Supporting Information for:

Dynamic Structural Flexibility of Fe-MOF-5 Evidenced by ^{57}Fe Mössbauer Spectroscopy

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Table S1. Hyperfine splitting parameters used for the simulation of the temperature-dependent, zero-field spectra recorded for the N_2(l)-soaked Fe-MOF-5 sample. The simulations were obtained using the Voigt based method developed by Rancourt et al., see reference 1.

T [K]	Site	Γ [mm/s]	$\Delta E_{Q,0}$ [mm/s]	$d(\Delta E_Q)$ [mm/s]	δ [mm/s]	%
4.2	blue	0.27	3.02	0.23	1.156	100
10	blue		2.94	0.24	1.15	65(3)
	pink		2.14	0.92		26(2)
	red		0.89	1.66		9(2)
20	blue		2.84	0.25	1.15	39(2)
	pink		2.08	1.00		45(3)
	red		0.98	1.60		16(3)
30	blue		2.71	0.43	1.15	29(2)
	pink		1.91	0.81		28(2)
	red		1.26	1.82		43(3)
50	blue		2.64	0.50	1.09	15(2)
	pink		1.87	0.87		33(3)
	red		0.92	1.15		52(3)
70	pink		1.79	1.01	1.07	44(3)
	red		0.71	1.01		56(3)
100	pink		1.53	1.67	1.07	42(3)
	red		0.56	0.73		58(3)

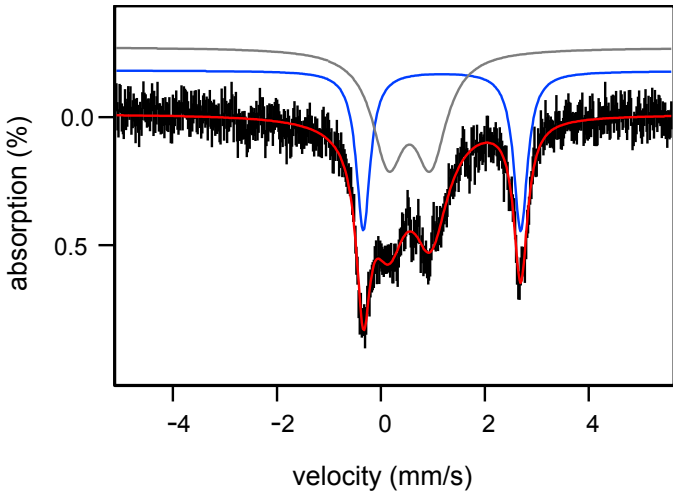


Figure S1. The 4.2-K, 0-T Mössbauer spectrum of Fe-MOF-5 after exposure to O_2. The simulated spectrum is shown in red and arises from the sum of two components. The blue trace accounts for the Fe^{2+} sites, which represent 40 % of the iron present in the sample. The component shown in gray accounts for the Fe^{3+} sites, which represent 60 % of the total iron.

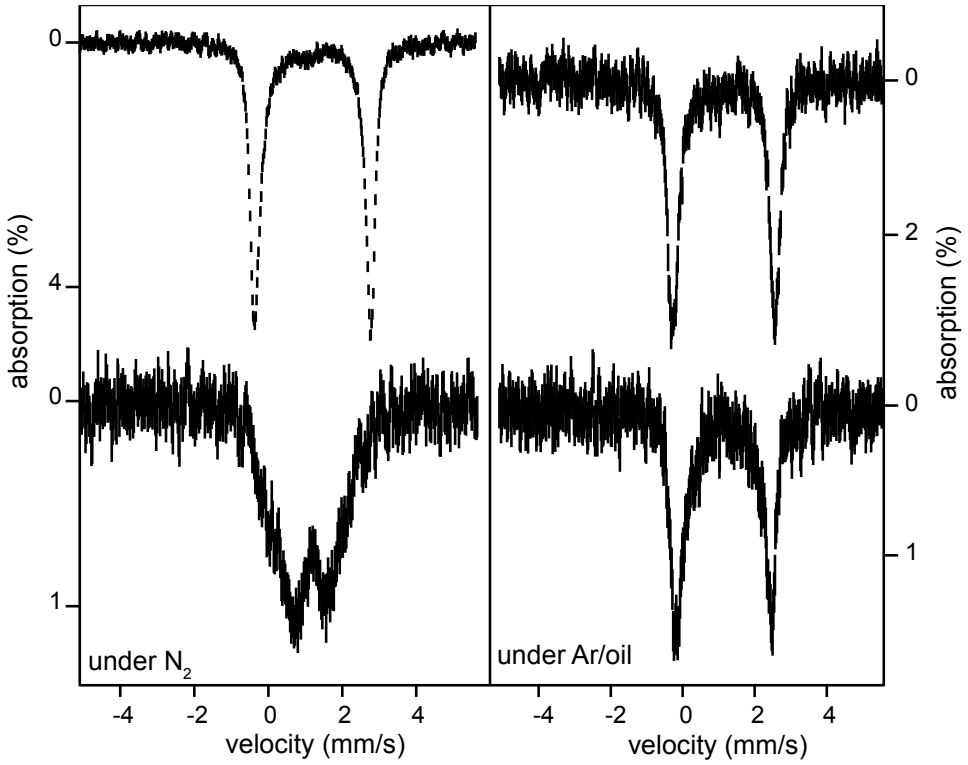


Figure S2. Comparison of the zero-field Mössbauer spectra recorded at 4.2 (top) and 70 K (bottom) of the evacuated (right) and non-evacuated (left) Fe-MOF-5 samples.

