718519000000
C	-2.422641000000	4.783538000000	14.721055000000	N	8.819438000000	12.117364000000	22.497362000000
H	-3.368799000000	5.929544000000	16.315478000000	O	14.380527000000	7.447933000000	19.711326000000
H	-1.927853000000	4.109475000000	15.428178000000	H	12.770332000000	9.018187000000	18.606705000000
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N	-1.604313000000	7.642602000000	16.853063000000	H	11.197903000000	8.496591000000	21.258349000000
C	-0.554937000000	8.559061000000	17.303256000000	H	9.614903000000	8.346977000000	20.526249000000
C	-0.117856000000	8.107730000000	18.703091000000	H	10.454135000000	10.267131000000	18.864489000000
O	-0.917601000000	7.493192000000	19.467783000000	H	11.690570000000	10.565032000000	20.089014000000
C	-1.017681000000	10.055828000000	17.316885000000	H	9.023899000000	11.507811000000	20.069542000000
C	-1.294057000000	10.559306000000	15.888432000000	H	11.603113000000	10.427986000000	22.473621000000
C	-2.231195000000	10.291943000000	18.235979000000	H	10.789201000000	11.423818000000	23.677407000000
H	-2.252111000000	7.351082000000	17.575171000000	H	7.946832000000	12.331620000000	22.012060000000
H	0.286182000000	8.479827000000	16.611116000000	H	8.977621000000	12.384611000000	23.475216000000
H	-0.160988000000	10.616708000000	17.716524000000	H	12.911236000000	8.022492000000	16.356298000000
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H	-1.554025000000	11.624710000000	15.909601000000	H	11.748725000000	6.898209000000	16.754771000000
H	-2.140790000000	10.021984000000	15.443474000000	O	13.102200000000	8.390195000000	14.474445000000
H	-2.055360000000	9.937884000000	19.256877000000	H	12.109605000000	8.264400000000	14.268509000000
H	-2.465759000000	11.361754000000	18.280289000000	H	13.657863000000	7.856662000000	13.879772000000
H	-3.118970000000	9.776630000000	17.847626000000	O	10.467066000000	5.851276000000	15.887186000000
N	1.145459000000	8.435741000000	19.059474000000	H	9.867805000000	6.261511000000	16.595201000000
C	1.669678000000	8.165704000000	20.400000000000	H	10.413854000000	6.373666000000	15.055089000000
C	2.180997000000	6.714097000000	20.608434000000	H	9.882172000000	-0.420136000000	20.167426000000
C	3.350926000000	6.326053000000	19.756390000000	H	2.720979000000	-1.585316000000	20.128344000000
N	3.234987000000	5.660477000000	18.526486000000	H	-1.654213000000	-0.496845000000	17.901820000000
C	4.703538000000	6.530921000000	19.933657000000	H	-0.062874000000	2.594138000000	14.720594000000
C	4.493145000000	5.493208000000	18.017526000000	H	4.644933000000	-1.759481000000	16.608552000000
N	5.402813000000	6.011902000000	18.845235000000	H	6.223791000000	-2.566005000000	16.442465000000
H	1.750064000000	8.877832000000	18.361388000000	H	-4.799465000000	6.033628000000	19.545178000000
H	0.871775000000	8.354109000000	21.125391000000	H	-4.127004000000	5.723283000000	21.151196000000
H	1.340085000000	6.029343000000	20.453621000000	H	2.484633000000	8.871395000000	20.585020000000
H	2.469738000000	6.621218000000	21.663107000000	H	-3.492040000000	6.667012000000	14.719058000000
H	5.228417000000	7.016756000000	20.738123000000	H	6.501515000000	6.283808000000	12.822058000000
H	4.704667000000	5.024922000000	17.073768000000	H	3.410912000000	11.558466000000	17.508926000000
C	10.163318000000	0.218582000000	19.321240000000	H	6.926027000000	17.151848000000	20.075113000000
C	9.974648000000	1.698611000000	19.685165000000	H	9.393569000000	10.659665000000	12.689804000000
N	10.313771000000	2.614252000000	18.587026000000	H	15.147492000000	4.186406000000	20.369013000000
C	11.552220000000	3.022734000000	18.289174000000	H	10.823206000000	4.045318000000	24.873822000000
N	12.624276000000	2.596588000000	19.006370000000	H	13.436799000000	13.745872000000	14.555567000000
N	11.779456000000	3.866329000000	17.264045000000	H	8.981055000000	13.174757000000	17.106763000000
H	11.207287000000	0.007950000000	19.066435000000	H	9.639779000000	20.045472000000	23.975614000000
H	9.540392000000	-0.050112000000	18.461625000000	H	8.132474000000	5.600863000000	24.281485000000
