Supporting Information for:

Unprecedented Fe(IV) Species in a Diheme Protein MauG: A Quantum Chemical Investigation on the Unusual Mössbauer Spectroscopic Properties

Yan Ling,[1] Victor L. Davidson,[2] and Yong Zhang[1,3]*

[1]Department of Chemistry and Biochemistry, University of Southern Mississippi, 118 College Drive #5043, Hattiesburg, MS 39406; [2]Department of Biochemistry, University of Mississippi Medical Center, 2500 N. State Street, Jackson, MS 39216; [3]Department of Chemistry, Chemical Biology, and Biomedical Engineering, Stevens Institute of Technology, Castle Point on Hudson, Hoboken, NJ 07030

Computational Details:

The ^{57}Fe quadrupole splitting arises from the non-spherical nuclear charge distribution in the I*=3/2 excited state in the presence of an electric field gradient at the ^{57}Fe nucleus, while the isomer shift arises from differences in the electron density at the nucleus between the absorber (the molecule or system of interest) and a reference compound (usually α-Fe at 300K). The former effect is related to the components of the electric field gradient (EFG) tensor at the nucleus as follows:[1]

$$\Delta E_Q = \frac{1}{2} eQV_{zz}\left(1+\frac{\eta^2}{3}\right)^{1/2} \quad (1)$$

where *e* is the electron charge, *Q* is the quadrupole moment of the E*=14.4 keV excited state, and the principal components of the EFG tensor are labeled according to the convention:

$$|V_{zz}|>|V_{yy}|>|V_{xx}| \quad (2)$$

with the asymmetry parameter being given by:

$$\eta = \frac{V_{xx}-V_{yy}}{V_{zz}} \quad (3)$$

The isomer shift in ^{57}Fe Mössbauer spectroscopy is given by:[1]

$$\delta_{Fe}=E_A-E_{Fe}=\frac{2\pi}{3}Ze^2\left(<R^2>^*-<R^2>\right)\left(|\psi(0)|^2_A-|\psi(0)|^2_{Fe}\right) \quad (4)$$

where Z represents the atomic number of the nucleus of interest (iron) and R, R* are average nuclear radii of the ground and excited states of ^{57}Fe. Since $|\psi(0)|^2_{Fe}$ is a constant, the isomer shift (from Fe) can be written as:

$$\delta_{Fe} = \alpha\,[\,\rho(0) - c\,] \quad (5)$$

where α is the so-called calibration constant and ρ(0) is the computed charge density at the iron nucleus. Both α and c can be obtained from the correlation between experimental δ_{Fe} values and the corresponding computed ρ(0) data in a training set. Then, one can use equation (5) to predict δ_{Fe} for a new molecule from its computed ρ(0), basically as described in detail elsewhere for a wide variety of heme and other model systems.[2]

The hybrid functional B3LYP[3] with a Wachter's basis (62111111/3311111/3111) for Fe,[4] 6-311G* for all the other heavy atoms and 6-31G* for hydrogens in the *Gaussian*

03 program[5] was used to predict Mössbauer quadrupole splittings and isomer shifts, the same approach used in the previous work for various iron-containing proteins and models.[2,6] To calculate ΔE_Q, we first evaluated the principal components of the electric field gradient tensor at the ^{57}Fe nucleus (V_{ii}), then we used equation (1) to deduce ΔE_Q, using a precise recent determination of Q = 0.16 (±5%) x 10^{-28}m^2,[7] a value previously found to permit excellent accord between theory and experiment in a broad range of systems.[2,6] To calculate δ_{Fe} values, we read the Kohn-Sham orbitals from the *Gaussian 03* results into the AIM 2000 program,[8] to evaluate the charge density at the iron nucleus, $\rho(0)$. Then, we evaluated the isomer shifts by using the equation derived previously:[2]

$$\delta_{Fe} = -0.404\ [\rho(0) - 11614.16] \qquad (6)$$

Charges were calculated using the natural bonding orbital analysis.[9]