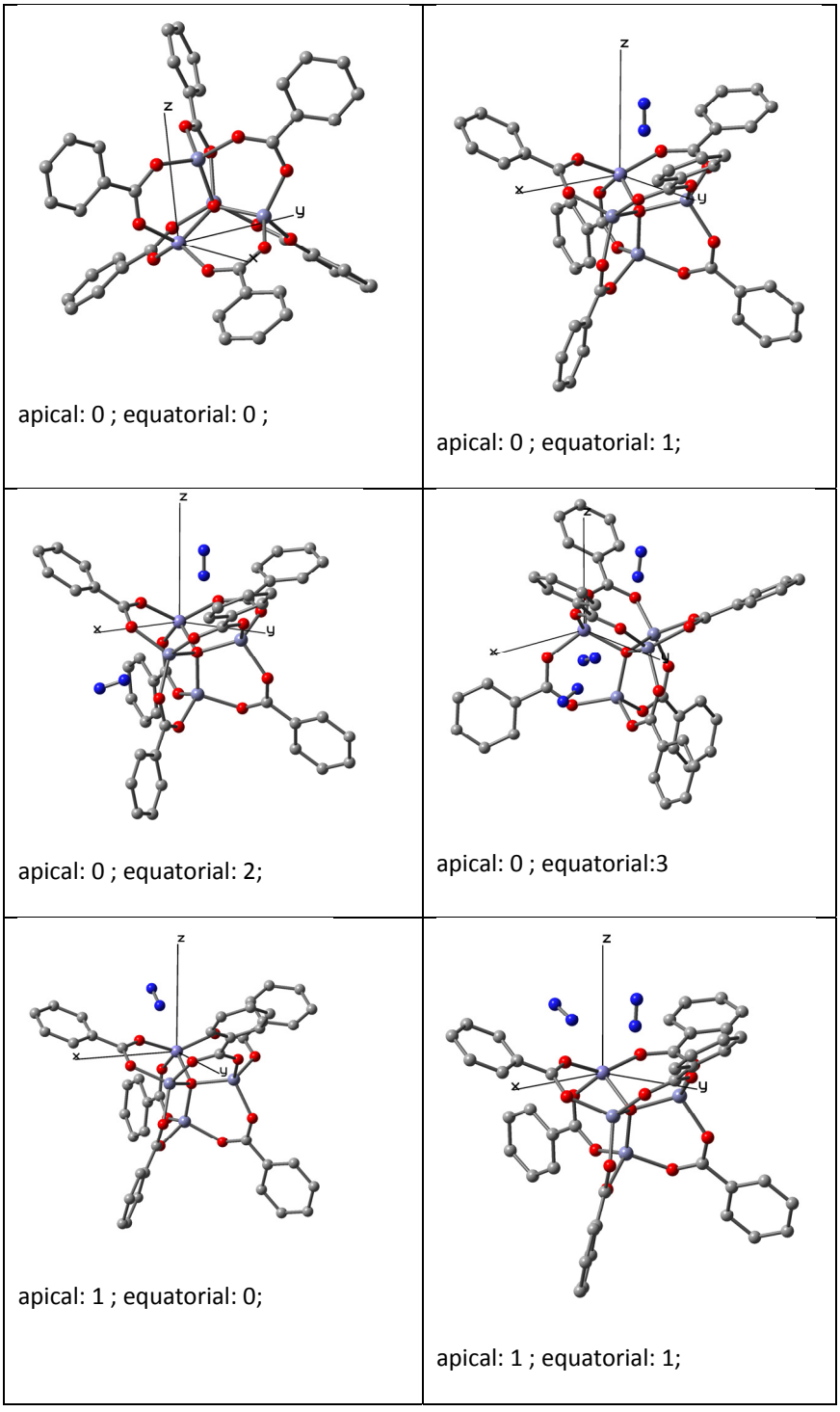
Table S2. Hyperfine splitting parameters used for the simulation of the temperature-dependent, zero-field spectra recorded for the evacuated Fe-MOF-5 sample. In contrast to the simulations of the zero-field, temperature-dependent N_2(l)-soaked Fe-MOF-5 sample that used three distinct spectral components these simulations were obtained using only one single component.

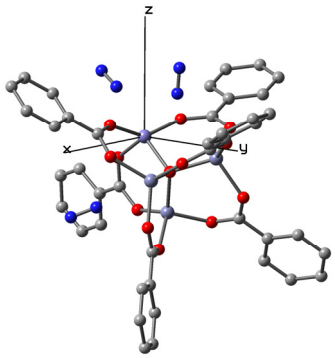
Temp. [K]	δ [mm/s]	ΔE_Q [mm/s]	Γ [mm/s]
4.2	1.149	2.83	0.35
50.0	1.147	2.68	0.40
70.0	1.145	2.59	0.55
100.0	1.145	2.32	0.80
150.0	1.1(1)	1.88	1.00

Table S3. Predicted Electric Field Gradient tensor components, zero-field Mössbauer parameters, average Fe-N bond energies (BE), and the TD-DFT predicted energy of the lowest excited state. The EFG tensor components are listed in the frame for which this tensor is diagonal. This frame is shown in Figure S3. The asymmetry parameter of the EFG tensor η is defined in the proper frame of the EFG tensor, i.e., the coordinate frame for which $|V_{ZZ}| \geq |V_{XX}| \geq |V_{YY}|$, as $\eta = |(V_{XX} - V_{YY})/V_{ZZ}|$. The quadrupole splitting ΔE_Q is proportional to both the V_{zz} component of the EFG tensor and η such that $\Delta E_Q = (eQV_{ZZ}/2)\sqrt{1+\eta^2/3}$.

