Electronic Supplementary Material (ESI) for ChemComm.
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Supporting information for

Assessing the Impacts of Dynamic Soft-Template Innate to Switchable Ionic Liquids on Nanoparticulate Green Rust Crystalline Structure

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Supplemental Experimental Details

Sample preparation

High-purity (99.999%) CO_2 and Ar were purchased from Matheson. $Fe(C_2H_3O_2)_2$ (99.99%) and Fe_2O_3 (99.995%) were obtained from Sigma-Aldrich. 1-hexanol and DBU were provided by Acros. All green rust was synthesized according to the synthetic procedure outlined in previous work.[1] Three 5 mL 0.1 M solutions were made by dissolving $Fe(C_2H_3O_2)_2$ (Sigma- Aldrich) equimolar mixture of oxygen-free 1-hexanol (Acros) and DBU (Acros) in a nitrogen-filled dry box. One sample was set aside and used as the non-ionic solvent for testing. The two remaining samples were loaded with CO_2 by sparging in the dry box for an hour at room temperature. CO_2 loading was confirmed gravimetrically. One sample was set aside as the ionic solvent for testing. The third clear, nearly colorless sample was diluted to 0.05 M with dry, oxygen-free methanol, which resulted in a clear, dark green solution immediately upon mixing. The three samples were placed in glass 1 dram vials fitted with a gas-tight screw cap and sealed with parafilm prior to shipping to the beamline. Once received at the beamline at Brookhaven National Laboratory, the vials were stored in glove box. The sample injection into the SALVI device was all handled in the glove box.

XAS experiment

The details of vacuum compatible microfluidic reactor, SALVI fabrication can be found in our previous publications.[2-4] Briefly, soft lithography was applied to make a 500 µm wide by 300 µm deep channel on a silicon wafer as the microfluidic mold. The wider channel was selected because the beam size was about 300 µm. The XAS measurements were conducted in the X18A beamline at National Synchrotron Light Source (NSLS) at the Brookhaven National Laboratory (BNL). The beam energy was selected using a Si(111) monochromator with channel-cut crystal. The beam has x-ray energies ranging from 4.7 keV to 31 keV. Polydimethylsiloxane (PDMS) was filled in the mold to form the block with the channel after it is hardened. A 100 nm thick SiN membrane window supported on a silicon frame (frame size 7.5×7.5 mm^2, window size 1.5×1.5 mm^2, Norcada) was bonded to the PDMS block after oxygen plasma treatment. The channel length was between 2.5 mm and 3.0 mm. The two pieces were attached to each other by immediate contact to seal the microchannel and form the detection area. The microfluidic device was attached to a sample holder (Figure. S3) and inserted in the existing setup. During an experiment, the device was moved vertically along the channel relative to the beam to obtain multiple measurements. The spectra were collected with the SALVI device integrated to the synchrotron beam in the fluorescence mode using a passivated implanted planar silicon (PIPS) detector.[5] The distance of the fluorescence detector to the sample was adjusted to a suitable value to maximize the signal but to avoid self-sorption by the liquid sample.

In situ liquid SIMS experiment

ToF-SIMS V spectrometer (IONTOF GmbH, Münster, Germany) was employed for *in situ* liquid SIMS analysis of SWILs. In this study, a 25 keV Bi_3^+ cluster ion beam was applied as the primary ion beam. During the measurement, the Bi_3^+ beam made an aperture with 2 µm in diameter. The pulse width of ~180 ns was used for sputtering through the SiN membrane. After punch-through, the ion beam bombarded on the sample surface for about 200 s and then the pulse width was changed to 80 ns to obtain better mass resolution. The maximum chamber pressure during analysis was 8.4×10^{-7} mbar, indicating that there was no spraying or fast spreading of aqueous solutions from the aperture occurred.[3] Before SIMS analysis, a 1 KeV O_2^+ beam was scanned on the SiN window for ~20 s to remove surface contamination. Also, an electron flood gun was used to compensate surface charging during all measurements. A total measurement time is 400 s after punch-through. The raster resolution was 64 × 64 pixels. The same instrument settings were applied to all the samples measurement. The mass resolution was approximately 500 in the positive mode and 370 in the negative mode, based on the half peak width of the peak Si^+ (m/z^+ 28) and CN^- (m/z^- 26), respectively.

Data analysis

Details analysis of raw data can be found in our previous work.[1] In general, the XAFS software package of Athena is used to process the collected spectra and to remove the background. Data fitting was performed using FEFF9 code and Artemis. [4, 6] Iron oxide (Fe_2O_3, Alfa Aesar, 99.995%) was used as a reference to calibrate the possible energy shift (ΔE_0).

FEFF simulation

To generate an EXAFS spectrum of DFT optimized structures, firstly, all the atom positions and coordination numbers were adopted from the simulated structure. These coordinates were used as the primary input for the ab initio EXAFS scattering code (FEFF9) that includes all the single- and multiple-scattering paths out to 6 Å.[7-8] Next, an approximate treatment of the bond disorder at 300 K is applied by setting a universal value of Debye–Waller Factor (DWF) of all paths to 0.0035. The obtained spectra for each Fe atom in the cluster are then averaged, and an overall E^0 is applied to match experimental values (oscillations in χ(k) converge at k = 0). While the global DWF is a good estimate of the first shell disorder, it is an overestimation of the order in the higher shells which manifests as an over-prediction of these amplitudes, although the atom positions predicted by the theory are correctly represented.

DFT calculation

Density functional theory calculations were performed with the CP2K package[9], using the PBE-D3 density functional[10-11]. The Gaussian plane wave hybrid basis set scheme was employed[12], in which the DZVP Gaussian basis sets[13] in conjunction with an energy cutoff of 420 Ry were used. Spin-polarization together with different starting spin configurations were considered in the calculations. In systems of molecules bonded to Fe, the binding energy per molecule is computed as

$$\delta E_b = (E(Fe - n\,Mol) - E(Fe) - n\,E(Mol))/n$$

Where E(Fe -*n* Mol) is the energy of the bound system, *E*(Fe) is the energy of an iron atom, and E(*Mol*) is the energy of one molecule, and *n* is the number of molecules binding to the Fe site.

