Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Can an External Electric Field Switch between Ethylene Formation and L-Arginine Hydroxylation in the Ethylene Forming Enzyme?

Shobhit S. Chaturvedi, ‡[a] Simahudeen Bathir Jaber Sathik Rifayee, ‡[a] Rajeev Ramanan,[b] Joel A. Rankin,[c] Jian Hu,[d,e] Robert P. Hausinger,[c,d] Christo Z. Christov[a,*]

[a] Department of Chemistry, Michigan Technological University, Houghton, MI 49931, USA.

[b] Department of Chemistry, National Institute of Technology, Rourkela, OR 769008, India.

[c] Department of Microbiology and Molecular Genetics, Michigan State University, East Lansing, MI 48824, USA.

[d] Department of Biochemistry and Molecular Biology, and [e] Department of Chemistry, Michigan State University, East Lansing, MI 48824, USA.

*Corresponding Author: Christo Z. Christov: christov@mtu.edu

‡ Authors with equal contribution.

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Mutagenesis, protein purification, and assays for product formation

The E84A, R171A, R184A, and E285A variants of EFE were previously characterized and the R277A protein was shown to form insoluble inclusions in the cells.[1] Three new variants (D91A, D253A, and K269A) were created by site-directed mutagenesis using a gap-repair method[2] with the template pET28a:His6-TEV-EFE[3] and the following primers: CGCTGGGAAACCCGCCTTTCCCGAAATTTTTACCGTGTGTAAAG, D91A-F; GGGTTTCCC-AGCGGTAACTTC, D91A-R; ACCGTTTTTCCCGGAGCTATTCTGCAATTTATGACCGGGGGAC, D253A-F; TCCGGGAAAAACGGTCCAC, D253A-R; CTGTCCACTCCCCATGCAGTGAAATTGAATACCCGTGAACGG, K269A-F; and ATGGGGAGTGGACAGTAACTG, K269A-R. The DpnI-digested products were transformed into *Escherichia coli* DH5α.

The new EFE variants were expressed as previously described.[1] Cells were suspended in buffer A [50 mM NaH_2PO_4, 100 mM NaCl, 10 mM imidazole titrated to a pH of 7.5 with sodium hydroxide] supplemented with 1 mM phenylmethylsulfonyl fluoride and 1 U/mL Benzonase (EMD Millipore). Cells were lysed using two passes through a French pressure cell at 16,000 psi and clarified by ultracentrifugation at 146,000 rcf for 45 min at 4 °C. Nickel-nitrilotriacetic acid (Ni-NTA) resin was equilibrated in buffer A and the clarified lysate was applied to the resin by gravity flow. The column was washed with five column volumes of buffer A and the sample was eluted with three column volumes of buffer A containing 250 mM imidazole titrated with HCl to pH 7.5. Tobacco etch virus protease[4] and 5 mM ethylenediaminetetraacetic acid were added and digestion was continued overnight at 4 °C. The sample was exchanged into Buffer A using a PD-10 column (Cytiva), TEV and uncleaved EFE were removed using a Ni-NTA column equilibrated in buffer A, and the flow through fraction was collected by gravity flow. The preparation was concentrated using an Amicon Ultra-4 10 kDa cutoff spin filter (MilliporeSigma) and exchanged using a PD-10 column into 25 mM 4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid (HEPES) buffer adjusted to pH 8.0 with sodium hydroxide.

EFE (1 µM final concentration) was assayed in 2 mL of 25 mM HEPES titrated to pH 7.5 with sodium hydroxide, 0.5 mM 2OG, 0.5 mM L-Arg, 0.2 mM ammonium ferrous sulfate and 0.4 mM sodium L-ascorbate. After 80 min, the reactions were terminated with 100 µL of 3.6 M hydrochloric acid. The amounts of ethylene and P5C were determined as previously reported.[3]

Two-Dimensional Reaction Coordinate Scan.

We are particularly grateful to the reviewer for this very relevant and important point. We performed 2D PES calculations as the reviewer suggested. The calculated overall 2D PES is shown in **Figure S12**. We used an initial structure of **AI** (L-Arg in conformation A, in-line 2OG) complex, which leads to the ferryl intermediate's formation on applying -0.010 ExtEF (**Figure 2** in the manuscript and **Figure S16**). The reaction coordinate for the PES calculations in the first dimension was the decrease of the distance between O_d and C_2 of 2OG. During the scan, the bond between Fe and O_p breaks during step 13 (**Figure S13 and S16e**), and is created again at step 21, where Fe(II)-succinyl-peroxide intermediate is formed (**Figure S13 and S16b**). At step 23 from the scan, the ferryl is finally formed (**Figures S12, S16c**).

As the initial structure for the scans in the second dimension, the structure from each other step from the scan from the first dimension was taken. The reaction coordinate for the scans in the second dimension increased the Op-Od distance without restraining the O_d-C_2 bond (the reaction coordinate in the first dimension). In all second-dimension scans that started from structures up to 12 (from the first-dimension scan), the reaction proceeds through a very high barrier of 65-70 kcal/mol, breaking the high-energy O_p-O_d bond but not leading to the expected products (**Figures S12 and S14**). The second-dimension scans starting from steps 14 through 20 lead to very exothermic Fe(II)-succinyl-peroxide (with about -75 kcal/mol change in energy from the TS) (**Figure S15 and S16b**). The second-dimension scan starting from point 24 (from the first scan) forms the ferryl intermediate at the beginning (**Figures S15 and S16c**).

The high exothermicity of the Fe(II)-succinyl-peroxide intermediate in the 2D scans is consistent with the scans performed with the combined coordinate in the present manuscript and our prior

study, [5] with another computational study of the EFE, [6] and with studies of many different Fe(II)/2OG enzymes.[7–12]

Nonetheless, the fact that 2D PES show high energy jumps during the reaction path suggests that more complex conformational changes in the active site might contribute to the reaction. Such effects can be explored, for example, using QM/MM Meta dynamics simulations of the free energy surface of the reaction path [13–17], which could be a subject of future study. However, we should be cautious that the QM/MM MetD simulations are much more computationally demanding; they do not provide well-defined energy minima and transition state structures, which in this study are vital.

Table S1. Peroxosuccinate intermediate (IM) exothermicity from the TS state during O_2 activation, as reported in the literature.

Publication by Other Groups	**Energy jump from TS to IM (peroxosuccinate)**
Xue, J.; Lu, J.; Lai, W., Phys Chem Chem Phys 2019, 21 (19), 9957–9968.	34.7
Rugg, G.; Senn, H. M., Phys Chem Chem Phys 2017, 19 (44), 30107–30119.	62.6
Song, X.; Lu, J.; Lai, W., Phys Chem Chem Phys 2017, 19 (30), 20188–20197.	58.9
Wójcik, A.; Radoń, M.; Borowski, T., J. Phys. Chem. A 2016, 120 (8), 1261–1274.	57.2
Our earlier Publications	
Waheed, S. O.; Ramanan, R.; Chaturvedi, S. S.; Lehnert, N.; Schofield, C. J.; Christov, C. Z.; Karabencheva-Christova, T. G., ACS Cent. Sci. 2020, 6 (5), 795–814.	46.1
S. Chaturvedi, S.; Ramanan, R.; Hu, J.; P. Hausinger, R.; Z. Christov, C.. ACS Catal. 2021, 11 (3), 1578–1592.	AO-35.8 BO-37.9
S. Chaturvedi, S.; Ramanan, R.; Lehnert, N.; J. Schofield, C.; G. Karabencheva-	49.7

Christova, T.; Z. Christov, C., ACS Catal. 2019, 10 (2), 1195–1209.	
Current Manuscript	40 to 45

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(1) Martinez, S.; Fellner, M.; Herr, C. Q.; Ritchie, A.; Hu, J.; Hausinger, R. P. Structures and Mechanisms of the Non-Heme Fe(II)- and 2-Oxoglutarate-Dependent Ethylene-Forming Enzyme: Substrate Binding Creates a Twist. *J. Am. Chem. Soc.* **2017**, *139* (34), 11980–11988. https://doi.org/10.1021/jacs.7b06186.

(2) García-Nafría, J.; Watson, J. F.; Greger, I. H. IVA Cloning: A Single-Tube Universal Cloning System Exploiting Bacterial In Vivo Assembly. *Sci. Rep.* **2016**, *6* (1), 27459. https://doi.org/10.1038/srep27459.

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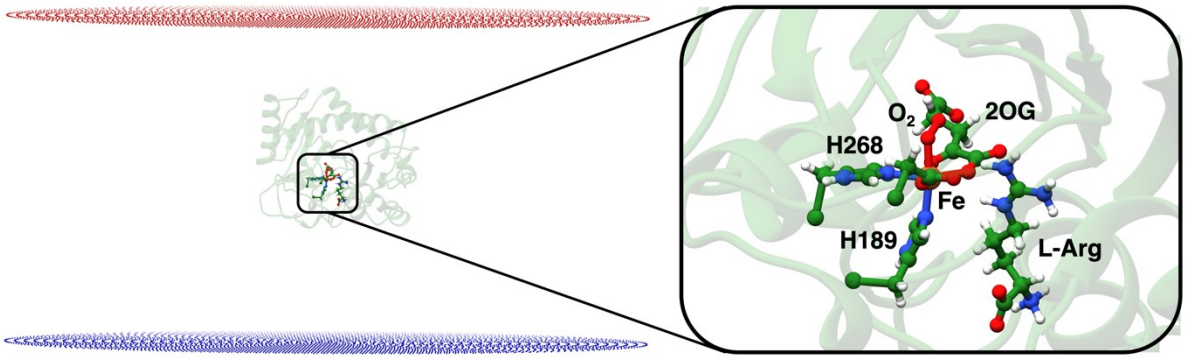

Figure S1. Figure showing the orientation of the external electric field (ExtEF) is along the Fe-O_2 bond.

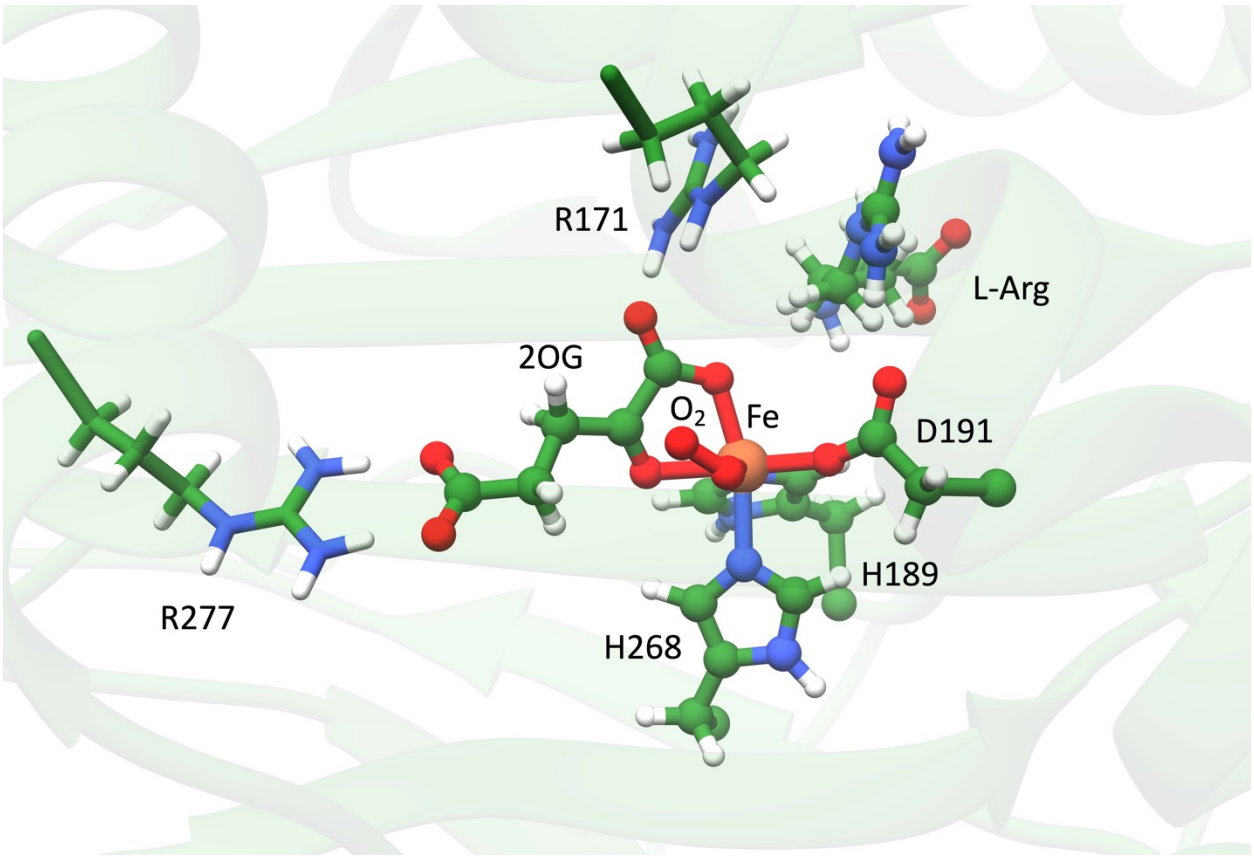

Figure S2. The QM region used for the expanded QM region calculations with the **AO+0.0025** structure. The new added salt-bridge forming residues with 2OG - R277 and R171 are shown in sticks.

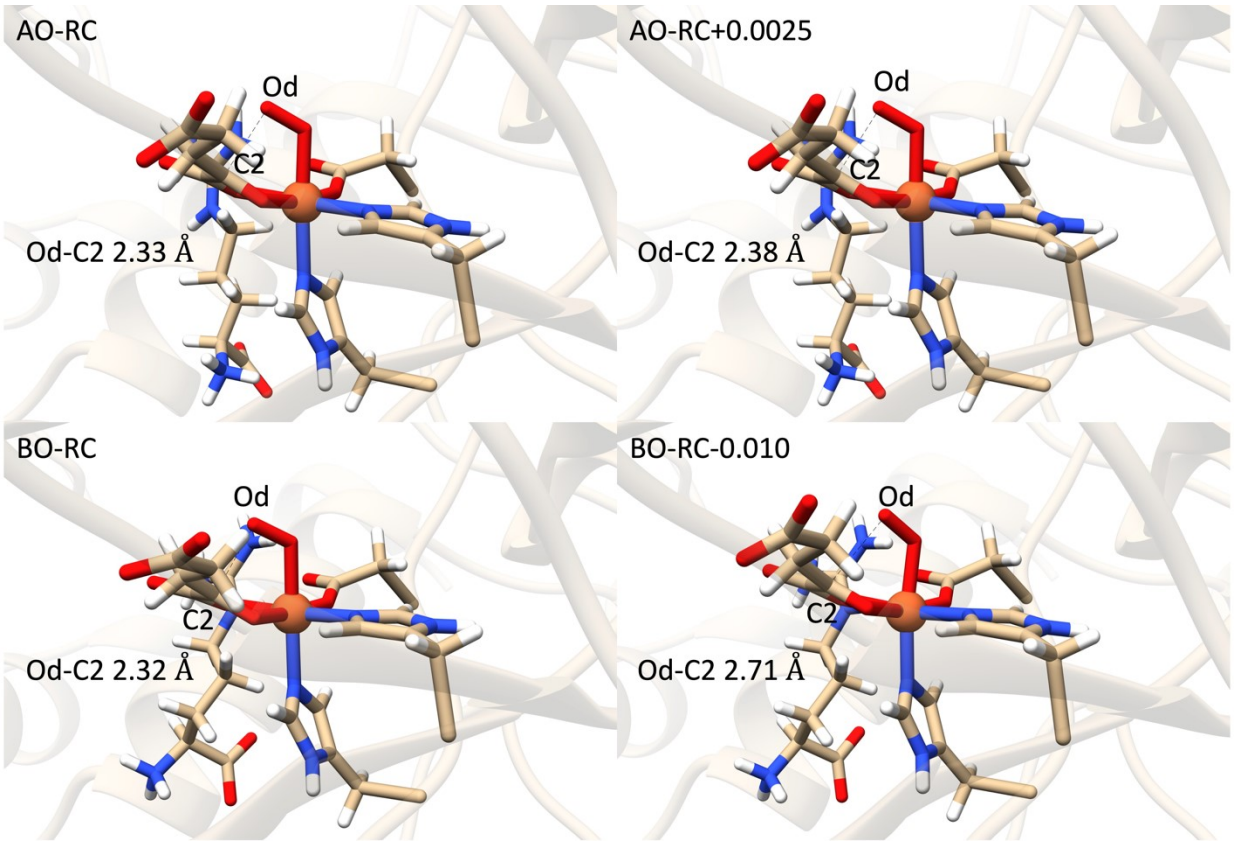

Figure S3. The change in the distance between the distal oxygen (Od) of the superoxo complex and C2 of 2OG upon application of an ExtEF.

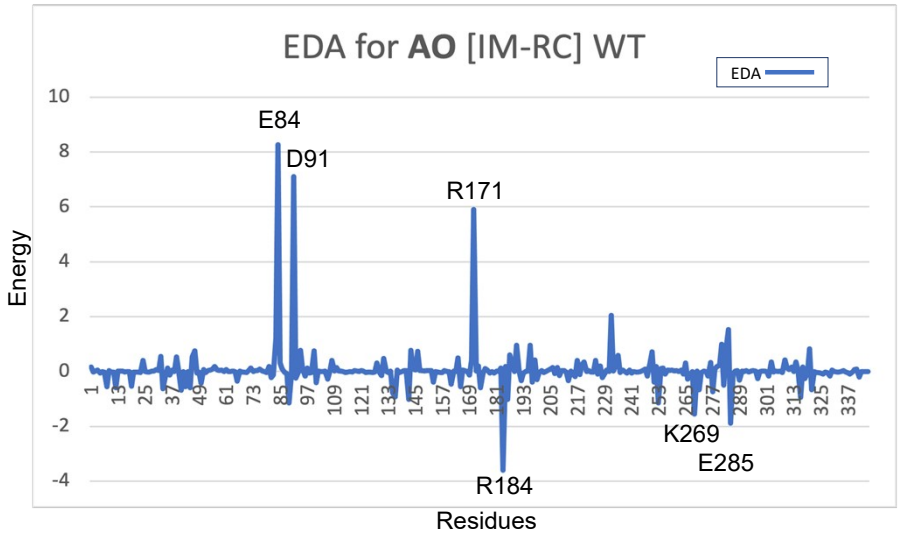

Figure S4. Total energy decomposition analysis (EDA) for the residues stabilizing/de-stabilizing the **AO-IM** with respect to the **AO-RC**.

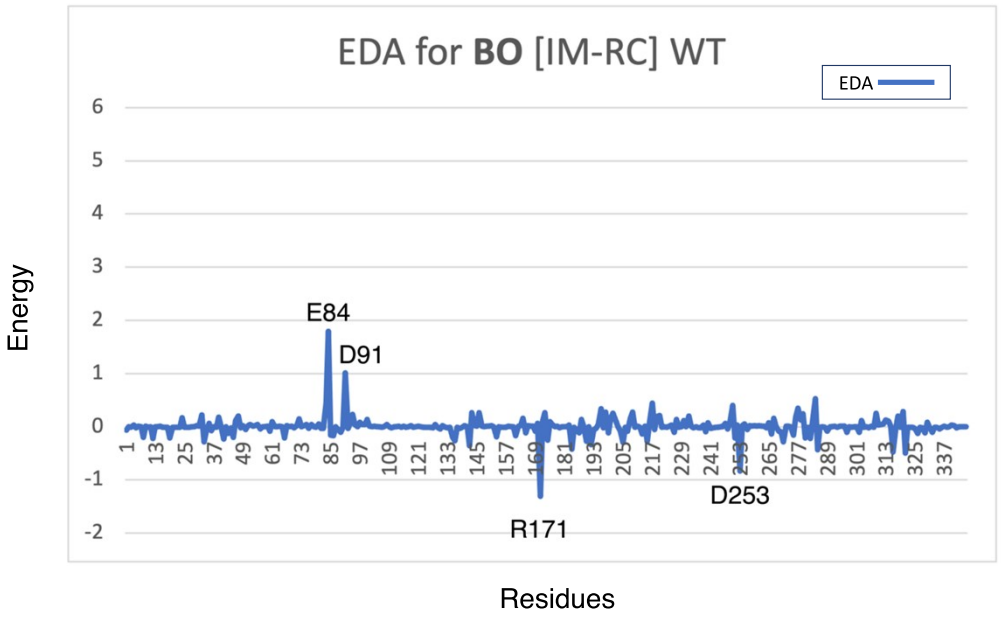

Figure S5. Total EDA for the residues stabilizing/de-stabilizing the **BO-IM** with respect to the **BO-RC**.

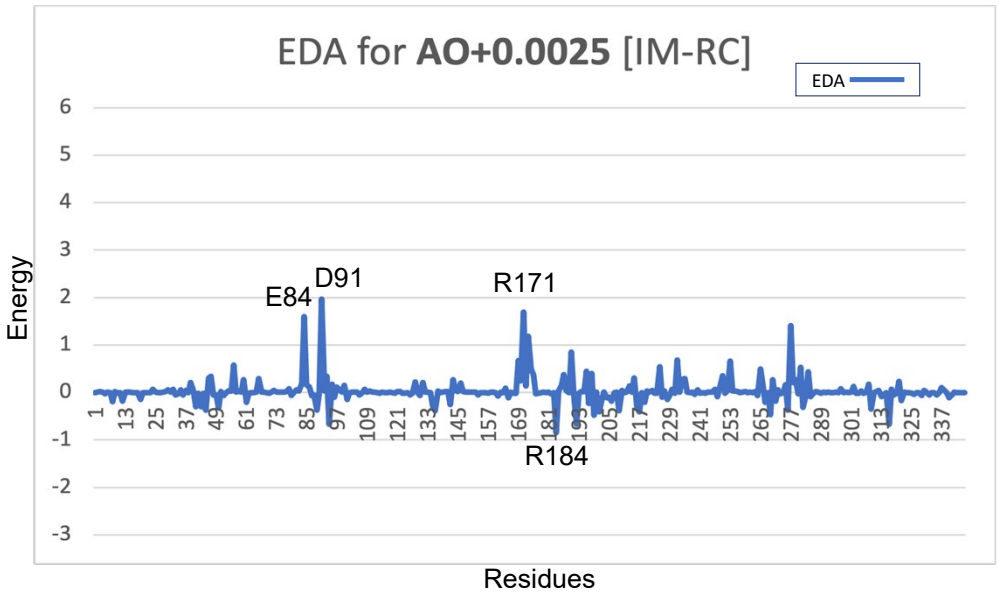

Figure S6. Total EDA for the residues stabilizing/de-stabilizing the **AO-IM+0.0025** with respect to the **AO-RC+0.0025**.

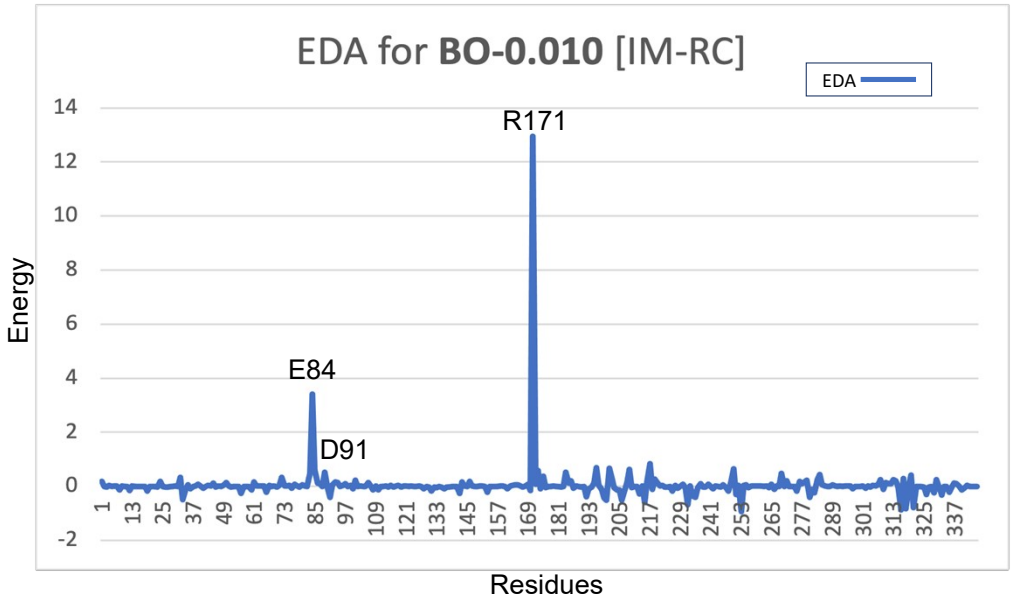

Figure S7. Total EDA for the residues stabilizing/de-stabilizing the **BO-IM-0.010** with respect to the **BO-RC-0.010**.

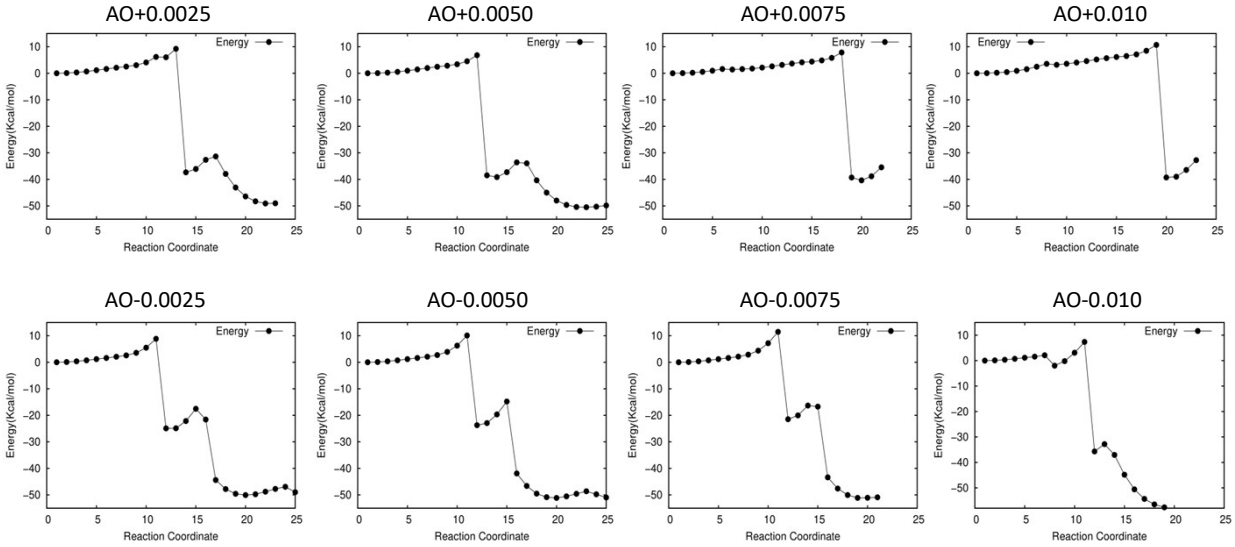

Figure S8. Potential Energy Surface profiles of EFE-AO systems.