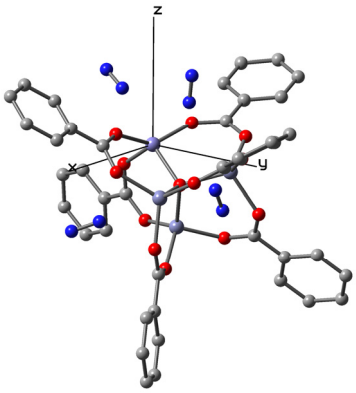
Model/ Nr. of N_2 per minimum		**Average BE**(FeN) kcal/mol	δ [mm/s]	**EFG tensor components** [mm/s]			η	**ΔEQ** [mm/s]	**TD** Energy of the 1st excited state [cm^{-1}]
Apical	Equatorial			V_{xx}	V_{yy}	V_{zz}			
0	0	-	0.992	2.166	0.804	-2.970	0.459	-3.073	1399
0	1	-3.64	0.989	2.265	0.456	-2.722	0.665	-2.915	1616
0	2	-3.24	0.994	2.431	0.417	-2.849	0.707	-3.077	1327
0	3	-2.76	0.997	3.660	-1.431	-2.229	0.218	3.689	1083
1	0	-2.92	1.023	2.519	0.055	-2.574	0.957	-2.941	1874
1	1	-3.34	1.028	2.579	-0.250	-2.329	0.806	2.845	2017
1	2	-3.10	1.031	2.662	-0.266	-2.396	0.800	2.932	1826
1	3	-2.65	1.033	2.699	-0.290	-2.409	0.785	2.963	1770
Expt. N_2 –soaked Fe-MOF-5		-	*1.156*	-				*3.02*	-
Expt. evacuated Fe-MOF-5			*1.149*					*2.83*	

Figure S3. Geometry optimized structure of Fe-MOF-5 incorporating up to four N_2 molecules. The Cartesian coordinates corresponding to these structures are listed in Table S4. The iron ion is found at the center of the coordinate frame.





apical: 1 ; equatorial: 2;



apical: 1 ; equatorial: 3;

Table S4. Cartesian coordinates of the geometry-optimized structures of Fe-MOF-5 model incorporating up to N_2 molecules. The coordinate frames are illustrated in Figure S3 and were chosen such that the respective ground state EFG tensors are diagonal in these frames.

Apical: 0; Equatorial: 0.

Fe	0.	0.	0.
Zn	-1.80825	2.70574	0.69673
Zn	1.39721	2.9433	0.59999
Zn	-0.01095	1.21384	2.94184
C	-5.23444	3.94915	6.61478
C	-5.30997	4.51375	5.33716
C	-4.27161	2.97361	6.89415
O	-0.11447	1.74236	1.03563
O	-3.12178	1.56745	-0.2067
O	-1.46684	4.26118	-0.43104
O	-2.59959	3.24894	2.3978
O	2.01044	3.7744	2.25968
O	0.79382	4.30907	-0.65491
O	2.90543	1.96854	-0.17427
O	1.44656	2.19923	3.7965
O	0.22311	-0.70066	3.17542
O	-1.65429	1.77509	3.84457
O	-1.76986	-0.13168	-0.85946
O	0.12916	-1.66031	1.11444
O	1.78927	0.10771	-0.83077
C	-2.92465	0.449	-0.81733
C	-0.38393	4.77114	-0.91324
C	-2.5175	2.69177	3.5601
C	2.05919	3.28284	3.4532
C	2.86662	0.8186	-0.75904
C	0.22641	-1.73484	2.40089
C	-4.06571	-0.19718	-1.50268
C	-0.49736	5.94054	-1.8148
C	-3.45883	3.12697	4.61688
C	2.85242	3.99978	4.47721
C	4.10505	0.2926	-1.37339
C	4.34396	5.35915	6.41328
C	6.44884	-0.70052	-2.53105
C	0.35183	-3.07275	3.02323
C	0.58427	-5.60141	4.19656
C	-5.3262	0.41929	-1.49973
C	-1.75853	6.47318	-2.12108
C	-4.42576	4.10494	4.3397
C	3.53523	5.1781	4.14024
C	0.65672	6.52182	-2.36121
C	4.27757	5.855	5.10695
C	6.45211	0.55475	-1.91363
C	2.92067	3.50529	5.78826
C	0.46445	-3.19481	4.41634
C	-3.38555	2.56288	5.89924
C	3.66536	4.18381	6.75206
C	0.58062	-4.45593	4.9994

C	-3.89242	-1.42678	-2.15595
C	0.35614	-4.22377	2.22091
C	4.10525	-0.96643	-1.99282
C	5.27468	-1.45994	-2.56931
C	0.47189	-5.48333	2.8073
C	-6.22528	-1.4145	-2.79685
C	-6.40146	-0.18894	-2.14586
C	-4.97023	-2.03224	-2.80043
C	-0.71033	8.1554	-3.50843
C	-1.86282	7.57777	-2.96539
C	0.54852	7.62585	-3.20572
C	5.28476	1.05151	-1.33563
H	-5.92146	4.26764	7.38778
H	-6.05447	5.26825	5.12169
H	-4.21337	2.53714	7.8821
H	4.92057	5.8855	7.16256
H	7.35575	-1.08492	-2.97892
H	0.67414	-6.57953	4.65056
H	-5.44021	1.36432	-0.99002
H	-2.63488	6.01241	-1.69034
H	-4.46597	4.52824	3.3472
H	3.47009	5.54376	3.12639
H	1.61844	6.09788	-2.11377
H	4.80195	6.76412	4.84526
H	7.36043	1.14114	-1.88335
H	2.38831	2.59712	6.02842
H	0.4589	-2.29828	5.01797
H	-2.63485	1.81133	6.09281
H	3.71683	3.80051	7.7622
H	0.66771	-4.54713	6.07367
H	-2.91603	-1.88775	-2.14666
H	0.2676	-4.11044	1.1508
H	3.18907	-1.53759	-2.01047
H	5.27279	-2.43092	-3.04578
H	0.47466	-6.36904	2.1864
H	-7.06084	-1.8855	-3.29768
H	-7.37221	0.28803	-2.14257
H	-4.83451	-2.98029	-3.30307
H	-0.79263	9.01269	-4.16358
H	-2.83607	7.98741	-3.19969
H	1.43943	8.07251	-3.62611
H	5.26545	2.01696	-0.8525

Apical: 0; Equatorial: 1

Fe	0.	0.	0.
Zn	2.13818	2.38768	-0.88334
Zn	-0.95893	3.10083	-0.51923
Zn	-0.03075	1.17172	-2.97202
C	5.25254	3.11849	-7.06205
C	5.5249	3.64052	-5.79314
C	4.12067	2.32169	-7.26385
O	0.30151	1.69143	-1.0879
O	3.31584	1.09741	-0.00036