Supplemental Figures

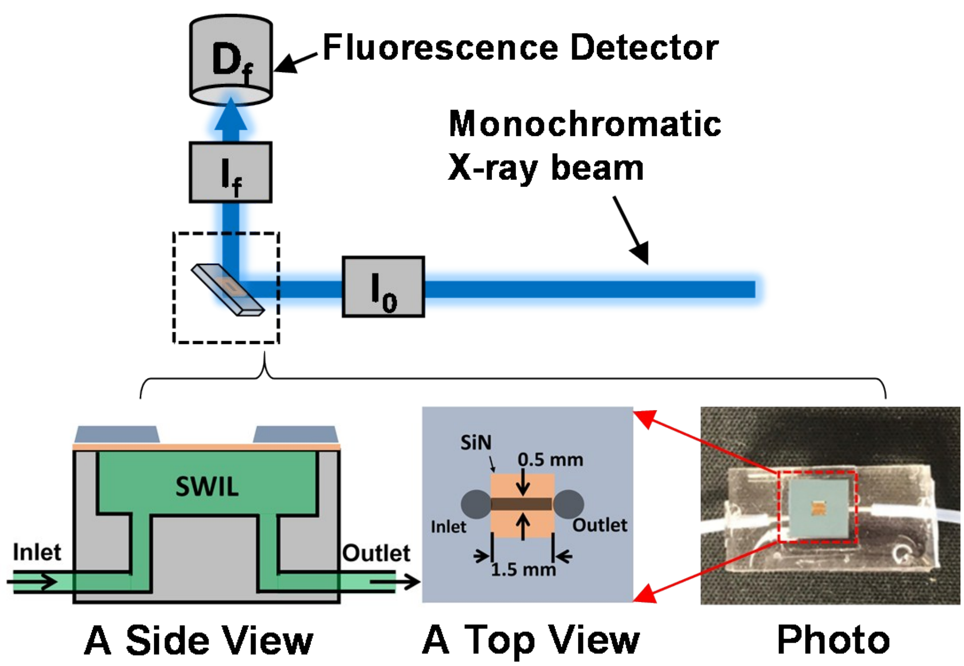

Figure S1. The schematic showing the top and side view of the SALVI cell in relation to the overall beamline setup; and a photo of the SALVI device is also shown.[4]

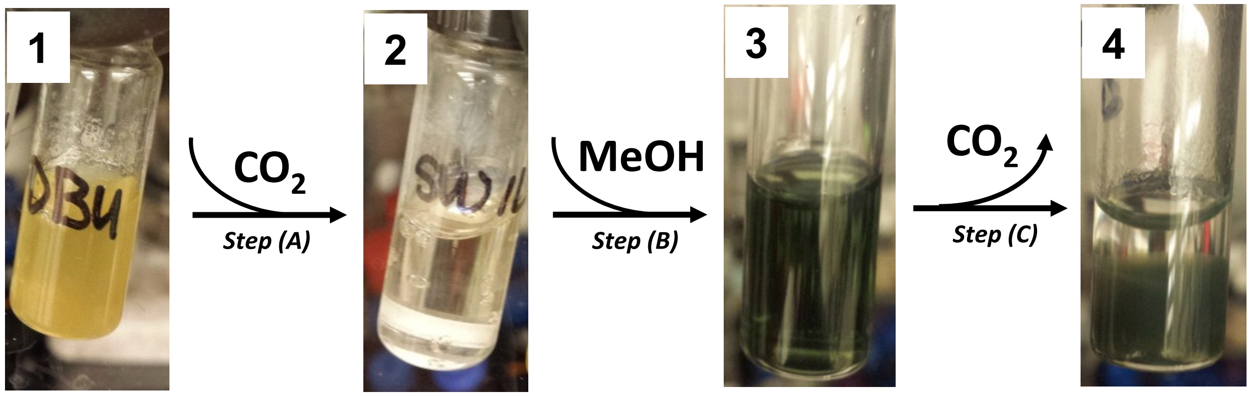

Figure S2. SWIL sample preparation and relationship to each other: (**1**) $Fe(OAc)_2$ dissolved in DBU and 1-hexanol (light brown solution); (**2**) CO_2 added to solution **1** to form ionic liquid (colorless solution); (**3**) methanol added to **2** to form carbonate green rust solution; and (**4**) CO_2 removed to form green rust suspension/precipitation

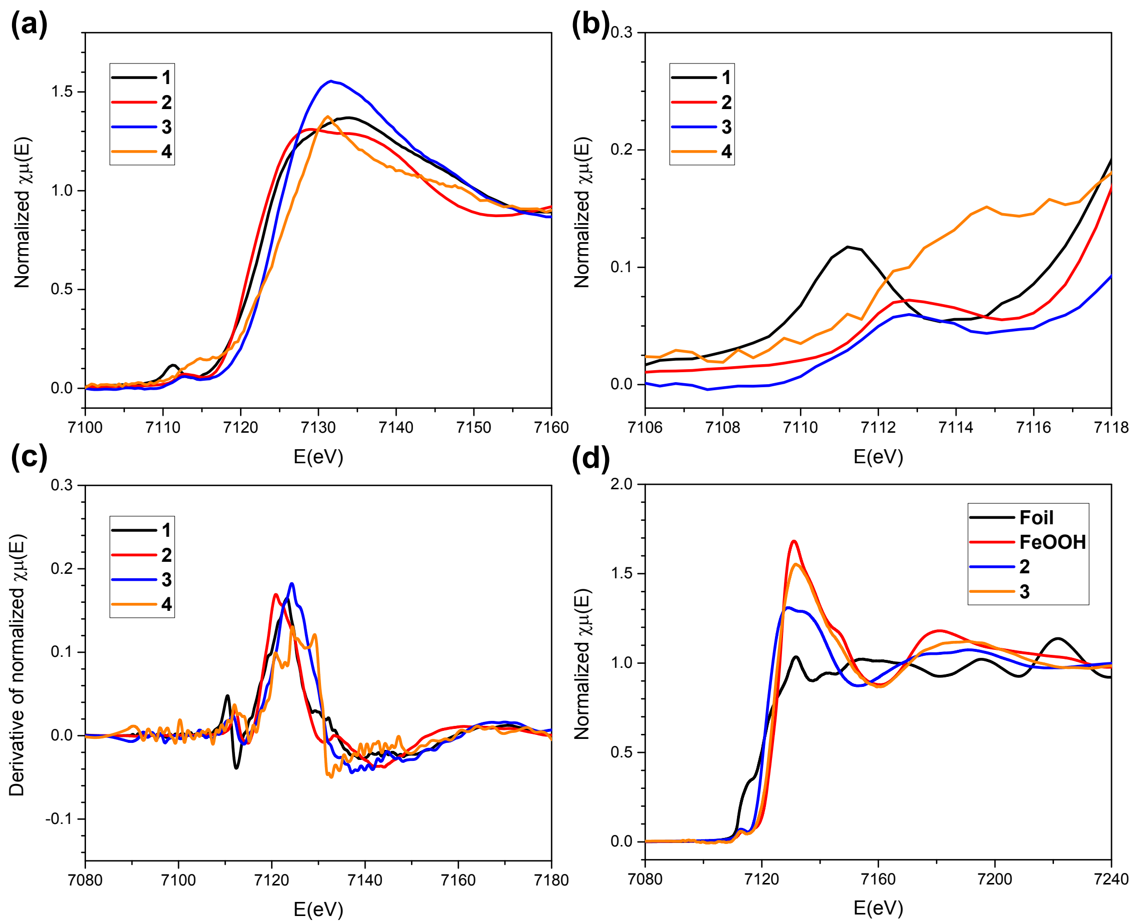

Figure S3. (a) Normalized and (c) first derivative spectra of Fe-XANES of the as-prepared 1, 2, 3, and 4. (b) The pre-edge feature at 7106–7118 eV, corresponding to the 1s→3d electronic transition for Fe. (d) XANES spectra comparison of Fe foil and FeOOH (Lepidocrocite) references with 2 and 3.