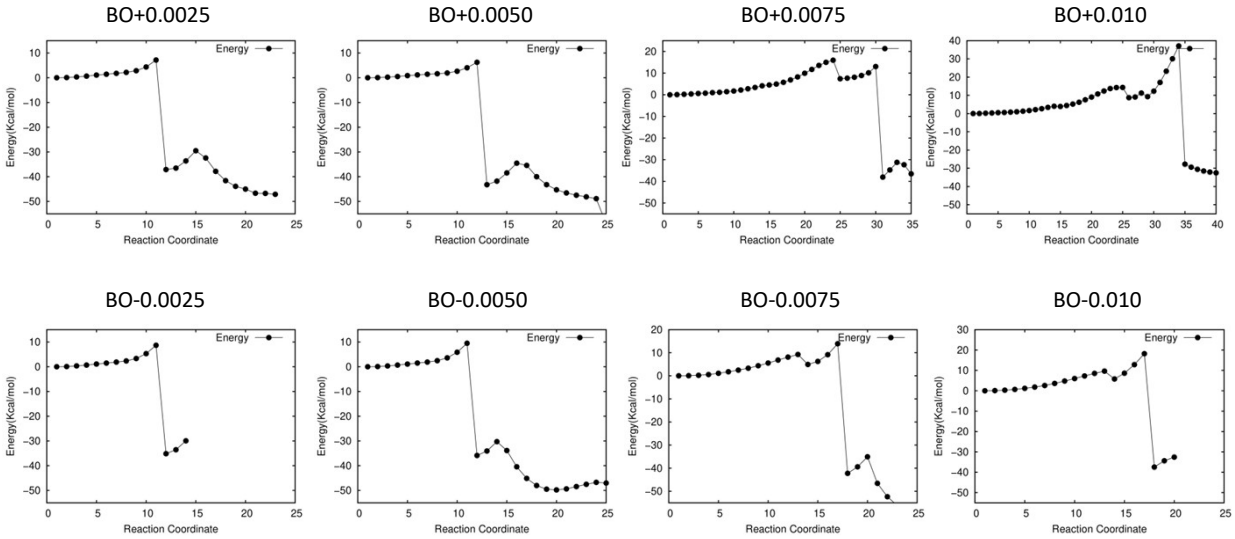

Figure S9. Potential Energy Surface profiles of EFE-BO systems.

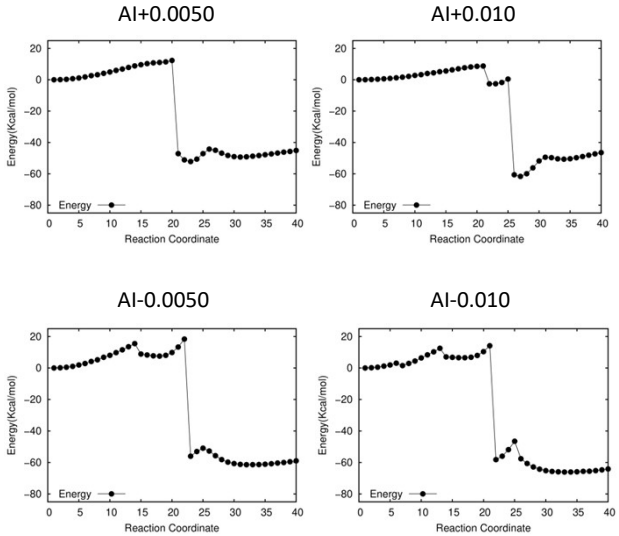

Figure S10. Potential Energy Surface profiles of EFE-AI systems.

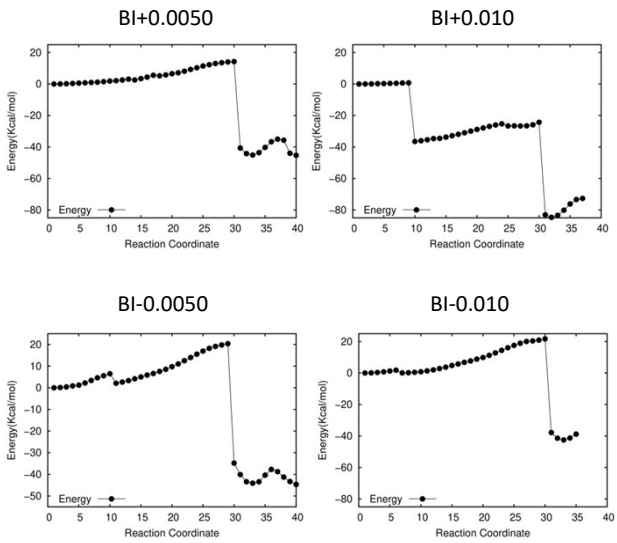

Figure S11. Potential Energy Surface profiles of EFE-BI systems.

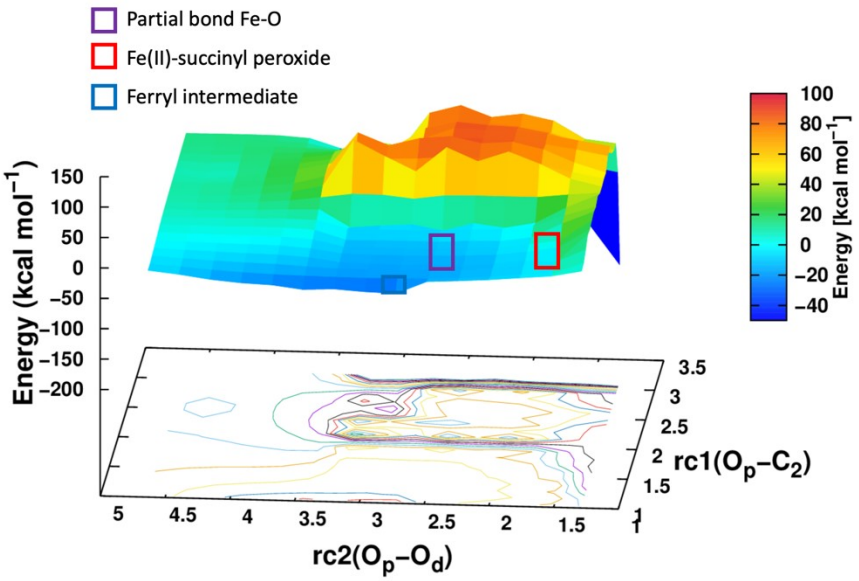

Figure S12. Potential Energy Surface obtained from 2D scans in the AI-0.010 system.

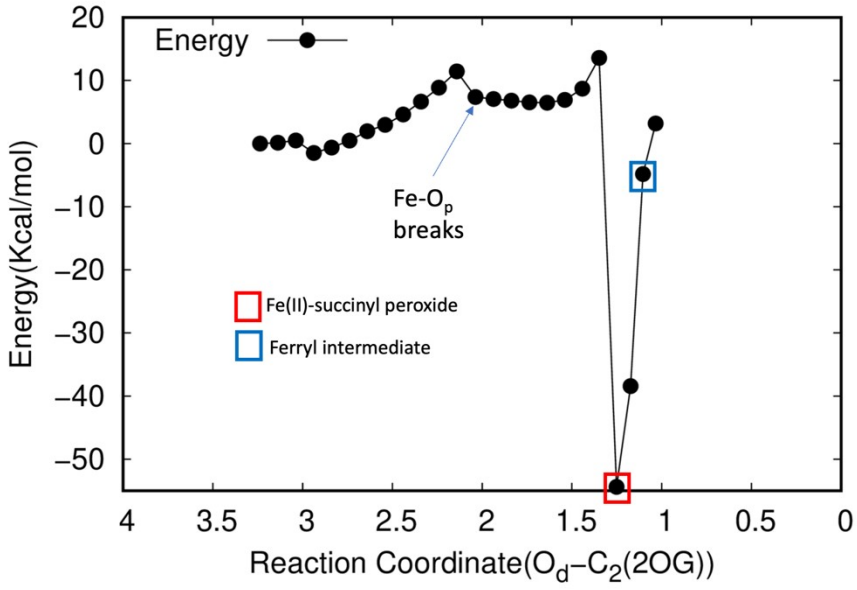

Figure S13. Energy profile of the scan in the first dimension with the reaction coordinate O_d-C_2(2OG) distance for AI-0.010 ExtEF.

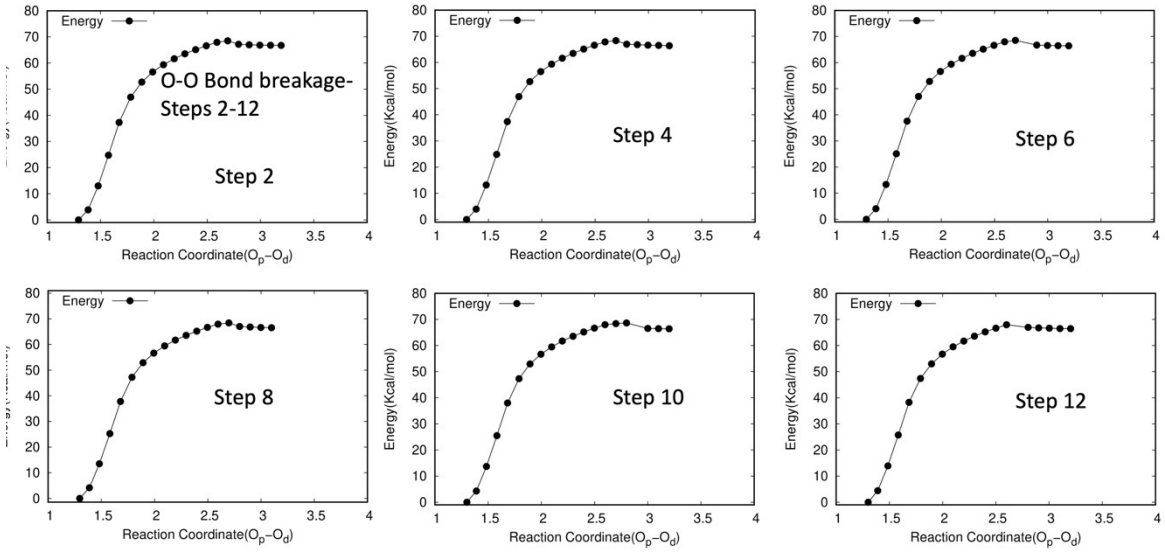

Figure S14. Energy profiles of the scans in the second dimension with a reaction coordinate O_p-O_d distance starting from steps 2 to 12 from the first scan for AI-0.010 ExtEF.

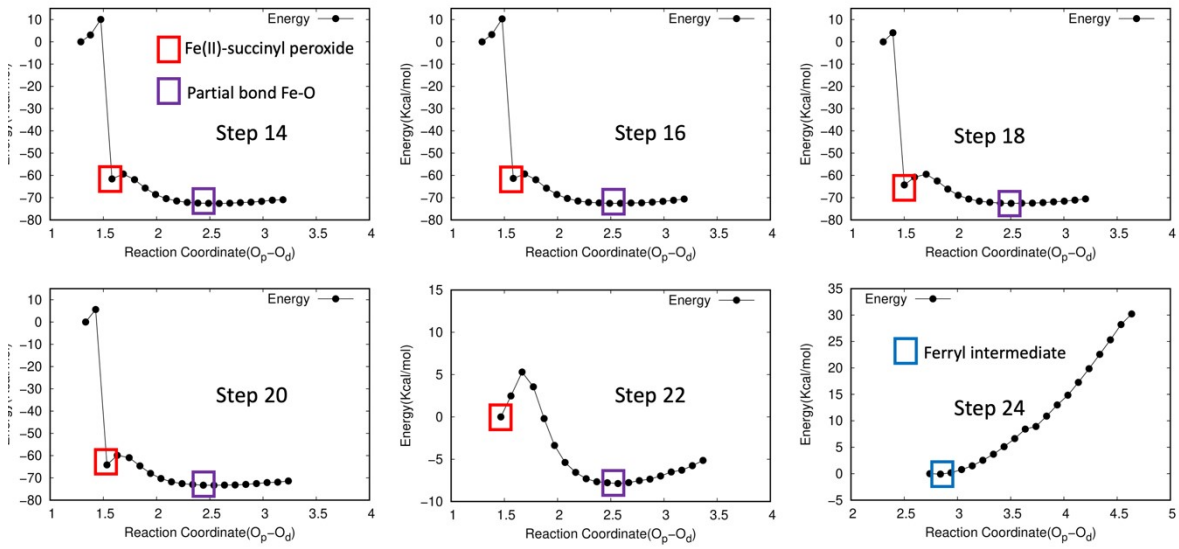

Figure S15. Energy profiles of the scans in the second dimension with a reaction coordinate O_p-O_d distance starting from steps 14 to 24 from the first scan for AI-0.010 ExtEF.

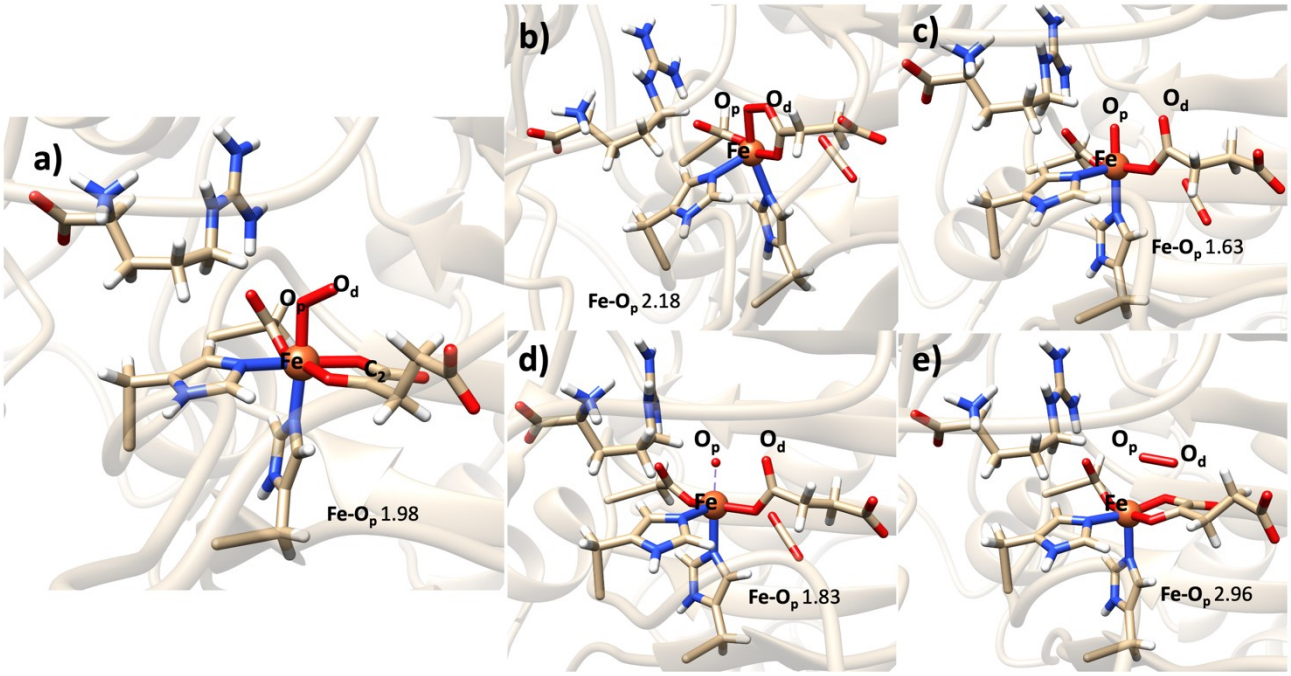

Figure S16. Figure showing the stationary points on the PES obtained from 2D scan. a) Initial Fe(III)-superoxo with inline 2OG with L-Arg in A conformation, b) Fe(II)-succinyl peroxide, c) Ferryl, d) Partial bond Fe-O_p intermediates, and e) Fe-O_p bond breakage.

Table S2. Spin densities of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.0025 au along the Fe-O bond. CO2 is the C1 carboxylate of 2OG. 2OG-CO2 is the rest of 2OG except the C1 carboxylate.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC+0.0025	4.18	-0.21	-0.48	0.14	0.09	0.00	0.14	0.05	0.06
AO-TS+0.0025	4.18	0.08	-0.19	-0.24	-0.11	0.00	0.13	0.05	0.07
AO-IM+0.0025	4.24	-0.19	-0.56	0.19	0.02	0.00	0.15	0.07	0.05

Table S3. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.0025 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC+0.0025	0.94	-0.19	-0.12	-0.51	-1.01	0.88	-0.48	0.25	0.25
AO-TS+0.0025	0.95	-0.28	-0.11	-0.36	-1.08	0.87	-0.49	0.25	0.25
AO-IM+0.0025	0.93	-0.35	-0.13	-0.45	-0.90	0.86	-0.47	0.27	0.23

Table S4. Spin densities of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.0050 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC+0.0050	4.15	-0.16	-0.45	0.13	0.08	0.00	0.12	0.04	0.05
AO-TS+0.0050	4.23	-0.45	-0.35	0.07	0.22	0.00	0.13	0.06	0.06
AO-IM+0.0050	3.82	0.02	0.02	0.01	0.00	0.05	0.02	0.02	0.00

Table S5. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.0050 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-	0.93	-0.17	-0.09	-0.52	-0.99	0.87	-0.49	0.22	0.24

RC+0.0050									
AO-TS+0.0050	0.95	-0.16	-0.07	-0.46	-1.14	0.87	-0.49	0.25	0.25
AO-IM+0.0050	0.86	-0.25	-0.09	-0.39	-0.79	0.84	-0.55	0.20	0.18

Table S6. Spin densities of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.0075 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC+0.0075	3.83	0.03	-0.08	0.06	0.03	0.00	0.05	0.02	0.03
AO-TS+0.0075	4.23	-0.42	-0.35	0.07	0.20	0.00	0.12	0.06	0.06
AO-IM+0.0075	3.82	0.02	0.02	0.01	0.00	0.04	0.02	0.02	0.00

Table S7. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.0075 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC+0.0075	0.85	-0.07	0.02	-0.54	-0.95	0.85	-0.54	0.18	0.21
AO-TS+0.0075	0.95	-0.16	-0.07	-0.46	-1.11	0.86	-0.49	0.23	0.25
AO-IM+0.0075	0.87	-0.25	-0.08	-0.39	-0.78	0.83	-0.55	0.18	0.18

Table S8. Spin densities of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.010 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC+0.010	3.80	0.04	-0.04	0.05	0.03	0.00	0.04	0.02	0.03
AO-TS+0.010	4.22	-0.25	-0.30	0.01	0.07	0.00	0.11	0.05	0.06
AO-IM+0.010	3.82	0.02	0.03	0.02	0.00	0.04	0.02	0.02	0.00

Table S9. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.010 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC+0.010	0.85	-0.06	0.04	-0.55	-0.94	0.85	-0.55	0.16	0.20
AO-TS+0.010	0.94	-0.20	-0.07	-0.45	-1.02	0.85	-0.49	0.20	0.24
AO-IM+0.010	0.87	-0.26	-0.07	-0.40	-0.77	0.83	-0.55	0.17	0.18

Table S10. Spin densities of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.0025 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC-0.0025	4.21	-0.28	-0.50	0.14	0.09	0.00	0.16	0.07	0.06
AO-TS-0.0025	4.20	0.05	-0.19	-0.25	-0.11	0.00	0.14	0.06	0.07
AO-IM-0.0025	3.80	0.06	0.00	0.03	0.00	0.02	0.02	0.01	0.00

Table S11. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.0025 au along the Fe-O bond.

Charge Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC-0.0025	0.95	-0.20	-0.15	-0.51	-1.05	0.88	-0.47	0.30	0.25
AO-TS-0.0025	0.95	-0.30	-0.13	-0.36	-1.10	0.88	-0.49	0.29	0.26
AO-IM-0.0025	0.83	-0.40	-0.13	-0.04	-0.93	0.84	-0.59	0.23	0.20

Table S12. Spin densities of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.0050 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC-0.0050	4.22	-0.32	-0.50	0.14	0.09	0.00	0.16	0.07	0.07

AO-TS-0.0050	4.25	-0.43	-0.30	-0.01	0.17	0.00	0.14	0.10	0.07
AO-IM-0.0050	3.80	0.06	0.00	0.03	0.00	0.02	0.03	0.01	0.00

Table S13. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.0050 au along the Fe-O bond.

Charge Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC-0.0050	0.95	-0.20	-0.17	-0.51	-1.07	0.89	-0.47	0.32	0.26
AO-TS-0.0050	0.96	-0.20	-0.11	-0.45	-1.20	0.88	-0.49	0.35	0.26
AO-IM-0.0050	0.83	-0.41	-0.14	-0.04	-0.94	0.85	-0.60	0.25	0.20

Table S14. Spin densities of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.0075 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC-0.0075	4.23	-0.35	-0.49	0.14	0.09	0.00	0.17	0.10	0.07
AO-TS-0.0075	4.21	0.05	-0.18	-0.29	-0.12	0.00	0.15	0.08	0.08
AO-IM-0.0075	3.82	0.01	0.01	0.00	0.05	0.02	0.02	0.00	0.00

Table S15. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.0075 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC-0.0075	0.95	-0.20	-0.18	-0.51	-1.09	0.89	-0.48	0.35	0.26
AO-TS-0.0075	0.95	-0.33	-0.16	-0.35	-1.13	0.89	-0.49	0.34	0.27
AO-IM-0.0075	0.87	-0.25	-0.14	-0.42	-0.81	0.86	-0.58	0.29	0.18

Table S16. Spin densities of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.010 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC-0.010	4.23	-0.38	-0.49	0.14	0.10	0.00	0.17	0.13	0.07
AO-TS-0.010	4.25	-0.33	-0.24	-0.02	0.15	-0.15	0.14	0.12	0.07
AO-IM-0.010	3.83	0.01	0.01	0.00	0.05	0.03	0.02	0.00	0.00

Table S17. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.010 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AO-RC-0.010	0.95	-0.21	-0.20	-0.51	-1.11	0.89	-0.47	0.38	0.27
AO-TS-0.010	0.96	-0.25	-0.16	-0.47	-1.24	1.03	-0.50	0.37	0.26
AO-IM-0.010	0.88	-0.25	-0.15	-0.42	-0.82	0.86	-0.59	0.31	0.18

Table S18. Spin densities of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.0025 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC+0.0025	4.19	-0.23	-0.49	0.13	0.09	0.00	0.13	0.06	0.07
BO-TS+0.0025	4.24	-0.42	-0.32	0.03	0.16	0.00	0.12	0.07	0.07
BO-IM+0.0025	3.82	0.02	0.02	0.01	0.00	0.06	0.02	0.02	0.00

Table S19. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.0025 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC+0.0025	0.93	-0.19	-0.13	-0.52	-1.01	0.85	-0.46	0.27	0.26

BO-TS+0.0025	0.94	-0.18	-0.09	-0.47	-1.13	0.85	-0.48	0.29	0.26
BO-IM+0.0025	0.86	-0.25	-0.10	-0.41	-0.80	0.82	-0.54	0.23	0.18

Table S20. Spin densities of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.0050 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC+0.0050	4.16	-0.16	-0.47	0.12	0.09	0.00	0.11	0.05	0.06
BO-TS+0.0050	4.21	-0.04	-0.23	-0.08	-0.12	0.00	0.11	0.05	0.07
BO-IM+0.0050	4.18	0.24	-0.37	0.26	-0.53	0.00	0.09	0.06	0.05

Table S21. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.0050 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC+0.0050	0.92	-0.17	-0.09	-0.52	-0.98	0.84	-0.48	0.22	0.25
BO-TS+0.0050	0.94	-0.26	-0.10	-0.44	-0.96	0.84	-0.49	0.22	0.25
BO-IM+0.0050	0.87	-0.41	-0.16	-0.54	-0.52	0.83	-0.51	0.22	0.21

Table S22. Spin densities of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.0075 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC+0.0075	3.81	0.04	-0.07	0.06	0.03	0.00	0.04	0.02	0.03
BO-TS+0.0075	4.16	0.25	-0.09	-0.17	-0.37	0.00	0.09	0.04	0.07
BO-IM+0.0075	3.82	0.02	0.02	0.01	0.00	0.04	0.02	0.02	0.00

Table S23. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.0075 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC+0.0075	0.84	-0.08	0.04	-0.56	-0.91	0.83	-0.55	0.18	0.22
BO-TS+0.0075	0.93	-0.28	-0.11	-0.43	-0.85	0.83	-0.51	0.18	0.24
BO-IM+0.0075	0.87	-0.25	-0.07	-0.41	-0.77	0.82	-0.55	0.18	0.19

Table S24. Spin densities of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.010 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC+0.010	3.79	0.04	-0.04	0.06	0.03	0.00	0.03	0.02	0.02
BO-TS+0.010	3.76	0.00	0.00	-0.01	0.03	0.00	0.05	0.01	0.02
BO-IM+0.010	3.82	0.02	0.02	0.02	0.00	0.04	0.02	0.02	0.00

Table S25. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of +0.010 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC+0.010	0.84	-0.07	0.07	-0.58	-0.90	0.82	-0.55	0.16	0.22
BO-TS+0.010	0.81	-0.09	-0.09	-0.04	-0.90	0.81	-0.54	0.11	0.21
BO-IM+0.010	0.87	-0.06	-0.06	-0.43	-0.75	0.81	-0.54	0.17	0.20

Table S26. Spin densities of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.0025 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC-0.0025	4.21	-0.27	-0.50	0.14	0.09	0.00	0.14	0.07	0.07
BO-TS-0.0025	4.24	-0.39	-0.31	-0.01	0.16	0.00	0.13	0.09	0.07

BO-IM-0.0025	3.82	0.01	0.02	0.01	0.00	0.05	0.02	0.02	0.00

Table S27. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.0025 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC-0.0025	0.93	-0.19	-0.14	-0.52	-1.02	0.85	-0.46	0.30	0.26
BO-TS-0.0025	0.94	-0.20	-0.10	-0.46	-1.15	0.85	-0.48	0.32	0.26
BO-IM-0.0025	0.86	-0.25	-0.12	-0.41	-0.80	0.83	-0.54	0.25	0.18

Table S28. Spin densities of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.0050 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC-0.0050	4.22	-0.30	-0.50	0.14	0.09	0.00	0.14	0.07	0.07
BO-TS-0.0050	4.24	-0.38	-0.30	-0.03	0.14	0.00	0.13	0.11	0.07
BO-IM-0.0050	3.82	0.01	0.02	0.01	0.00	0.05	0.03	0.02	0.00

Table S29. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.0050 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC-0.0050	0.93	-0.20	-0.16	-0.52	-1.04	0.85	-0.46	0.32	0.26
BO-TS-0.0050	0.95	-0.21	-0.11	-0.45	-1.16	0.85	-0.48	0.34	0.26
BO-IM-0.0050	0.86	-0.26	-0.12	-0.39	-0.81	0.83	-0.55	0.27	0.18

Table S30. Spin densities of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.0075 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC-0.0075	3.44	0.14	0.26	0.05	0.02	0.00	0.05	-0.01	0.02
BO-TS-0.0075	2.89	0.57	0.42	-0.03	0.10	0.00	0.10	-0.01	-0.05
BO-IM-0.0075	3.82	0.01	0.02	0.01	0.00	0.05	0.03	0.02	0.00

Table S31. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.0075 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC-0.0075	0.81	-0.11	-0.12	-0.52	-1.01	0.84	-0.51	0.36	0.26
BO-TS-0.0075	0.79	-0.15	-0.15	-0.44	-1.15	0.85	-0.50	0.39	0.35
BO-IM-0.0075	0.86	-0.26	-0.13	-0.39	-0.82	0.84	-0.55	0.29	0.18

Table S32. Spin densities of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.010 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC-0.010	3.30	0.20	0.36	0.05	0.02	0.00	0.05	-0.02	0.01
BO-TS-0.010	2.88	0.63	0.37	-0.02	0.08	0.00	0.09	0.02	-0.06
BO-IM-0.010	3.95	-0.17	0.00	0.04	0.00	0.05	0.04	0.04	0.00

Table S33. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and off-line 2OG bound to EFE with an ExtEF of -0.010 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BO-RC-0.010	0.80	-0.13	-0.16	-0.51	-1.02	0.85	-0.50	0.41	0.27

BO-TS-0.010	0.80	-0.15	-0.16	-0.44	-1.16	0.86	-0.49	0.38	0.36
BO-IM-0.010	0.88	-0.42	-0.20	-0.07	-0.99	0.83	-0.54	0.30	0.21

Table S34. Spin densities of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and in-line 2OG bound to EFE with an ExtEF of +0.0050 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AI-RC+0.0050	4.16	-0.47	-0.15	0.16	0.06	0.00	0.12	0.05	0.05
AI-TS+0.0050	4.24	-0.35	-0.48	0.12	0.19	0.00	0.11	0.05	0.08
AI-IM+0.0050	3.81	0.01	0.07	0.00	0.03	0.00	0.03	0.02	0.02

Table S35. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and in-line 2OG bound to EFE with an ExtEF of +0.0050 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AI-RC+0.0050	0.93	-0.21	-0.19	-0.40	-0.97	0.90	-0.47	0.24	0.19
AI-TS+0.0050	0.92	-0.12	-0.20	-0.34	-1.17	0.90	-0.48	0.25	0.23
AI-IM+0.0050	0.83	-0.16	-0.42	0.01	-0.90	0.88	-0.54	0.19	0.12

Table S36. Spin densities of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and in-line 2OG bound to EFE with an ExtEF of +0.010 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AI-RC+0.010	3.97	-0.27	-0.02	0.11	0.04	0.00	0.09	0.04	0.03
AI-TS+0.010	4.23	-0.44	-0.44	0.20	0.19	0.00	0.11	0.05	0.07
AI-IM+0.010	3.78	0.09	0.00	0.03	0.00	0.04	0.02	0.02	0.00

Table S37. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and in-line 2OG bound to EFE with an ExtEF of +0.010 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AI-RC+0.010	0.89	-0.07	-0.12	-0.44	-1.00	0.92	-0.51	0.20	0.13
AI-TS+0.010	0.91	-0.10	-0.16	-0.37	-1.14	0.94	-0.48	0.23	0.18
AI-IM+0.010	0.82	-0.10	-0.39	0.00	-0.93	0.94	-0.55	0.15	0.07

Table S38. Spin densities of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and in-line 2OG bound to EFE with an ExtEF of -0.0050 au along the Fe-O bond.