O	2.11459	4.03996	0.16002
O	2.9019	2.77468	-2.63804
O	-1.67732	3.91736	-2.15588
O	-0.08164	4.52223	0.48759
O	-2.5161	2.37299	0.41647
O	-1.46112	2.27701	-3.71239
O	-0.45159	-0.71702	-3.16152
O	1.58529	1.53985	-4.01648
O	1.77877	-0.37345	0.78603
O	-0.27672	-1.66108	-1.09924
O	-1.84288	0.22582	0.69657
C	3.00021	0.03175	0.65329
C	1.17493	4.79334	0.62102
C	2.6207	2.27719	-3.79634
C	-1.9253	3.41692	-3.31855
C	-2.73298	1.15876	0.79541
C	-0.47486	-1.74011	-2.37295
C	4.07902	-0.75785	1.28744
C	1.55215	6.02132	1.35767
C	3.53266	2.56886	-4.9265
C	-2.78174	4.18706	-4.25017
C	-4.04884	0.82208	1.38178
C	-4.39718	5.64398	-6.00795
C	-6.53773	0.18941	2.48789
C	-0.74707	-3.07143	-2.96391
C	-1.25965	-5.58619	-4.07724
C	5.41168	-0.3291	1.19122
C	2.90487	6.35116	1.53019
C	4.66906	3.36688	-4.72699
C	-3.31158	5.42498	-3.85677
C	0.55749	6.85952	1.88359
C	-4.1162	6.1503	-4.73457
C	-6.26721	1.5	2.08032
C	-3.06472	3.68234	-5.52804
C	-0.96568	-3.19924	-4.34371
C	3.26189	2.04744	-6.20034
C	-3.87082	4.40965	-6.40296
C	-1.22126	-4.45336	-4.89694
C	3.7746	-1.9367	1.98499
C	-0.78604	-4.20977	-2.14468
C	-4.32388	-0.49211	1.7897
C	-5.56535	-0.8055	2.34112
C	-1.04171	-5.46237	-2.70108
C	6.12117	-2.24605	2.48572
C	6.42822	-1.07204	1.7898
C	4.79393	-2.67724	2.58175
C	2.26359	8.34152	2.74731
C	3.2576	7.50835	2.22336
C	0.91401	8.01552	2.57668
C	-5.02741	1.81728	1.52751
H	5.91811	3.33143	-7.88829
H	6.39999	4.25703	-5.63767
H	3.91021	1.91795	-8.24502

H	-5.02195	6.20789	-6.68816
H	-7.50092	-0.05544	2.91579
H	-1.45801	-6.55886	-4.50802
H	5.62658	0.57879	0.64769
H	3.6561	5.69473	1.11707
H	4.86044	3.75948	-3.73951
H	-3.0814	5.79751	-2.86978
H	-0.478	6.58988	1.73913
H	-4.52264	7.10518	-4.42952
H	-7.02005	2.26844	2.19233
H	-2.64797	2.72769	-5.81228
H	-0.93165	-2.31231	-4.95849
H	2.38258	1.4351	-6.33341
H	-4.08803	4.01819	-7.38764
H	-1.3898	-4.54885	-5.96113
H	2.7443	-2.25405	2.04586
H	-0.61403	-4.09219	-1.08521
H	-3.5611	-1.24613	1.66438
H	-5.77592	-1.81925	2.65375
H	-1.07102	-6.33832	-2.06708
H	6.91128	-2.82182	2.94942
H	7.45472	-0.73969	1.71457
H	4.55702	-3.586	3.11827
H	2.53902	9.23938	3.28479
H	4.30102	7.7611	2.35485
H	0.14555	8.66011	2.98145
H	-4.7986	2.82171	1.20402
N	0.24819	1.90309	2.18801
N	0.3277	1.98743	3.29463

Apical: 0; Equatorial: 2.

Fe	0.	0.	0.
Zn	2.52744	1.89577	-0.96854
Zn	-0.36497	3.23314	-0.48288
Zn	0.09118	1.16644	-2.95533
C	5.30538	2.77576	-7.30249
C	5.81342	2.91882	-6.00699
C	3.98326	2.36138	-7.49512
O	0.58134	1.60646	-1.08825
O	3.45245	0.58709	0.15477
O	2.83174	3.62768	-0.08548
O	3.31632	2.0822	-2.74517
O	-1.02903	4.13535	-2.10377
O	0.79938	4.51153	0.41425
O	-1.99778	2.79479	0.50868
O	-1.30604	2.40874	-3.55178
O	-0.60403	-0.64161	-3.16671
O	1.60381	1.5472	-4.14013
O	1.66787	-0.61321	0.87948
O	-0.61545	-1.57283	-1.09001
O	-1.74846	0.55406	0.75642
C	2.9364	-0.36218	0.86127
C	2.09282	4.55419	0.4174