H	8.929758000000	1.907573000000	19.929501000000	C	2.003385000000	5.195213000000	17.886822000000
H	10.561405000000	1.957765000000	20.574491000000	H	2.247016000000	4.850807000000	16.880992000000
H	9.533269000000	3.015362000000	18.048638000000	H	1.554719000000	4.377959000000	18.460277000000

H	1.285249000000	6.011196000000	17.813557000000	H	7.675683000000	9.227153000000	19.819920000000
⁵P_{me} – VioC MeHis Product bound state							
C	11.631838000000	4.681801000000	25.719405000000	H	6.887455000000	11.451280000000	18.819463000000
C	11.775286000000	6.012046000000	24.997853000000	N	3.479426000000	9.643190000000	14.758840000000
O	11.568011000000	6.130131000000	23.763484000000	C	3.156657000000	8.365784000000	14.118710000000
C	12.922140000000	3.821973000000	25.813252000000	C	4.513201000000	7.826294000000	13.630700000000
O	13.419805000000	3.457598000000	24.497386000000	O	5.375242000000	8.632151000000	13.180751000000
C	12.656111000000	2.527403000000	26.581563000000	C	2.099095000000	8.565939000000	12.994924000000
H	11.255141000000	4.847000000000	26.737768000000	O	0.896760000000	9.134361000000	13.553677000000
H	13.700197000000	4.403754000000	26.328601000000	C	1.800163000000	7.272165000000	12.227455000000
H	14.137928000000	4.099071000000	24.221559000000	H	4.121444000000	10.216174000000	14.223656000000
H	13.575677000000	1.938416000000	26.644090000000	H	2.731431000000	7.709521000000	14.882001000000
H	12.295404000000	2.729890000000	27.596747000000	H	2.486646000000	9.324866000000	12.306242000000
H	11.903024000000	1.929121000000	26.056191000000	H	0.345765000000	8.443136000000	14.005537000000
N	12.150555000000	7.098982000000	25.744232000000	H	1.017928000000	7.467992000000	11.488197000000
C	12.129443000000	8.460571000000	25.172889000000	H	2.689850000000	6.903746000000	11.702659000000
C	13.196364000000	8.623967000000	24.078388000000	H	1.439508000000	6.494481000000	12.910583000000
O	13.002509000000	9.357181000000	23.074599000000	N	4.763157000000	6.507466000000	13.799453000000
C	12.281462000000	9.518921000000	26.291511000000	C	6.136686000000	5.981643000000	13.689817000000
C	11.232909000000	9.425794000000	27.432594000000	C	6.187647000000	4.480572000000	14.014137000000
C	11.506542000000	10.531624000000	28.473306000000	C	7.579707000000	4.016292000000	14.505359000000
C	9.789410000000	9.526811000000	26.899661000000	C	7.819820000000	4.227230000000	16.003268000000
H	12.194691000000	7.019883000000	26.750655000000	O	8.061985000000	3.213350000000	16.722480000000
H	11.174503000000	8.605955000000	24.658542000000	O	7.806089000000	5.470966000000	16.446241000000
H	13.293528000000	9.448151000000	26.716890000000	H	4.023479000000	5.870575000000	14.093283000000
H	12.191973000000	10.507518000000	25.827445000000	H	6.769202000000	6.528521000000	14.397146000000
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H	11.312266000000	11.518456000000	28.034179000000	C	6.130324000000	-0.457033000000	16.614864000000
H	10.847166000000	10.407006000000	29.341647000000	C	7.552037000000	-0.451678000000	16.021015000000
N	14.363781000000	7.954108000000	24.267654000000	C	5.304774000000	0.723687000000	16.066433000000
C	15.291693000000	7.684101000000	23.158534000000	H	5.308533000000	-1.987020000000	15.292001000000
C	15.186949000000	6.175783000000	22.928292000000	H	6.221471000000	-0.317043000000	17.704403000000
O	15.170309000000	5.393766000000	23.943555000000	H	8.167465000000	-1.250442000000	16.454671000000
C	16.740297000000	8.185481000000	23.421014000000	H	7.515198000000	-0.614684000000	14.934408000000
C	16.773408000000	9.725468000000	23.418636000000	H	8.047167000000	0.508957000000	16.202838000000
C	17.351974000000	7.617953000000	24.716201000000	H	5.797462000000	1.675906000000	16.291738000000
H	14.402978000000	7.282152000000	25.024856000000	H	4.299210000000	0.727650000000	16.505871000000
H	14.892316000000	8.209205000000	22.285673000000	H	5.202394000000	0.640016000000	14.974008000000
H	17.337980000000	7.824635000000	22.569368000000	C	-3.851694000000	5.172602000000	19.509693000000