In MauG models **1a-1e** and **2a-2e**, the heme group is represented by a porphyrin with original eight β substituents replaced by methyl groups. As shown in Figure 2 in the Text, the amino acids used in the calculations are basically truncated to leave the C_β moiety to be CH_3 with the exception of Pro107 due to its ring structure. Unless otherwise stated below or in the Text, the geometries of the structural models investigated in this work were optimized (see Tables S1-S11 for the optimized coordinates) with the terminal C atoms and their attached hydrogen atoms fixed at the x-ray crystal structure positions to mimic the protein environment effect. Optimizations were done using the DFT method BPW91[10] with the Wachters' basis for Fe, 6-311G* for other heavy atoms and 6-31G* for hydrogens, which is the same approach used previously to investigate other heme protein systems.[6e,6h] Then, the Mössbauer properties of these optimized structures were calculated using above methods. Previous investigations suggest that the residual errors in ΔE_Q calculations can be decreased upon using better quality x-ray structures[6a,6b] or properly optimized structures for proteins.[6b,6e,6f] For heme site **1**, calculations done using the partially optimized porphyrin structures (**1c-1e**) only have errors of 0.03-0.15 mm/s and no further improvement was found by using full optimization. For heme site **2**, the porphyrin moiety in **2e** was subjected to full optimization, which has a decreased error of 0.06 mm/s compared to an error of 0.34 mm/s from the partial optimization. For Fe^{IV}=O and Fe^{IV}=OH systems such as heme **1** models, the calculated asymmetry parameters are in a range of 0.03 to 0.16, indicating basically an axial symmetry. In contrast, for heme **2e** and **2f** models, the calculated asymmetry parameters are larger. For instance, for the protein based model **2e**, the asymmetry parameter is 0.76, which may help enhance the ΔE_Q value by 9% based on equation (1).

In addition, we used Bader's Atoms-in-Molecules (AIM) theory[8b,11] to help analyze the interactions between Gln103/Pro107 and the oxo group for heme site **1**. For convenience, we give here a very brief overview of this approach. According to the AIM theory, every chemical bond has a bond critical point at which the first derivative of the charge density, $\rho(\mathbf{r})$, is zero. The $\rho(\mathbf{r})$ topology is described by a real, symmetric, second-rank Hessian-of-$\rho(\mathbf{r})$ tensor, and the tensor trace is related to the bond interaction energy by a local expression of the virial theorem:

$$\mathrm{Tr(Hessian)} = \nabla^2\rho(\mathbf{r}) = [2G(\mathbf{r}) + V(\mathbf{r})]\ (4m/\hbar^2) \qquad (7)$$

where $\nabla^2\rho(\mathbf{r})$ is the Laplacian of $\rho(\mathbf{r})$, $G(\mathbf{r})$ and $V(\mathbf{r})$ are electronic kinetic and electronic potential energy densities, and m is the electron mass, respectively. Negative and positive $\nabla^2\rho(\mathbf{r})$ values are associated with shared-electron (covalent) interactions and closed-shell

(electrostatic) interactions, respectively. In the latter case, one can further evaluate the total energy density, H(**r**), at the bond critical point:

$$H(\mathbf{r}) = G(\mathbf{r}) + V(\mathbf{r}) \quad (8)$$

A negative H(**r**) is termed partial covalence, while a positive H(**r**) indicates a purely closed-shell, electrostatic interaction.[8b,11,12] All critical point properties were calculated by using the AIM2000 program[8a] and are shown in Table S8. These results suggest that the interactions between Gln103/Pro107 and the oxo group are similar to some hydrogen bonds in biomolecules.[12]

References cited in this supporting information:

(1) Debrunner, P. G. In *Iron Porphyrins*; Lever, A. B. P., Gray, H. B., Eds.; VCH Publishers: New York, **1989**; Vol.3, pp139-234.

(2) Zhang, Y.; Mao, J.; Oldfield, E. *J. Am. Chem. Soc.* **2002**, *124*, 7829-7839.

(3) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-52.

(4) Wachters, A. J. *J. Chem. Phys.* **1970,** 52, 1033-1036. http://www.emsl.pnl.gov/forms/basisform.html

(5) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.;Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Gaussian 03, Revision D.01; Gaussian, Inc.: Wallingford CT, 2004.

(6) a) Zhang, Y.; Mao, J.; Godbout, N.; Oldfield, E. *J. Am. Chem. Soc.* **2002**, *124*, 13921-13930. b) Zhang, Y.; Gossman, W.; Oldfield, E. *J. Am. Chem. Soc.* **2003**, *125*, 16387-16396. c) Zhang, Y.; Oldfield, E. *J. Phys. Chem. B.*, **2003**, *107*, 7180-7188. d) Zhang, Y.; Oldfield, E. *J. Phys. Chem. A.*, **2003**, *107*, 4147-4150. e) Zhang, Y.; Oldfield, E. *J. Am. Chem. Soc.* **2004**, *126*, 4470-4471. f) Zhang, Y.; Oldfield, E. *J. Am. Chem. Soc.* **2004**, *126*, 9494-9495. g) Ling, Y.; Zhang, Y. *J. Am. Chem. Soc.* **2009**, *131*, 6386-6388. h) Ling, Y.; Zhang, Y.; *Ann. Rep. Comput. Chem.* **2010**, in press.

(7) Dufek, P.; Blaha, P.; Schwarz, K. *Phys. Rev. Lett.* **1995**, *75*, 3545-3548.