It needs to note that, for the XANES spectra of 4, during CO_2 removal, the solvated iron complex in green solution 3 started to precipitate and settled to the bottom of the cell, which led to poor signal to noise ratio (less iron species in the solution to absorb photons); Secondly, the spectra collected in this step give only averaged information of solution 3 and following formed GR suspended in the liquid.

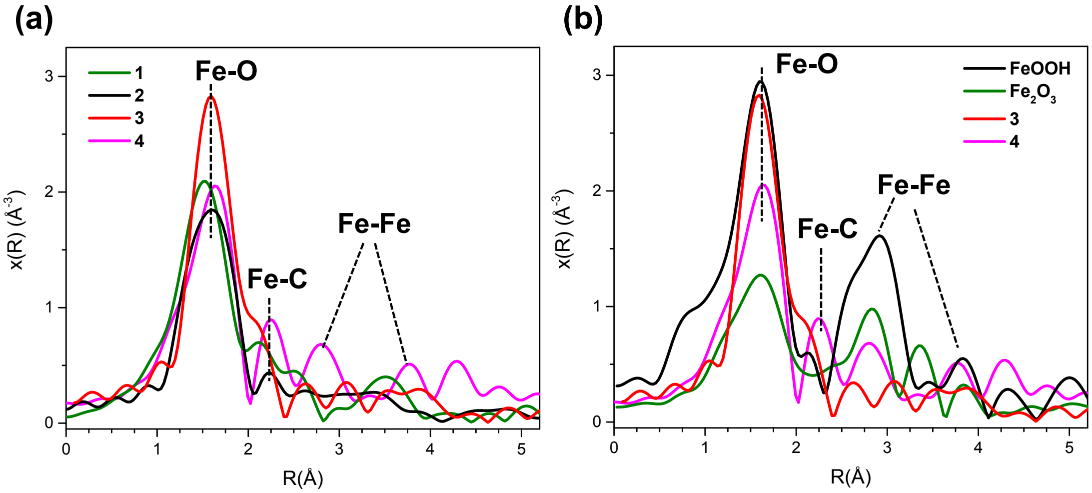

Figure S4. The k^2-weighted Fe-EXAFS $\chi(R)$ spectra of the as-prepared 1, 2, 3, 4, and Fe_2O_3 and FeOOH (Lepidocrocite) references.

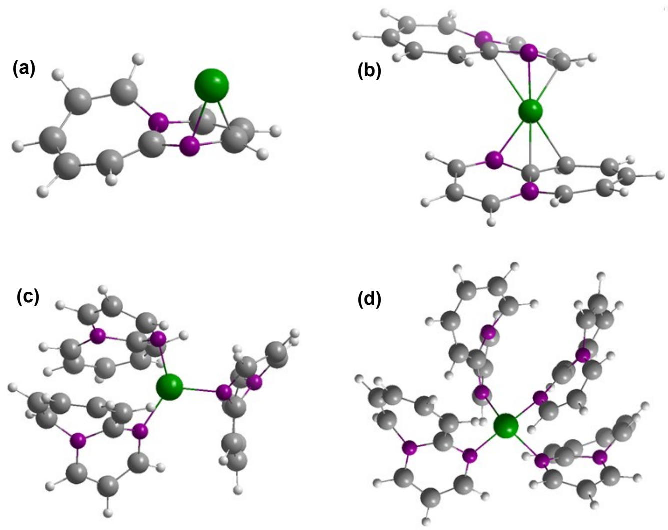

Figure S5. Considered structures of $(DBU)_n$-Fe systems, n =1, 2, 3, and 4. Green, purple, grey and white spheres represent Fe, N, C and H atoms, respectively.

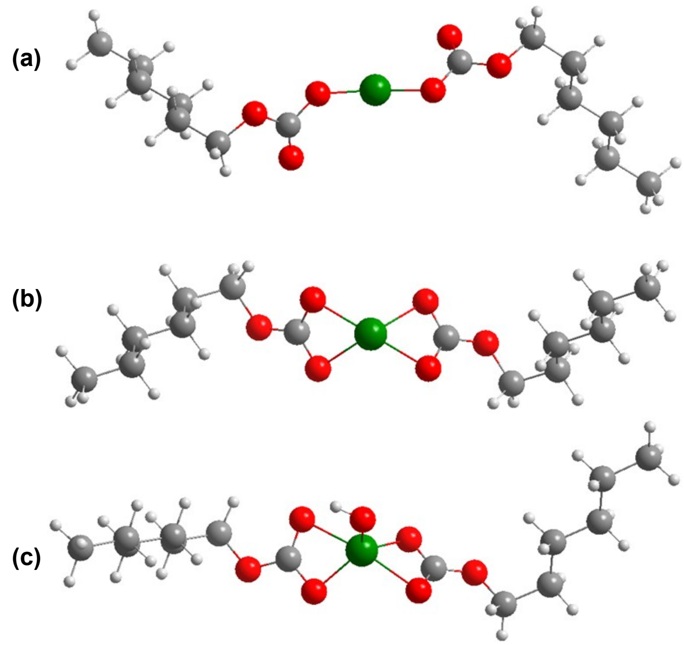

Figure S6. Possible structures of the Fe-hexylcarbonate cluster in the ionic solution: Fe in Sol-(a), Sol-(b), and Sol-(c) is 2, 4, and 5 coordinated. Green, red, grey and white spheres represent Fe, O, C and H atoms, respectively.