Spin Density	FE	Op	Od	CO2	2OG-CO2	L-ARG	D191	H189	H268
AI-RC-0.0050	3.14	0.43	0.27	0.09	0.03	0.00	0.04	0.00	-0.03
AI-TS-0.0050	2.90	0.28	0.43	0.21	0.06	0.00	-0.02	0.01	0.10
AI-IM-0.0050	3.82	0.05	0.00	0.02	0.00	0.03	0.02	0.02	0.00

Table S39. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and in-line 2OG bound to EFE with an ExtEF of -0.0050 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AI-RC-0.0050	0.81	-0.27	-0.16	-0.36	-1.00	0.81	-0.48	0.29	0.36
AI-TS-0.0050	0.80	-0.12	-0.36	-0.27	-1.10	0.82	-0.43	0.35	0.31
AI-IM-0.0050	0.84	-0.21	-0.45	0.02	-0.88	0.79	-0.52	0.21	0.21

Table S40. Spin densities of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and in-line 2OG bound to EFE with an ExtEF of -0.010 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AI-RC-0.010	3.04	0.48	0.33	0.09	0.04	0.00	0.05	0.00	-0.04
AI-TS-0.010	2.91	0.37	0.46	0.27	0.11	0.00	-0.01	-0.01	0.15

AI-IM-0.010	3.82	0.04	0.00	0.02	0.00	0.03	0.02	0.03	0.00

Table S41. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation A of L-Arg and in-line 2OG bound to EFE with an ExtEF of -0.010 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
AI-RC-0.010	0.80	-0.32	-0.18	-0.34	-1.00	0.76	-0.47	0.31	0.44
AI-TS-0.010	0.93	0.24	0.01	1.37	-0.75	0.81	-0.26	0.38	0.36
AI-IM-0.010	0.84	-0.22	-0.48	0.02	-0.87	0.74	-0.50	0.22	0.25

Table S42. Spin densities of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and in-line 2OG bound to EFE with an ExtEF of +0.0050 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BI-RC+0.0050	3.92	-0.23	0.02	0.09	0.03	0.00	0.08	0.03	0.03
BI-TS+0.0050	4.24	-0.33	-0.44	0.10	0.16	0.00	0.11	0.06	0.08
BI-IM+0.0050	3.80	0.01	0.07	0.00	0.00	0.00	0.03	0.02	0.02

Table S43. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and in-line 2OG bound to EFE with an ExtEF of +0.0050 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BI-RC+0.0050	0.86	-0.04	-0.13	-0.42	-1.06	0.90	-0.50	0.22	0.18
BI-TS+0.0050	0.92	-0.17	-0.17	-0.34	-1.16	0.91	-0.47	0.24	0.23
BI-IM+0.0050	0.84	-0.19	-0.47	0.01	-0.89	0.91	-0.52	0.19	0.13

Table S44. Spin densities of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and in-line 2OG bound to EFE with an ExtEF of +0.010 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BI-RC+0.010	2.25	0.91	0.75	0.02	0.02	0.00	0.08	0.00	-0.03
BI-TS+0.010	4.24	-0.33	-0.38	0.04	0.17	0.00	0.12	0.06	0.07
BI-IM+0.010	3.78	0.10	0.00	0.03	0.00	0.03	0.02	0.02	0.00

Table S45. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and in-line 2OG bound to EFE with an ExtEF of +0.010 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BI-RC+0.010	0.75	0.01	-0.07	-0.43	-1.08	0.94	-0.52	0.22	0.19
BI-TS+0.010	0.92	-0.06	-0.17	-0.36	-1.19	0.94	-0.48	0.23	0.17
BI-IM+0.010	0.82	-0.08	-0.39	-0.00	-0.96	0.94	-0.55	0.15	0.07

Table S46. Spin densities of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and in-line 2OG bound to EFE with an ExtEF of -0.0050 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BI-RC-0.0050	4.21	-0.51	-0.22	0.19	0.05	0.00	0.12	0.06	0.08
BI-TS-0.0050	4.24	-0.34	-0.52	0.16	0.18	0.00	0.09	0.05	0.12
BI-IM-0.0050	3.81	0.06	0.00	0.02	0.00	0.03	0.01	0.02	0.00

Table S47. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and in-line 2OG bound to EFE with an ExtEF of -0.0050 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BI-RC-0.0050	0.94	-0.18	-0.31	-0.36	-1.01	0.81	-0.43	0.25	0.30

BI-TS-0.0050	0.92	-0.22	-0.17	-0.33	-1.13	0.82	-0.46	0.24	0.33
BI-IM-0.0050	0.83	-0.17	-0.48	0.01	-0.89	0.80	-0.52	0.20	0.22

Table S48. Spin densities of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and in-line 2OG bound to EFE with an ExtEF of -0.010 au along the Fe-O bond.

Spin Density	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BI-RC-0.010	4.24	-0.56	-0.25	0.21	0.05	0.00	0.12	0.06	0.12
BI-TS-0.010	4.23	-0.31	-0.54	0.12	0.18	0.00	0.07	0.05	0.17
BI-IM-0.010	3.81	0.01	0.06	0.00	0.00	0.00	0.03	0.02	0.03

Table S49. Mulliken charges of stationary points in the O_2 attack on 2OG for conformation B of L-Arg and in-line 2OG bound to EFE with an ExtEF of -0.010 au along the Fe-O bond.

Charge Distribution	**FE**	**Op**	**Od**	**CO2**	**2OG-CO2**	**L-ARG**	**D191**	**H189**	**H268**
BI-RC-0.010	0.95	-0.22	-0.33	-0.34	-1.01	0.75	-0.42	0.26	0.36
BI-TS-0.010	0.94	-0.24	-0.19	-0.34	-1.13	0.75	-0.45	0.26	0.40
BI-IM-0.010	0.83	-0.19	-0.50	0.02	-0.89	0.74	-0.49	0.21	0.27

Table S50. The occupation numbers of the Fe-O bonding natural orbitals in off-line 2OG with L-Arg conformation A and B under varying ExtEF conditions.

ExtEF (au)	Fe-based natural orbital & occupation number	O_2-based natural orbital & occupation number
AO-RC+0.0025	$d_{xz} + \pi^*_{\perp}$ (1.22)	$d_{xz} - \pi^*_{\perp}$ (0.78)
AO-RC+0.0050	$d_{xz} + \pi^*_{\perp}$ (1.23)	$d_{xz} - \pi^*_{\perp}$ (0.77)
AO-RC+0.0075	$d_{xz} + \pi^*_{\perp}$ (1.36)	$d_{xz} - \pi^*_{\perp}$ (0.64)
AO-RC+0.010	$d_{xz} + \pi^*_{\perp}$ (1.35)	$d_{xz} - \pi^*_{\perp}$ (0.65)
AO-RC-0.0025	$d_{xz} + \pi^*_{\perp}$ (1.18)	$d_{xz} - \pi^*_{\perp}$ (0.82)
AO-RC-0.0050	$d_{xz} + \pi^*_{\perp}$ (1.17)	$d_{xz} - \pi^*_{\perp}$ (0.83)
AO-RC-0.0075	$d_{xz} + \pi^*_{\perp}$ (1.15)	$d_{xz} - \pi^*_{\perp}$ (0.85)
AO-RC-0.010	$d_{xz} + \pi^*_{\perp}$ (1.13)	$d_{xz} - \pi^*_{\perp}$ (0.87)

BO-RC+0.0025	$d_{x^2-y^2} + \pi^*_{\|\|}$ (1.22)	$d_{x^2-y^2} - \pi^*_{\|\|}$ (0.78)
BO-RC+0.0050	$d_{x^2-y^2} + \pi^*_{\|\|}$ (1.26)	$d_{x^2-y^2} - \pi^*_{\|\|}$ (0.74)
BO-RC+0.0075	$d_{xz} + \pi^*_{\perp}$ (1.34)	$d_{xz} - \pi^*_{\perp}$ (0.66)
BO-RC+0.010	$d_{xz} + \pi^*_{\perp}$ (1.32)	$d_{xz} - \pi^*_{\perp}$ (0.68)
BO-RC-0.0025	$d_{x^2-y^2} + \pi^*_{\|\|}$ (1.21)	$d_{x^2-y^2} - \pi^*_{\|\|}$ (0.79)
BO-RC-0.0050	$d_{x^2-y^2} + \pi^*_{\|\|}$ (1.19)	$d_{x^2-y^2} - \pi^*_{\|\|}$ (0.81)
BO-RC-0.0075	$d_{xz} + \pi^*_{\perp}$ (0.30)	$d_{xz} - \pi^*_{\perp}$ (1.70)
BO-RC-0.010	$d_{xz} + \pi^*_{\perp}$ (0.20)	$d_{xz} - \pi^*_{\perp}$ (1.80)

Table S51. Ethylene and P5C production by selected EFE variants described in the text compared to the WT enzyme. The assays were carried out in 2 mL reactions consisting of 0.5 mM 2OG, 0.5 mM L-Arg, 0.2 mM Fe(II), 0.4 mM L-ascorbic acid, and 1 µM EFE in 25 mM HEPES, pH 7.5. The samples were incubated at 25 °C for 80 min and terminated with 100 µL of 3.6 M HCl. Standard error of the mean is given in *parentheses*. N = two or greater. ND, not detected.

Sample	Ethylene (% vs WT)	P5C (% vs WT)	Reference
E84A	ND	3.8 (±0.7)	[Ref. 1]
D91A	ND	ND	This study
R171A	ND	3.2 (±1.7)	[Ref. 1]
R184A	76.5 (±6.9)	77.6 (±9.4)	[Ref. 1]
D253A	0.3 (±0.1)	ND	This study
K269A	94.8 (±12.7)	91.9 (±10.9)	This study
E285A	0.2 (±0.2)	9.0 (±4.1)	[Ref. 1]

AO-RC+0.0025

1 C	41.8893920	28.4300325	29.9172203
2 H	40.8811875	28.8349910	29.7519956
3 H	41.8123956	27.3379204	29.7911616
4 C	42.3104145	28.7989521	31.3055500
5 N	43.3857109	28.2695408	31.9981845
6 H	44.0501834	27.5612010	31.6685902
7 C	43.4633529	28.8839242	33.1964061
8 H	44.2389842	28.6811546	33.9316813
9 N	42.4917165	29.7742674	33.3286432
10 C	41.7620754	29.7261980	32.1604442
11 H	40.9143704	30.3830247	31.9928005
12 C	40.1630731	34.3559415	32.3775172
13 H	41.1924408	34.4973371	32.0282880
14 H	39.8594898	35.2753968	32.9024161
15 C	40.0436790	33.1801166	33.3497732
16 O	38.9741810	32.9897044	33.9334406
17 O	41.0947901	32.4389304	33.4545071
18 C	47.4039475	32.1387099	31.6008286
19 H	48.0925356	31.9064790	32.4257136
20 H	47.7521533	33.0839677	31.1522702
21 C	46.0077392	32.2886084	32.1141553
22 N	45.0204236	32.9594314	31.4192106
23 H	45.1389708	33.4464060	30.5236781
24 C	43.8736013	32.8725172	32.1155318
25 H	42.9234409	33.2790101	31.7829299
26 N	44.0635026	32.2048009	33.2440964
27 C	45.3928629	31.8382731	33.2622240
28 H	45.8167400	31.2868966	34.0983286
29 Fe	42.4377849	31.5766167	34.5429112
30 O	42.7592407	33.2700181	35.6875833
31 O	42.8929346	33.1714211	36.9436648
32 C	41.9368905	30.7088769	37.1974482
33 O	41.3295787	30.8664250	36.0746048
34 O	41.4209601	30.4235690	38.2761548
35 C	43.4730034	30.8653514	37.0732266
36 O	43.9131900	30.8550342	35.9061759
37 C	44.3390819	30.8226171	38.2844901
38 C	45.6628582	31.5777836	38.1748189
39 C	46.7803134	31.0389610	39.1023091

40 O 47.7615528 31.8044926 39.2683045
41 O 46.6402877 29.8779376 39.5628671
42 H 46.0487049 31.4951300 37.1441290
43 H 45.5295922 32.6544339 38.3614111
44 H 43.7357022 31.1306857 39.1509082
45 H 44.5927144 29.7592661 38.4766887
46 N 38.0811541 26.0776320 32.6441386
47 C 36.7514919 26.7306373 32.8367694
48 C 35.8964533 26.4917876 31.5591015
49 O 36.5263774 26.0634551 30.5469382
50 C 36.9010078 28.2256889 33.1631269
51 C 37.8844277 28.5501513 34.3016106
52 C 37.8654128 30.0107219 34.7538725
53 N 36.5967256 30.2990958 35.4135769
54 C 36.2418769 31.4309019 36.0355551
55 N 35.0793739 31.4273581 36.7029065
56 N 37.0234283 32.5123387 36.0225516
57 O 34.6885036 26.7644250 31.6368435
58 H 36.2726459 26.2111576 33.6812381
59 H 37.1974256 28.7753798 32.2534866
60 H 35.8871918 28.5709580 33.4128161
61 H 37.6859479 27.9053299 35.1765734
62 H 38.9175999 28.3286780 33.9905314
63 H 38.7086783 30.1956585 35.4418494
64 H 38.0121781 30.6897066 33.8976353
65 H 35.9293789 29.5321497 35.5344026
66 H 34.5014993 30.5885359 36.6824781
67 H 34.7334922 32.2878105 37.1302066
68 H 37.8290385 32.5956895 35.3909829
69 H 36.7258910 33.3486165 36.5210379
70 H 37.9653223 25.0591801 32.4999179
71 H 38.5549541 26.4571044 31.8084950
72 H 38.7083882 26.1653296 33.4730547
73 H 39.5166747 34.1876472 31.5161734
74 H 47.5381477 31.3900105 30.8201195
75 H 42.5439014 28.7845697 29.1209867

AO-TS+0.0025

1 C 41.8816909 28.4430024 29.9286085
2 H 40.8734940 28.8418894 29.7483343
3 H 41.8088943 27.3493854 29.8131763
4 C 42.2862320 28.8247217 31.3189994
5 N 43.3546331 28.2978678 32.0261898
6 H 44.0214351 27.5881890 31.7036569
7 C 43.4170676 28.9166742 33.2238141
8 H 44.1774778 28.7206441 33.9769147
9 N 42.4442623 29.8084438 33.3397907
10 C 41.7296349 29.7583729 32.1630956
11 H 40.8815596 30.4129300 31.9882601
12 C 40.1754005 34.3516376 32.3954546
13 H 41.2047021 34.4926170 32.0454948
14 H 39.8725937 35.2750545 32.9138522
15 C 40.0639490 33.1832176 33.3802702
16 O 38.9845935 32.9751480 33.9434247
17 O 41.1304517 32.4761702 33.5221233
18 C 47.4188959 32.1412947 31.5869078
19 H 48.1026288 31.9052261 32.4146896
20 H 47.7758564 33.0828669 31.1375023
21 C 46.0218350 32.2962804 32.0962728
22 N 45.0358019 32.9685457 31.4012011
23 H 45.1560878 33.4589276 30.5078837
24 C 43.8873528 32.8805299 32.0947651
25 H 42.9394062 33.2909812 31.7605582
26 N 44.0760697 32.2097241 33.2211247
27 C 45.4046049 31.8432322 33.2415526
28 H 45.8269064 31.2856485 34.0742801
29 Fe 42.5083051 31.5955086 34.5678303
30 O 42.7349247 33.0890904 35.8427353
31 O 43.1178706 32.6447891 37.0806991
32 C 41.7820710 30.7212745 37.2645545
33 O 41.2254669 30.7747474 36.1574192
34 O 41.4396399 30.4230022 38.3921086
35 C 43.4744394 31.2710304 37.0617764
36 O 43.8055275 30.8149071 35.8887305
37 C 44.3302128 30.9508416 38.2768042
38 C 45.7029311 31.6229202 38.1802942
39 C 46.7951873 31.0578873 39.1192338
40 O 47.7912631 31.8083287 39.2761514
41 O 46.6323801 29.9068822 39.5891399
42 H 46.0905125 31.4929968 37.1545606
43 H 45.6272974 32.7089413 38.3417413
44 H 43.7861921 31.2608714 39.1812101
45 H 44.4602889 29.8611174 38.3381269
46 N 38.0810394 26.0772668 32.6455965
47 C 36.7508037 26.7300052 32.8341239
48 C 35.8978272 26.4901096 31.5554668
49 O 36.5282292 26.0581582 30.5455220
50 C 36.8991367 28.2252201 33.1602255
51 C 37.8818186 28.5489285 34.2989669
52 C 37.8640452 30.0094977 34.7501197
53 N 36.5975250 30.2990586 35.4129436
54 C 36.2450985 31.4325270 36.0332716
55 N 35.0850522 31.4303890 36.7052675
56 N 37.0292430 32.5121652 36.0180974
57 O 34.6904130 26.7661248 31.6309800
58 H 36.2705969 26.2111537 33.6782449
59 H 37.1960830 28.7755485 32.2512376
60 H 35.8852526 28.5702819 33.4095947
61 H 37.6815957 27.9044688 35.1738453
62 H 38.9149092 28.3260051 33.9888878
63 H 38.7081155 30.1928897 35.4370246
64 H 38.0112343 30.6888540 33.8943693
65 H 35.9289734 29.5330709 35.5341177
66 H 34.5033731 30.5942599 36.6811126
67 H 34.7374957 32.2936183 37.1254988
68 H 37.8274210 32.5981753 35.3757136
69 H 36.7287109 33.3515858 36.5097198
70 H 37.9669033 25.0585771 32.5014295
71 H 38.5570991 26.4569659 31.8113310
72 H 38.7056199 26.1654983 33.4764256
73 H 39.5284872 34.1846469 31.5342435
74 H 47.5495144 31.3894522 30.8086156
75 H 42.5393262 28.7895127 29.1314175

AO-IM+0.0025

1 C 41.9087404 28.3770595 29.8687346

2	H	40.8891403	28.7588579	29.7176869
3	H	41.8553815	27.2838242	29.7454067
4	C	42.3547230	28.7678590	31.2422237
5	N	43.4476020	28.2522068	31.9154836
6	H	44.0934574	27.5243626	31.5937399
7	C	43.5879187	28.9240447	33.0761587
8	H	44.3836002	28.7362541	33.7931399
9	N	42.6390045	29.8368393	33.1961408
10	C	41.8562272	29.7457966	32.0699317
11	H	41.0092707	30.4054495	31.9110679
12	C	40.0929819	34.4281120	32.4237142
13	H	41.0629638	34.7767875	32.0475172
14	H	39.6660676	35.2350716	33.0401347
15	C	40.2234933	33.1846676	33.3057276
16	O	39.2588845	32.8024764	33.9664411
17	O	41.3862411	32.6145122	33.2639318
18	C	47.4674522	32.1236441	31.5957519
19	H	48.1636734	31.8716104	32.4078243
20	H	47.8306442	33.0626987	31.1459551
21	C	46.0847984	32.3075737	32.1323319
22	N	45.1065123	33.0052979	31.4501175
23	H	45.2236648	33.4878467	30.5518829
24	C	43.9718519	32.9642476	32.1674911
25	H	43.0256555	33.3916440	31.8526804
26	N	44.1570341	32.2971551	33.2992036
27	C	45.4752905	31.8862202	33.2942085
28	H	45.8953177	31.3221102	34.1237652
29	Fe	42.4681521	31.5284987	34.4896818
30	O	41.4856565	32.4340179	36.0533502
31	O	42.7973450	31.8813479	37.6941558
32	C	40.7085815	31.3447229	36.2469988
33	O	41.0242322	30.3985639	35.4185646
34	O	39.8295378	31.2929921	37.0983911
35	C	43.7675638	31.2977435	37.1427580
36	O	43.9058250	31.0960219	35.9006681
37	C	44.8368201	30.8350267	38.1135057
38	C	46.0085011	31.8136630	38.1749110
39	C	47.1766346	31.2422941	39.0134167
40	O	48.1560937	32.0047994	39.1786335
41	O	47.0439725	30.0688311	39.4345016
42	H	46.3861837	32.0420500	37.1644660
43	H	45.7011156	32.7778839	38.6113197
44	H	44.3964135	30.7104005	39.1116893
45	H	45.1899959	29.8515881	37.7767730
46	N	38.0301987	26.0693587	32.5880524
47	C	36.6878483	26.6991119	32.7713020
48	C	35.8420422	26.4505289	31.4928161
49	O	36.4798153	26.0329667	30.4811170
50	C	36.8138042	28.1960690	33.0907748
51	C	37.7735920	28.5318196	34.2420215
52	C	37.7514782	29.9942065	34.6757520
53	N	36.4755045	30.3056748	35.3093934
54	C	36.1513751	31.4314816	35.9562704
55	N	34.9863637	31.4421332	36.6199357
56	N	36.9488721	32.5010510	35.9476449
57	O	34.6307771	26.7117815	31.5675378
58	H	36.2139352	26.1759800	33.6162719
59	H	37.1198559	28.7437960	32.1831485
60	H	35.7931064	28.5340841	33.3214707
61	H	37.5552970	27.8961766	35.1192391
62	H	38.8145143	28.3102255	33.9587690
63	H	38.5723036	30.1693568	35.3839375
64	H	37.9278210	30.6627203	33.8163863
65	H	35.7969063	29.5492978	35.4311691
66	H	34.3891631	30.6173184	36.5747119
67	H	34.6546240	32.3005991	37.0608028
68	H	37.8351485	32.5165159	35.4384212
69	H	36.7176601	33.3143299	36.5132458
70	H	37.9341371	25.0491035	32.4459062
71	H	38.5052710	26.4592729	31.7573784
72	H	38.6477541	26.1684150	33.4232559
73	H	39.4501791	34.2176740	31.5689700
74	H	47.5753576	31.3777269	30.8083313
75	H	42.5527694	28.7523693	29.0734760

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1	C	41.9050535	28.4403665	29.9121272
2	H	40.8942780	28.8372016	29.7414710
3	H	41.8376486	27.3472516	29.7844471
4	C	42.3153104	28.8129187	31.3027748
5	N	43.3918026	28.2913178	31.9995496
6	H	44.0667344	27.5940520	31.6706094
7	C	43.4585939	28.9090804	33.1983199
8	H	44.2332075	28.7155238	33.9374038
9	N	42.4810180	29.7909043	33.3251388
10	C	41.7576048	29.7378459	32.1546951
11	H	40.9106664	30.3952387	31.9821339
12	C	40.1205651	34.3628067	32.3655388
13	H	41.1489974	34.5241887	32.0215918
14	H	39.7973194	35.2759628	32.8898938
15	C	40.0144806	33.1791354	33.3293231
16	O	38.9431327	32.9710778	33.9069161
17	O	41.0698975	32.4459160	33.4284245
18	C	47.3977051	32.1609965	31.6295939
19	H	48.0816294	31.9222570	32.4566468
20	H	47.7519843	33.1084832	31.1907682
21	C	45.9994163	32.3133445	32.1376231
22	N	45.0218920	33.0053007	31.4492782
23	H	45.1507048	33.5105871	30.5652273
24	C	43.8714438	32.9196993	32.1402363
25	H	42.9282499	33.3467918	31.8135006
26	N	44.0487334	32.2295050	33.2570665
27	C	45.3745499	31.8499785	33.2750284
28	H	45.7908798	31.2868226	34.1071935
29	Fe	42.4129737	31.6064805	34.5482780
30	O	42.7353961	33.2770114	35.6943401
31	O	42.8296482	33.2011438	36.9492395
32	C	41.9000491	30.6838601	37.1877685
33	O	41.3001752	30.8659265	36.0648814
34	O	41.3785849	30.3820823	38.2584559
35	C	43.4413843	30.8239639	37.0787185
36	O	43.8871815	30.8459247	35.9165374
37	C	44.2937461	30.7665614	38.2961198
38	C	45.6110505	31.5366199	38.2129566
39	C	46.7357998	30.9660947	39.1129647
40	O	47.7208958	31.7228946	39.2770724