H	17.313570000000	6.525064000000	24.740279000000	C	-3.577076000000	3.666819000000	19.661297000000
H	18.397752000000	7.934250000000	24.807678000000	C	-2.563032000000	3.320481000000	20.779598000000
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N	15.038067000000	5.747136000000	21.670518000000	H	-3.204521000000	3.252399000000	18.712708000000
C	14.617223000000	4.366636000000	21.409717000000	H	-2.873353000000	3.849051000000	21.695742000000
C	13.092966000000	4.267681000000	21.608597000000	H	-1.863579000000	1.542686000000	21.860736000000
O	12.677542000000	2.874132000000	21.767724000000	H	-3.580013000000	1.481707000000	21.417146000000
H	14.847309000000	6.407611000000	20.892178000000	H	-2.349609000000	1.236114000000	20.171353000000
H	15.129607000000	3.692875000000	22.101006000000	H	-1.081065000000	4.864419000000	20.265789000000
H	12.779185000000	4.841283000000	22.479169000000	H	-0.428739000000	3.520787000000	21.220652000000
H	12.569439000000	4.664521000000	20.739725000000	H	-0.803330000000	3.291343000000	19.494987000000
H	12.763591000000	2.665628000000	22.729459000000	C	8.693064000000	11.090677000000	13.306690000000
C	3.774544000000	11.279481000000	16.542365000000	C	8.889629000000	12.389198000000	14.088427000000
C	3.185591000000	9.970727000000	16.035997000000	O	8.649551000000	13.491001000000	13.538483000000
O	2.482657000000	9.222311000000	16.775938000000	C	8.433846000000	9.791635000000	14.112630000000
C	5.326465000000	11.347212000000	16.432845000000	C	9.689895000000	9.185135000000	14.705367000000
C	6.030527000000	10.267098000000	17.198349000000	O	10.005492000000	9.477845000000	15.934040000000
N	6.646738000000	10.509628000000	18.422128000000	O	10.415720000000	8.412567000000	13.962264000000
C	6.199527000000	8.915918000000	16.958318000000	H	7.844394000000	11.270223000000	12.640151000000
C	7.155852000000	9.341631000000	18.885978000000	H	7.720819000000	9.982930000000	14.917487000000
N	6.911447000000	8.351060000000	18.013746000000	H	7.981278000000	9.060457000000	13.438438000000
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H	5.625395000000	11.313402000000	15.377565000000	C	9.679333000000	13.469361000000	16.171942000000
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H	5.879604000000	8.327192000000	16.117328000000	O	11.567163000000	14.645620000000	17.129666000000
				H	9.510755000000	11.372642000000	15.789506000000

H	9.246189000000	14.337048000000	15.665430000000	H	2.358945000000	2.276179000000	18.898591000000
N	12.017570000000	12.932025000000	15.659874000000	H	3.817353000000	2.863140000000	19.699916000000
C	13.471443000000	13.016832000000	15.710775000000	H	2.380077000000	2.479233000000	20.662026000000
C	14.046907000000	11.611683000000	15.554856000000	N	0.137553000000	0.018030000000	18.857626000000
O	13.483925000000	11.060289000000	14.339651000000	C	-0.774525000000	-0.037892000000	17.706842000000
H	11.651370000000	12.247663000000	15.011296000000	C	-0.669581000000	1.189349000000	16.791574000000
H	13.765725000000	13.469962000000	16.661557000000	O	-1.584123000000	2.048879000000	16.736454000000
H	13.775758000000	11.002486000000	16.430777000000	H	-0.233894000000	0.340076000000	19.739986000000
H	15.144478000000	11.660935000000	15.499631000000	H	-0.552909000000	-0.947643000000	17.139065000000
H	13.440835000000	10.067851000000	14.358036000000	N	0.478903000000	1.260936000000	16.067566000000
C	6.549637000000	16.124924000000	20.542106000000	C	0.775168000000	2.415885000000	15.220758000000
C	6.619007000000	16.335642000000	22.054101000000	C	1.929509000000	2.099238000000	14.255187000000
O	6.910613000000	17.462652000000	22.546250000000	C	2.479128000000	3.366915000000	13.626743000000
C	7.543981000000	15.121990000000	19.907893000000	O	2.805758000000	4.356930000000	14.336388000000
C	7.205766000000	13.641526000000	20.044332000000	N	2.620045000000	3.380849000000	12.277615000000
O	7.715811000000	12.837613000000	19.156089000000	H	1.202623000000	0.570131000000	16.273132000000
O	6.500492000000	13.216601000000	21.030731000000	H	1.045046000000	3.282429000000	15.833507000000