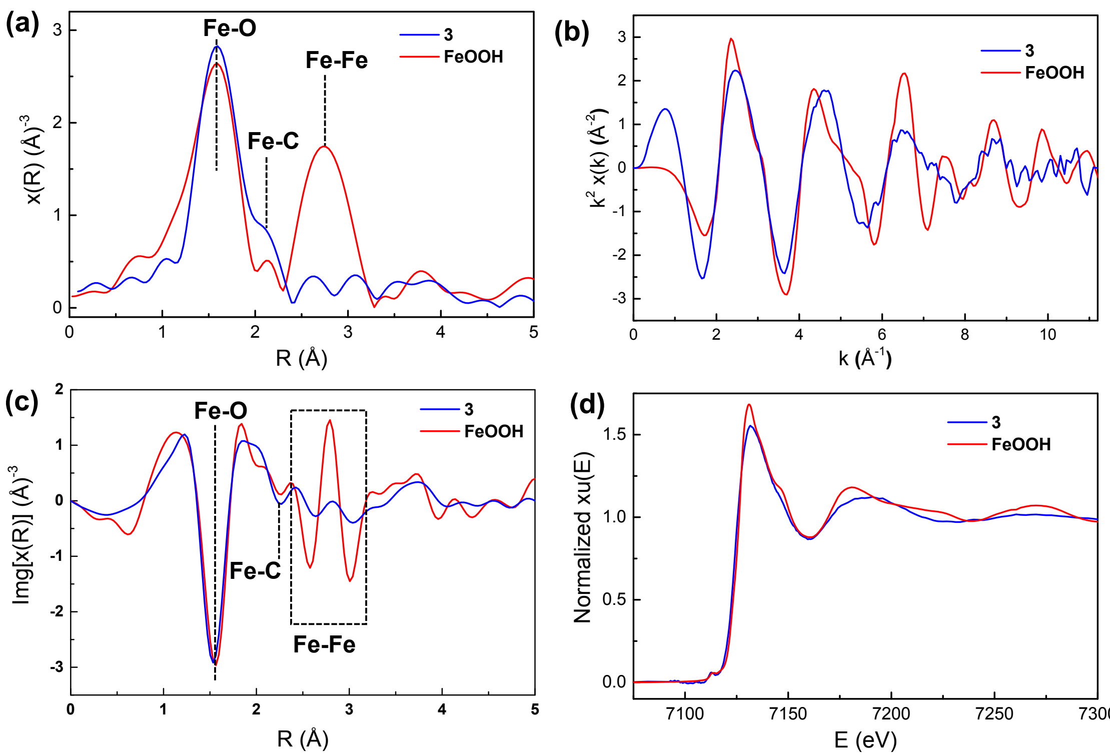

Figure S7. Comparison of Fe k-edge EXAFS (a) Mag χ(R), (b) χ(k) and (c) Img χ(R) spectra and (d) XANES spectra for solution **3** and FeOOH (Lepidocrocite) reference.

The intensive feature at ~1.5 Å is assigned to the first shell Fe-O path. A weak bump appeared at 2.2 Å might be a Fe-C signal. The peak for Fe-Fe scattering centers at ~2.6 Å. However, this peak is very weak in 3 (a and c. blue curves).

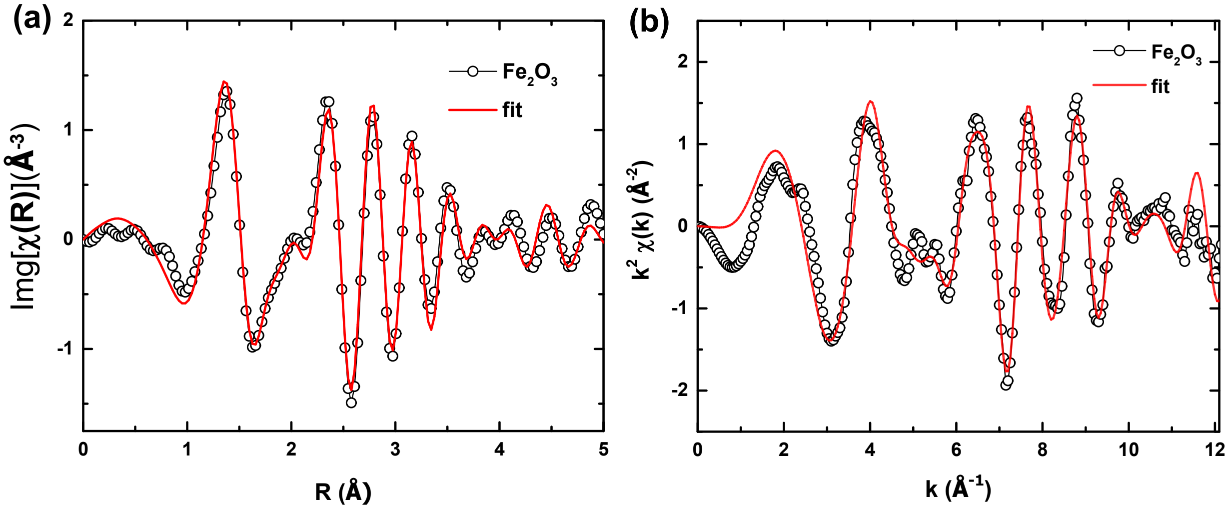

Figure S8. k^2-weighted Fe K-edge (a) Img[χ(R)] and (b) χ(k) spectra of Fe_2O_3 reference and the obtained FEFF fits.