C	2.81374	1.94156	-3.92676
C	-1.5082	3.63285	-3.19146
C	-2.4384	1.64062	0.88112
C	-0.85221	-1.62017	-2.35924
C	3.83602	-1.20355	1.68129
C	2.75066	5.72261	1.04772
C	3.67694	2.23056	-5.09542
C	-2.32878	4.49998	-4.0692
C	-3.78296	1.55875	1.49398
C	-3.8755	6.13907	-5.72584
C	-6.32539	1.4085	2.64814
C	-1.42151	-2.86513	-2.92528
C	-2.49535	-5.21786	-3.99158
C	5.21518	-0.94412	1.70052
C	4.15059	5.79664	1.10086
C	5.00285	2.64815	-4.90541
C	-2.57996	5.83129	-3.70567
C	1.97679	6.75927	1.59063
C	-3.35064	6.64733	-4.53296
C	-5.81486	2.64579	2.24149
C	-2.8558	3.99354	-5.26644
C	-1.69429	-2.95545	-4.29862
C	3.16984	2.08961	-6.39596
C	-3.62745	4.81167	-6.09082
C	-2.22958	-4.12886	-4.82831
C	3.3157	-2.26293	2.44058
C	-1.69052	-3.95908	-2.08873
C	-4.29863	0.31882	1.90097
C	-5.56636	0.24603	2.47647
C	-2.22516	-5.13111	-2.62184
C	5.54137	-2.79246	3.22723
C	6.06342	-1.73708	2.47192
C	4.16729	-3.05408	3.21017
C	3.99481	7.92894	2.23358
C	4.76915	6.89694	1.69298
C	2.59874	7.8585	2.18141
C	-4.54798	2.72269	1.66479
H	5.9356	2.98679	-8.15642
H	6.83538	3.2405	-5.85841
H	3.59024	2.25235	-8.49689
H	-4.47378	6.77331	-6.36685
H	-7.30933	1.35026	3.09457
H	-2.91064	-6.12793	-4.40416
H	5.59747	-0.12518	1.10973
H	4.72908	4.9899	0.676
H	5.37369	2.75386	-3.89689
H	-2.16411	6.20308	-2.78111
H	0.90086	6.6851	1.53887
H	-3.54194	7.67402	-4.25108
H	-6.40296	3.54402	2.37249
H	-2.65177	2.96605	-5.5283
H	-1.48244	-2.10322	-4.92679
H	2.14595	1.77081	-6.52209

H	-4.03364	4.41854	-7.01312
H	-2.43943	-4.19552	-5.88729
H	2.25265	-2.45037	2.41318
H	-1.4745	-3.87114	-1.03447
H	-3.69815	-0.56691	1.75617
H	-5.96271	-0.71073	2.78852
H	-2.43109	-5.97305	-1.97474
H	6.20106	-3.40728	3.82518
H	7.12585	-1.53499	2.48549
H	3.76394	-3.8705	3.79372
H	4.4763	8.78275	2.69197
H	5.84868	6.9519	1.7329
H	2.00001	8.65686	2.59867
H	-4.13579	3.66674	1.34119
N	0.59397	1.99795	2.18599
N	0.70607	2.10379	3.28777
N	2.94248	-1.74538	-2.72542
N	2.37692	-0.86812	-2.34078

Apical: 0, Equatorial: 3.

Fe	0.	0.	0.
Zn	-0.77335	1.22429	-2.86013
Zn	-0.91584	3.09088	-0.18693
Zn	-3.13809	0.78593	-0.68597
C	-6.48457	0.40591	-6.7934
C	-5.13528	0.63373	-7.08386
C	-6.90431	0.28354	-5.46462
O	-1.23842	1.28622	-0.9357
O	0.53221	-0.16708	-3.28321
O	-0.15834	2.96736	-3.5103
O	-2.40021	0.92177	-3.91579
O	-2.50433	3.88656	0.6226
O	-0.50999	4.28489	-1.6944
O	0.61006	3.13705	1.03594
O	-4.06127	2.29716	0.16913
O	-3.40728	-0.78122	0.44745
O	-4.06194	0.6073	-2.40041
O	1.12541	-1.05444	-1.27518
O	-1.2404	-1.24827	0.92282
O	1.23403	0.96119	1.23838
C	1.22207	-0.98813	-2.56277
C	-0.2036	4.12403	-2.93575
C	-3.63853	0.72593	-3.61444
C	-3.72154	3.45131	0.62884
C	1.37581	2.21602	1.51805
C	-2.5019	-1.4945	1.03414
C	2.16345	-1.90252	-3.24837
C	0.12836	5.32197	-3.74296
C	-4.62406	0.6148	-4.71575
C	-4.77268	4.31922	1.21047
C	2.4622	2.61369	2.44181
C	-6.75835	5.95479	2.3081
C	4.51451	3.36579	4.18706

C	-2.9351	-2.64072	1.86441
C	-3.75915	-4.80734	3.43019
C	2.28769	-1.86599	-4.64577
C	0.48846	5.18418	-5.0918
C	-4.20633	0.73838	-6.04932
C	-4.44042	5.58258	1.72206
C	0.08187	6.59749	-3.16081
C	-5.43157	6.39635	2.26943
C	3.6674	4.3378	3.64451
C	-6.10437	3.8798	1.2496
C	-4.30123	-2.93176	2.00093
C	-5.97821	0.3881	-4.42761
C	-7.09298	4.69623	1.79741
C	-4.7098	-4.01227	2.7815
C	2.93457	-2.80855	-2.50398
C	-1.98409	-3.44021	2.51697
C	3.3143	1.64126	2.98775
C	4.33673	2.01797	3.8573
C	-2.39663	-4.51968	3.29681
C	3.94151	-3.62891	-4.54522
C	3.17429	-2.72733	-5.29043
C	3.82052	-3.66796	-3.15213
C	0.755	7.58263	-5.26574
C	0.80172	6.31214	-5.84919
C	0.39396	7.72347	-3.92164
C	2.64396	3.96503	2.77431
H	-7.20436	0.32511	-7.59737
H	-4.81111	0.72974	-8.11135
H	-7.94786	0.10852	-5.24014
H	-7.52647	6.5876	2.733
H	5.30824	3.65673	4.86244
H	-4.07784	-5.6455	4.03576
H	1.68597	-1.16283	-5.20194
H	0.5164	4.19438	-5.52237
H	-3.1604	0.9156	-6.25077
H	-3.41061	5.90454	1.6808
H	-0.20033	6.68331	-2.12206
H	-5.17305	7.36998	2.6635
H	3.80547	5.37982	3.89936
H	-6.34072	2.90538	0.84885
H	-5.01834	-2.30492	1.49236
H	-6.28059	0.29863	-3.39494
H	-8.11905	4.35511	1.82656
H	-5.76325	-4.23457	2.88494
H	2.82516	-2.82363	-1.4299
H	-0.93699	-3.20255	2.40179
H	3.15957	0.60634	2.72155
H	4.992	1.26665	4.27677
H	-1.66154	-5.13444	3.79842
H	4.62919	-4.29696	-5.04684
H	3.26779	-2.69747	-6.36754
H	4.41376	-4.36537	-2.57633
H	0.99749	8.45734	-5.85485

H	1.08008	6.20341	-6.88878
H	0.35616	8.70612	-3.47106
H	1.97924	4.69927	2.34428
N	2.01892	2.01831	-1.63835
N	3.0589	2.32449	-1.88761
N	-2.19252	-2.72494	-2.60228
N	-1.99607	-1.71459	-2.18041
N	-1.89775	1.46052	3.46085
N	-1.70485	1.48156	2.36552

Apical: 1, Equatorial: 0.