H	5.524936000000	15.827787000000	20.281409000000	H	1.608518000000	1.379374000000	13.494408000000
H	7.631909000000	15.335730000000	18.837846000000	H	2.756561000000	1.638479000000	14.813258000000
H	8.553138000000	15.276652000000	20.315781000000	H	2.349085000000	2.600371000000	11.701374000000
N	6.308243000000	15.262569000000	22.831705000000	H	2.984704000000	4.209437000000	11.829138000000
C	6.080194000000	15.384166000000	24.268642000000	C	-2.833637000000	6.197775000000	15.298544000000
C	7.305368000000	15.697218000000	25.136673000000	C	-1.611591000000	7.049046000000	15.613327000000
O	7.146685000000	16.139054000000	26.296308000000	O	-0.695149000000	7.209967000000	14.755011000000
H	6.167959000000	14.371423000000	22.338471000000	C	-2.478575000000	4.863356000000	14.622997000000
H	5.364607000000	16.187174000000	24.473640000000	H	-3.422410000000	6.024476000000	16.206867000000
H	5.642739000000	14.444761000000	24.621582000000	H	-2.019299000000	4.165827000000	15.331162000000
N	8.517038000000	15.456969000000	24.565914000000	H	-3.381805000000	4.385502000000	14.228369000000
C	9.796704000000	15.764051000000	25.204384000000	H	-1.787718000000	5.041588000000	13.792875000000
C	10.331946000000	17.160385000000	24.816977000000	N	-1.595593000000	7.637963000000	16.834283000000
O	11.487169000000	17.507785000000	25.179500000000	C	-0.513837000000	8.491591000000	17.326400000000
C	10.843450000000	14.681660000000	24.865391000000	C	-0.071021000000	7.950515000000	18.693423000000
C	10.554940000000	13.346578000000	25.573127000000	O	-0.866364000000	7.288132000000	19.420195000000
O	10.776296000000	13.280882000000	26.813721000000	C	-0.925372000000	9.999128000000	17.418137000000
O	10.094273000000	12.361307000000	24.832900000000	C	-1.191611000000	10.578791000000	16.016689000000
H	8.535888000000	15.064607000000	23.634206000000	C	-2.124700000000	10.229368000000	18.356865000000
H	9.632023000000	15.769563000000	26.287567000000	H	-2.268622000000	7.350304000000	17.533990000000
H	10.890894000000	14.537823000000	23.778755000000	H	0.314473000000	8.422708000000	16.618073000000
H	11.811116000000	15.057268000000	25.207963000000	H	-0.049101000000	10.511736000000	17.839307000000
N	9.512088000000	17.957462000000	24.082599000000	H	-0.337620000000	10.436650000000	15.346152000000
C	9.932637000000	19.272321000000	23.602837000000	H	-1.401470000000	11.653080000000	16.086345000000
C	9.864351000000	19.384574000000	22.067078000000	H	-2.065935000000	10.100749000000	15.557604000000
C	10.689590000000	18.368709000000	21.289658000000	H	-1.955278000000	9.814749000000	19.356078000000
C	11.897499000000	17.839048000000	21.776879000000	H	-2.320204000000	11.302762000000	18.461459000000
C	10.237271000000	17.940103000000	20.027262000000	H	-3.033143000000	9.768662000000	17.948284000000
C	12.624605000000	16.908934000000	21.021357000000	N	1.195936000000	8.256444000000	19.059547000000
C	10.960281000000	17.010104000000	19.272490000000	C	1.748567000000	7.872205000000	20.359787000000
C	12.160938000000	16.488494000000	19.770413000000	C	2.284853000000	6.416040000000	20.422716000000
H	8.592408000000	17.634036000000	23.794636000000	C	3.467498000000	6.119873000000	19.550244000000
H	10.944857000000	19.436706000000	23.979408000000	N	3.379200000000	5.681881000000	18.218970000000
H	8.814775000000	19.287497000000	21.761287000000	C	4.819818000000	6.199500000000	19.818170000000
H	10.175957000000	20.406764000000	21.796265000000	C	4.652270000000	5.525029000000	17.745792000000
H	12.256980000000	18.111908000000	22.763702000000	N	5.547653000000	5.832766000000	18.686134000000
H	9.301128000000	18.337748000000	19.640700000000	H	1.796409000000	8.733800000000	18.381961000000
H	13.547700000000	16.502313000000	21.425217000000	H	0.959762000000	7.977994000000	21.111570000000
H	10.600281000000	16.662042000000	18.310723000000	H	1.452601000000	5.737585000000	20.202098000000
H	12.698838000000	15.754353000000	19.181389000000	H	2.574997000000	6.224387000000	21.463405000000
C	2.274537000000	-0.272481000000	20.033219000000	H	5.330393000000	6.510439000000	20.714021000000