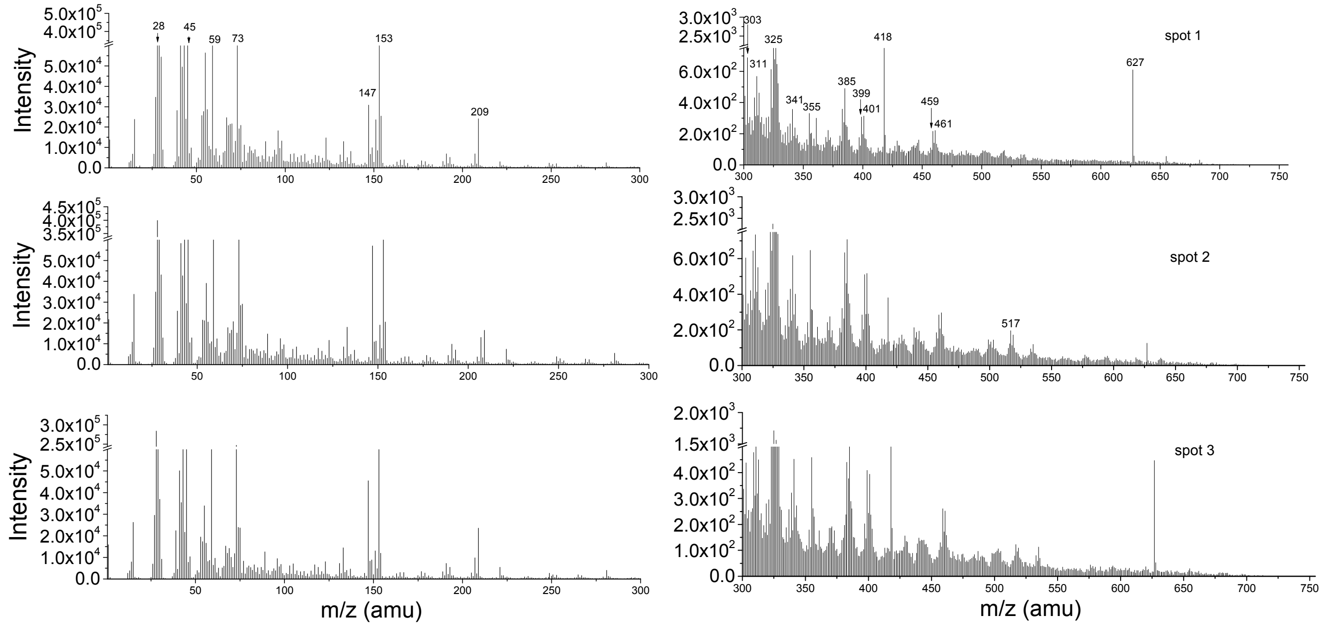

Figure S9. In situ liquid ToF-SIMS spectral analysis of the green rust in DBU and hexanol SWIL in the positive ion mode.

Three replicates were shown to confirm data reproducibility.

Supplemental Tables

Table S1. The Fe-N bonding distance, and the binding energy per molecule.

	d_{FeN} (Å)	δE_b (eV)
$(DBU)_1$-Fe	2.1	-1.13
$(DBU)_2$-Fe	1.9	-1.87
$(DBU)_3$-Fe	2.0	-1.56
$(DBU)_4$-Fe	2.0	-1.49

Based on Figure S4 and Table S1, it appears that in the case of $(DBU)_2$-Fe the FeN bond is shortest (1.9 Å) and the binding energy (per molecule) is highest (-1.87 eV), and in the case of $(DBU)_1$-Fe the FeN bond is longest (2.1 Å) and the binding energy is lowest (-1.13 eV). In the $(DBU)_3$-Fe and $(DBU)_4$-Fe systems, the Fe-N bond is 2.0 Å, while the binding energy is -1.56 and -1.49 eV respectively.

Table S2. The Fe-O bonding distance, and the relative energy to Sol-(b).

	d_{FeO} (Å)	Relative E (eV)
Sol-(a)	1.8	0.65
Sol-(b)	2.0	0
Sol-(c)	2.1 (1.8)	
* The distance of additional Fe-OH		

The structure of Sol-(a) is 0.65 eV less stable than that of Sol-(b). The Fe-O bond length clearly changes from one structure to another. In Sol-(b), there are 4 oxygen atoms of hexanol bonded to Fe, the Fe-O bond is 2.0 Å which is considerably longer than the one in the structure with 2 oxygen atoms of hexanol bonded to Fe in Sol-(a), 1.8 Å. When one more OH group is attached to the Fe site in Sol-(c), the Fe-O (O of hexanol) becomes longer, 2.1 Å. The Fe-OH distance in this case is just 1.8 Å.

Table S3. The parameters determined by fitting the experimental spectrum of Fe_2O_3. Other parameters: amplitude reduction factor (amp) $S_0^2 = 0.84 \pm 0.2$, R-factor = 0.01, and $E_0 = -2.3$.

Shell	CN	Distance (Å)	DWF
Fe-O_1	3	1.914 ± 0.036	0.0024± 0.0008
Fe-O_2	3	2.070 ± 0.043	0.0033±0.0010
Fe-Fe_1	3	2.949 ± 0.019	0.0063±0.0029
Fe-Fe_2	3	3.380 ± 0.024	0.0066±0.0030
Fe-Fe_3	6	3.678 ± 0.024	0.0089±0.0035
Fe-Fe_4	6	5.000 ± 0.033	0.0116±0.0052

Standard Fe_2O_3 is fitted to determine the necessary paths and fitting parameters that are then used to analyze the Fe spectra of the solutions. Therefore, during the fit of Fe samples, we fixed the value of reduction factor ($S_0^2 = 0.84$) for the fits of samples.

Table S4. Cartesian coordinates

XYZ coordinates for all DFT-optimized structures.

(DBU) molecule

C	6.3303719936	8.9477050060	8.8799372030
C	6.9685007502	7.7354514302	8.9048938954
C	6.8522012324	10.1368195212	9.5170003227
C	8.1481367046	10.4289686934	9.7339091120
C	8.2855988636	7.4226643992	9.3745767315
C	9.3651156759	8.2702768364	9.4509169732
N	9.2337108793	9.6644286270	9.1486797857
N	10.6367938995	7.8026901350	9.7468839267
C	10.2984826317	10.3189640143	8.6201973237
C	11.5282336001	9.7044643432	8.5322770854
C	11.6521867401	8.4839274245	9.2604642782
H	12.3842019155	10.2133633744	8.1023059088
H	12.6470526787	8.0980558206	9.4960832253
H	10.1217737169	11.3610170135	8.3571151798
H	8.4642894707	11.2317931614	10.3958254326
H	6.1276234111	10.8288077076	9.9533965940
H	5.3072566700	8.9863350816	8.5111196609
H	6.3920506656	6.8759493920	8.5565620560
H	8.5199569023	6.3824168347	9.5916270978

$C_6H_{12}OCO_2^{2-}$

C	7.3215984274	6.1086461125	10.9988243949
H	7.5949748155	5.6262197725	11.9475144231
H	6.2771718955	6.4382569772	11.0860366593
H	7.3525013218	5.3377309065	10.2166084964
C	8.2526792385	7.2823667844	10.6632680789
H	8.2306571079	8.0224133216	11.4760865416
H	9.2940213780	6.9329485420	10.6150732506
C	7.8881389838	7.9706414294	9.3388778866
H	6.8460130753	8.3210996205	9.3824778356
H	7.9122746909	7.2308349618	8.5247643605
C	8.8164498819	9.1428846367	8.9923604939
H	9.8560902409	8.7881332233	8.9499034998
C	8.4571521859	9.8106449201	7.6579550838
C	9.3796118559	10.9648096564	7.2911312493
O	10.7266175876	10.4258957493	7.0488022772
C	11.8049031210	10.8344273760	7.7354478989
O	12.9054611002	10.3476001658	7.5744019618
O	11.5445899989	11.8503251919	8.6252543309
H	8.7896403507	9.8932470110	9.7965680054
H	8.4705883667	9.0674502930	6.8480401825
H	7.4288246815	10.2046867914	7.6943475518
H	9.4172419728	11.7261630305	8.0756253817
H	9.0835159521	11.4400281208	6.3469424338
H	12.4065233587	12.0304517104	9.0461384242