Fe	0.	0.	0.
Zn	1.53633	2.86478	-0.79765
Zn	-1.65533	2.7792	-0.86205
Zn	0.03787	1.1131	-3.03644
C	4.60574	4.81899	-6.70975
C	4.52744	5.41926	-5.44869
C	3.9057	3.63562	-6.96722
O	-0.02345	1.70231	-1.15144
O	3.05045	1.86733	-0.05858
O	1.02027	4.25795	0.46832
O	2.15861	3.62393	-2.49015
O	-2.29299	3.47746	-2.57307
O	-1.25118	4.21236	0.40224
O	-3.12716	1.72288	-0.11754
O	-1.51595	1.86426	-3.97059
O	0.08228	-0.80726	-3.27029
O	1.58837	1.94278	-3.90699
O	1.86934	0.07515	0.66876
O	0.01502	-1.66486	-1.16267
O	-1.86243	0.02472	0.69004
C	2.97965	0.72402	0.53221
C	-0.13677	4.69631	0.83793
C	2.219	3.037	-3.6403
C	-2.24862	2.89823	-3.72791
C	-3.00242	0.61309	0.52526
C	0.05508	-1.80145	-2.44422
C	4.22227	0.13188	1.07713
C	-0.18763	5.80464	1.81906
C	3.04736	3.65274	-4.70152
C	-3.07594	3.45187	-4.82393
C	-4.21567	-0.01178	1.09921
C	-4.63447	4.4985	-6.89682
C	-6.51592	-1.18222	2.17858
C	0.07199	-3.17108	-3.01257
C	0.10138	-5.75474	-4.08709
C	5.43479	0.82973	0.96731
C	1.00096	6.36469	2.31083
C	3.75188	4.8387	-4.44602
C	-3.9031	4.5608	-4.59138
C	-1.42517	6.29727	2.25948
C	-4.67906	5.08162	-5.62607
C	-6.60449	0.03952	1.50313

C	-3.03343	2.86942	-6.09944
C	0.12311	-3.35571	-4.40239
C	3.1277	3.05348	-5.96738
C	-3.8111	3.39232	-7.13168
C	0.13807	-4.6438	-4.93607
C	4.19672	-1.12477	1.70021
C	0.0356	-4.28787	-2.16453
C	-4.13119	-1.23736	1.77651
C	-5.27828	-1.81971	2.31383
C	0.05004	-5.57474	-2.70089
C	6.57805	-0.97724	2.09924
C	6.60774	0.27562	1.47779
C	5.37158	-1.67651	2.20905
C	-0.28511	7.89691	3.6719
C	0.95032	7.40803	3.23432
C	-1.47189	7.34007	3.1837
C	-5.45934	0.624	0.96411
H	5.20822	5.27069	-7.48692
H	5.06841	6.33461	-5.24996
H	3.96637	3.17142	-7.94233
H	-5.23737	4.90361	-7.69894
H	-7.40553	-1.63494	2.59622
H	0.11264	-6.7538	-4.50264
H	5.43532	1.79417	0.48193
H	1.94367	5.97196	1.96014
H	3.67695	5.2858	-3.46605
H	-3.92126	4.99591	-3.60335
H	-2.32887	5.85353	1.86922
H	-5.31544	5.93728	-5.4447
H	-7.5616	0.53207	1.39761
H	-2.39072	2.0165	-6.25866
H	0.15012	-2.48499	-5.04014
H	2.5783	2.141	-6.14468
H	-3.77664	2.9416	-8.11438
H	0.17783	-4.78253	-6.00806
H	3.25683	-1.65062	1.77391
H	-0.00426	-4.12835	-1.0975
H	-3.16805	-1.7159	1.86942
H	-5.20983	-2.76508	2.83485
H	0.02152	-6.43344	-2.04369
H	7.48926	-1.40642	2.49456
H	7.54089	0.8156	1.39169
H	5.34892	-2.646	2.68804
H	-0.32274	8.70683	4.38852
H	1.86786	7.83895	3.61167
H	-2.42712	7.71818	3.52211
H	-5.50539	1.56533	0.43727
N	0.03569	-1.94878	1.76295
N	0.04855	-2.88731	2.35975

Apical: 1; Equatorial: 1.