41 O 46.5939852 29.7959053 39.5524173
42 H 45.9957712 31.5052462 37.1792133
43 H 45.4705663 32.6019871 38.4509398
44 H 43.6788822 31.0504756 39.1625952
45 H 44.5626592 29.7033532 38.4735078
46 N 38.0918382 26.1183784 32.6190361
47 C 36.7481971 26.7449271 32.8060452
48 C 35.8976216 26.4740637 31.5325956
49 O 36.5298789 26.0359421 30.5240686
50 C 36.8753743 28.2428512 33.1331705
51 C 37.8563164 28.5738309 34.2737511
52 C 37.8399788 30.0356169 34.7250430
53 N 36.5708745 30.3320637 35.3787506
54 C 36.2290293 31.4606608 36.0202227
55 N 35.0719621 31.4526116 36.6963265
56 N 37.0126341 32.5378337 36.0120236
57 O 34.6836058 26.7227371 31.6054183
58 H 36.2805923 26.2206449 33.6540870
59 H 37.1643893 28.7976896 32.2239903
60 H 35.8583526 28.5753766 33.3861385
61 H 37.6555372 27.9290617 35.1484282
62 H 38.8905727 28.3529287 33.9649350
63 H 38.6832125 30.2146882 35.4148463
64 H 37.9976256 30.7138844 33.8704177
65 H 35.9033612 29.5667682 35.5050356
66 H 34.4927827 30.6162331 36.6807751
67 H 34.7352913 32.3095762 37.1398765
68 H 37.8167504 32.6244196 35.3780360
69 H 36.7316401 33.3664069 36.5348650
70 H 37.9979285 25.1030207 32.4523014
71 H 38.5749299 26.5253505 31.8006622
72 H 38.7014642 26.2000974 33.4622662
73 H 39.4819432 34.1813901 31.5010637
74 H 47.5324388 31.4170530 30.8444429
75 H 42.5605151 28.8007922 29.1193280

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1 C 41.8992345 28.4371036 29.8936105
2 H 40.8879364 28.8278018 29.7130076
3 H 41.8395700 27.3433483 29.7698130
4 C 42.2971158 28.8176633 31.2854734
5 N 43.3643787 28.2936770 31.9968331
6 H 44.0368755 27.5889499 31.6772200
7 C 43.4266549 28.9174279 33.1907949
8 H 44.1882255 28.7301481 33.9452074
9 N 42.4522197 29.8076426 33.2978272
10 C 41.7383798 29.7544452 32.1230699
11 H 40.8943783 30.4127111 31.9419631
12 C 40.1484129 34.3635799 32.3891285
13 H 41.1713357 34.5434810 32.0378182
14 H 39.8167419 35.2753579 32.9115817
15 C 40.0768406 33.1911676 33.3734914
16 O 38.9994474 32.9291267 33.9164688
17 O 41.1785319 32.5430311 33.5419660
18 C 47.4084419 32.1614633 31.6297009
19 H 48.0957337 31.9221252 32.4537039
20 H 47.7628032 33.1072673 31.1874575
21 C 46.0132021 32.3170173 32.1439666
22 N 45.0331782 33.0083737 31.4569987
23 H 45.1597564 33.5134341 30.5724919
24 C 43.8849998 32.9247442 32.1508562
25 H 42.9409374 33.3538467 31.8301355
26 N 44.0671055 32.2361041 33.2676915
27 C 45.3925413 31.8564860 33.2845613
28 H 45.8064527 31.2958210 34.1199561
29 Fe 42.4891143 31.5284556 34.5699318
30 O 42.7866351 33.2025228 35.9585828
31 O 43.1728988 32.6984745 37.1312737
32 C 41.8382496 30.7648125 37.1990439
33 O 41.2363274 30.8704799 36.0704206
34 O 41.3717301 30.3762844 38.2611906
35 C 43.3596459 31.2547482 37.0783776
36 O 43.7890456 30.8909926 35.8528423
37 C 44.2633151 30.9021689 38.2546048
38 C 45.6333177 31.5729485 38.1714727
39 C 46.7303200 30.9870175 39.0917324
40 O 47.7313810 31.7277262 39.2515277
41 O 46.5652777 29.8295449 39.5517546
42 H 46.0186659 31.4846366 37.1399423
43 H 45.5633303 32.6527277 38.3744367
44 H 43.7332435 31.1651332 39.1834953
45 H 44.3922969 29.8104541 38.2708966
46 N 38.0907410 26.1120320 32.6233980
47 C 36.7478573 26.7401869 32.8101121
48 C 35.8983781 26.4724977 31.5354891
49 O 36.5317226 26.0364496 30.5266443
50 C 36.8768568 28.2374736 33.1388443
51 C 37.8581417 28.5654431 34.2797900
52 C 37.8452508 30.0268716 34.7312804
53 N 36.5775446 30.3253346 35.3865772
54 C 36.2359416 31.4572805 36.0213897
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56 N 37.0229494 32.5325282 36.0110144
57 O 34.6845412 26.7219668 31.6075718
58 H 36.2790058 26.2156256 33.6572573
59 H 37.1667470 28.7929870 32.2302895
60 H 35.8603293 28.5713332 33.3921097
61 H 37.6558378 27.9209329 35.1542888
62 H 38.8919932 28.3420792 33.9715466
63 H 38.6903880 30.2043108 35.4191350
64 H 38.0019511 30.7047513 33.8760836
65 H 35.9081301 29.5617180 35.5134186
66 H 34.4942402 30.6209248 36.6765677
67 H 34.7411061 32.3134983 37.1353734
68 H 37.8376063 32.6081462 35.3899748
69 H 36.7434906 33.3645111 36.5290799
70 H 37.9956156 25.0965117 32.4578187
71 H 38.5738071 26.5174082 31.8044568
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74 H 47.5369018 31.4159039 30.8450313
75 H 42.5602025 28.8002770 29.1066585

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1 C 41.9028465 28.3912351 29.8687148
2 H 40.8856504 28.7765664 29.7081226

3	H	41.8481447	27.2994080	29.7265516
4	C	42.3243834	28.7533354	31.2578285
5	N	43.4261634	28.2448504	31.9211066
6	H	44.1040257	27.5594949	31.5763566
7	C	43.5226664	28.8650722	33.1165118
8	H	44.3206660	28.6757541	33.8312900
9	N	42.5385106	29.7307013	33.2745770
10	C	41.7793557	29.6691720	32.1287627
11	H	40.9165444	30.3140644	31.9807677
12	C	40.0551690	34.5039045	32.3830024
13	H	41.0403575	34.8064383	32.0057706
14	H	39.6382680	35.3585786	32.9403373
15	C	40.1381465	33.3062123	33.3351726
16	O	39.1087184	32.9488481	33.9282872
17	O	41.2942622	32.7652932	33.4227457
18	C	47.4380914	32.1297113	31.6418248
19	H	48.1341925	31.8730857	32.4531348
20	H	47.7960141	33.0779542	31.2074619
21	C	46.0529741	32.2953978	32.1796135
22	N	45.0786132	33.0270899	31.5312877
23	H	45.1948962	33.5387560	30.6493196
24	C	43.9477916	32.9694620	32.2618731
25	H	43.0062573	33.4301518	31.9793062
26	N	44.1297108	32.2541902	33.3628577
27	C	45.4426855	31.8313125	33.3261420
28	H	45.8741351	31.2315726	34.1253830
29	Fe	42.3784020	31.4815109	34.4834481
30	O	41.8110858	32.3052312	36.5423743
31	O	42.8002551	32.2701820	37.5729391
32	C	40.8693153	31.1535443	36.7472262
33	O	40.6598398	30.6534025	35.6326113
34	O	40.5336289	30.9165374	37.8871419
35	C	43.7479463	31.3591659	37.2629838
36	O	43.7413731	30.7568169	36.1961611
37	C	44.7318892	31.2157652	38.3696221
38	C	46.1167955	31.7583252	38.0102312
39	C	47.1993716	31.1902942	38.9607697
40	O	48.2063930	31.9124340	39.1219908
41	O	46.9813704	30.0498719	39.4393352
42	H	46.3817077	31.4368256	36.9876175
43	H	46.1520414	32.8572841	38.0289260
44	H	44.3380031	31.6991135	39.2750154
45	H	44.8617094	30.1407298	38.5793832
46	N	38.0183622	26.0849512	32.5601013
47	C	36.6628239	26.6924730	32.7195863
48	C	35.8224327	26.3822644	31.4541291
49	O	36.4687509	25.9639671	30.4463577
50	C	36.7591307	28.2056768	32.9713845
51	C	37.7967317	28.6307754	34.0217798
52	C	37.7263929	30.1103971	34.3935356
53	N	36.5405232	30.3583194	35.2037433
54	C	36.2574568	31.4646541	35.9048786
55	N	35.1479041	31.4401404	36.6590471
56	N	37.0520202	32.5339479	35.8762535
57	O	34.6027499	26.6055596	31.5262739
58	H	36.2029613	26.1961175	33.5879441
59	H	36.9726355	28.7236277	32.0212726
60	H	35.7493282	28.5220788	33.2689972
61	H	37.6909285	28.0280039	34.9410780
62	H	38.8165868	28.4432971	33.6487865
63	H	38.6344157	30.3838936	34.9498792
64	H	37.7153388	30.7396885	33.4861285
65	H	35.8594443	29.6036223	35.3207608
66	H	34.5414203	30.6240811	36.6103544
67	H	34.8183236	32.2933462	37.1152688
68	H	37.8496346	32.6189230	35.2287988
69	H	36.8265602	33.3467734	36.4463819
70	H	37.9428502	25.0645827	32.4160266
71	H	38.5068270	26.4838929	31.7405183
72	H	38.6150976	26.1930034	33.4100202
73	H	39.4194029	34.2534718	31.5337957
74	H	47.5545890	31.3945111	30.8455987
75	H	42.5569223	28.7726883	29.0846578

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1	C	41.9148419	28.4521307	29.9089062
2	H	40.9032866	28.8440816	29.7302204
3	H	41.8529736	27.3581545	29.7781033
4	C	42.3120388	28.8257156	31.3033956
5	N	43.3951708	28.3158109	31.9988387
6	H	44.0830600	27.6343719	31.6673535
7	C	43.4510257	28.9356323	33.1989473
8	H	44.2310607	28.7514211	33.9352698
9	N	42.4623780	29.8018149	33.3286090
10	C	41.7415683	29.7417453	32.1581833
11	H	40.8967431	30.4030084	31.9860873
12	C	40.1066358	34.3838417	32.3473786
13	H	41.1259712	34.5940750	31.9994166
14	H	39.7526151	35.2712405	32.8953164
15	C	40.0450407	33.1639485	33.2743278
16	O	38.9761584	32.9360643	33.8677639
17	O	41.0943362	32.4371620	33.3152594
18	C	47.4188978	32.1794446	31.6499935
19	H	48.1082297	31.9362401	32.4715667
20	H	47.7746935	33.1272485	31.2130896
21	C	46.0251773	32.3361419	32.1687507
22	N	45.0485330	33.0423171	31.4948786
23	H	45.1747855	33.5563952	30.6157124
24	C	43.9031684	32.9617141	32.1976477
25	H	42.9588286	33.3970338	31.8846797
26	N	44.0817573	32.2586574	33.3055525
27	C	45.4040788	31.8669237	33.3065049
28	H	45.8270234	31.2969708	34.1311887
29	Fe	42.4258207	31.6084233	34.5630860
30	O	42.5375896	33.4954955	35.5076483
31	O	42.5453570	33.6828159	36.7120904
32	C	41.8877897	30.6860577	37.2556179
33	O	41.3227217	30.9196276	36.1348567
34	O	41.3500210	30.3378970	38.3056339
35	C	43.4430956	30.8333280	37.2095379
36	O	43.9267385	30.9747056	36.0815236
37	C	44.2351484	30.7562275	38.4594441
38	C	45.5030250	31.6140761	38.4872410
39	C	46.6934822	30.9339129	39.2082881
40	O	47.7078427	31.6528650	39.3315593
41	O	46.5581597	29.7343592	39.5683538

42 H	45.8438200	31.8354039	37.4628776
43 H	45.3210138	32.5896219	38.9650642
44 H	43.5627619	30.9293922	39.3115401
45 H	44.5923765	29.7077716	38.5851065
46 N	38.1208515	26.1405999	32.5827476
47 C	36.7679282	26.7478133	32.7716928
48 C	35.9105336	26.4450415	31.5108808
49 O	36.5363879	25.9977850	30.5002825
50 C	36.8841555	28.2484843	33.0942588
51 C	37.8745709	28.5787855	34.2284887
52 C	37.8734983	30.0388474	34.6862169
53 N	36.6052017	30.3499276	35.3335206
54 C	36.2844744	31.4848969	35.9812759
55 N	35.1382248	31.4845457	36.6753547
56 N	37.0748696	32.5533653	35.9533421
57 O	34.6918835	26.6694568	31.5910113
58 H	36.3158984	26.2244708	33.6288335
59 H	37.1615710	28.8049954	32.1822310
60 H	35.8683043	28.5749548	33.3588559
61 H	37.6745138	27.9319259	35.1020743
62 H	38.9059565	28.3542385	33.9118171
63 H	38.7158700	30.1999544	35.3819489
64 H	38.0518224	30.7231886	33.8407516
65 H	35.9410773	29.5862695	35.4829531
66 H	34.5560623	30.6519104	36.6778883
67 H	34.8117462	32.3426884	37.1267114
68 H	37.8727386	32.6328553	35.3047914
69 H	36.8199085	33.3844226	36.4866077
70 H	38.0425871	25.1295912	32.3951698
71 H	38.6092009	26.5693288	31.7773555
72 H	38.7185416	26.2139303	33.4358141
73 H	39.4718321	34.1932283	31.4820706
74 H	47.5436439	31.4379916	30.8608465
75 H	42.5737079	28.8157340	29.1203915

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1 C	41.9162205	28.4616706	29.9050220
2 H	40.9033942	28.8448517	29.7156817
3 H	41.8641782	27.3664687	29.7850480
4 C	42.3039943	28.8518221	31.2975706
5 N	43.3648955	28.3276650	32.0182792
6 H	44.0380106	27.6225249	31.7040513
7 C	43.4228847	28.9621359	33.2084841
8 H	44.1779085	28.7796152	33.9709512
9 N	42.4537803	29.8568671	33.3022459
10 C	41.7468382	29.7993488	32.1250411
11 H	40.9110607	30.4660968	31.9353739
12 C	40.1531408	34.4025793	32.3934130
13 H	41.1737130	34.6046152	32.0471357
14 H	39.8002330	35.3066274	32.9154950
15 C	40.0960810	33.2224434	33.3681908
16 O	39.0192391	32.9345001	33.9014564
17 O	41.2050067	32.5874551	33.5323794
18 C	47.4305751	32.1840633	31.6585627
19 H	48.1186604	31.9367717	32.4796607
20 H	47.7914215	33.1294883	31.2210798
21 C	46.0381892	32.3492043	32.1771781
22 N	45.0675877	33.0650770	31.5018002
23 H	45.2001390	33.5834032	30.6257666
24 C	43.9193345	32.9881016	32.1961286
25 H	42.9822006	33.4395576	31.8860961
26 N	44.0916166	32.2769489	33.3002735
27 C	45.4116967	31.8788889	33.3106263
28 H	45.8193004	31.3049224	34.1402808
29 Fe	42.4995532	31.5840162	34.5942463
30 O	42.7934038	33.2108854	35.9846308
31 O	43.1584729	32.6836352	37.1623511
32 C	41.8052563	30.7623643	37.1906649
33 O	41.2141063	30.8986227	36.0566981
34 O	41.3241718	30.3521369	38.2372031
35 C	43.3289859	31.2402663	37.0970094
36 O	43.7704880	30.8838599	35.8718593
37 C	44.2167384	30.8729919	38.2784759
38 C	45.5938085	31.5286050	38.2022176
39 C	46.6921787	30.9099433	39.0971467
40 O	47.7131624	31.6243326	39.2300760
41 O	46.5110435	29.7562460	39.5629933
42 H	45.9737258	31.4630097	37.1669089
43 H	45.5400414	32.6034991	38.4349356
44 H	43.6860107	31.1428636	39.2046392
45 H	44.3291377	29.7783006	38.2893863
46 N	38.1164927	26.1371164	32.5999595
47 C	36.7642880	26.7456290	32.7888393
48 C	35.9105447	26.4491006	31.5234288
49 O	36.5400033	26.0062869	30.5130816
50 C	36.8797827	28.2451811	33.1175046
51 C	37.8666478	28.5758901	34.2551820
52 C	37.8644099	30.0374582	34.7102338
53 N	36.6016775	30.3450714	35.3694469
54 C	36.2743762	31.4788420	36.0149291
55 N	35.1165264	31.4812744	36.6885805
56 N	37.0675296	32.5468627	36.0050661
57 O	34.6919719	26.6738386	31.6002744
58 H	36.3092414	26.2189631	33.6423494
59 H	37.1589862	28.8044724	32.2074864
60 H	35.8625601	28.5692753	33.3798860
61 H	37.6651554	27.9308881	35.1296656
62 H	38.8989457	28.3503407	33.9424939
63 H	38.7150868	30.2045832	35.3943753
64 H	38.0270520	30.7167152	33.8570083
65 H	35.9299140	29.5850480	35.5026699
66 H	34.5300996	30.6514712	36.6775090
67 H	34.7892069	32.3385848	37.1409181
68 H	37.8857112	32.6181043	35.3872609
69 H	36.8056338	33.3777190	36.5359422
70 H	38.0367355	25.1252642	32.4158350
71 H	38.6032816	26.5621856	31.7921263
72 H	38.7166797	26.2127026	33.4511193
73 H	39.5204910	34.1981753	31.5296767
74 H	47.5489958	31.4410359	30.8699221
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47 C	36.7767665	26.7033600	32.9164525
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71 H	38.3486607	26.1798868	31.8034860
72 H	38.7679073	26.0764307	33.4613373
73 H	39.6103399	34.2134953	31.5400892
74 H	47.5186277	31.2889638	30.7665142
75 H	42.4422175	28.7288489	29.1506028

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1 C	41.7972145	28.4145350	29.9934816
2 H	40.7928223	28.8319796	29.8381337
3 H	41.6987719	27.3226790	29.8863203
4 C	42.2473244	28.7901709	31.3721870
5 N	43.3158647	28.2390972	32.0607868
6 H	43.9410678	27.4891572	31.7345722
7 C	43.4227942	28.8440431	33.2554384
8 H	44.1954371	28.6135208	33.9860745
9 N	42.4677136	29.7629089	33.3993783
10 C	41.7226994	29.7252867	32.2339359
11 H	40.8662943	30.3717925	32.0819023
12 C	40.2822468	34.3351397	32.4036097
13 H	41.3157909	34.3866328	32.0435162
14 H	40.0591087	35.2805113	32.9229791
15 C	40.1000357	33.1942960	33.4143148
16 O	39.0233344	33.0824939	34.0043949
17 O	41.1249588	32.4268401	33.5563952
18 C	47.4091915	32.0590343	31.4976744
19 H	48.1062637	31.8508356	32.3211109
20 H	47.7438899	32.9906121	31.0112207
21 C	46.0192643	32.2140145	32.0193912
22 N	45.0064410	32.8080486	31.2942467
23 H	45.0958333	33.2166974	30.3582977
24 C	43.8647239	32.7176989	31.9957531
25 H	42.8930240	33.0380106	31.6322061
26 N	44.0890151	32.1356155	33.1637462
27 C	45.4278404	31.8118784	33.1961186
28 H	45.8666554	31.2981456	34.0482762
29 Fe	42.5542495	31.5521769	34.5242671
30 O	42.7874576	33.1708346	35.7209167
31 O	43.2487920	32.8146254	36.9797771
32 C	41.8925525	30.8560236	37.3339571
33 O	41.3253104	30.8792591	36.2418381
34 O	41.6021395	30.5864499	38.4840759
35 C	43.6308541	31.4563650	37.0273690
36 O	43.9305715	30.9245784	35.8910842
37 C	44.4990115	31.2002850	38.2528146
38 C	45.8744445	31.8635775	38.1211238
39 C	46.9444652	31.3848747	39.1300436
40 O	47.9384977	32.1509483	39.3007799
41 O	46.7839888	30.2639556	39.6603774
42 H	46.2791774	31.6376038	37.1193520
43 H	45.8015782	32.9625260	38.1712627
44 H	43.9727998	31.5356055	39.1604290
45 H	44.6394787	30.1136125	38.3473213
46 N	38.0168500	25.9434108	32.7523392
47 C	36.7564684	26.6937983	33.0143611
48 C	35.8771559	26.6063473	31.7257947
49 O	36.4877013	26.2842832	30.6826879
50 C	36.9900437	28.1709510	33.3507763
51 C	37.9756913	28.4814930	34.4838192
52 C	37.9292300	29.9419773	34.9220716
53 N	36.6433909	30.2094232	35.5645123
54 C	36.2268842	31.3614453	36.0756235
55 N	35.0351425	31.3855950	36.6936361
56 N	37.0012914	32.4602848	36.0377480
57 O	34.6828264	26.9250157	31.8681101
58 H	36.2453139	26.1856137	33.8443157
59 H	37.3110532	28.7078386	32.4431259
60 H	35.9850190	28.5538250	33.5865425
61 H	37.7878157	27.8385328	35.3620157
62 H	39.0085893	28.2706762	34.1684676
63 H	38.7511080	30.1625888	35.6254543
64 H	38.0609323	30.6133076	34.0564871
65 H	35.9772516	29.4345849	35.6591801
66 H	34.4601222	30.5386862	36.6594050
67 H	34.6432630	32.2701377	37.0082441
68 H	37.7995095	32.5295980	35.3950983
69 H	36.6134404	33.3310183	36.3858492
70 H	37.8332593	24.9186771	32.7374372
71 H	38.3438727	26.1723872	31.8003256
72 H	38.7696735	26.0750829	33.4573947
73 H	39.6159930	34.2159171	31.5492334
74 H	47.5411027	31.2867038	30.7399329
75 H	42.4423624	28.7378094	29.1765697

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1 C	41.7121094	28.3383480	29.7838550
2 H	40.7215513	28.7785911	29.6068050
3 H	41.6027535	27.2550132	29.6206841
4 C	42.1151071	28.6395903	31.1932148
5 N	43.1918717	28.0858071	31.8609834
6 H	43.8465674	27.3718329	31.5158422
7 C	43.2698677	28.6319272	33.0858684

8 H 44.0519074 28.3878529 33.8004711
9 N 42.2862372 29.5057973 33.2735147
10 C 41.5533142 29.5093240 32.1005837
11 H 40.6759344 30.1352289 31.9704205
12 C 40.2256310 34.3908567 32.3605010
13 H 41.2585813 34.4296149 31.9945660
14 H 40.0057140 35.3671363 32.8242538
15 C 40.0591281 33.3113101 33.4457419
16 O 38.9403347 33.1525271 33.9552555
17 O 41.1388478 32.7032088 33.7566950
18 C 47.2923327 32.0178215 31.5549095
19 H 47.9840694 31.8090424 32.3838951
20 H 47.6121935 32.9675019 31.0939643
21 C 45.8914149 32.1296042 32.0635123
22 N 44.8809635 32.7641563 31.3721304
23 H 44.9727251 33.2070237 30.4518521
24 C 43.7399118 32.6443947 32.0824572
25 H 42.7709614 33.0023065 31.7464690
26 N 43.9542845 31.9988480 33.2184052
27 C 45.2936610 31.6704319 33.2176970
28 H 45.7448997 31.0947490 34.0229598
29 Fe 42.2573393 31.2302977 34.4463079
30 O 42.2833048 32.4344292 36.5657296
31 O 43.4829970 32.2835336 37.3372905
32 C 41.2135785 31.4968974 37.1275661
33 O 40.8243821 30.7662665 36.2065595
34 O 40.9383502 31.6412262 38.2983597
35 C 44.2143577 31.2537066 36.8562871
36 O 43.8568834 30.5774639 35.9120865
37 C 45.4757553 31.0190841 37.6292500
38 C 46.0987711 32.1783363 38.4012747
39 C 47.3002178 31.6733575 39.2318517
40 O 48.2649427 32.4605671 39.4112972
41 O 47.2157633 30.5005039 39.6653630
42 H 46.4298378 32.9914730 37.7362194
43 H 45.3567580 32.6119866 39.0950011
44 H 45.2701834 30.2068997 38.3478785
45 H 46.1862610 30.5909621 36.9076776
46 N 37.9607347 25.9606927 32.6447704
47 C 36.6793178 26.6737694 32.9136360
48 C 35.7816859 26.5542294 31.6418467
49 O 36.3842515 26.2338179 30.5937725
50 C 36.8707574 28.1612417 33.2256538
51 C 37.8806794 28.5229533 34.3181528
52 C 37.8131250 29.9961305 34.7069226
53 N 36.5538469 30.2515614 35.4028454
54 C 36.1771776 31.3870299 35.9777046
55 N 35.0046785 31.4010786 36.6338086
56 N 36.9656189 32.4748396 35.9565325
57 O 34.5855087 26.8582187 31.7985819
58 H 36.1979827 26.1597844 33.7577107
59 H 37.1419455 28.6985204 32.3022806
60 H 35.8624099 28.5141529 33.4896672
61 H 37.7263845 27.9057899 35.2207107
62 H 38.9079163 28.3180819 33.9795424
63 H 38.6559518 30.2636602 35.3628883
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67 H 34.6315642 32.2765030 36.9926103
68 H 37.7511829 32.5653371 35.2960422
69 H 36.6084741 33.3313866 36.3663214
70 H 37.8006849 24.9327539 32.6160572
71 H 38.2979034 26.2204158 31.7049245
72 H 38.7010315 26.0970006 33.3628896
73 H 39.5572267 34.2330257 31.5141013
74 H 47.4582633 31.2654700 30.7838703
75 H 42.4020960 28.6931240 29.0182705