$(DBU)_1$-Fe

C	6.1131546899	8.9038911676	8.6846181337
C	6.7875197660	7.7174402003	8.8277616994
C	6.6285235116	10.1874207310	9.0812248642
C	7.9227664148	10.5443749152	9.2624892936
C	8.1182391175	7.4981953539	9.3008725979
C	9.1799063219	8.3759739184	9.3589577819
N	9.0685238560	9.7524498536	8.9219468060
N	10.4083172338	7.9396480666	9.8152745834
C	10.2032044316	10.4077839792	8.5092785811
C	11.4539108420	9.8909458732	8.7348357722
C	11.5484980849	8.6941616382	9.5156686208
H	12.3416993928	10.3987474867	8.3718545378
H	12.4920350713	8.1427428270	9.5529854847
H	10.0328498481	11.3743486016	8.0402179714
H	8.1729949251	11.5131283265	9.6884513305
H	5.8981390689	10.9595216776	9.3307307315
H	5.0758158283	8.8670875198	8.3569319594
H	6.2291078819	6.8080942336	8.5999800245
H	8.3826819817	6.4848560725	9.5965903500
Fe	11.0276382976	8.7006548309	11.5528864555

$(DBU)_2$-Fe

C	6.8698983984	7.6328349100	9.4864194384
C	7.6233407538	6.6796727429	10.1597556856
C	7.3284694338	8.9090613592	9.0579312950
C	8.5856135025	9.4501442733	9.1028588347
C	8.9707551444	6.7526675265	10.5485786648
C	9.9911644296	7.7035793430	10.2877807999
N	9.8115673787	8.9193129656	9.5238486852
N	11.1803007018	7.5110935708	10.9511421817
C	10.9690847015	9.6143003902	9.1426307464
C	12.2074216190	9.2415111913	9.5496358345
C	12.3449440606	8.1317292086	10.4697447740
H	13.0815375620	9.7774080952	9.1910177003
H	13.1994646594	8.0837539426	11.1446424370
H	10.7960206649	10.4500124910	8.4722042007
H	8.7094975749	10.4604000501	8.7193049316
H	6.5826592808	9.5800850922	8.6327538768
H	5.8215148683	7.4048820805	9.3014784114
H	7.1061998644	5.7709330445	10.4665622782
H	9.3461347390	5.9406805139	11.1699080864
Fe	11.8554647782	6.3713161804	9.6000281790
C	15.3549086781	4.4449873871	10.0497096271
C	14.8344095719	5.4344164573	9.2681417815
C	14.7233121025	3.2067000083	10.4180707827
C	13.5190555571	2.6695405991	10.0580846457
C	13.5147652337	5.4894400801	8.6663836759
C	12.4530463630	4.5204376172	8.7225128449
N	12.5153260385	3.1658366403	9.2210261539
N	11.2547885257	5.0203152583	8.2886588178
C	11.4244254460	2.3503497762	8.9024067002
C	10.2522237608	2.8589068087	8.3817074048
C	10.1469417995	4.2336597380	8.1335461824
H	9.4283523140	2.1831114913	8.1691756805
H	9.2375618473	4.7313806961	7.8133537540
H	11.5638427831	1.2960769992	9.1190567588
H	13.2461200145	1.7019838018	10.4725334766
H	15.2855891984	2.5716820944	11.1022963892
H	16.3573374206	4.5986291703	10.4468457959
H	15.4551021006	6.3075591348	9.0711548854
H	13.4260687579	6.1383737130	7.7868646496

$(DBU)_3$-Fe

Fe	10.9459402511	5.6552272371	8.6323493402
C	7.3470735485	4.1369001324	9.3380826160
C	8.0269952439	4.5038585593	8.1938458909
C	7.2031083159	4.9142486344	10.5268021385
C	7.6489932849	6.1697233858	10.8525851781
C	8.8231252265	5.6724209425	7.9622503784
C	9.1783907996	6.6996052117	8.8981917899
N	8.4284414424	7.0633785143	10.0942040419
N	10.2453931251	7.5225408547	8.5735187476
C	8.4795534215	8.3941036966	10.4406685974
C	9.4142397850	9.2772318295	9.9288802980
C	10.3979525189	8.7472032645	9.0814932847
H	9.4185668495	10.3150537458	10.2485185729
H	11.3357169825	9.2507457387	8.8625716411
H	7.7525687064	8.7058016990	11.1841490776
H	7.3703274766	6.6004375974	11.8170596864
H	6.6169340211	4.4568837817	11.3238742749
H	6.8322742961	3.1778025020	9.3311294807
H	7.9907307784	3.8075861904	7.3558352261
H	9.1160380112	5.8850230703	6.9085294314
C	11.3833531630	7.8242485315	13.4359739225
C	12.2039230616	7.6660147851	12.3485208625
C	10.1860758288	7.0558297926	13.7073101264
C	9.9118963985	5.8042913382	13.2675549251
C	12.0924780557	6.7031113029	11.2933272598

C	11.4415796071	5.5029993612	11.3503570194
N	10.8670779175	5.0097392087	12.5541567709
N	11.3956267021	4.6380868236	10.2421364628
C	11.0811780910	3.6744542017	12.8381454469
C	11.5512506288	2.8357527234	11.8441074612
C	11.5743364853	3.3255022412	10.5166392954
H	11.8188321697	1.8067865711	12.0689037106
H	11.6551850684	2.6636957264	9.6573336797
H	10.8272293110	3.3601494521	13.8500229593
H	8.9452781068	5.3306659654	13.4320190860
H	9.4073715845	7.5371820590	14.3028120924
H	11.6003864316	8.6475179578	14.1154045058
H	13.0220659575	8.3809032281	12.2394652274
H	12.6122623817	6.9077312542	10.3608655544
C	10.8929981631	1.3022574861	6.0826894357
C	12.0419099482	1.7121963397	6.7083106945
C	9.8752409316	2.1508496629	5.5295645952
C	9.9810649740	3.4469139402	5.1474888257
C	12.4206605951	3.0573204086	7.0312079456
C	11.9097726450	4.2123428623	6.4940332827
N	11.1698290267	4.2073963898	5.2422068807
N	12.1458108952	5.4696367413	7.0410235455
C	11.4530086569	5.2150476947	4.3628727551
C	12.1833490803	6.3223701937	4.7814624006
C	12.3922112960	6.4784761081	6.1628497285
H	12.4535248938	7.1092923908	4.0785209152
H	12.6502851645	7.4403691600	6.5961464714
H	11.0018886391	5.1333486467	3.3766920296
H	9.1224489658	3.9829829902	4.7538775431
H	8.8874917092	1.7153693317	5.3870290331
H	10.6922077363	0.2333700145	6.0448639105
H	12.7024415570	0.9347066460	7.0909971528
H	13.1497446021	3.2051745393	7.8262659378