Fe	0.	0.	0.
Zn	2.00021	2.44844	-1.13559

Zn	-1.09528	3.04157	-0.66416
Zn	-0.1921	1.06023	-3.0572
C	4.70559	3.26679	-7.48823
C	5.01004	3.84043	-6.24926
C	3.62517	2.38622	-7.60616
O	0.19637	1.6559	-1.21238
O	3.31958	1.24813	-0.32901
O	1.951	4.08416	-0.0591
O	2.63698	2.87902	-2.92974
O	-1.82666	3.83668	-2.30707
O	-0.24816	4.46159	0.37137
O	-2.66063	2.30687	0.25719
O	-1.69732	2.09699	-3.76211
O	-0.50676	-0.84531	-3.218
O	1.34636	1.50445	-4.19577
O	1.878	-0.20639	0.64463
O	-0.15579	-1.6883	-1.13351
O	-1.93448	0.17108	0.47823
C	3.07698	0.21148	0.39656
C	1.001	4.78362	0.46048
C	2.33108	2.32518	-4.05663
C	-2.12935	3.26706	-3.42529
C	-2.85759	1.07189	0.57282
C	-0.40667	-1.83259	-2.39005
C	4.222	-0.52979	0.97344
C	1.35546	6.00861	1.21349
C	3.15314	2.6524	-5.24462
C	-3.01195	3.99094	-4.36926
C	-4.19092	0.67295	1.07701
C	-4.67326	5.36191	-6.15342
C	-6.71259	-0.07262	2.02868
C	-0.59597	-3.20437	-2.92285
C	-0.95172	-5.79118	-3.92984
C	5.53105	-0.07467	0.75323
C	2.6993	6.38968	1.34494
C	4.23758	3.53479	-5.12945
C	-3.50557	5.26126	-4.03673
C	0.34811	6.79327	1.7949
C	-4.33288	5.94375	-4.92769
C	-6.45545	1.26347	1.7036
C	-3.3548	3.41039	-5.59938
C	-0.86451	-3.39925	-4.28587
C	2.85	2.07932	-6.48859
C	-4.18382	4.09479	-6.48738
C	-1.04173	-4.68881	-4.78606
C	4.00749	-1.6864	1.73772
C	-0.50583	-4.31259	-2.06753
C	-4.45302	-0.66673	1.40153
C	-5.7107	-1.03681	1.87569
C	-0.68354	-5.60094	-2.57028
C	6.39388	-1.92137	2.05667
C	6.61207	-0.76902	1.29438
C	5.09064	-2.37916	2.27679

C	2.02412	8.32457	2.63121
C	3.03072	7.54463	2.05221
C	0.68334	7.94735	2.50174
C	-5.19964	1.63688	1.22728
H	5.30642	3.5047	-8.35624
H	5.84528	4.52178	-6.15864
H	3.38966	1.94273	-8.56421
H	-5.31548	5.89269	-6.84399
H	-7.68834	-0.36114	2.3967
H	-1.08922	-6.79139	-4.31925
H	5.6771	0.8155	0.1599
H	3.46027	5.774	0.88906
H	4.45495	3.96629	-4.16383
H	-3.22938	5.69217	-3.08596
H	-0.68039	6.48493	1.68116
H	-4.71086	6.9239	-4.66981
H	-7.23128	2.00807	1.81945
H	-2.96513	2.43187	-5.83708
H	-0.93006	-2.53488	-4.92948
H	2.01174	1.4021	-6.55641
H	-4.44713	3.6448	-7.43513
H	-1.24892	-4.8352	-5.83759
H	2.99519	-2.02691	1.8947
H	-0.29626	-4.14564	-1.02163
H	-3.66818	-1.39672	1.27127
H	-5.9112	-2.07051	2.12279
H	-0.61292	-6.45301	-1.90756
H	7.23381	-2.45982	2.47541
H	7.61982	-0.41564	1.123
H	4.92183	-3.27155	2.86416
H	2.28295	9.22093	3.17936
H	4.06731	7.83699	2.15184
H	-0.09491	8.55093	2.94886
H	-4.98062	2.66166	0.96705
N	0.08531	1.80347	2.07446
N	0.16392	1.95336	3.17442
N	-0.25552	-1.87211	1.80767
N	-0.35495	-2.86807	2.29262

Apical:1, Equatorial: 2.

Fe	0.	0.	0.
Zn	2.1681	2.21012	-1.27279
Zn	-0.85055	3.12036	-0.64987
Zn	-0.23613	1.04797	-3.0454
C	4.18201	3.6401	-7.79185
C	4.7683	3.86494	-6.54183
C	2.94808	2.98715	-7.87996
O	0.29231	1.61825	-1.23077
O	3.40574	1.0879	-0.252
O	2.26196	3.95136	-0.34632
O	2.76718	2.55983	-3.09769
O	-1.64123	3.91051	-2.27526
O	0.15028	4.50737	0.28105

O	-2.43056	2.51783	0.34845
O	-1.86094	2.04236	-3.54609
O	-0.59464	-0.85149	-3.2184
O	1.07479	1.70719	-4.3526
O	1.85451	-0.26925	0.69761
O	-0.32188	-1.67943	-1.11451
O	-1.90545	0.31917	0.51788
C	3.07612	0.12447	0.53969
C	1.42414	4.73643	0.23408
C	2.19992	2.32704	-4.23526
C	-2.14787	3.27303	-3.2783
C	-2.7378	1.30107	0.64524
C	-0.60335	-1.82337	-2.36464
C	4.14888	-0.5663	1.29186
C	1.93618	5.95853	0.89749
C	2.88707	2.78137	-5.46665
C	-3.10133	3.98555	-4.16016
C	-4.09371	1.01933	1.16884
C	-4.8961	5.33416	-5.82885
C	-6.65829	0.4966	2.15378
C	-0.94203	-3.17823	-2.86511
C	-1.58	-5.73358	-3.81148
C	5.47932	-0.13802	1.16402
C	3.3122	6.23162	0.9014
C	4.12374	3.43845	-5.38142
C	-3.44071	5.32076	-3.89604
C	1.04753	6.84697	1.52133
C	-4.33458	5.99208	-4.72949
C	-6.28281	1.80803	1.84392
C	-3.66579	3.32889	-5.26373
C	-1.2564	-3.37044	-4.21893
C	2.30114	2.55835	-6.72175
C	-4.56115	4.00216	-6.09402
C	-1.57425	-4.64422	-4.68878
C	3.84486	-1.64808	2.13199
C	-0.94974	-4.27345	-1.98833
C	-4.47435	-0.2952	1.47844
C	-5.75337	-0.5541	1.96909
C	-1.26736	-5.5461	-2.46103
C	6.18504	-1.8646	2.705
C	6.49243	-0.78594	1.86919
C	4.86039	-2.29474	2.8349
C	2.90483	8.26628	2.14584
C	3.7934	7.38225	1.5247
C	1.53215	7.99708	2.1431
C	-5.00543	2.0704	1.35108
H	4.68314	3.97263	-8.69144
H	5.72178	4.37122	-6.47406
H	2.49392	2.81504	-8.84643
H	-5.59006	5.85609	-6.47474
H	-7.65072	0.2941	2.53441
H	-1.82653	-6.72162	-4.17741
H	5.69519	0.69593	0.51314