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1 C 41.7681682 28.3859612 29.9934711
2 H 40.7678601 28.8143570 29.8424293
3 H 41.6611251 27.2950999 29.8828890
4 C 42.2281858 28.7504343 31.3713308
5 N 43.3135752 28.2045932 32.0376895
6 H 43.9361629 27.4547065 31.6999406
7 C 43.4416954 28.8037921 33.2295744
8 H 44.2338789 28.5729497 33.9374006
9 N 42.4801597 29.7155296 33.3991040
10 C 41.7119185 29.6776592 32.2464335
11 H 40.8452749 30.3146007 32.1142732
12 C 40.3106646 34.3398411 32.4261076
13 H 41.3486451 34.3993831 32.0800218
14 H 40.0807105 35.2764464 32.9587851
15 C 40.1109279 33.1934791 33.4264853
16 O 39.0255850 33.0723756 33.9924342
17 O 41.1432650 32.4376694 33.6108540
18 C 47.3676550 32.0229163 31.5123917
19 H 48.0726741 31.8248743 32.3315714
20 H 47.6902351 32.9548577 31.0180066
21 C 45.9813729 32.1692513 32.0480108
22 N 44.9508432 32.7329034 31.3247296
23 H 45.0190980 33.1004152 30.3696455
24 C 43.8228352 32.6554215 32.0503108
25 H 42.8412071 32.9484309 31.6901215
26 N 44.0716173 32.1133344 33.2349601
27 C 45.4154078 31.8041271 33.2501060
28 H 45.8754506 31.3195050 34.1077485
29 Fe 42.4938193 31.4636698 34.5571674
30 O 42.8986527 33.3269005 35.6786058
31 O 43.1388948 33.2430380 36.9328991
32 C 42.0974229 30.8921600 37.3232465
33 O 41.4547190 30.9443402 36.2147199
34 O 41.6131692 30.7040929 38.4421094
35 C 43.6182975 31.0722667 37.1242658
36 O 44.0301841 30.9407427 35.9525512
37 C 44.5329884 31.0891700 38.3170804
38 C 45.8545086 31.8364216 38.1315087
39 C 46.9716106 31.4393192 39.1235952
40 O 47.9347222 32.2502487 39.2684551
41 O 46.8762996 30.3233782 39.6826980
42 H 46.2404229 31.6183675 37.1209796
43 H 45.7080403 32.9286655 38.1611926
44 H 43.9558496 31.4517122 39.1810180
45 H 44.7745982 30.0347552 38.5494649
46 N 38.0103154 25.9020762 32.7748825

47 C 36.7668747 26.6792984 33.0299505
48 C 35.9107716 26.6269035 31.7207427
49 O 36.5494577 26.3304429 30.6866893
50 C 37.0227417 28.1515395 33.3707651
51 C 37.9876082 28.4557380 34.5226741
52 C 37.9316560 29.9169718 34.9571567
53 N 36.6313018 30.1839120 35.5713145
54 C 36.1928468 31.3416513 36.0447589
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56 N 36.9576919 32.4486151 35.9941300
57 O 34.7172921 26.9534088 31.8418744
58 H 36.2271558 26.1804565 33.8468017
59 H 37.3733583 28.6806508 32.4702104
60 H 36.0200265 28.5541741 33.5822356
61 H 37.7853582 27.8123180 35.3973874
62 H 39.0257627 28.2464289 34.2249915
63 H 38.7380395 30.1443865 35.6764302
64 H 38.0760812 30.5844530 34.0904379
65 H 35.9719258 29.4031401 35.6699160
66 H 34.4240432 30.5170115 36.6191481
67 H 34.5873086 32.2581804 36.9289571
68 H 37.7600494 32.5104303 35.3575267
69 H 36.5486274 33.3229886 36.3051149
70 H 37.8138534 24.8793637 32.7979765
71 H 38.3004618 26.0880424 31.7992726
72 H 38.7869491 26.0461306 33.4500862
73 H 39.6561767 34.2462774 31.5595290
74 H 47.5088824 31.2481080 30.7588706
75 H 42.4192136 28.7072777 29.1804751

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1 C 41.7696098 28.3899525 30.0294756
2 H 40.7665439 28.8125442 29.8785192
3 H 41.6676778 27.2977427 29.9263562
4 C 42.2324585 28.7647560 31.4041404
5 N 43.3105771 28.2116720 32.0777039
6 H 43.9297733 27.4576541 31.7433746
7 C 43.4352945 28.8138959 33.2692670
8 H 44.2189479 28.5815207 33.9862845
9 N 42.4806738 29.7337433 33.4297393
10 C 41.7201662 29.7006603 32.2730481
11 H 40.8640882 30.3503802 32.1340139
12 C 40.3325208 34.3315843 32.4583168
13 H 41.3697823 34.3943598 32.1106397
14 H 40.1036086 35.2676261 32.9923833
15 C 40.1402384 33.1836075 33.4630712
16 O 39.0399317 33.0549985 34.0071900
17 O 41.1763538 32.4504492 33.6676356
18 C 47.3615748 32.0272059 31.4889816
19 H 48.0676288 31.8339207 32.3085959
20 H 47.6847933 32.9557691 30.9882596
21 C 45.9769808 32.1780855 32.0278809
22 N 44.9416351 32.7321872 31.3031893
23 H 45.0033674 33.0898744 30.3441740
24 C 43.8166709 32.6581788 32.0354976
25 H 42.8322431 32.9475745 31.6799983
26 N 44.0732104 32.1293614 33.2231754
27 C 45.4168725 31.8243384 33.2361623
28 H 45.8774432 31.3502782 34.0999615
29 Fe 42.5608593 31.4568774 34.6179718
30 O 42.8282547 33.3489073 35.7831243
31 O 43.3468419 32.9674520 37.0555224
32 C 42.0218169 31.0590852 37.3985004
33 O 41.3855930 30.9847004 36.3016141
34 O 41.6144876 30.8241708 38.5339356
35 C 43.5404679 31.5988631 37.1327678
36 O 43.9333568 31.0653326 35.9622656
37 C 44.4851500 31.3432288 38.3209317
38 C 45.8615170 31.9969388 38.1689035
39 C 46.9545308 31.5144164 39.1492612
40 O 47.9597391 32.2757983 39.3039431
41 O 46.8093803 30.3960762 39.6887296
42 H 46.2380247 31.7762527 37.1547457
43 H 45.7999455 33.0973505 38.2261602
44 H 43.9748317 31.6725453 39.2403259
45 H 44.6112969 30.2549124 38.4090537
46 N 38.0383628 25.8969463 32.7749866
47 C 36.7863868 26.6582142 33.0356323
48 C 35.9129544 26.5811817 31.7498088
49 O 36.5100202 26.2932067 30.6923047
50 C 37.0261357 28.1374649 33.3662761
51 C 38.0048570 28.4523562 34.5035852
52 C 37.9537152 29.9162532 34.9294405
53 N 36.6616092 30.1878042 35.5587335
54 C 36.2316180 31.3506828 36.0311286
55 N 35.0351242 31.3827250 36.6410178
56 N 36.9967362 32.4540487 35.9668064
57 O 34.7123397 26.8954637 31.8829551
58 H 36.2694787 26.1547787 33.8649548
59 H 37.3569050 28.6677653 32.4591354
60 H 36.0233578 28.5307289 33.5945848
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67 H 34.6358967 32.2706142 36.9335890
68 H 37.8065015 32.5122206 35.3351318
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72 H 38.7878703 26.0225433 33.4859964
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1 C 41.6939319 28.3146594 29.7786149
2 H 40.7069859 28.7626242 29.6003135
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6 H 43.8320072 27.3444150 31.5040238
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8 H 44.0519860 28.3600218 33.7829699

9 N	42.2789127	29.4770626	33.2699107
10 C	41.5392666	29.4806732	32.0992623
11 H	40.6558319	30.0992812	31.9750223
12 C	40.2731182	34.3756887	32.3748124
13 H	41.3131040	34.3945564	32.0287920
14 H	40.0679863	35.3519295	32.8456057
15 C	40.0660910	33.2967215	33.4544821
16 O	38.9306376	33.1447857	33.9285073
17 O	41.1338608	32.6927519	33.8122422
18 C	47.2729854	31.9906261	31.5173498
19 H	47.9683145	31.7984673	32.3475583
20 H	47.5847279	32.9360865	31.0417694
21 C	45.8739837	32.0989280	32.0314817
22 N	44.8492968	32.6967980	31.3293533
23 H	44.9248498	33.1016971	30.3903094
24 C	43.7142966	32.5772635	32.0481858
25 H	42.7367315	32.9009158	31.7021719
26 N	43.9465238	31.9713030	33.2027461
27 C	45.2915210	31.6656607	33.2033826
28 H	45.7567070	31.1167140	34.0194627
29 Fe	42.2644020	31.1944704	34.4322401
30 O	42.3054764	32.4434729	36.5846199
31 O	43.5072241	32.2902102	37.3536151
32 C	41.2405830	31.5018060	37.1512925
33 O	40.8618114	30.7529439	36.2433149
34 O	40.9576877	31.6655870	38.3197852
35 C	44.2427986	31.2658548	36.8633215
36 O	43.8888819	30.5916334	35.9191242
37 C	45.5105181	31.0411442	37.6348774
38 C	46.1365022	32.2204299	38.3756346
39 C	47.3524666	31.7574685	39.2097613
40 O	48.2878963	32.5789254	39.3966625
41 O	47.3107240	30.5831990	39.6464432
42 H	46.4514411	33.0214227	37.6878308
43 H	45.3974501	32.6675756	39.0647595
44 H	45.3080925	30.2436860	38.3699842
45 H	46.2170262	30.5993158	36.9182288
46 N	37.9749239	25.9176035	32.6832941
47 C	36.7101916	26.6574269	32.9475959
48 C	35.8328265	26.5694470	31.6576046
49 O	36.4575718	26.2734019	30.6154055
50 C	36.9208602	28.1419289	33.2599056
51 C	37.9136931	28.5035366	34.3666929
52 C	37.8350180	29.9793948	34.7417536
53 N	36.5597573	30.2374603	35.4086032
54 C	36.1631501	31.3814122	35.9473424
55 N	34.9846139	31.4002699	36.5946424
56 N	36.9412072	32.4777167	35.9086083
57 O	34.6371490	26.8812124	31.7981796
58 H	36.2036366	26.1520283	33.7813679
59 H	37.2156217	28.6725813	32.3409328
60 H	35.9127418	28.5098807	33.5033971
61 H	37.7465240	27.8905393	35.2698669
62 H	38.9461356	28.2996081	34.0446590
63 H	38.6620060	30.2581880	35.4134861
64 H	37.9197663	30.6140933	33.8426592
65 H	35.8953400	29.4615987	35.5079745
66 H	34.4114143	30.5510599	36.5668954
67 H	34.5964835	32.2822747	36.9168405
68 H	37.7267056	32.5629743	35.2462836
69 H	36.5613523	33.3406593	36.2818830
70 H	37.8039713	24.8903567	32.7026604
71 H	38.2675744	26.1217022	31.7134808
72 H	38.7438587	26.0754265	33.3646550
73 H	39.6177481	34.2490738	31.5131129
74 H	47.4451318	31.2275384	30.7583176
75 H	42.3875915	28.6599500	29.0120134

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1 C	47.6606909	33.0308853	32.4754096
2 H	47.4105862	32.4789723	33.3942800
3 H	48.7498106	33.1938237	32.4928134
4 C	46.8834785	34.3137479	32.4582695
5 N	47.0871066	35.3468971	31.5597262
6 H	47.8429766	35.4276805	30.8704984
7 C	46.1334426	36.2739519	31.7440517
8 H	46.0254763	37.1658591	31.1336453
9 N	45.3218159	35.9131185	32.7285464
10 C	45.7820033	34.6972473	33.1891323
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13 H	40.9281816	33.2712866	33.3299879
14 H	40.0735531	33.5077580	34.8692846
15 C	41.9873645	34.4651317	34.8345123
16 O	42.0428259	34.7703222	36.0317964
17 O	42.6761658	35.0193030	33.9050816
18 C	43.3012797	35.0406241	27.4050237
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32 C	43.5028248	39.2454737	33.8021366
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19 H	43.2513211	36.0543705	26.9241362
20 H	42.5548814	34.4318887	26.8057103
21 C	42.9463408	35.0996666	28.8063945
22 N	42.4051146	34.0554051	29.5316029
23 H	42.1502594	33.1251025	29.1829911
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25 H	41.8926066	33.8348275	31.6144816
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27 C	43.0941512	36.1223399	29.7098983
28 H	43.4684970	37.1269537	29.5378470
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33 O	44.2690416	38.0730921	33.9257018
34 O	43.2427989	39.8875148	34.7773084
35 C	41.7278035	38.7900170	31.1386434
36 O	42.8915590	38.4023384	31.4727735
37 C	41.6012217	40.1535419	30.3801943
38 C	42.7249672	41.0858349	30.7600080
39 C	42.9753577	42.1527608	29.5901917
40 O	43.5398136	43.1682535	30.0503146
41 O	42.6637255	41.8597212	28.4367160
42 H	42.5540156	41.6071868	31.7103273
43 H	43.6817307	40.5471299	30.8378545
44 H	41.6488252	39.8968705	29.3093991
45 H	40.6074643	40.5775403	30.5745520
46 N	49.2440572	37.2877377	37.7269844
47 C	48.0258102	36.4271513	37.8595531
48 C	48.4259302	34.9341396	37.8205477
49 O	49.5715925	34.6685323	37.3832391
50 C	47.0593745	36.8311086	36.7343063
51 C	45.6560169	36.2259775	36.7635579
52 C	44.8992865	36.4750975	38.0687116
53 N	43.4893955	36.1813625	37.8836638
54 C	42.5507026	36.3056429	38.8264132
55 N	42.8478635	36.7263931	40.0649396
56 N	41.2820764	36.0093632	38.5244438
57 O	47.5419780	34.1417770	38.2062044
58 H	47.5975945	36.6543483	38.8475308
59 H	46.9727696	37.9289082	36.7551887
60 H	47.5346407	36.5784535	35.7706015
61 H	45.0998992	36.6779463	35.9248299
62 H	45.7068706	35.1408699	36.5826712
63 H	45.3220933	35.8359317	38.8636824
64 H	45.0280264	37.5211781	38.4020661
65 H	43.1545672	35.8540590	36.9629290
66 H	42.0873608	36.7125709	40.7464138
67 H	43.8089653	36.7669558	40.4146146
68 H	41.0156512	35.8998755	37.5473510
69 H	40.5513997	36.2436773	39.1982971
70 H	50.0179553	36.9783325	38.3326331
71 H	49.6145076	37.2450321	36.7581820
72 H	49.0209571	38.2758115	37.9722124
73 H	41.3360170	32.5193819	34.8962409
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1 C	47.4122754	33.1637061	32.5545452
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4 C	46.6111676	34.4279928	32.5186813
5 N	46.8566403	35.4873062	31.6629057
6 H	47.6514516	35.5834382	31.0245693
7 C	45.8487559	36.3750861	31.7971275
8 H	45.7512271	37.2821252	31.2048930
9 N	44.9784821	35.9606197	32.6996035
10 C	45.4358926	34.7502480	33.1606246
11 H	44.8737711	34.1684352	33.8877481
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13 H	40.5924801	33.1445947	33.4988411
14 H	39.9039814	33.4989510	35.0914702
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16 O	42.0008675	34.8399438	35.9506254
17 O	42.3271659	34.9867988	33.7373947
18 C	43.2405715	35.1463688	27.3768418
19 H	43.2234133	36.1542063	26.9385789
20 H	42.5032137	34.5418060	26.8235979
21 C	42.8779349	35.2129480	28.8215598
22 N	42.3648418	34.1469708	29.5390444
23 H	42.1401757	33.2102581	29.1862222
24 C	42.1976662	34.5386276	30.8150535
25 H	41.8432162	33.8955447	31.6141910
26 N	42.5531937	35.8067567	30.9648949
27 C	42.9705300	36.2447072	29.7256838
28 H	43.2839770	37.2730386	29.5633720
29 Fe	42.9563402	36.7161651	32.8594869
30 O	40.9929902	37.4915102	32.9816395
31 O	40.0205095	37.0962283	32.3670600
32 C	43.4634856	39.3897328	33.8115157
33 O	43.4125484	38.1709455	34.2024862
34 O	43.7664441	40.3707713	34.4888732
35 C	43.1588880	39.5849832	32.3003901
36 O	43.3251475	38.5772050	31.6058931
37 C	42.7161322	40.9043019	31.8085621
38 C	42.1496223	40.9576925	30.3929284
39 C	42.9753880	41.8581971	29.4372558
40 O	43.7510587	42.7023143	29.9639430
41 O	42.7720505	41.6798478	28.2204624
42 H	42.0598121	39.9605617	29.9385962
43 H	41.1304888	41.3780853	30.4116108
44 H	42.0521616	41.3238155	32.5844043
45 H	43.5888972	41.6020865	31.8243614
46 N	49.1958453	37.2998954	37.7175440
47 C	47.9997409	36.4054484	37.8405518
48 C	48.4391641	34.9213656	37.8184672
49 O	49.6189471	34.6742235	37.4562875

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62 H 45.6677434 35.1037706 36.5538065
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5 N 46.9177644 35.4388601 31.7787833
6 H 47.7149355 35.5632644 31.1481833
7 C 45.9083815 36.3200271 31.9492922
8 H 45.7989196 37.2628048 31.4191145
9 N 45.0282970 35.8553144 32.8166327
10 C 45.4809716 34.6250668 33.2215803
11 H 44.9168630 34.0087096 33.9179175
12 C 40.8367091 33.2963665 34.5665798
13 H 40.6015692 33.1575159 33.5039804
14 H 39.8888904 33.4887885 35.0927645
15 C 41.7765865 34.4822646 34.8062479
16 O 41.9682127 34.8427481 35.9791915
17 O 42.3394303 34.9834932 33.7756829
18 C 43.2523783 35.0832078 27.3771069
19 H 43.2231985 36.1019084 26.9644703
20 H 42.5114294 34.4878023 26.8194396
21 C 42.9177853 35.1054702 28.8297161
22 N 42.3669976 34.0366293 29.5125864
23 H 42.0892295 33.1280761 29.1266723
24 C 42.2647063 34.3723613 30.8116368
25 H 41.8838196 33.7159673 31.5875702
26 N 42.7016743 35.6056129 31.0043801
27 C 43.1026956 36.0817942 29.7783835
28 H 43.4762654 37.0959009 29.6654020
29 Fe 42.9701227 36.6260194 32.8573251
30 O 41.3421154 37.6336817 32.9033160
31 O 41.6352180 39.0445376 32.6590635
32 C 43.6104688 39.2140288 33.9805026
33 O 43.6401938 38.0310358 34.4008803
34 O 43.9499271 40.2717290 34.4875517
35 C 42.9524045 39.2438152 32.4013462
36 O 43.5784867 38.2258257 31.8127415
37 C 43.1246140 40.6280993 31.7613126
38 C 42.5815938 40.6211543 30.3306248
39 C 43.0130087 41.8133677 29.4741083
40 O 43.6405874 42.7751501 29.9692596
41 O 42.7046536 41.7184550 28.2588110
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43 H 41.4796663 40.5889002 30.3354265
44 H 42.6231758 41.3786920 32.3862705
45 H 44.1969936 40.8611252 31.7766444
46 N 49.1989109 37.3003428 37.7235395
47 C 48.0037769 36.4045512 37.8484646
48 C 48.4445306 34.9210536 37.8293376
49 O 49.6238978 34.6735196 37.4657112
50 C 47.0313924 36.7839823 36.7173099
51 C 45.6252756 36.1839435 36.7592781
52 C 44.8748680 36.4381257 38.0660607
53 N 43.4681418 36.1336190 37.8937539
54 C 42.5246352 36.3460043 38.8203846
55 N 42.8337471 36.8257007 40.0343218
56 N 41.2519380 36.0842305 38.5217005
57 O 47.5605514 34.1088980 38.1655202
58 H 47.5616186 36.6231339 38.8324931
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60 H 47.5051918 36.5194247 35.7559727
61 H 45.0567439 36.6431058 35.9337603
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64 H 44.9986688 37.4893308 38.3850950
65 H 43.1242741 35.7676897 36.9913876
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67 H 43.7925658 36.8491382 40.3882776
68 H 40.9839739 35.8950273 37.5573274
69 H 40.5230661 36.3536669 39.1853399
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72 H 48.9611197 38.2803728 37.9882872
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7 C 45.8991535 36.3253585 31.8442938
8 H 45.7915292 37.2403182 31.2666947
9 N 45.0494431 35.9099796 32.7655428
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12 C	40.7506150	33.2373621	34.5961390
13 H	40.4962432	33.0752490	33.5409692
14 H	39.8061934	33.3941459	35.1410197
15 C	41.6395591	34.4687144	34.7990343
16 O	41.8966705	34.8146620	35.9680364
17 O	42.0707705	35.0253174	33.7399099
18 C	43.2524769	35.2082253	27.4526948
19 H	43.2465042	36.2221477	27.0274239
20 H	42.4947681	34.6255952	26.9038136
21 C	42.9032012	35.2588829	28.9024791
22 N	42.3331037	34.2050915	29.5925926
23 H	42.0802229	33.2832486	29.2201835
24 C	42.1631026	34.5835494	30.8739047
25 H	41.7587975	33.9467092	31.6538025
26 N	42.5758048	35.8300477	31.0576632
27 C	43.0331194	36.2658738	29.8313983
28 H	43.4047913	37.2769977	29.6837263
29 Fe	43.0520318	36.6124562	33.0252496
30 O	42.0830303	38.4506989	33.8406347
31 O	41.8742944	39.5342267	32.9355171
32 C	43.2820927	38.7144682	34.6846206
33 O	43.7380240	37.6034471	34.9930922
34 O	43.6014924	39.8735301	34.8490624
35 C	42.8300393	39.5215114	31.9831325
36 O	43.6505528	38.6091231	31.9265137
37 C	42.7226669	40.7145004	31.1098079
38 C	42.9581381	40.4136376	29.6379178
39 C	43.2034145	41.7157112	28.8317346
40 O	43.6722726	42.6937500	29.4679148
41 O	42.9433296	41.6287969	27.6192544
42 H	43.8573206	39.7814694	29.5214838
43 H	42.1134622	39.8730465	29.1860295
44 H	41.7558204	41.2091502	31.2870985
45 H	43.4956913	41.4419886	31.4252517
46 N	49.2068306	37.2746592	37.6654103
47 C	48.0650568	36.3254616	37.8700590
48 C	48.5745114	34.8663668	37.9106622
49 O	49.7366923	34.6460409	37.4798292
50 C	47.0523183	36.5607255	36.7359672
51 C	45.6923364	35.8743580	36.8652800
52 C	44.8898465	36.3312470	38.0833796
53 N	43.4926708	35.9735960	37.9270362
54 C	42.5402448	36.2493568	38.8298646
55 N	42.8443734	36.7605524	40.0331145
56 N	41.2662338	36.0183614	38.5153103
57 O	47.7475587	34.0394951	38.3387551
58 H	47.6291627	36.5746010	38.8492481
59 H	46.8869464	37.6477643	36.6478789
60 H	47.5272893	36.2432651	35.7907870
61 H	45.1226334	36.1429319	35.9653322
62 H	45.8135718	34.7807680	36.8884802
63 H	45.2975348	35.8649122	38.9966246
64 H	44.9926836	37.4246563	38.2150626
65 H	43.1418763	35.6848235	37.0007290
66 H	42.0747473	36.8382282	40.7018343
67 H	43.7998337	36.7739271	40.3969643
68 H	41.0217293	35.7742908	37.5556921
69 H	40.5299419	36.3207542	39.1553765
70 H	50.0395834	37.0128776	38.2129033
71 H	49.5146785	37.2624107	36.6745302
72 H	48.9430853	38.2483137	37.9313901
73 H	41.2783331	32.3596064	34.9691346
74 H	44.2009531	34.7280355	27.2121167
75 H	47.2465193	32.4716537	31.6878948

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1 C	47.3593412	33.1997433	32.5331963
2 H	47.1029610	32.6572265	33.4559227
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4 C	46.5633397	34.4665541	32.4826295
5 N	46.8131582	35.5188109	31.6183693
6 H	47.6058679	35.6056945	30.9780291
7 C	45.8057967	36.4106134	31.7466521
8 H	45.7098145	37.3141117	31.1482147
9 N	44.9356295	36.0056818	32.6515846
10 C	45.3879908	34.7977559	33.1205905
11 H	44.8191768	34.2228365	33.8479320
12 C	40.8200582	33.3320284	34.4884497
13 H	40.5924187	33.1961238	33.4233105
14 H	39.8660889	33.5328551	35.0006889
15 C	41.7679484	34.5116633	34.7415071
16 O	41.9694744	34.8335355	35.9337741
17 O	42.3085565	35.0453723	33.7284401
18 C	43.2243410	35.1603539	27.3540350
19 H	43.2088366	36.1652199	26.9090549
20 H	42.4897607	34.5533062	26.7997796
21 C	42.8506749	35.2367937	28.7956423
22 N	42.3380523	34.1729414	29.5172296
23 H	42.1120087	33.2353600	29.1680766
24 C	42.1561260	34.5747747	30.7882820
25 H	41.7952629	33.9362583	31.5881875
26 N	42.5018782	35.8460594	30.9309263
27 C	42.9270996	36.2771688	29.6920027
28 H	43.2280632	37.3086618	29.5232561
29 Fe	42.9000590	36.7725375	32.8182507
30 O	40.8917741	37.5447553	32.9529936
31 O	39.9292108	37.1783351	32.3137354
32 C	43.4512653	39.4196241	33.8037807
33 O	43.3817086	38.1987946	34.1868393
34 O	43.8170849	40.3827879	34.4770394
35 C	43.0879979	39.6361900	32.3087894
36 O	43.2352339	38.6370912	31.5949834
37 C	42.6148099	40.9561856	31.8558302
38 C	42.0771239	41.0525328	30.4331340
39 C	43.0015968	41.8725339	29.4960217
40 O	43.7993243	42.6845017	30.0415631
41 O	42.8513050	41.6803603	28.2734810
42 H	41.8930928	40.0678133	29.9805315
43 H	41.1052924	41.5732696	30.4392950
44 H	41.9201704	41.3196001	32.6351387
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46 N	49.1650432	37.3019823	37.6480296
47 C	47.9934019	36.3746723	37.7882555
48 C	48.4758325	34.9042354	37.8015216
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57 O 47.6200991 34.0753024 38.1612062
58 H 47.5431264 36.5989805 38.7671716
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6 H 47.7028193 35.5501669 31.0772952
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8 H 45.7857680 37.2483866 31.3423394
9 N 45.0306719 35.8637802 32.7715530
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12 C 40.8544103 33.3456874 34.5067886
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16 O 41.9512126 34.8559425 35.9921262
17 O 42.5064379 34.9008975 33.8247995
18 C 43.2226597 35.0997374 27.3927951
19 H 43.1891163 36.1189374 26.9815335
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21 C 42.8805863 35.1215429 28.8384825
22 N 42.3468514 34.0431668 29.5199194
23 H 42.0921556 33.1282240 29.1405584
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25 H 41.8393684 33.7342267 31.5996458
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27 C 43.0221391 36.1115753 29.7776268
28 H 43.3785085 37.1345798 29.6713063
29 Fe 42.8611333 36.5380079 32.7859525
30 O 41.5353673 37.7794152 33.3710486
31 O 41.7697896 39.1547018 32.8603060
32 C 43.9512572 39.2135749 34.2870548
33 O 43.9765566 38.0807864 34.4885462
34 O 44.1513852 40.3773179 34.4177663
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36 O 43.5719078 38.2694833 31.8331523
37 C 43.2189913 40.6572002 31.7779006
38 C 42.4425791 40.7826351 30.4595349
39 C 42.9499708 41.9319526 29.5516739
40 O 43.6342871 42.8487876 30.0635175
41 O 42.5888054 41.7928427 28.3654066
42 H 42.5010193 39.8426129 29.8876932
43 H 41.3812185 40.9495215 30.7029778
44 H 42.8981665 41.4055022 32.5061735
45 H 44.3000309 40.7597031 31.6342037
46 N 49.1518456 37.3414840 37.5261082
47 C 47.9989299 36.4022796 37.7196266
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49 O 49.6755633 34.7072161 37.4006467
50 C 46.9885696 36.6801997 36.5921767
51 C 45.6001780 36.0525187 36.7053614
52 C 44.8684887 36.3945267 38.0024816
53 N 43.4647677 36.0732708 37.8704515
54 C 42.5273486 36.3682213 38.7833810
55 N 42.8617016 36.8756621 39.9805859
56 N 41.2472184 36.1638451 38.4857193
57 O 47.6485861 34.1174191 38.1770462
58 H 47.5582389 36.6531917 38.6962864
59 H 46.8747635 37.7749014 36.5204885
60 H 47.4474656 36.3607097 35.6403851
61 H 45.0140175 36.4426171 35.8599764
62 H 45.6601519 34.9595797 36.5954429
63 H 45.3292186 35.8356654 38.8379712
64 H 44.9972487 37.4675782 38.2438438
65 H 43.0928699 35.7060164 36.9704821
66 H 42.0998222 37.0210935 40.6472653
67 H 43.8216422 36.8778503 40.3265749
68 H 40.9686493 35.9537769 37.5263250
69 H 40.5260956 36.4882316 39.1336217
70 H 50.0023959 37.0296656 38.0180005
71 H 49.4169333 37.3705858 36.5233294
72 H 48.9141325 38.3052509 37.8452509
73 H 41.3048045 32.4262963 34.8808638
74 H 44.1848156 34.6466062 27.1540583
75 H 47.2456244 32.4484721 31.6494444