$(DBU)_4$-Fe

C	14.5129327170	10.4896878433	11.3367573701
C	13.6518207684	10.4577981883	10.2700115679
C	15.2998917761	9.3723020137	11.7943146463
C	15.6946670469	8.2993655157	11.0668404510
C	13.3969324110	9.3712760781	9.3684127370
C	14.2033575764	8.2980924245	9.0883608332
N	15.5238671147	8.1805410998	9.6511252493
N	13.7991882163	7.2826063753	8.2208676575
C	16.4878641761	7.5421522260	8.9064435297
C	16.1377163824	6.8261565778	7.7776475748
C	14.7687561428	6.6348014187	7.5186242820
H	16.8960298323	6.3441673427	7.1689467375
H	14.4171625488	5.9130379449	6.7845715710
H	17.4986129215	7.5966783805	9.3021461652
H	16.1725434754	7.4431148313	11.5387323059
H	15.5588021115	9.3451451760	12.8543751101
H	14.5241014947	11.3863382917	11.9547267677
H	13.0286842753	11.3396761139	10.1149192224
H	12.4543208676	9.3874789104	8.8239059005
Fe	12.1563611507	6.2262271725	8.6246284664
C	6.9522273293	4.3082766728	10.3932444530
C	8.1650824959	4.0040398062	9.8261988025
C	6.5484785165	5.6341091275	10.7868224247
C	7.0273959419	6.8031435727	10.3002381566
C	9.2214100515	4.8850866165	9.4270996087
C	9.1377168988	6.2180644213	9.1049149528
N	7.8735576982	6.9044311230	9.1440091959
N	10.2281252235	6.9510279886	8.6469028966
C	7.6473316406	7.9111425779	8.2444831014
C	8.6874055411	8.4347624894	7.5027339634
C	9.9864296767	7.9985164494	7.8281120664
H	8.5203225132	9.2317902948	6.7862708008
H	10.8624920450	8.5333567129	7.4675273500
H	6.6320782901	8.3003264783	8.2230257436
H	6.7865492037	7.7564749774	10.7656297187
H	5.8425440750	5.7190838164	11.6157421627
H	6.2996817503	3.4840024484	10.6762570584
H	8.3953847009	2.9457679694	9.6929361250
H	10.1961053498	4.4250284470	9.2798650779
C	10.3395029592	7.7783928609	13.7342198906
C	11.4705308708	8.0641108707	13.0179909793
C	9.4131501250	6.7247806254	13.3975607093
C	9.6817421877	5.5921690493	12.7145948044
C	12.0130640059	7.3539456943	11.8958766318
C	11.8224985605	6.0438358046	11.5646623764
N	11.0179678141	5.1741235440	12.3735447571
N	12.4440495726	5.4500974190	10.4487142794
C	11.3519212298	3.8582714984	12.4508209158
C	12.3436701233	3.3393402786	11.6349770586
C	12.7917842989	4.1530322802	10.5791336737
H	12.6506538956	2.3023757471	11.7173435295
H	13.3920554145	3.7417469396	9.7705628789
H	10.7500055793	3.2588606869	13.1298665696
H	8.8953947663	4.9392383276	12.3425362023
H	8.3612167665	6.8855055000	13.6430202679
H	10.0422436375	8.4691281851	14.5217228771
H	12.0107182454	8.9756683794	13.2790159318
H	12.7049971573	7.8971088388	11.2554581319
C	10.0511600600	1.1437764101	7.0283313588
C	11.3245837770	1.5921785621	7.2704177329
C	8.9048742199	1.9928615444	6.8286775740
C	8.9002621047	3.2845897691	6.4226913193
C	11.8051454002	2.9424524567	7.2950657093
C	11.2475196300	4.0560852592	6.7217830852
N	10.0524059408	3.9786210249	5.9243123624
N	11.8441023796	5.3117964388	6.8342789362
C	9.9072431607	4.8659178715	4.8919741020
C	10.7743920055	5.9333313700	4.7530972068
C	11.6743777615	6.1792766276	5.8061093955
H	10.6868181893	6.6162607912	3.9146631183
H	12.2497163711	7.1016020129	5.8637220556
H	9.0484640498	4.6974359774	4.2471622992
H	7.9946475486	3.8858770624	6.4572150694
H	7.9298424968	1.5876323839	7.1066697102
H	9.8652379917	0.0738887024	7.1071525403
H	12.0693612268	0.8368020451	7.5247264508
H	12.7641816567	3.1249307994	7.7756470851

Sol-(a)

C	6.4726942803	6.9126364303	11.0477594266
H	6.5842698688	6.4035910117	12.0152147740
H	5.5685051963	7.5342652282	11.1054403193
H	6.2850943213	6.1400344101	10.2892904074
C	7.7086629993	7.7535827439	10.6959835496
H	7.8910152133	8.4991047087	11.4834274494
H	8.6047895679	7.1164317480	10.6854025154
C	7.5782722887	8.4674547902	9.3414176382
H	6.6821083281	9.1059721125	9.3497847669
H	7.3960369755	7.7222128440	8.5523816621
C	8.8107229073	9.3084589477	8.9792430760
H	9.7046962016	8.6688606030	8.9736164523
C	8.6775589153	10.0010055439	7.6155690850
C	9.8870577581	10.8476033900	7.2410577573
O	11.0492370431	9.9751850687	7.0533185967
C	12.1201687646	10.2090217299	7.8558019412
O	13.0633420790	9.2949333858	7.5733791455
O	12.2153483628	11.0926558227	8.6958081151
H	8.9928510350	10.0642290757	9.7574247704
H	8.4990448524	9.2541892011	6.8286681112
H	7.7967271107	10.6630945626	7.6123628515
H	10.1283572486	11.5905164610	8.0101851962
H	9.7433097717	11.3581514755	6.2800241955
C	23.4337441637	11.7804583975	10.8646458900
H	23.3478817187	12.3865574528	11.7772495748
H	24.2949420638	11.1105263363	10.9943050306