(8) (a) AIM2000, Version 1.0, written by Biegler-König F., University of Applied Science, Bielefeld, Germany. (b) Bader, R. F. W. *Atoms in Molecules: A Quantum Theory*; Oxford Univ. Press: Oxford, 1990.

(9) NBO Version 3.1, Glendening, E. D.; Reed, A. E.; Carpenter, J. E.; Weinhold, F., Theoretical Chemistry Institute, University of Wisconsin, Madison, WI.

(10) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098-3100. Perdew, J. P.; Burke, K.; Wang, Y. *Phys. Rev. B* **1996**, *54*, 16533-16539.
(11) Bader, R. F. W. *J. Phys. Chem. A*. **1998**, *102*, 7314-7323.
(12) Arnold, W. E.; Oldfield, E. *J. Am. Chem. Soc.* **2000**, *122*, 12835-12841.

Table S1. Cartesian coordinates of the MauG-**1a** model

C	-2.316459	-0.581241	4.961015
C	-1.354293	-0.303212	3.818388
N	0.019289	-0.16188	3.999758
C	0.611429	-0.011864	2.776745
N	-0.294615	-0.050825	1.810657
C	-1.514893	-0.229493	2.445621
H	-1.874751	-0.283667	5.912221
H	-3.245656	-0.033078	4.804568
H	0.503528	-0.163033	4.894156
H	-2.433539	-0.301002	1.868823
H	1.680933	0.122129	2.635067
H	-2.52432	-1.651559	4.975303
C	2.921817	2.034016	-0.371202
C	1.68107	2.684562	-0.261549
C	1.476586	4.136201	-0.161218
C	2.507628	5.239405	-0.094542
C	0.119323	4.353517	-0.12857
C	-0.569173	5.711233	0.005143
C	-0.504839	3.034821	-0.24291
N	0.456599	2.046145	-0.271501
C	-1.870353	2.812915	-0.428991
C	-2.486258	1.58791	-0.689714
C	-3.890821	1.429429	-1.04559
C	-4.906504	2.546384	-1.136501
C	-4.103795	0.079963	-1.234431
C	-5.398507	-0.602966	-1.651062
C	-2.819019	-0.572376	-0.981791
N	-1.859467	0.36378	-0.658716
C	-2.597818	-1.949959	-0.99513
C	-1.39455	-2.600497	-0.714837
C	-1.243435	-4.053925	-0.65557
C	-2.42203	-5.009641	-0.856949
C	0.086303	-4.290058	-0.333107
C	0.85222	-5.593027	-0.080677
C	0.724393	-2.966382	-0.260581
N	-0.20288	-1.968644	-0.451782
C	2.100957	-2.747248	-0.14174
C	2.768495	-1.52104	-0.21584
C	4.217132	-1.384053	-0.375744
C	5.228607	-2.548392	-0.407222
C	4.458193	-0.022487	-0.532358
C	5.81111	0.642377	-0.836261
C	3.151972	0.648291	-0.394836
N	2.151115	-0.288925	-0.220643
Fe	0.131866	0.037034	-0.481459
H	3.799149	2.683573	-0.442922
H	-2.518054	3.693207	-0.444141
H	-3.451952	-2.587591	-1.233374
H	2.74315	-3.628716	-0.079715
H	-1.64719	5.54953	-0.015394
H	-0.288747	6.170072	0.95296
H	-0.285183	6.369644	-0.816063
H	1.993633	6.192228	0.032472
H	3.170997	5.069592	0.753315

H	-5.840492	2.13739	-1.522295
H	-5.068665	2.937665	-0.132095
H	-4.564673	3.350576	-1.78871
H	-5.262042	-1.683743	-1.622771
H	-2.051852	-6.034679	-0.845173
H	-3.115179	-4.864245	-0.028258
H	-2.936661	-4.820344	-1.799165
H	1.868881	-5.328822	0.210368
H	6.205804	-2.09792	-0.581449
H	5.241362	-3.087509	0.5403
H	4.997787	-3.241299	-1.216826
H	5.720925	1.725138	-0.924513
H	6.495305	0.39959	-0.022626
O	0.34049	0.078624	-2.120546
H	3.092201	5.26101	-1.014486
H	-6.210775	-0.321567	-0.981608
H	-5.641919	-0.294442	-2.667267
H	0.382417	-6.166248	0.718573
H	0.878721	-6.193289	-0.990003
H	6.197214	0.233001	-1.769302