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1 C 47.4189185 33.1250958 32.5024117
2 H 47.1721633 32.5791484 33.4256567
3 H 48.5102833 33.2851568 32.5012045
4 C 46.6418302 34.4037811 32.4764336
5 N 46.8764486 35.4529705 31.6054033
6 H 47.6555287 35.5380196 30.9483131
7 C 45.8796965 36.3518332 31.7536106
8 H 45.7785836 37.2617288 31.1658115
9 N 45.0296134 35.9521962 32.6792493

10 C	45.4847118	34.7432385	33.1415441
11 H	44.9351391	34.1700182	33.8853452
12 C	40.7521038	33.2977832	34.5276897
13 H	40.5193104	33.1541900	33.4651319
14 H	39.7971673	33.4642299	35.0503898
15 C	41.6550452	34.5103094	34.7705393
16 O	41.8813512	34.8360907	35.9536347
17 O	42.1363826	35.0698380	33.7370719
18 C	43.2324492	35.2172828	27.4349144
19 H	43.2261734	36.2285021	27.0033973
20 H	42.4752699	34.6323240	26.8877505
21 C	42.8778862	35.2789827	28.8832273
22 N	42.3081822	34.2299570	29.5817500
23 H	42.0520363	33.3067132	29.2154673
24 C	42.1308591	34.6214827	30.8582939
25 H	41.7248764	33.9907282	31.6420583
26 N	42.5388948	35.8710555	31.0308953
27 C	42.9989608	36.2963154	29.8019258
28 H	43.3597037	37.3099927	29.6449016
29 Fe	43.0422746	36.6817812	32.9801046
30 O	42.1655093	38.5031193	33.9289852
31 O	41.8845782	39.5971244	33.0532481
32 C	43.4253666	38.7498934	34.6728277
33 O	43.8970327	37.6342904	34.9428328
34 O	43.7709373	39.9050350	34.8196062
35 C	42.7457886	39.5750413	32.0144639
36 O	43.5530217	38.6533653	31.8916313
37 C	42.5771748	40.7629787	31.1478801
38 C	42.7332554	40.4656779	29.6637914
39 C	43.1588049	41.7260132	28.8656132
40 O	43.6631151	42.6761416	29.5177323
41 O	42.9919313	41.6304153	27.6374301
42 H	43.5262539	39.7129507	29.5050583
43 H	41.8100379	40.0641933	29.2213278
44 H	41.6249399	41.2608856	31.3859692
45 H	43.3730460	41.4908070	31.4093225
46 N	49.1394409	37.3015690	37.4669190
47 C	48.0333621	36.3222353	37.7344722
48 C	48.5920205	34.8856907	37.8526318
49 O	49.7482653	34.6691945	37.3958110
50 C	46.9996632	36.4533004	36.6007220
51 C	45.6534407	35.7625854	36.8154348
52 C	44.8632465	36.3338899	37.9928213
53 N	43.4692201	35.9567595	37.8859572
54 C	42.5300600	36.2996040	38.7812153
55 N	42.8589778	36.8396649	39.9658872
56 N	41.2492519	36.1044047	38.4766211
57 O	47.8110989	34.0629964	38.3619439
58 H	47.5931073	36.6086594	38.7011774
59 H	46.8103459	37.5264989	36.4277588
60 H	47.4646946	36.0684610	35.6758596
61 H	45.0688210	35.9381161	35.9026227
62 H	45.7862403	34.6769725	36.9407127
63 H	45.2828374	35.9635429	38.9446699
64 H	44.9648821	37.4354270	38.0085669
65 H	43.0958971	35.6549416	36.9687745
66 H	42.0942531	36.9850134	40.6297754
67 H	43.8144072	36.8319519	40.3252479
68 H	40.9900408	35.8520092	37.5224436
69 H	40.5241141	36.4559985	39.1050137
70 H	50.0202665	37.0340155	37.9327998
71 H	49.3634638	37.3252439	36.4542084
72 H	48.8814822	38.2655092	37.7730030
73 H	41.2584281	32.4078649	34.9015191
74 H	44.1809510	34.7354138	27.1978201
75 H	47.2103790	32.4855317	31.6447777

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1 C	47.6215718	33.0577244	32.5083385
2 H	47.3654221	32.5086092	33.4270076
3 H	48.7112275	33.2146117	32.5310822
4 C	46.8501684	34.3437034	32.4830417
5 N	47.0633786	35.3740181	31.5829696
6 H	47.8283087	35.4500279	30.9013103
7 C	46.1096736	36.3021678	31.7517787
8 H	46.0093730	37.1908368	31.1357752
9 N	45.2866735	35.9466292	32.7313650
10 C	45.7433420	34.7318412	33.2028724
11 H	45.2386914	34.2067634	34.0065807
12 C	41.0305615	33.3420170	34.4124943
13 H	40.8969012	33.2891586	33.3255524
14 H	40.0449165	33.5307482	34.8665872
15 C	41.9569621	34.4851460	34.8269280
16 O	42.0272624	34.7841140	36.0244327
17 O	42.6187601	35.0569374	33.8883734
18 C	43.3031246	35.0382920	27.4037257
19 H	43.2503884	36.0567123	26.9933661
20 H	42.5558312	34.4274809	26.8707844
21 C	43.0245294	35.0617354	28.8665784
22 N	42.5908085	33.9702182	29.5961577
23 H	42.3689561	33.0353881	29.2374638
24 C	42.5539013	34.3186441	30.8954095
25 H	42.3000316	33.6411135	31.7047087
26 N	42.9082260	35.5856538	31.0421014
27 C	43.1952192	36.0667244	29.7859017
28 H	43.5069953	37.0952521	29.6297900
29 Fe	43.2664137	36.5813140	32.9005847
30 O	41.3381027	37.3583401	32.6129837
31 O	41.1901496	38.6205163	32.5582263
32 C	43.4150798	39.2696580	33.7875324
33 O	43.4782015	38.0695925	34.2463662
34 O	43.4485320	40.3101107	34.4429292
35 C	43.3485723	39.3276538	32.2503729
36 O	43.6985114	38.2803122	31.6693747
37 C	43.1173386	40.6253642	31.5528445
38 C	42.7221295	40.5094936	30.0873939
39 C	42.7794279	41.8355399	29.2905498
40 O	43.4956537	42.7616763	29.7526094
41 O	42.1282509	41.8385444	28.2210502
42 H	43.4062010	39.8109417	29.5731539
43 H	41.7150768	40.0767619	29.9805895
44 H	42.3889798	41.2005409	32.1451199
45 H	44.0469574	41.2203954	31.6259575
46 N	49.3477943	37.1955379	37.7942399
47 C	48.0978765	36.3872957	37.9215393
48 C	48.4246013	34.8748145	37.8181327

49 O	49.5420052	34.5876225	37.3421249
50 C	47.1332826	36.8596802	36.8236948
51 C	45.7256359	36.2604545	36.8326608
52 C	44.9959559	36.3952052	38.1679902
53 N	43.5833325	36.0860073	37.9845221
54 C	42.6361643	36.2139667	38.9124487
55 N	42.9075549	36.6863521	40.1407941
56 N	41.3725083	35.9057678	38.5979437
57 O	47.5039827	34.1124792	38.1871690
58 H	47.6956729	36.6029486	38.9226646
59 H	47.0599054	37.9563776	36.8947224
60 H	47.5963894	36.6331757	35.8468909
61 H	45.1407924	36.7745770	36.0513380
62 H	45.7754895	35.1920656	36.5715184
63 H	45.4482175	35.7016936	38.8942845
64 H	45.1013048	37.4164518	38.5759740
65 H	43.2664159	35.6965269	37.0875258
66 H	42.1522471	36.6288859	40.8215329
67 H	43.8668835	36.7071006	40.5062869
68 H	41.1450632	35.6223364	37.6479355
69 H	40.6353773	36.0723606	39.2801888
70 H	50.0968383	36.8834745	38.4319240
71 H	49.7579373	37.1050714	36.8439166
72 H	49.1597170	38.1971125	38.0068781
73 H	41.4354512	32.3927518	34.7632463
74 H	44.2677898	34.6055662	27.1387037
75 H	47.4323254	32.4249567	31.6412411

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1 C	47.6166683	33.0744827	32.5053346
2 H	47.3704412	32.5231844	33.4253377
3 H	48.7048471	33.2405818	32.5223324
4 C	46.8351676	34.3545347	32.4878735
5 N	47.0396137	35.3959451	31.5960620
6 H	47.8010987	35.4770317	30.9104446
7 C	46.0844476	36.3189197	31.7790151
8 H	45.9696340	37.2194191	31.1820139
9 N	45.2680108	35.9457001	32.7600115
10 C	45.7304657	34.7284578	33.2171618
11 H	45.2355766	34.1960182	34.0220044
12 C	41.0219390	33.3661102	34.4020605
13 H	40.8782687	33.3094560	33.3164684
14 H	40.0381637	33.5508447	34.8629657
15 C	41.9384970	34.5245606	34.8044343
16 O	42.0476889	34.7959052	36.0066722
17 O	42.5338938	35.1418476	33.8526567
18 C	43.3009507	35.0429063	27.4025365
19 H	43.2504138	36.0615264	26.9925437
20 H	42.5552546	34.4328973	26.8661885
21 C	43.0159732	35.0652672	28.8643337
22 N	42.5845582	33.9691822	29.5901178
23 H	42.3659207	33.0350987	29.2280860
24 C	42.5370180	34.3144090	30.8896638
25 H	42.2822593	33.6341473	31.6967341
26 N	42.8803301	35.5835998	31.0395669
27 C	43.1730914	36.0699823	29.7868407
28 H	43.4792879	37.1027083	29.6430221
29 Fe	43.2920724	36.6308419	32.8522989
30 O	41.3272265	37.5628124	32.5801649
31 O	41.5429287	38.9076706	32.3657836
32 C	43.2968381	39.2703311	33.8649743
33 O	43.3789659	38.0863421	34.3330437
34 O	43.4695769	40.3370575	34.4389470
35 C	42.9081090	39.2318657	32.2959815
36 O	43.6381887	38.2318319	31.7764040
37 C	42.9967427	40.5863371	31.5922429
38 C	42.6659571	40.4987491	30.1054574
39 C	42.7750649	41.8196721	29.3068881
40 O	43.4663312	42.7517299	29.7890936
41 O	42.1743277	41.8142698	28.2056457
42 H	43.3525297	39.7828545	29.6189881
43 H	41.6526391	40.0947856	29.9477971
44 H	42.3229059	41.2817837	32.1160395
45 H	44.0111095	40.9812818	31.7374219
46 N	49.3515091	37.1959479	37.7973369
47 C	48.1010168	36.3885880	37.9236836
48 C	48.4259088	34.8759063	37.8183796
49 O	49.5429338	34.5878500	37.3420376
50 C	47.1374584	36.8633012	36.8260562
51 C	45.7294389	36.2653058	36.8326999
52 C	44.9975607	36.3981793	38.1669603
53 N	43.5855250	36.0894187	37.9796170
54 C	42.6372960	36.2097219	38.9072112
55 N	42.9054803	36.6771919	40.1382219
56 N	41.3752525	35.8976780	38.5899001
57 O	47.5042723	34.1141546	38.1861718
58 H	47.6987533	36.6033765	38.9250051
59 H	47.0653326	37.9598665	36.8983956
60 H	47.6015471	36.6380329	35.8494870
61 H	45.1452978	36.7810196	36.0518431
62 H	45.7783449	35.1973834	36.5695405
63 H	45.4481392	35.7033096	38.8930139
64 H	45.1027801	37.4187101	38.5769456
65 H	43.2696486	35.7071125	37.0785914
66 H	42.1493235	36.6145492	40.8176052
67 H	43.8641999	36.7010134	40.5048348
68 H	41.1515449	35.6209460	37.6367842
69 H	40.6354605	36.0651150	39.2690018
70 H	50.1007286	36.8820570	38.4338756
71 H	49.7608098	37.1078013	36.8464108
72 H	49.1643173	38.1971371	38.0124717
73 H	41.4309633	32.4184789	34.7524334
74 H	44.2659215	34.6095348	27.1396916
75 H	47.4290643	32.4383706	31.6403299

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1 C	47.6311313	33.0606396	32.5184532
2 H	47.3855545	32.5075633	33.4376453
3 H	48.7226058	33.2071151	32.5242484
4 C	46.8695648	34.3521824	32.5135693
5 N	47.0647648	35.3796850	31.6078864
6 H	47.8148300	35.4534348	30.9101892
7 C	46.1195014	36.3135507	31.8038283
8 H	46.0131826	37.2082605	31.1973958
9 N	45.3218618	35.9654316	32.8049881
10 C	45.7853832	34.7483973	33.2637686

11	H	45.3055642	34.2229375	34.0836492
12	C	40.8536232	33.2625315	34.4610677
13	H	40.6417113	33.1538437	33.3902015
14	H	39.8913891	33.4128147	34.9782731
15	C	41.7281679	34.4847726	34.7504305
16	O	41.9662303	34.7729057	35.9357635
17	O	42.1170032	35.1259679	33.7211799
18	C	43.3180795	35.1292667	27.4394952
19	H	43.2846762	36.1408513	27.0099816
20	H	42.5561984	34.5253460	26.9193393
21	C	43.0328356	35.1803239	28.9011157
22	N	42.5424193	34.1116352	29.6267540
23	H	42.3205400	33.1750835	29.2722892
24	C	42.4560833	34.4854419	30.9190059
25	H	42.1400793	33.8348766	31.7284150
26	N	42.8363882	35.7455524	31.0715438
27	C	43.1952915	36.1915081	29.8195144
28	H	43.5597698	37.2024093	29.6518509
29	Fe	43.3198393	36.5440835	33.0349414
30	O	42.0185891	38.3766436	33.5401444
31	O	41.9021060	39.4573971	32.6199130
32	C	43.0218868	38.7361007	34.5983938
33	O	43.4917257	37.6720024	35.0110782
34	O	43.2008944	39.9222019	34.7955068
35	C	43.0283013	39.5426951	31.8671448
36	O	43.8877456	38.6808434	31.8986912
37	C	43.0055317	40.7938901	31.0569362
38	C	42.6063959	40.5579783	29.6004565
39	C	42.6416059	41.8778363	28.7943321
40	O	43.3623193	42.7957353	29.2615637
41	O	41.9588545	41.8846059	27.7498851
42	H	43.3083139	39.8519239	29.1214863
43	H	41.6009391	40.1171746	29.5153815
44	H	42.3153108	41.5076089	31.5273987
45	H	44.0077284	41.2425987	31.0769903
46	N	49.3511079	37.1521630	37.7900183
47	C	48.1229313	36.3167350	37.9473518
48	C	48.4865039	34.8128163	37.8726252
49	O	49.5934520	34.5445346	37.3605606
50	C	47.1428935	36.7231732	36.8384439
51	C	45.7667269	36.0573750	36.8580316
52	C	44.9889572	36.2773317	38.1540388
53	N	43.5814810	35.9565060	37.9494679
54	C	42.6238628	36.1079887	38.8617732
55	N	42.8862920	36.5882405	40.0906802
56	N	41.3604712	35.8108969	38.5340973
57	O	47.5987841	34.0369889	38.2873656
58	H	47.7181841	36.5465739	38.9442561
59	H	47.0149354	37.8171787	36.8817115
60	H	47.6212590	36.4950626	35.8693098
61	H	45.1878745	36.4845598	36.0269325
62	H	45.8713657	34.9751777	36.6881021
63	H	45.4114407	35.6372350	38.9447244
64	H	45.0846741	37.3246656	38.4946535
65	H	43.2622739	35.6396472	37.0243866
66	H	42.1274959	36.5272983	40.7678353
67	H	43.8430425	36.6168179	40.4614060
68	H	41.1545337	35.5207063	37.5782792
69	H	40.6138206	36.0185289	39.1933679
70	H	50.1110621	36.8772537	38.4315954
71	H	49.7567135	37.0467622	36.8393752
72	H	49.1389944	38.1558429	37.9696967
73	H	41.3400509	32.3520879	34.8111357
74	H	44.2697956	34.6700292	27.1722791
75	H	47.4202363	32.4361188	31.6503724

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1	C	47.6283243	33.0847145	32.4999891
2	H	47.3787345	32.5389417	33.4222971
3	H	48.7177859	33.2436500	32.5188767
4	C	46.8550108	34.3694054	32.4719042
5	N	47.0678848	35.4004973	31.5718606
6	H	47.8364406	35.4773144	30.8927156
7	C	46.1105317	36.3246653	31.7338941
8	H	46.0115834	37.2125114	31.1166820
9	N	45.2835667	35.9678003	32.7123377
10	C	45.7452759	34.7549212	33.1883881
11	H	45.2449631	34.2307663	33.9950062
12	C	41.0246613	33.3434444	34.3866726
13	H	40.8971073	33.2914350	33.2990241
14	H	40.0375160	33.5317179	34.8379973
15	C	41.9462203	34.4894445	34.8057647
16	O	42.0092146	34.7901212	36.0028830
17	O	42.6060623	35.0653067	33.8683247
18	C	43.3045692	35.0314254	27.3884694
19	H	43.2485554	36.0492901	26.9769689
20	H	42.5621630	34.4148770	26.8550980
21	C	43.0246792	35.0540265	28.8504501
22	N	42.6031883	33.9586177	29.5811784
23	H	42.3918539	33.0220490	29.2204925
24	C	42.5699857	34.3063672	30.8810270
25	H	42.3326222	33.6256798	31.6928334
26	N	42.9115184	35.5770946	31.0253815
27	C	43.1897336	36.0605958	29.7686835
28	H	43.4985037	37.0899977	29.6123474
29	Fe	43.2693188	36.5785281	32.8784595
30	O	41.3030364	37.3221500	32.5673052
31	O	41.1331565	38.5839718	32.5073912
32	C	43.3232686	39.2659026	33.7785310
33	O	43.4097017	38.0653743	34.2294108
34	O	43.3227383	40.3017757	34.4436042
35	C	43.2695415	39.3304911	32.2404270
36	O	43.6510230	38.2975438	31.6539498
37	C	43.0241001	40.6342999	31.5535947
38	C	42.5832103	40.5355138	30.0983850
39	C	42.6315856	41.8693137	29.3140940
40	O	43.3941564	42.7699680	29.7509602
41	O	41.9267745	41.9118013	28.2770230
42	H	43.2469398	39.8359472	29.5594203
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47	C	48.1039245	36.3572618	37.8946550
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58 H 47.7007224 36.6179818 38.8845263
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12 C 41.0094621 33.3674043 34.3793697
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41 O 41.9408125 41.9005255 28.2648842
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44 H 42.2186344 41.2802475 32.1430576
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66 H 42.1854965 36.5750348 40.8173422
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68 H 41.1696564 35.5773393 37.6438706
69 H 40.6571320 36.0368773 39.2761428
70 H 50.0973010 36.8748492 38.4007395
71 H 49.7876908 36.9948426 36.7974930
72 H 49.1647130 38.1647127 37.8474197
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6 H 47.8706974 35.4078889 30.9931358
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8 H 46.0933538 37.1685644 31.3306127
9 N 45.4127198 35.9169239 32.9344881
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12 C	40.8571129	33.2963838	34.4506978
13 H	40.6741419	33.2170202	33.3719645
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15 C	41.7289775	34.5091591	34.7947379
16 O	41.9449417	34.7524355	35.9951632
17 O	42.1324309	35.1896932	33.7986032
18 C	43.3141230	35.1415153	27.5105399
19 H	43.2672878	36.1555189	27.0873133
20 H	42.5422983	34.5373982	27.0052215
21 C	43.0650959	35.1827842	28.9797551
22 N	42.5763480	34.1166936	29.7104400
23 H	42.3485088	33.1823540	29.3544653
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25 H	42.2307852	33.8316003	31.8224754
26 N	42.9367387	35.7356741	31.1601490
27 C	43.2700209	36.1825146	29.9017312
28 H	43.6626497	37.1815698	29.7293574
29 Fe	43.4289054	36.5551668	33.1410981
30 O	42.0945180	38.4638197	33.4546490
31 O	42.1112434	39.4827394	32.4538903
32 C	42.9898250	38.8451466	34.6200031
33 O	43.4413484	37.7823118	35.0594211
34 O	43.0911174	40.0280888	34.8618925
35 C	43.2679377	39.4129224	31.7537032
36 O	44.0912645	38.5411716	31.9631263
37 C	43.3862705	40.5190305	30.7537018
38 C	42.1191475	40.8459502	29.9640229
39 C	42.3262784	42.0760234	29.0505895
40 O	43.1918328	42.9053237	29.4319035
41 O	41.6019396	42.1370752	28.0319947
42 H	41.7870456	39.9953866	29.3480614
43 H	41.2922079	41.0752375	30.6576446
44 H	43.6902463	41.4328005	31.2923815
45 H	44.2237248	40.2589578	30.0905750
46 N	49.3406443	37.1145969	37.7129929
47 C	48.1152223	36.2899879	37.9349202
48 C	48.4903929	34.7864207	37.9801921
49 O	49.5907836	34.4938846	37.4694573
50 C	47.1393955	36.5928410	36.7900935
51 C	45.7632803	35.9315435	36.8766102
52 C	44.9987508	36.2484911	38.1610749
53 N	43.5851135	35.9353127	37.9806067
54 C	42.6342571	36.0995978	38.8949514
55 N	42.8957734	36.6050035	40.1144047
56 N	41.3693398	35.7932944	38.5773750
57 O	47.6156188	34.0418518	38.4719951
58 H	47.7051818	36.5964394	38.9085239
59 H	47.0110549	37.6851417	36.7218501
60 H	47.6167892	36.2718259	35.8475262
61 H	45.1751542	36.2935944	36.0197666
62 H	45.8654590	34.8393971	36.7895995
63 H	45.4183246	35.6541302	38.9882996
64 H	45.1099441	37.3144384	38.4300155
65 H	43.2553987	35.6085401	37.0627833
66 H	42.1485478	36.5227891	40.8011773
67 H	43.8548804	36.6531199	40.4792349
68 H	41.1655239	35.4677293	37.6324640
69 H	40.6277732	35.9924038	39.2434004
70 H	50.1036628	36.8890834	38.3704392
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1 C	47.5613682	33.1395110	32.5354953
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18 C	43.3052420	35.0347572	27.3397322
19 H	43.2526527	36.0451191	26.9091443
20 H	42.5757897	34.4039734	26.8051664
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33 O	43.3556313	38.1313371	34.0705892
34 O	43.2845203	40.3580246	34.3457917
35 C	43.2014460	39.4719414	32.1118861
36 O	43.4627244	38.4674782	31.4609745
37 C	42.8733092	40.7987726	31.5065320
38 C	42.2563686	40.7405564	30.1126627
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40 O	43.2553665	42.8710622	29.6749403
41 O	41.5920418	42.1739630	28.3290090
42 H	42.7744099	39.9681639	29.5181873
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27 C 43.1988992 36.0927851 29.7191556
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2 H 47.4092382 32.4394015 33.4489939
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15 C	41.6955834	34.5346363	34.7626929
16 O	41.9151638	34.7704269	35.9638352
17 O	42.0869337	35.2260161	33.7692434
18 C	43.3118676	35.1303996	27.4884167
19 H	43.2606740	36.1424564	27.0609103
20 H	42.5471488	34.5173641	26.9827908
21 C	43.0577389	35.1758588	28.9561958
22 N	42.5785505	34.1089015	29.6916751
23 H	42.3711605	33.1679179	29.3408457
24 C	42.5337313	34.4810956	30.9886007
25 H	42.2474582	33.8275838	31.8069315
26 N	42.9236069	35.7382969	31.1333178
27 C	43.2526218	36.1820345	29.8728572
28 H	43.6443254	37.1806768	29.6958709
29 Fe	43.4176669	36.5622808	33.1103360
30 O	41.9945050	38.4452887	33.3758669
31 O	41.9850514	39.4526073	32.3619297
32 C	42.8569870	38.8716883	34.5574642
33 O	43.3600377	37.8343413	34.9983803
34 O	42.8816892	40.0566923	34.8108148
35 C	43.1447289	39.4074941	31.6630744
36 O	44.0028720	38.5793622	31.8935112
37 C	43.2233591	40.4963026	30.6356355
38 C	41.9234197	40.8688617	29.9217318
39 C	42.1145818	42.1101747	29.0200144
40 O	43.0077656	42.9151841	29.3868586
41 O	41.3577028	42.2156234	28.0250508
42 H	41.5319483	40.0369511	29.3146310
43 H	41.1442756	41.1108600	30.6652047
44 H	43.5990221	41.4014646	31.1431789
45 H	44.0100463	40.2044095	29.9248346
46 N	49.3631707	37.1178433	37.7017501
47 C	48.1252777	36.3128353	37.9215463
48 C	48.4782551	34.8038111	37.9956216
49 O	49.5979224	34.4939244	37.5482094
50 C	47.1632157	36.6145179	36.7649927
51 C	45.7791779	35.9675103	36.8422980
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57 O	47.5649211	34.0781639	38.4485419
58 H	47.7115204	36.6381629	38.8876302
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61 H	45.1940711	36.3449407	35.9888227
62 H	45.8726871	34.8757247	36.7439684
63 H	45.4371677	35.6602652	38.9466224
64 H	45.1339191	37.3329528	38.4167840
65 H	43.2732757	35.6376175	37.0322174
66 H	42.1698858	36.5112398	40.7784272
67 H	43.8698124	36.6612918	40.4535453
68 H	41.1853945	35.4661304	37.6072086
69 H	40.6473934	35.9771594	39.2255719
70 H	50.1286902	36.8675688	38.3490166
71 H	49.7696407	36.9504420	36.7599733
72 H	49.1630758	38.1353907	37.7894047
73 H	41.2791101	32.3949237	34.7516062
74 H	44.2636482	34.6850133	27.1989139
75 H	47.4147036	32.4259426	31.6565511