H	23.6769975298	12.4625176712	10.0382621758
C	22.1486563683	10.9904963595	10.5781146462
H	21.9095669409	10.3418738802	11.4331218238
H	21.2969274049	11.6800047856	10.4888288604
C	22.2444734397	10.1362137006	9.3043510332
H	23.0982308822	9.4471680030	9.3897508409
H	22.4792691028	10.7843878249	8.4466287553
C	20.9635441372	9.3416448216	9.0136261320
H	20.1126658006	10.0313649109	8.9224569179
C	21.0635890890	8.4932260167	7.7377111138
C	19.8064152970	7.6869970559	7.4466519336
O	18.7186743643	8.6200787249	7.1341830338
C	17.5217449333	8.3677725947	7.7158406584
O	16.6462618413	9.3080912737	7.3439950300
O	17.2625878410	7.4309126284	8.4696573315
H	20.7271559540	8.6891049476	9.8673706815
H	21.2946124494	9.1331064925	6.8740692153
H	21.9005339597	7.7817597396	7.8220148005
H	19.5013022039	7.0658785953	8.2969362485
H	19.9264191852	7.0434287755	6.5647715580
Fe	14.8610140797	9.1967095670	7.6917313088

Sol-(b)

C	7.2721225921	6.0819563051	11.1169904813
H	7.5732485570	5.6336036119	12.0740167397
H	6.2238728907	6.3958947680	11.2157132662
H	7.3013972859	5.2878917397	10.3581002570
C	8.1758690616	7.2603731747	10.7269618146
H	8.1577601718	8.0247804571	11.5169687859
H	9.2217381485	6.9263135811	10.6683795440
C	7.7750318199	7.9009320438	9.3889941377
H	6.7307719850	8.2433132847	9.4439267282
H	7.7884151810	7.1340764565	8.5998792281
C	8.6852631893	9.0681525517	8.9815713389
H	9.7273670470	8.7213801014	8.9370968685
C	8.3000198326	9.6767173182	7.6255450936
C	9.2141577250	10.8120085699	7.1885361842
O	10.5658905409	10.2663677778	6.9800098440
C	11.5883684534	10.8312002580	7.6221489987
O	12.7398563566	10.2895704045	7.5012635642
O	11.4451865917	11.9198024854	8.3182139317
H	8.6638394607	9.8503767524	9.7549564776
H	8.2942857626	8.8967680116	6.8508524410
H	7.2735937072	10.0753547363	7.6652444493
H	9.2696317748	11.6161750443	7.9299802315
H	8.9131430430	11.2363029941	6.2222215680
C	19.5490237737	18.0811401140	11.1675083874
H	19.2199836969	18.5396152774	12.1104504442
H	20.5991657767	17.7842099154	11.2946619363
H	19.5256417784	18.8630838817	10.3959512825
C	18.6713958886	16.8838556244	10.7752811026
H	18.6813397603	16.1323230146	11.5777202175
H	17.6226754663	17.2019631873	10.6866948776
C	19.1134624690	16.2279813936	9.4576301281
H	20.1593441401	15.8974593314	9.5450218286
H	19.1131463125	16.9832425669	8.6572967482
C	18.2253124571	15.0454524083	9.0448356236
H	17.1820293842	15.3824753967	8.9652941787
C	18.6535976164	14.4150173065	7.7117455734
C	17.7590313257	13.2667713788	7.2674886658
O	16.4169234930	13.8015486479	6.9860331956
C	15.3720163569	13.2694356076	7.6232314118
O	14.2283214044	13.7991739469	7.4233891744
O	15.4771332071	12.2268100449	8.3916208093
H	18.2313800635	14.2774554036	9.8325479411
H	18.6770839523	15.1803221601	6.9228229110
H	19.6807246062	14.0238064543	7.7882923106
H	17.6727328036	12.4817924993	8.0264828219
H	18.1002976180	12.8189357812	6.3255086950
Fe	13.4595896049	12.0756969799	8.3185155004

Sol-(c)

C	6.4324400928	7.0357828636	10.8839839266
H	6.4352916250	6.4928629832	11.8393034710
H	5.6453869250	7.8000925699	10.9421070709
H	6.1343101348	6.3239964254	10.1019127779
C	7.8007246500	7.6614063104	10.5770351758
H	8.0934697454	8.3402664919	11.3909175319
H	8.5731987472	6.8793112830	10.5574997059
C	7.8211923498	8.4268503808	9.2447672194
H	7.0634367385	9.2245055079	9.2692912824
H	7.5090537423	7.7539633432	8.4318940435
C	9.1955996574	9.0263146115	8.9146903193
H	9.9464464241	8.2246802676	8.8702014094
C	9.2047014610	9.8009895438	7.5892254533
C	10.5590812234	10.3999023641	7.2463263287
O	11.4966799807	9.2980237323	6.9651009078
C	12.7074525481	9.3576228351	7.5124985329
O	13.5273671895	8.3996325968	7.2037546889
O	13.0769808511	10.2763619848	8.3139585604
H	9.5184765113	9.6933006605	9.7280181060
H	8.8752497754	9.1518112217	6.7655404807
H	8.4807053152	10.6303972902	7.6314047066
H	10.9676406600	11.0076118207	8.0612371203
H	10.5253847619	11.0044425719	6.3307332351
C	23.5288159099	11.1836263769	10.9842333675
H	23.5432452773	11.6014857209	12.0005271921
H	24.3313223212	10.4356512208	10.9246128706
H	23.7911829766	11.9950404527	10.2914225632
C	22.1637381144	10.5725510614	10.6370937740
H	21.9097154723	9.7855875041	11.3616737322
H	21.3762909275	11.3322214806	10.7447766635
C	22.1113244608	9.9910788996	9.2154740273
H	22.8843648994	9.2155428289	9.1061643239
H	22.3799987547	10.7744212835	8.4908063934
C	20.7353059219	9.4131114477	8.8569799497
H	19.9690458422	10.1926382408	8.9705366972
C	20.6726957092	8.8528852893	7.4282418844
C	19.3005503830	8.3150448768	7.0557652264
O	18.3667076137	9.4561201161	7.0425149901
C	17.1285427795	9.2476878465	7.4751350321
O	16.3370511069	10.2717216528	7.5060373720
O	16.7072515085	8.1078266315	7.8749952749
H	20.4625828465	8.6219173952	9.5713586657
H	20.9688476043	9.6247986101	6.7036843848
H	21.3944870303	8.0291211409	7.3091131036
H	18.9320779400	7.5712748062	7.7711489822
H	19.2789250705	7.8800471912	6.0481665517
Fe	14.9333331619	9.1424962955	8.4123715457
O	14.9392250218	8.9972665125	10.2157182276
H	14.1080801804	9.0764404312	10.7123623800

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