H	3.98009	5.5367	0.41451
H	4.55702	3.60422	-4.40643
H	-2.99464	5.80906	-3.04249
H	-0.00806	6.62044	1.50639
H	-4.59316	7.02233	-4.52479
H	-6.98383	2.61966	1.98391
H	-3.39302	2.30076	-5.44966
H	-1.24684	-2.51639	-4.87935
H	1.34732	2.05425	-6.76664
H	-4.99589	3.49317	-6.94381
H	-1.81667	-4.78838	-5.73303
H	2.81743	-1.96779	2.21907
H	-0.70523	-4.10911	-0.94963
H	-3.76323	-1.09284	1.32362
H	-6.04566	-1.5685	2.20452
H	-1.27165	-6.3881	-1.78198
H	6.97238	-2.3671	3.25116
H	7.51661	-0.45324	1.76872
H	4.62264	-3.12966	3.48003
H	3.2797	9.15939	2.62832
H	4.85478	7.59088	1.52643
H	0.84493	8.68103	2.62261
H	-4.69598	3.0742	1.10114
N	0.20273	1.92284	2.06763
N	0.29912	2.10824	3.16055
N	-0.37639	-1.83425	1.82192
N	-0.57658	-2.79873	2.33845
N	3.10148	-1.27729	-3.07613
N	2.42685	-0.49343	-2.66655

Apical: 1; Equatorial: 3.

Fe	0.	0.	0.
Zn	2.25164	2.1368	-1.25027
Zn	-0.74748	3.13878	-0.68386
Zn	-0.15505	1.04224	-3.06066
C	4.49052	3.33947	-7.74186
C	5.04646	3.58085	-6.48111
C	3.23894	2.7242	-7.84977
O	0.35844	1.5998	-1.23946
O	3.43816	0.98852	-0.1987
O	2.37643	3.8858	-0.34353
O	2.90418	2.43506	-3.06543
O	-1.44569	3.96914	-2.3319
O	0.27539	4.49516	0.26991
O	-2.36915	2.57834	0.2645
O	-1.70144	2.12551	-3.63172
O	-0.62396	-0.83447	-3.22508
O	1.21946	1.60805	-4.34707
O	1.83444	-0.32435	0.72494
O	-0.36106	-1.66704	-1.12147
O	-1.88586	0.3801	0.53606
C	3.06871	0.03608	0.58867
C	1.55482	4.69237	0.23082

C	2.36183	2.19186	-4.21282
C	-1.93806	3.36745	-3.36289
C	-2.7032	1.3794	0.60299
C	-0.66202	-1.8029	-2.36724
C	4.10874	-0.68135	1.36158
C	2.09329	5.90167	0.89665
C	3.09948	2.58921	-5.43469
C	-2.81602	4.13415	-4.27715
C	-4.0741	1.14308	1.10981
C	-4.46915	5.58581	-6.00476
C	-6.66567	0.70563	2.06615
C	-1.06334	-3.1437	-2.85948
C	-1.8228	-5.67199	-3.78894
C	5.45263	-0.29091	1.25522
C	3.47584	6.13912	0.9108
C	4.35409	3.2083	-5.32971
C	-3.09824	5.48289	-4.01377
C	1.22326	6.81338	1.51312
C	-3.92139	6.20548	-4.87655
C	-6.25821	1.99774	1.71797
C	-3.36632	3.51603	-5.40991
C	-1.39749	-3.32741	-4.20984
C	2.54402	2.34967	-6.70054
C	-4.19134	4.24068	-6.26936
C	-1.77597	-4.58767	-4.67125
C	3.76015	-1.75091	2.20006
C	-1.11214	-4.23398	-1.97779
C	-4.48692	-0.15198	1.45734
C	-5.77914	-0.36846	1.93381
C	-1.49032	-5.49309	-2.44206
C	6.08316	-2.03034	2.81425
C	6.43496	-0.96408	1.98002
C	4.74495	-2.42279	2.92274
C	3.11185	8.18456	2.15104
C	3.9819	7.2774	1.5371
C	1.73272	7.95105	2.13791
C	-4.96727	2.21749	1.23946
H	5.02887	3.62999	-8.63448
H	6.01366	4.05799	-6.39812
H	2.80835	2.53915	-8.8246
H	-5.10828	6.14759	-6.67336
H	-7.66828	0.53621	2.43612
H	-2.11646	-6.64949	-4.14827
H	5.70281	0.53414	0.60527
H	4.12918	5.42681	0.42937
H	4.7636	3.38752	-4.34686
H	-2.66424	5.94097	-3.13754
H	0.1623	6.61421	1.4905
H	-4.13578	7.2459	-4.67232
H	-6.94465	2.82758	1.81779
H	-3.13927	2.47696	-5.59599
H	-1.35539	-2.47766	-4.87453
H	1.57587	1.87538	-6.76074

H	-4.61564	3.76107	-7.14116
H	-2.03355	-4.72512	-5.71273
H	2.72281	-2.04145	2.27038
H	-0.85149	-4.07646	-0.94197
H	-3.78948	-0.96813	1.34255
H	-6.09589	-1.36807	2.19909
H	-1.52618	-6.33126	-1.75923
H	6.84662	-2.55241	3.37572
H	7.46964	-0.66057	1.89606
H	4.4729	-3.24814	3.56665
H	3.50606	9.06799	2.63593
H	5.04828	7.45847	1.54678
H	1.05979	8.6529	2.61178
H	-4.633	3.20587	0.96159
N	0.24904	1.93596	2.06088
N	0.33338	2.1204	3.15493
N	-0.44976	-1.84387	1.81811
N	-0.6943	-2.80182	2.32767
N	3.08299	-1.43029	-2.98962
N	2.43158	-0.61445	-2.60567
N	-4.3903	-0.10492	-3.5032
N	-3.79881	0.00889	-2.56783

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