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1 C	47.5556805	33.1676231	32.5542315
2 H	47.3051521	32.6259438	33.4785075
3 H	48.6442120	33.3324425	32.5825784
4 C	46.7708854	34.4448088	32.5059548
5 N	46.9952393	35.4744231	31.6049412
6 H	47.7896836	35.5564762	30.9528034
7 C	46.0112591	36.3746543	31.7127537
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9 N	45.1558605	36.0083959	32.6696707
10 C	45.6297895	34.8126754	33.1824374
11 H	45.1116141	34.2865654	33.9748124
12 C	40.9721572	33.3563792	34.3626027
13 H	40.7998595	33.2711059	33.2821659
14 H	40.0111378	33.5939417	34.8468963
15 C	41.9473399	34.4930176	34.6996684
16 O	41.9985442	34.8840523	35.8790726
17 O	42.6347114	34.9460354	33.7322010
18 C	43.3067685	35.0284082	27.3476750
19 H	43.2471091	36.0365437	26.9127564
20 H	42.5817268	34.3887177	26.8176321
21 C	43.0084848	35.0788883	28.8040309
22 N	42.6025158	33.9938579	29.5571680
23 H	42.4370621	33.0392073	29.2201517
24 C	42.5566695	34.3685624	30.8489710
25 H	42.3514060	33.7058395	31.6841202
26 N	42.8686055	35.6515384	30.9632218
27 C	43.1492793	36.1104812	29.6976398
28 H	43.4560264	37.1356083	29.5156105
29 Fe	43.2354129	36.5944123	32.7899193
30 O	41.2405550	36.9853263	32.7518638
31 O	40.8281827	38.1633363	32.5979047
32 C	43.2345375	39.3412121	33.6282522
33 O	43.3857558	38.1440227	34.0359346
34 O	43.1938681	40.3606826	34.3220320
35 C	43.1423857	39.4799676	32.0830663
36 O	43.4463682	38.4954016	31.4220181
37 C	42.7666991	40.8029030	31.4898011
38 C	42.1533517	40.7446163	30.0933687
39 C	42.2458016	42.0694623	29.3009376
40 O	43.1276542	42.8853776	29.6690979
41 O	41.4579970	42.2017374	28.3271417
42 H	42.6911633	39.9876580	29.4962989
43 H	41.1028148	40.4102954	30.1227384
44 H	42.1395594	41.3381636	32.2187012
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46 N	49.4103696	37.1521930	37.7137237
47 C	48.1440573	36.3896056	37.9069060
48 C	48.4373556	34.8656927	37.9638534
49 O	49.5655244	34.5208398	37.5748098
50 C	47.2007603	36.7627044	36.7553222
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25 H 42.4168778 33.7016702 31.7149338
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29 Fe 43.2082200 36.6956990 32.6210748
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31 O 41.1258994 38.8231561 32.2291663
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54 C 42.6877469 36.1753402 38.8117569
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65 H 43.3408213 35.7466263 36.9751940
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67 H 43.8849894 36.6739128 40.4294875
68 H 41.2387244 35.5276752 37.5267778
69 H 40.6845615 35.9645582 39.1575609
70 H 50.1665792 36.8651751 38.3752641
71 H 49.8403111 36.9859668 36.7819548
72 H 49.2454136 38.1714893 37.8206161
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75 H 47.3799170 32.5476339 31.6898056

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5 N 46.9373989 35.5256019 31.6089400
6 H 47.7281881 35.5979523 30.9527400
7 C 45.9627579 36.4385395 31.7310813
8 H 45.8714142 37.3214568 31.1073558
9 N 45.1014770 36.0809882 32.6832347
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12 C 40.8359172 33.3667779 34.3639279
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14 H	39.9067417	33.6048230	34.9079731
15 C	41.8110148	34.5310751	34.5908097
16 O	41.9848889	34.9250522	35.7594413
17 O	42.3531291	35.0049056	33.5474825
18 C	43.2917780	35.0446692	27.2601313
19 H	43.2578802	36.0487946	26.8135078
20 H	42.5927950	34.4044733	26.6960971
21 C	42.9074955	35.1115568	28.6947980
22 N	42.4926358	34.0293676	29.4463335
23 H	42.3865955	33.0601527	29.1289226
24 C	42.3325182	34.4348803	30.7190720
25 H	42.0985355	33.7809016	31.5537836
26 N	42.5767340	35.7332041	30.8258986
27 C	42.9372318	36.1675713	29.5703967
28 H	43.2472609	37.1923322	29.3866561
29 Fe	43.0899756	36.6672548	32.6671234
30 O	41.8965755	37.9310841	33.2816723
31 O	41.7684641	39.2755883	32.2129251
32 C	43.1321314	38.9604857	35.0489296
33 O	43.5571430	37.9325332	35.3890730
34 O	42.8307902	40.0853780	34.9079726
35 C	42.8106853	39.3029900	31.4577043
36 O	43.6944723	38.4273804	31.4509045
37 C	42.9116156	40.5075108	30.5412832
38 C	41.6260979	40.8893686	29.8055791
39 C	41.8095927	42.1492743	28.9324640
40 O	42.7200695	42.9370879	29.2953732
41 O	41.0395762	42.2987969	27.9483991
42 H	41.2608551	40.0684681	29.1659933
43 H	40.8235261	41.0875731	30.5395918
44 H	43.2354174	41.3716899	31.1433655
45 H	43.7287872	40.3028449	29.8347574
46 N	49.4480209	37.0665000	37.7100810
47 C	48.1837787	36.3084600	37.9367815
48 C	48.4982375	34.7983877	38.1294057
49 O	49.6588011	34.4491718	37.8623533
50 C	47.2470058	36.5626209	36.7482559
51 C	45.8714554	35.8928267	36.8093906
52 C	45.0751647	36.2208111	38.0721072
53 N	43.6582569	35.9122454	37.8628520
54 C	42.6880573	36.0721157	38.7539439
55 N	42.9165965	36.5780671	39.9814493
56 N	41.4255826	35.7751976	38.4031910
57 O	47.5173530	34.1136310	38.5034094
58 H	47.7561674	36.6961365	38.8736636
59 H	47.1157199	37.6530205	36.6327605
60 H	47.7561919	36.2083961	35.8347468
61 H	45.3054104	36.2254954	35.9253343
62 H	45.9909587	34.8014449	36.7515132
63 H	45.4798019	35.6242731	38.9041601
64 H	45.1767202	37.2879111	38.3405150
65 H	43.3547197	35.5820541	36.9382549
66 H	42.1671771	36.4584458	40.6592381
67 H	43.8689341	36.6156504	40.3700873
68 H	41.2486897	35.4390306	37.4539666
69 H	40.6748598	35.9366277	39.0663903
70 H	50.2428457	36.6651419	38.2402237
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73 H	41.2589050	32.4293868	34.7251016
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1 C	48.4058673	34.0990476	39.1293371
2 H	48.1967576	34.0644299	38.0481662
3 H	49.0888211	33.2591561	39.3310992
4 C	47.1147841	33.9462831	39.8702093
5 N	46.9837731	33.5174848	41.1815997
6 H	47.7407031	33.2386666	41.8149344
7 C	45.6718666	33.5467031	41.5060847
8 H	45.2758958	33.2774454	42.4826314
9 N	44.9479219	33.9644319	40.4761878
10 C	45.8319081	34.2068674	39.4488103
11 H	45.4962784	34.5249410	38.4655476
12 C	42.4917483	36.5149210	36.5191034
13 H	42.1983326	37.4510318	37.0137004
14 H	41.6423428	36.1366900	35.9348383
15 C	42.8679048	35.4314128	37.5407169
16 O	42.9889525	34.2628877	37.1952005
17 O	43.0291810	35.8477447	38.7642618
18 C	45.9052452	38.4396035	43.9229505
19 H	45.4474038	38.0577402	44.8471224
20 H	45.8033833	39.5383332	43.9351491
21 C	45.2053612	37.8495516	42.7487750
22 N	45.1827536	38.3861590	41.4748837
23 H	45.6349218	39.2494296	41.1609210
24 C	44.4636921	37.5551208	40.6874913
25 H	44.2734439	37.7035610	39.6275516
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28 H	44.2619427	35.9779097	43.4545617
29 Fe	42.9456531	34.8127002	40.4468013
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31 O	42.1536216	33.0079864	40.0677804
32 C	40.8735243	35.5028275	42.3098635
33 O	41.2206287	35.5474356	41.0674108
34 O	39.9530792	36.0849565	42.8510553
35 C	41.8354459	34.6330087	43.1685783
36 O	42.8337258	34.1778172	42.6042754
37 C	41.5715704	34.4512659	44.6189202
38 C	40.5533020	33.3298483	44.9173993
39 C	40.4284148	33.1197692	46.4510326
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41 O	40.4108413	31.9385651	46.8404823
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43 H	40.8517475	32.3802327	44.4511070
44 H	42.5280117	34.2183346	45.1112428
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6 H 47.8492981 33.2782603 41.8305720
7 C 45.7709350 33.5060286 41.5207093
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39 C 40.2862775 32.8887970 46.3305514
40 O 40.2948302 33.9414632 47.0185424
41 O 40.3286722 31.7116125 46.7615322
42 H 39.4753994 33.8311588 44.5957516
43 H 39.9627387 32.1229577 44.2884969
44 H 42.3856668 32.8883793 44.6036193
45 H 41.8177103 34.5267672 44.6832276
46 N 47.0878011 28.7510843 37.4250891
47 C 46.9006037 30.1097199 36.8167500
48 C 48.0968599 30.4299344 35.8701518
49 O 48.0690397 31.5659462 35.3551078
50 C 46.6696233 31.1529506 37.9062332
51 C 45.4159047 30.9658465 38.7819754
52 C 44.1079871 31.4888424 38.1876154
53 N 43.5366879 30.6183800 37.1515047
54 C 42.5724258 31.0304324 36.3024216
55 N 41.9739955 30.1415334 35.4862486
56 N 42.1830377 32.2958860 36.2759574
57 O 48.9307763 29.5150593 35.6686191
58 H 46.0148376 30.0334779 36.1685867
59 H 47.5625221 31.1782163 38.5555545
60 H 46.6302481 32.1311563 37.4066916
61 H 45.3012778 29.9171633 39.1152877
62 H 45.5694958 31.5434655 39.7048245
63 H 43.3765129 31.6623250 38.9965427
64 H 44.2921487 32.4799913 37.7517941
65 H 43.6889742 29.6157848 37.2348586
66 H 42.2258494 29.1510323 35.5023469
67 H 41.2135747 30.4772279 34.8895190
68 H 41.5246728 32.5896320 35.5587800
69 H 42.6312204 33.0887637 36.7912756
70 H 47.6930244 28.1876448 36.7968896
71 H 47.5759674 28.7987958 38.3402809
72 H 46.1764912 28.2730433 37.5599080
73 H 43.3583288 36.8776435 36.0554534
74 H 47.0172180 38.3095720 44.0711411
75 H 48.9836472 35.3031577 39.3749863

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1 C 48.4187413 34.3513888 39.1131378
2 H 48.1354737 34.3948807 38.0499127
3 H 49.1285815 33.5173680 39.2228200
4 C 47.1751481 34.1320968 39.9162401
5 N 47.1235746 33.7689059 41.2508325
6 H 47.9131639 33.6316098 41.8910679
7 C 45.8266513 33.7258312 41.6252970
8 H 45.5070997 33.5220196 42.6448358
9 N 45.0306712 34.0098369 40.6033122
10 C 45.8601129 34.2656511 39.5329824
11 H 45.4636782 34.5363786 38.5572408
12 C 42.4874373 36.6523309 36.6744244
13 H 42.1524798 37.6029519 37.1082938
14 H 41.6485072 36.2318085 36.0945911
15 C 42.8359858 35.6324498 37.7694492
16 O 43.2811595 34.5103552 37.4496078

17 O	42.6039140	35.9791843	38.9710204
18 C	45.8485017	38.4244287	43.9885923
19 H	45.4067896	38.0391170	44.9190630
20 H	45.7536059	39.5226456	44.0087469
21 C	45.1172664	37.8555938	42.8228536
22 N	45.0999617	38.3980853	41.5519372
23 H	45.5843775	39.2480655	41.2349518
24 C	44.3313111	37.6126007	40.7717109
25 H	44.1462017	37.7935820	39.7169082
26 N	43.8287859	36.5983210	41.4667124
27 C	44.3167944	36.7410141	42.7486923
28 H	44.0580364	36.0449621	43.5413327
29 Fe	43.0140325	34.7782499	40.6099124
30 O	41.5196640	32.4572048	41.8193249
31 O	41.8365170	33.0413003	40.5305806
32 C	40.8610676	36.6619010	43.2712380
33 O	40.4275301	36.2645121	42.2646959
34 O	41.2740205	37.0638664	44.2786493
35 C	41.9549572	33.1621274	42.8603526
36 O	42.6405309	34.1675746	42.7146700
37 C	41.5501281	32.6057504	44.1963605
38 C	40.4865296	33.4258839	44.9412401
39 C	40.2844095	32.9484657	46.4065836
40 O	39.8165445	33.8086074	47.1881127
41 O	40.5972231	31.7694933	46.6928903
42 H	40.7677910	34.4875872	44.9859956
43 H	39.5157378	33.3725601	44.4169916
44 H	41.2225047	31.5651905	44.0968040
45 H	42.4604808	32.6153394	44.8093659
46 N	47.0773397	28.7166658	37.3939754
47 C	46.9101907	30.0809363	36.7910664
48 C	48.1083206	30.3842480	35.8432256
49 O	48.0998366	31.5208485	35.3318575
50 C	46.7038562	31.1189307	37.8889599
51 C	45.4443405	30.9445168	38.7578579
52 C	44.1543377	31.5125622	38.1677907
53 N	43.5533972	30.6578145	37.1372928
54 C	42.6082935	31.0961569	36.2826168
55 N	41.9964070	30.2169578	35.4679335
56 N	42.2575422	32.3747165	36.2491357
57 O	48.9282980	29.4550019	35.6392825
58 H	46.0200518	30.0257190	36.1464322
59 H	47.5958894	31.1162778	38.5394802
60 H	46.6853008	32.1028920	37.4002098
61 H	45.2991565	29.8903241	39.0604316
62 H	45.6090911	31.4896961	39.6976416
63 H	43.4254263	31.7027909	38.9751522
64 H	44.3651341	32.4960492	37.7290315
65 H	43.6738765	29.6511118	37.2227460
66 H	42.2214924	29.2202335	35.5092894
67 H	41.2096211	30.5487969	34.9037801
68 H	41.6129189	32.6930407	35.5293072
69 H	42.7352240	33.1516802	36.7587144
70 H	47.6821901	28.1505905	36.7676670
71 H	47.5615169	28.7566152	38.3117265
72 H	46.1605820	28.2466605	37.5226899
73 H	43.3185349	36.8580648	35.9998745
74 H	46.9216336	38.2349095	44.0117760
75 H	48.9625575	35.2603513	39.3702724

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1 C	48.3524665	34.4648389	39.1492374
2 H	48.0374207	34.5183842	38.0955426
3 H	49.0445515	33.6150351	39.2451467
4 C	47.1253125	34.2890173	39.9892911
5 N	47.0930096	33.9433963	41.3308542
6 H	47.8949146	33.7898600	41.9538143
7 C	45.8144551	33.9843347	41.7535571
8 H	45.5056531	33.8178249	42.7822445
9 N	45.0082889	34.3042859	40.7468756
10 C	45.8109996	34.4944026	39.6429739
11 H	45.3983588	34.7782866	38.6808852
12 C	42.5950527	36.7152387	36.7359755
13 H	42.2720849	37.6622945	37.1856352
14 H	41.7401347	36.2753682	36.1945317
15 C	43.0266990	35.7038095	37.8035229
16 O	43.3046351	34.5322841	37.4613336
17 O	43.0676572	36.1194915	39.0004078
18 C	45.9457620	38.5951357	44.0614435
19 H	45.4970689	38.2080056	44.9875926
20 H	45.8933572	39.6948140	44.0968817
21 C	45.2008761	38.0595828	42.8919033
22 N	45.1389706	38.6285463	41.6326103
23 H	45.5922512	39.5043283	41.3226686
24 C	44.4146603	37.8319046	40.8352237
25 H	44.2202561	38.0150161	39.7840525
26 N	43.9799872	36.7723574	41.5213471
27 C	44.4643588	36.9076828	42.8073908
28 H	44.2777606	36.1832740	43.5912034
29 Fe	43.0981069	35.1485546	40.8191981
30 O	41.5506507	32.7595067	40.8816802
31 O	42.3982817	33.4172394	40.1600760
32 C	40.9083729	35.4839692	42.5801392
33 O	41.3406721	35.6563667	41.3704801
34 O	39.8632306	35.8839228	43.0488953
35 C	41.8828596	34.6710613	43.4732747
36 O	42.9460214	34.3078134	42.9746334
37 C	41.4869657	34.3786647	44.8810299
38 C	40.6516372	33.0872424	45.0024831
39 C	40.3088718	32.7779883	46.4841048
40 O	40.0407862	33.7627032	47.2096045
41 O	40.3268522	31.5734089	46.8340012
42 H	39.7068973	33.2186614	44.4453904
43 H	41.1792970	32.2224356	44.5691031
44 H	42.4043705	34.2899676	45.4790498
45 H	40.8784493	35.2055482	45.2718537
46 N	46.9919193	28.6039768	37.4526032
47 C	46.9655038	29.9413585	36.7664732
48 C	48.1643784	30.0047241	35.7742763
49 O	48.3443811	31.1032543	35.2270485
50 C	46.9197792	31.0716426	37.7887923
51 C	45.6996070	31.0726328	38.7247324
52 C	44.4080575	31.6370821	38.1403513
53 N	43.7424747	30.7300625	37.1923367
54 C	42.7514210	31.1401050	36.3753991
55 N	42.1049255	30.2158721	35.6227936

56 N	42.3775952	32.4037531	36.3239116
57 O	48.7927232	28.9239458	35.5850013
58 H	46.0576218	29.9540440	36.1449630
59 H	47.8408482	31.0343865	38.3944078
60 H	46.9630218	32.0173003	37.2297367
61 H	45.5221190	30.0678682	39.1572084
62 H	45.9435916	31.7142642	39.5834240
63 H	43.7134366	31.8994602	38.9542778
64 H	44.6197474	32.5847882	37.6262158
65 H	43.8318352	29.7279630	37.3469697
66 H	42.4862173	29.2827682	35.4760156
67 H	41.3080969	30.5303718	35.0631559
68 H	41.7177750	32.6994639	35.6062840
69 H	42.8049748	33.2249458	36.8488626
70 H	47.5793947	27.9905040	36.8526881
71 H	47.4615040	28.6565613	38.3774389
72 H	46.0420453	28.2053115	37.5699496
73 H	43.3926538	36.9378825	36.0272235
74 H	47.0090072	38.3551992	44.0641523
75 H	48.9229706	35.3638515	39.3824083

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1 C	48.5366658	34.4362838	39.0988595
2 H	48.2474618	34.4744802	38.0368855
3 H	49.2519149	33.6089987	39.2105354
4 C	47.2960746	34.2295153	39.9083531
5 N	47.2365187	33.9025887	41.2533249
6 H	48.0246088	33.7604593	41.8957222
7 C	45.9458272	33.9369765	41.6422190
8 H	45.6178601	33.7829440	42.6674630
9 N	45.1573857	34.2362385	40.6159007
10 C	45.9882758	34.4193819	39.5347622
11 H	45.5994890	34.7121332	38.5668209
12 C	42.5496917	36.5597337	36.6524691
13 H	42.1370412	37.5282570	36.9678290
14 H	41.7607364	35.9869467	36.1426083
15 C	43.0051442	35.7896471	37.8888101
16 O	42.9537118	34.5216182	37.9229601
17 O	43.3731057	36.4528495	38.8874833
18 C	46.1019563	38.6721129	44.2084215
19 H	45.6827244	38.2433957	45.1298189
20 H	46.0788014	39.7680497	44.3071296
21 C	45.3065464	38.2229629	43.0394860
22 N	45.2875484	38.8472681	41.8071520
23 H	45.7776694	39.7098731	41.5260839
24 C	44.5433576	38.1183448	40.9683189
25 H	44.3849891	38.3611847	39.9221752
26 N	44.0437741	37.0555634	41.5980035
27 C	44.5108805	37.1152681	42.8954835
28 H	44.2580339	36.3625310	43.6382381
29 Fe	43.3807335	35.3650716	40.6741738
30 O	40.1832676	32.1153564	41.9615011
31 O	41.4479252	32.4602089	42.0648887
32 C	40.4989690	35.3523687	41.4228371
33 O	41.2578396	35.4095266	40.4739367
34 O	40.4871219	34.7435130	42.5105008
35 C	41.8357883	33.7190991	42.9119882
36 O	42.8985328	34.1540843	42.4599915
37 C	41.5927083	33.5033122	44.3948264
38 C	40.2302090	32.9940357	44.8716386
39 C	40.2378838	32.7622981	46.4053258
40 O	40.1765404	33.7890846	47.1215145
41 O	40.3299580	31.5748046	46.8076649
42 H	39.4590798	33.7372994	44.6227708
43 H	39.9876961	32.0509022	44.3657752
44 H	42.3862847	32.8061444	44.7092278
45 H	41.8196882	34.4694667	44.8739785
46 N	46.9436996	28.6418670	37.5139880
47 C	46.8820405	29.9731291	36.8188975
48 C	48.0723930	30.0488212	35.8128080
49 O	48.2181285	31.1381810	35.2369982
50 C	46.8264419	31.1135666	37.8320403
51 C	45.6412395	31.0864116	38.8158208
52 C	44.3236849	31.6765361	38.3150255
53 N	43.6376863	30.8203607	37.3425108
54 C	42.6687324	31.2530424	36.5063889
55 N	42.0332460	30.3210804	35.7487536
56 N	42.3071202	32.5179434	36.4462124
57 O	48.7317162	28.9829187	35.6448946
58 H	45.9667824	29.9605428	36.2081992
59 H	47.7673217	31.1131750	38.4081688
60 H	46.8229426	32.0553071	37.2648433
61 H	45.4718069	30.0660739	39.2134958
62 H	45.9239939	31.6888855	39.6899464
63 H	43.6649663	31.8711740	39.1798856
64 H	44.5015451	32.6576262	37.8553573
65 H	43.7042602	29.8148596	37.4787448
66 H	42.4695205	29.4196353	35.5570786
67 H	41.2859454	30.6438662	35.1269101
68 H	41.6541514	32.8063973	35.7176485
69 H	42.6390538	33.3484571	37.0613835
70 H	47.5375816	28.0372533	36.9116108
71 H	47.4229848	28.7067386	38.4329745
72 H	46.0032965	28.2251567	37.6437841
73 H	43.3467719	36.7893697	35.9453640
74 H	47.1580056	38.4096967	44.1454553
75 H	49.0603267	35.3583145	39.3512597

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1 C	48.3789249	34.4200958	39.0976071
2 H	48.0612810	34.4841396	38.0451963
3 H	49.0966770	33.5891502	39.1723592
4 C	47.1590684	34.1781617	39.9313202
5 N	47.1428066	33.8325642	41.2712012
6 H	47.9449351	33.7487665	41.9055347
7 C	45.8567843	33.7547543	41.6729508
8 H	45.5660151	33.5718153	42.7051529
9 N	45.0312620	33.9939605	40.6619194
10 C	45.8326540	34.2636098	39.5730657
11 H	45.4096747	34.5229037	38.6061404
12 C	42.4886334	36.6255362	36.7507127
13 H	42.1982357	37.5618579	37.2432341
14 H	41.6094033	36.2581641	36.1916254
15 C	42.8355889	35.5417883	37.7769218
16 O	43.2919660	34.4409274	37.3817118
17 O	42.5762026	35.8025237	38.9890471

18 C	45.8469981	38.4821693	43.9848228
19 H	45.3993637	38.1125321	44.9188306
20 H	45.7694061	39.5816061	43.9917661
21 C	45.1132980	37.9055601	42.8255820
22 N	45.0986413	38.4284404	41.5469750
23 H	45.5828732	39.2801024	41.2245137
24 C	44.3453149	37.6264143	40.7718334
25 H	44.1732705	37.7944569	39.7122408
26 N	43.8435481	36.6159262	41.4797867
27 C	44.3203072	36.7847962	42.7655174
28 H	44.0650096	36.1009196	43.5701049
29 Fe	43.0281978	34.7953715	40.7224227
30 O	41.4893575	32.4562480	41.9113269
31 O	41.8541255	33.0002862	40.6146775
32 C	40.8254967	36.6480359	43.3031348
33 O	40.4908671	36.2181553	42.2705811
34 O	41.1425484	37.0677864	44.3362040
35 C	41.9678541	33.1435408	42.9475498
36 O	42.6899276	34.1195030	42.7972939
37 C	41.5601390	32.5949157	44.2864964
38 C	40.4656888	33.3887132	45.0133287
39 C	40.2295763	32.8656358	46.4561874
40 O	39.7958830	33.7118793	47.2678694
41 O	40.4850458	31.6602798	46.7024766
42 H	40.7319958	34.4520090	45.0939817
43 H	39.5128406	33.3382140	44.4563216
44 H	41.2538965	31.5463993	44.1963276
45 H	42.4668814	32.6318727	44.9044594
46 N	46.9751012	28.5523653	37.4607523
47 C	46.9397066	29.8936609	36.7829427
48 C	48.1419143	29.9694248	35.7953333
49 O	48.3212442	31.0697904	35.2528065
50 C	46.8727575	31.0121977	37.8174916
51 C	45.6586693	30.9683448	38.7623184
52 C	44.3537577	31.5208247	38.1955904
53 N	43.7088041	30.6145855	37.2321791
54 C	42.7389932	31.0243326	36.3921491
55 N	42.1056509	30.1024304	35.6216402
56 N	42.3573005	32.2849343	36.3389496
57 O	48.7735495	28.8894819	35.6021028
58 H	46.0344657	29.9002358	36.1574957
59 H	47.7977352	30.9914119	38.4175528
60 H	46.8879339	31.9665855	37.2722656
61 H	45.5002878	29.9503866	39.1701667
62 H	45.8942222	31.5924683	39.6347470
63 H	43.6569869	31.7554322	39.0193776
64 H	44.5476737	32.4794012	37.6961115
65 H	43.8117481	29.6111095	37.3784034
66 H	42.5176765	29.1887144	35.4416754
67 H	41.3503464	30.4388261	35.0185595
68 H	41.7181990	32.5698756	35.5999469
69 H	42.7891256	33.1141517	36.8546719
70 H	47.5634428	27.9459507	36.8550576
71 H	47.4473700	28.6056925	38.3841221
72 H	46.0255010	28.1553976	37.5800752
73 H	43.2893124	36.8471008	36.0451000
74 H	46.9169763	38.2756154	44.0082594
75 H	48.9268680	35.3284126	39.3481789