C	1.460598000000	-0.296967000000	18.757186000000	H	4.877470000000	5.216372000000	16.741108000000
O	1.975756000000	-0.590461000000	17.639080000000	C	10.446150000000	0.089775000000	19.409313000000
C	3.470313000000	0.716345000000	19.964424000000	C	9.920740000000	1.513048000000	19.647301000000
C	4.367859000000	0.539812000000	21.212424000000	N	10.096988000000	2.392378000000	18.483676000000
C	2.979614000000	2.166572000000	19.795948000000	C	11.223121000000	3.073903000000	18.223686000000
C	5.684357000000	1.332296000000	21.158738000000	N	12.330494000000	2.953876000000	18.985489000000
H	1.640890000000	-0.027281000000	20.896123000000	N	11.294288000000	3.897371000000	17.160025000000
H	4.060642000000	0.443003000000	19.078486000000	H	11.519964000000	0.098350000000	19.194325000000
H	4.599396000000	-0.529583000000	21.326907000000	H	9.932087000000	-0.374500000000	18.560886000000
H	3.798076000000	0.830775000000	22.108701000000	H	8.846863000000	1.492721000000	19.853282000000
H	6.309199000000	1.104737000000	22.029888000000	H	10.400411000000	1.959528000000	20.527301000000
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H	5.515569000000	2.414011000000	21.149085000000	H	12.319737000000	2.556327000000	19.925177000000

H	13.078451000000	3.609949000000	18.778796000000
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H	12.024616000000	4.610615000000	17.165385000000
Fe	7.641270000000	6.385429000000	18.373897000000
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O	9.669593000000	7.629212000000	18.138879000000
C	8.369204000000	5.695491000000	20.788498000000
O	7.721972000000	6.808937000000	20.726295000000
C	8.795360000000	5.098412000000	22.107755000000
C	7.890453000000	5.495905000000	23.281391000000
H	8.841874000000	4.010468000000	21.984222000000
H	9.822330000000	5.429081000000	22.320517000000
H	6.867656000000	5.124690000000	23.142299000000
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N	11.927403000000	7.727507000000	16.777806000000
C	12.177775000000	7.855191000000	18.248052000000
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O	13.231256000000	5.674799000000	18.149523000000
C	10.834355000000	7.654732000000	19.045056000000
C	10.654202000000	8.647242000000	20.211359000000
C	10.643266000000	10.155217000000	19.821888000000
N	9.656425000000	10.969086000000	20.554565000000
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N	10.806598000000	10.988219000000	22.628670000000
N	8.822264000000	12.113218000000	22.420969000000
O	13.999319000000	7.234767000000	19.656771000000
H	12.579134000000	8.855903000000	18.420054000000
H	9.540316000000	8.450848000000	17.609453000000
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H	10.380748000000	10.277864000000	18.765540000000
H	11.645506000000	10.586732000000	19.948415000000
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H	11.576572000000	10.377725000000	22.378858000000
H	10.791714000000	11.377144000000	23.588388000000
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H	9.001245000000	12.388031000000	23.401284000000
H	12.778928000000	7.785078000000	16.198626000000
H	11.296721000000	8.504679000000	16.443414000000
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O	13.024328000000	8.374255000000	14.320750000000
H	12.029842000000	8.392237000000	14.108925000000
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H	9.388806000000	6.023462000000	15.831508000000
H	10.300875000000	6.671455000000	14.659701000000
H	10.281945000000	-0.530798000000	20.298310000000
H	2.661303000000	-1.287903000000	20.190032000000
H	-1.798630000000	-0.082561000000	18.076806000000
H	-0.130415000000	2.687242000000	14.669817000000
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H	13.848054000000	13.655323000000	14.900055000000
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H	9.288365000000	20.047166000000	24.040154000000
C	8.276614000000	5.085467000000	24.221334000000
C	2.168565000000	5.482508000000	17.420448000000
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