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1 C	47.3514845	31.4349860	34.2290854
2 H	46.8750640	31.8366891	33.3255537
3 H	47.7384241	30.4458349	33.9407763
4 C	46.3173498	31.3144666	35.3056266
5 N	46.3611354	30.3984262	36.3408292
6 H	47.0983312	29.7035855	36.5040565
7 C	45.2676190	30.5717814	37.1121624
8 H	45.0487387	29.9869811	38.0030372
9 N	44.5121627	31.5507589	36.6325083
10 C	45.1504466	32.0185467	35.5030943
11 H	44.7230548	32.8075958	34.8883579
12 C	42.1476386	36.1267359	35.0315789
13 H	42.3244001	36.7636016	35.9092516
14 H	41.1115211	36.2758293	34.6870190
15 C	42.3274711	34.6374457	35.3682920
16 O	41.8897060	33.7834492	34.5946869
17 O	42.9496761	34.3835839	36.4703492
18 C	47.6196450	33.8773113	40.7689593
19 H	47.3164633	33.2452975	41.6168544
20 H	47.9058069	34.8640955	41.1709219
21 C	46.4839497	33.9898853	39.8181759
22 N	46.3311792	34.9909316	38.8792444
23 H	46.9543063	35.7902040	38.7292964
24 C	45.2028789	34.7371619	38.1818718
25 H	44.8094618	35.3435435	37.3698179
26 N	44.6204092	33.6366117	38.6239974
27 C	45.4052604	33.1600505	39.6421594
28 H	45.1711792	32.2442740	40.1788398
29 Fe	42.9514848	32.7005396	37.5926088
30 O	40.4334344	31.5995916	36.5306167
31 O	41.6666247	31.5733236	36.5724874
32 C	41.7078167	32.8929376	40.1985095
33 O	41.6391471	33.2737838	38.9721890
34 O	41.3216848	33.4771607	41.1967320
35 C	42.4314652	31.5200651	40.3676131
36 O	42.9718560	31.0445358	39.3644482
37 C	42.5093228	30.8739687	41.7169846
38 C	41.4962216	29.7307507	41.9539109
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45 H	42.3540886	31.6316257	42.4955023
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71 H 42.8278818 27.5101175 31.5542177
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28 H	45.2157046	32.1849321	40.0279830
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32 C	41.3313414	33.8502091	40.1993690
33 O	41.2395071	34.0184246	39.0526040
34 O	41.4253346	33.7586575	41.3563768
35 C	42.8994296	30.7252335	40.2646542
36 O	43.9248883	30.3503155	39.7370100
37 C	42.5639063	30.5731025	41.7317585
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39 C	41.6645754	28.8642243	43.4148831
40 O	41.8883576	29.6465912	44.3776214
41 O	41.5823334	27.6190253	43.4663089
42 H	40.4882052	29.9347894	41.9264282
43 H	41.5591860	28.6760093	41.2709134
44 H	43.5036557	30.2911021	42.2196617
45 H	42.2419791	31.5347878	42.1553950
46 N	43.7683293	27.9154719	31.3429024
47 C	43.8149927	29.4060237	31.5043505
48 C	45.0463634	30.0169085	30.7837524
49 O	45.2058585	31.2472145	30.9677805
50 C	43.7332236	29.8100319	32.9746503
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52 C	41.1663988	29.7894276	33.0289189
53 N	40.8146013	31.1744949	33.3112118
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56 N	39.5542300	33.0757992	33.0902188
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63 H	41.2458277	29.6561273	31.9391005
64 H	40.3502347	29.1301662	33.3416357
65 H	41.4037412	31.7406572	33.9179416
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68 H	40.2643474	33.5298202	33.6703952
69 H	38.8800379	33.7004823	32.6376299
70 H	44.4430469	27.4485334	31.9760759
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17 O 42.8058307 34.3280698 36.5196538
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23 H	46.8081574	35.7305665	38.7440661
24 C	44.9973774	34.7270109	38.2775275
25 H	44.5873093	35.3397314	37.4797722
26 N	44.4000786	33.6478252	38.7461583
27 C	45.2181118	33.1435264	39.7242022
28 H	44.9486954	32.2378698	40.2637577
29 Fe	42.8261179	32.5542109	37.6240105
30 O	40.7442295	31.0493670	39.0382614
31 O	41.0303893	31.9719631	37.9897233
32 C	42.3423789	33.4951815	41.8138092
33 O	41.3926991	33.5624336	41.1516665
34 O	43.2945664	33.4873537	42.4873882
35 C	41.7742200	30.7098172	39.7722937
36 O	42.9161891	31.1363891	39.5416650
37 C	41.4008189	29.7881814	40.9173567
38 C	41.8136135	30.3404848	42.2888220
39 C	41.8659993	29.3410698	43.4783272
40 O	42.0006533	29.8839307	44.6132202
41 O	41.8232762	28.1177798	43.2432810
42 H	42.8280250	30.7689218	42.2198076
43 H	41.1460912	31.1626694	42.5957662
44 H	40.3206823	29.5909528	40.8724699
45 H	41.9026466	28.8214275	40.7601573
46 N	43.6684293	27.9750829	31.3550415
47 C	43.6639168	29.4610338	31.5526215
48 C	44.8903820	30.1161805	30.8533148
49 O	45.0342205	31.3500450	31.0807972
50 C	43.5739810	29.8397357	33.0330033
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53 N	40.5714440	30.9223169	33.4063117
54 C	39.6047593	31.5358587	32.6982805
55 N	38.9765801	30.9098237	31.7039503
56 N	39.2931656	32.7887391	33.0628530
57 O	45.5909307	29.3830213	30.1264208
58 H	42.7766750	29.8345009	31.0176711
59 H	44.5059803	29.5270014	33.5368811
60 H	43.5647857	30.9388115	33.0488155
61 H	42.4766785	28.1729983	33.8805918
62 H	42.4143270	29.6289417	34.8501188
63 H	41.0332608	29.3465985	32.1304210
64 H	40.2796248	28.8386884	33.6374125
65 H	40.9463976	31.4469561	34.1931769
66 H	39.1124024	29.9097692	31.4930910
67 H	38.2786142	31.3874092	31.1372989
68 H	39.8917091	33.2376373	33.7562131
69 H	38.6826659	33.4188083	32.5404487
70 H	44.4075771	27.5145153	31.9157954
71 H	42.7474687	27.5285584	31.5871815
72 H	43.8750600	27.7354554	30.3740433
73 H	42.5339050	36.0063987	34.1864466
74 H	48.4118471	33.4430581	40.3534438
75 H	48.0967665	31.9459869	34.4262373

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1 C	47.4700667	31.5732007	34.3113375
2 H	46.9871743	31.9834578	33.4153097
3 H	47.8754780	30.5906992	34.0238680
4 C	46.4459325	31.4503204	35.3976452
5 N	46.5438471	30.6070213	36.4886121
6 H	47.3368116	29.9970448	36.7213083
7 C	45.4644182	30.7988034	37.2741156
8 H	45.2993054	30.2873500	38.2194716
9 N	44.6592527	31.7109504	36.7444451
10 C	45.2569185	32.1243775	35.5723006
11 H	44.8046201	32.8741884	34.9263430
12 C	42.4152240	36.2510713	35.1759808
13 H	42.6615052	36.8699197	36.0481128
14 H	41.3493004	36.4107682	34.9366788
15 C	42.5954696	34.7549865	35.4628925
16 O	42.3405517	33.9271054	34.5745166
17 O	42.9890755	34.4388668	36.6421786
18 C	47.7540333	33.8951175	40.8703567
19 H	47.4716903	33.2605973	41.7223611
20 H	48.0689993	34.8744059	41.2637641
21 C	46.5988431	34.0352643	39.9502873
22 N	46.4275027	35.0650346	39.0496389
23 H	47.0480175	35.8762024	38.9192308
24 C	45.2991303	34.8380767	38.3578834
25 H	44.9178163	35.4867245	37.5759069
26 N	44.7177047	33.7159971	38.7714093
27 C	45.5204842	33.2078510	39.7674408
28 H	45.2986354	32.2803714	40.2854184
29 Fe	43.0696683	32.8200818	37.7691736
30 O	40.9320526	31.8245942	36.4253766
31 O	41.8643572	31.2804820	37.1465065
32 C	41.7016028	32.8300749	40.3317018
33 O	41.7695924	33.3206288	39.1327660
34 O	41.1050963	33.2824948	41.2844873
35 C	42.5286901	31.5172018	40.4906804
36 O	43.2285744	31.1838140	39.5334012
37 C	42.4693116	30.7518936	41.7778949
38 C	41.5219651	29.5283998	41.7597833
39 C	41.6005159	28.7052365	43.0979729
40 O	41.7549220	29.3723228	44.1468412
41 O	41.4985564	27.4651090	42.9883347
42 H	40.4766758	29.8665529	41.6305414
43 H	41.7718955	28.8335827	40.9395279
44 H	43.4892124	30.3961672	41.9870199
45 H	42.1481307	31.4190951	42.5883286
46 N	43.5519071	28.0384248	31.4319988
47 C	43.6769118	29.5247242	31.6218496
48 C	44.8444334	30.0605631	30.7432272
49 O	45.1279953	31.2600791	30.9076980
50 C	43.8139996	29.9218180	33.0873697
51 C	42.6139489	29.5806775	33.9781829
52 C	41.2792665	30.1043907	33.4577075
53 N	41.2048782	31.5521183	33.4254574
54 C	40.1520156	32.2184528	32.9279883
55 N	39.1859332	31.5635855	32.2437788
56 N	40.0584990	33.5192732	33.1560350
57 O	45.3548408	29.2467549	29.9279690
58 H	42.7663464	29.9641128	31.1863153

59 H	44.7276249	29.4681354	33.5079479
60 H	43.9886719	31.0063872	33.0807390
61 H	42.5108352	28.4866520	34.0877172
62 H	42.7937521	29.9712926	34.9931222
63 H	41.1119461	29.7137546	32.4434675
64 H	40.4654762	29.7154791	34.0830409
65 H	41.7888486	32.1028396	34.0650447
66 H	39.3127800	30.6013582	31.9160110
67 H	38.5175850	32.1172352	31.7197173
68 H	40.8557015	33.9602822	33.6359926
69 H	39.3068269	34.1028991	32.7747087
70 H	44.2012693	27.5263224	32.0585044
71 H	42.5827880	27.6689137	31.5523890
72 H	43.8930607	27.8448085	30.4750877
73 H	43.0369846	36.5725856	34.3404515
74 H	48.6445507	33.4697885	40.4076029
75 H	48.3332411	32.1860200	34.5710481

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1 C	47.3896922	31.5504383	34.3858513
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3 H	47.7777633	30.5549824	34.1192386
4 C	46.3780488	31.4669434	35.4881880
5 N	46.4774137	30.6406126	36.5942675
6 H	47.2675174	30.0247800	36.8219400
7 C	45.4103949	30.8598777	37.3880241
8 H	45.2446738	30.3809334	38.3505598
9 N	44.6086189	31.7744158	36.8506375
10 C	45.1999257	32.1587409	35.6642952
11 H	44.7525126	32.9082430	35.0158389
12 C	42.3773742	36.2718944	35.2811353
13 H	42.6609121	36.9217065	36.1188590
14 H	41.3120059	36.4442080	35.0530792
15 C	42.5411931	34.7864133	35.6378411
16 O	42.0812981	33.9256477	34.8609836
17 O	43.1276895	34.5053097	36.7336804
18 C	47.9630988	33.9729269	40.9239059
19 H	47.6687688	33.3218059	41.7589221
20 H	48.3381017	34.9201114	41.3418207
21 C	46.7964782	34.1903637	40.0374313
22 N	46.6675526	35.2129039	39.1194965
23 H	47.3125034	35.9993284	38.9742559
24 C	45.5337796	35.0317964	38.4312457
25 H	45.1773614	35.6836423	37.6396761
26 N	44.9095512	33.9458716	38.8729996
27 C	45.6805580	33.4155415	39.8811853
28 H	45.3860272	32.5177364	40.4142439
29 Fe	43.2860553	32.9973771	38.0675497
30 O	41.2553791	31.0047061	39.0895976
31 O	41.5913697	31.3655130	37.8739176
32 C	41.6243347	33.0388210	40.2912884
33 O	41.8491097	33.7031878	39.1925290
34 O	41.0494318	33.4159861	41.2818914
35 C	42.2658556	31.5846382	40.1758202
36 O	43.4263411	31.6695954	39.5638205
37 C	42.1926966	30.7318556	41.4582911
38 C	41.3735670	29.4322672	41.5072333
39 C	41.4917882	28.6635373	42.8754458
40 O	41.6490102	29.3549057	43.9095332
41 O	41.4029326	27.4150162	42.8112892
42 H	40.2999057	29.6598783	41.3566025
43 H	41.6842963	28.7203679	40.7226826
44 H	43.2415925	30.4960035	41.6923105
45 H	41.8276636	31.3871310	42.2619242
46 N	43.5687420	28.0322429	31.4603236
47 C	43.6826792	29.5193875	31.6458139
48 C	44.8546114	30.0568290	30.7725021
49 O	45.1334220	31.2574537	30.9359943
50 C	43.7949307	29.9340092	33.1094515
51 C	42.5752732	29.6071296	33.9809671
52 C	41.2549412	30.1469708	33.4396431
53 N	41.1234692	31.5880720	33.5359416
54 C	40.0927179	32.2610255	32.9971018
55 N	39.1755376	31.6105842	32.2441703
56 N	39.9678090	33.5516462	33.2569187
57 O	45.3659404	29.2429423	29.9585682
58 H	42.7764866	29.9487134	31.1920379
59 H	44.6977321	29.4804304	33.5529541
60 H	43.9753742	31.0178271	33.0938298
61 H	42.4591685	28.5138230	34.0815616
62 H	42.7464049	29.9861921	35.0031232
63 H	41.1539883	29.8492212	32.3856065
64 H	40.4188064	29.6714580	33.9680441
65 H	41.7112777	32.1330650	34.1779093
66 H	39.3269823	30.6580633	31.8993645
67 H	38.5106895	32.1667292	31.7184250
68 H	40.7131223	33.9850611	33.8284069
69 H	39.2352637	34.1339444	32.8383663
70 H	44.2080182	27.5219897	32.0988138
71 H	42.5988877	27.6583037	31.5575121
72 H	43.9326546	27.8422000	30.5100734
73 H	42.9871730	36.5528101	34.4224742
74 H	48.8135609	33.5165955	40.4174051
75 H	48.2669624	32.1571005	34.6104066

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1 C	47.5183800	31.5543017	34.2521560
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3 H	47.9410352	30.5846010	33.9454851
4 C	46.4801067	31.3878390	35.3192470
5 N	46.5967153	30.5443655	36.4094653
6 H	47.4084219	29.9663741	36.6565015
7 C	45.4939810	30.6774750	37.1723154
8 H	45.3392902	30.1653703	38.1190857
9 N	44.6501627	31.5479613	36.6296809
10 C	45.2546522	31.9988859	35.4730769
11 H	44.7826538	32.7411494	34.8315897
12 C	42.3493814	36.2166534	35.1484393
13 H	42.5738509	36.8687507	36.0031639
14 H	41.2914786	36.3648467	34.8703429
15 C	42.5341813	34.7325263	35.5142682
16 O	42.1629854	33.8657730	34.6828474
17 O	43.0167375	34.4701269	36.6500064
18 C	47.7993061	33.9032817	40.8734260
19 H	47.5179881	33.2641235	41.7226192
20 H	48.1256064	34.8772710	41.2706707

21 C 46.6392570 34.0569518 39.9622713
22 N 46.4576089 35.1014242 39.0805460
23 H 47.0722571 35.9178518 38.9597526
24 C 45.3229186 34.8815447 38.3931859
25 H 44.9240033 35.5436771 37.6304398
26 N 44.7509320 33.7499278 38.7914174
27 C 45.5639253 33.2271719 39.7727304
28 H 45.3392903 32.2855534 40.2653811
29 Fe 43.2580683 32.7229118 37.7463526
30 O 41.4143960 31.6765057 39.7201987
31 O 41.5063756 31.9586509 38.2975387
32 C 41.6079227 34.4007329 40.5850261
33 O 41.7146834 34.7976627 39.4969983
34 O 41.5213099 34.0060983 41.6749379
35 C 42.5107119 31.0914134 40.2231182
36 O 43.5329706 30.9739497 39.5644557
37 C 42.3046803 30.5923989 41.6338351
38 C 41.4075579 29.3397803 41.7069210
39 C 41.5078032 28.5904247 43.0765733
40 O 41.6500574 29.3038841 44.0984654
41 O 41.4317963 27.3437342 43.0240040
42 H 40.3523702 29.6339061 41.5542157
43 H 41.6677253 28.6132259 40.9183734
44 H 43.3017896 30.3620777 42.0295375
45 H 41.8747847 31.3896478 42.2586475
46 N 43.5773876 28.0048422 31.3964241
47 C 43.6903086 29.4938777 31.5683704
48 C 44.8631548 30.0333294 30.7015490
49 O 45.1223107 31.2396938 30.8525540
50 C 43.7895595 29.9115563 33.0311367
51 C 42.5656897 29.5667758 33.8893918
52 C 41.2490333 30.1071156 33.3388914
53 N 41.0910874 31.5390342 33.5012473
54 C 40.0647310 32.2232390 32.9711019
55 N 39.1241168 31.5762381 32.2409457
56 N 39.9671267 33.5176365 33.2209941
57 O 45.3970893 29.2165726 29.9041416
58 H 42.7853274 29.9181399 31.1081995
59 H 44.6940529 29.4695792 33.4818513
60 H 43.9572041 30.9970506 33.0184033
61 H 42.4574684 28.4718719 33.9778780
62 H 42.7308019 29.9373898 34.9154927
63 H 41.1770958 29.8564302 32.2690641
64 H 40.4070576 29.5899360 33.8175977
65 H 41.7246178 32.0942753 34.0931442
66 H 39.2711569 30.6236537 31.8939132
67 H 38.4740916 32.1386999 31.7033345
68 H 40.7593115 33.9409842 33.7429890
69 H 39.2364818 34.1109676 32.8152649
70 H 44.2163381 27.5037327 32.0424684
71 H 42.6067009 27.6363296 31.5055069
72 H 43.9365042 27.7971260 30.4492532
73 H 42.9875028 36.5165015 34.3171997
74 H 48.6817797 33.4733597 40.3996385
75 H 48.3719541 32.1705281 34.5345446

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1 C 47.5111741 31.6453665 34.3410977
2 H 47.0234025 32.0871264 33.4605258
3 H 47.9185598 30.6715264 34.0277095
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5 N 46.6296373 30.6809864 36.5397943
6 H 47.4449224 30.1039110 36.7818517
7 C 45.5693532 30.8789927 37.3486395
8 H 45.4410616 30.3922034 38.3123580
9 N 44.7373152 31.7667347 36.8192573
10 C 45.3025047 32.1635713 35.6241724
11 H 44.8369757 32.9093569 34.9824423
12 C 42.5224904 36.3176217 35.2154089
13 H 42.7918946 36.9433800 36.0761698
14 H 41.4493556 36.4810444 35.0092625
15 C 42.6945071 34.8238568 35.5102824
16 O 42.4877381 33.9962442 34.5991380
17 O 43.0120940 34.4950463 36.7018823
18 C 47.8158053 33.9031171 40.9204414
19 H 47.5361310 33.2626317 41.7686683
20 H 48.1476476 34.8741606 41.3198568
21 C 46.6548305 34.0712230 40.0140828
22 N 46.4778709 35.1282405 39.1456450
23 H 47.1034536 35.9424528 39.0323505
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25 H 44.9685512 35.6088541 37.6997469
26 N 44.7613694 33.7929492 38.8407165
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28 H 45.3466707 32.3179720 40.3202587
29 Fe 43.1510585 32.8888664 37.8450322
30 O 40.8695220 31.7993492 36.4298981
31 O 41.9516931 31.3961225 37.0409995
32 C 41.6910689 32.7950670 40.3462574
33 O 41.7936470 33.3172801 39.1599600
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35 C 42.5398715 31.4966460 40.4973794
36 O 43.2515400 31.1886278 39.5383761
37 C 42.4615601 30.7036955 41.7668399
38 C 41.5461290 29.4581400 41.6862372
39 C 41.5711946 28.6061019 43.0104542
40 O 41.7091603 29.2472364 44.0736841
41 O 41.4412855 27.3693960 42.8740399
42 H 40.5009435 29.7739440 41.5080675
43 H 41.8463082 28.7808721 40.8670363
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46 N 43.5089838 28.0558790 31.4670868
47 C 43.6177167 29.5506267 31.6103975
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49 O 44.9658684 31.2647556 30.6667605
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57 O 45.1306276 29.2092218 29.7698337
58 H 42.6566786 29.9639934 31.2673840
59 H 44.8768904 29.5699359 33.3647502

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62 H 43.1596212 30.1311555 35.0457001
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67 H 38.6796766 32.1983667 31.8755976
68 H 41.0759854 34.0599053 33.6510437
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70 H 44.1573759 27.5618622 32.1094117
71 H 42.5446669 27.6783500 31.5757452
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1 C 47.5072002 31.7194876 34.3555969
2 H 47.0208880 32.1481711 33.4677284
3 H 47.8740969 30.7206330 34.0724947
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5 N 46.6306688 30.8398854 36.5872442
6 H 47.4182043 30.2173991 36.8071961
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9 N 44.8338078 32.0630981 36.9209774
10 C 45.3772482 32.4039488 35.6996192
11 H 44.9370937 33.1724257 35.0686221
12 C 42.5894225 36.4985344 35.3972891
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14 H 41.5122507 36.6651996 35.2225534
15 C 42.7622922 35.0304634 35.8079122
16 O 42.3522654 34.1418911 35.0174393
17 O 43.2824392 34.7717508 36.9311274
18 C 48.1188142 33.9870956 41.0289657
19 H 47.8419803 33.3116326 41.8500372
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25 H 45.2273758 36.0116090 38.0328302
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29 Fe 43.4973960 33.1790719 38.1948412
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41 O 41.3396281 27.3718787 42.7156471
42 H 40.3551140 29.8867451 41.4604126
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46 N 43.4664625 28.1265571 31.6315294
47 C 43.5463795 29.6224565 31.7802716
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56 N 40.3508655 33.7197806 33.3876735
57 O 45.0250463 29.2750567 29.9125110
58 H 42.5632103 30.0175753 31.4796080
59 H 44.9091039 29.6837581 33.4491178
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63 H 40.9778436 29.7963768 33.4015989
64 H 41.0097992 30.1845563 35.1419058
65 H 42.0440173 32.4092509 34.4539834
66 H 39.6592821 30.7994216 32.2288271
67 H 38.8336149 32.2860074 32.0770333
68 H 41.0794655 34.1874443 33.9709068
69 H 39.5729352 34.2427961 32.9725043
70 H 44.1187992 27.6329130 32.2699925
71 H 42.5105427 27.7238935 31.7125831
72 H 43.8617121 27.9696447 30.6784190
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74 H 48.9323306 33.5306560 40.4651208
75 H 48.3919494 32.3097133 34.5941755

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1 C 47.6222439 31.6862321 34.2201010
2 H 47.1625466 32.1371767 33.3287595
3 H 48.0438871 30.7182618 33.9072010
4 C 46.5716163 31.5244189 35.2769807
5 N 46.6733853 30.6920548 36.3775279
6 H 47.4834505 30.1191066 36.6450288
7 C 45.5782194 30.8614493 37.1439738
8 H 45.4114196 30.3671149 38.0986477
9 N 44.7517920 31.7446574 36.5916870
10 C 45.3632213 32.1681382 35.4283846
11 H 44.9137491 32.9249698 34.7873353
12 C 42.4939816 36.4072200 35.1326985
13 H 42.7418855 37.0772530 35.9667328
14 H 41.4259515 36.5534840 34.8897332
15 C 42.6774170 34.9345457 35.5178874
16 O 42.4008236 34.0564031 34.6477362
17 O 43.0420741 34.6719746 36.6887114
18 C 47.8584314 33.9039058 40.9294275
19 H 47.5763997 33.2501626 41.7669557
20 H 48.2058270 34.8624199 41.3446390
21 C 46.6958008 34.1068851 40.0325854

22	N	46.5119678	35.2068479	39.2222278
23	H	47.1345758	36.0259625	39.1425693
24	C	45.3823905	35.0371324	38.5201568
25	H	44.9900353	35.7603755	37.8112892
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30	O	41.6617185	31.6131966	39.6439918
31	O	41.8310852	31.7635839	38.2080262
32	C	41.5092123	34.2593907	40.4688297
33	O	41.6749287	34.5765593	39.3595425
34	O	41.3440420	33.9445303	41.5730286
35	C	42.6687184	30.9314312	40.2449901
36	O	43.6965000	30.6433609	39.6699817
37	C	42.2969841	30.5351663	41.6563535
38	C	41.4223882	29.2617066	41.6716013
39	C	41.4599874	28.4880422	43.0317810
40	O	41.6119750	29.1777688	44.0638393
41	O	41.3287903	27.2450153	42.9587332
42	H	40.3698608	29.5315147	41.4599343
43	H	41.7412439	28.5451247	40.8938446
44	H	43.2357596	30.3446933	42.1914058
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46	N	43.4810966	28.0853900	31.5058926
47	C	43.5585951	29.5839795	31.6311937
48	C	44.5948785	30.0955911	30.5809771
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50	C	43.8962709	30.0666629	33.0373515
51	C	42.8762563	29.7745952	34.1411332
52	C	41.4577710	30.2948689	33.8942324
53	N	41.4043454	31.7190287	33.6219203
54	C	40.3470908	32.3545108	33.0828797
55	N	39.3382722	31.6584238	32.4826319
56	N	40.2824039	33.6664426	33.1836427
57	O	45.0643690	29.2317951	29.7868277
58	H	42.5804054	29.9725661	31.3077857
59	H	44.8767553	29.6616148	33.3387651
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61	H	42.7943718	28.6874973	34.3263358
62	H	43.2605900	30.2098942	35.0777457
63	H	40.9995202	29.7424130	33.0600885
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65	H	42.0109208	32.3537740	34.1763427
66	H	39.5232167	30.7326566	32.0858222
67	H	38.7055769	32.2200753	31.9225263
68	H	41.0763140	34.1217754	33.6943116
69	H	39.5069268	34.2111734	32.7924309
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72	H	43.8731475	27.9045744	30.5579862
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