Table S2. Cartesian coordinates of the MauG-**1b** model

C	-2.316459	-0.58124	4.961015
C	-1.3578945845	-0.3062868083	3.8032503416
N	0.0092866084	-0.1010929396	3.9741446147
C	0.6036477423	0.0460082394	2.7585162543
N	-0.3033567304	-0.0547307875	1.7894781279
C	-1.5226678754	-0.2723895752	2.4275396346
H	-1.874751	-0.283666	5.912221
H	-3.245656	-0.033076	4.804568
H	0.4936222495	-0.057809474	4.8686840389
H	-2.4379739823	-0.396545614	1.8565929531
H	1.6661070959	0.2237548816	2.6187684969
H	-2.524321	-1.651557	4.975303
C	2.9153782059	2.0374442242	-0.3482309816
C	1.6770662301	2.6819592893	-0.2214601788
C	1.4755637273	4.1335581988	-0.1473201707
C	2.507631	5.239403	-0.094542
C	0.1154884574	4.3532570469	-0.1118246665
C	-0.56917	5.711233	0.005143
C	-0.5142833958	3.0385280315	-0.1984970767
N	0.444097219	2.0408089701	-0.2053696949
C	-1.8784159262	2.8206494258	-0.3918714396
C	-2.4889070106	1.597337954	-0.6593443195
C	-3.884211147	1.4339177723	-1.0332995035
C	-4.906502	2.546387	-1.136501
C	-4.0978235412	0.0746117768	-1.2275840631
C	-5.398507	-0.602963	-1.651062
C	-2.8249959906	-0.5789710137	-0.9592588361
N	-1.8523512033	0.3660932246	-0.622085216
C	-2.6055145412	-1.9522469884	-0.9672889355
C	-1.4039438644	-2.6006520312	-0.6755073226
C	-1.247892515	-4.0517340318	-0.6411646593
C	-2.422033	-5.00964	-0.856949
C	0.084769652	-4.2895862333	-0.3176098038
C	0.852217	-5.593028	-0.080677
C	0.7196342049	-2.9673115087	-0.2180341976
N	-0.2156238985	-1.9649845125	-0.3892266088
C	2.0957958423	-2.7542460831	-0.1145215149
C	2.7638784186	-1.5294238899	-0.2030536203
C	4.2056047339	-1.3893937444	-0.3728561615
C	5.228605	-2.548395	-0.407222
C	4.4486242473	-0.0167266848	-0.5314895789
C	5.81111	0.642373	-0.836261
C	3.1471455974	0.6524233886	-0.3837284645
N	2.1337981104	-0.2897991911	-0.211793411
Fe	0.0966324162	0.044028647	-0.3737773889
H	3.789717173	2.6883474126	-0.4282067555
H	-2.5237507064	3.7010137452	-0.4176056259
H	-3.4547036132	-2.5897514873	-1.218625269
H	2.7357801236	-3.6360994644	-0.0556681813
H	-1.647187	5.549531	-0.015394
H	-0.288743	6.170072	0.95296
H	-0.285179	6.369644	-0.816063
H	1.993637	6.192227	0.032472
H	3.171	5.06959	0.753315

H	-5.840491	2.137394	-1.522295
H	-5.068663	2.937668	-0.132095
H	-4.564671	3.350579	-1.78871
H	-5.262043	-1.68374	-1.622771
H	-2.051856	-6.034678	-0.845173
H	-3.115182	-4.864243	-0.028258
H	-2.936664	-4.820342	-1.799165
H	1.868878	-5.328823	0.210368
H	6.205803	-2.097924	-0.581449
H	5.24136	-3.087512	0.5403
H	4.997785	-3.241302	-1.216826
H	5.720926	1.725134	-0.924513
H	6.495305	0.399586	-0.022626
O	0.2839497802	0.0851306234	-2.1604869467
H	3.092204	5.261008	-1.014486
H	-6.210775	-0.321563	-0.981608
H	-5.641919	-0.294439	-2.667267
H	0.382413	-6.166248	0.718573
H	0.878717	-6.19329	-0.990003
H	6.197214	0.232997	-1.769302
H	1.1794837053	-0.2454738358	-2.3887570402

Table S3. Cartesian coordinates of the MauG-**1c** model

C	2.538426388	-2.3725491284	4.8366366637
C	2.0188860874	-1.3823245033	3.8092819014
N	2.1972276635	-0.006263504	3.9327237757
C	1.7271939128	0.6015634896	2.8025330357
N	1.2585769266	-0.2974850048	1.9492354601
C	1.4331483212	-1.5289746921	2.5643047482
H	2.5900340487	-1.9090113947	5.8219885901
H	1.8882163286	-3.2464654219	4.8797897719
H	2.6025182177	0.4706604491	4.7344330799
H	1.130259528	-2.4458060553	2.0654837794
H	1.7432807479	1.6766318707	2.6418748765
H	3.5377459231	-2.6785157269	4.5256143054
C	-1.1162132584	3.1052633688	0.4488044575
C	-1.8039347097	1.929968399	0.7973215198
C	-3.1694843994	1.8590620233	1.3333782944
C	-4.1053831658	2.9890149218	1.7023404829
C	-3.4845977201	0.5267573029	1.4699567841
C	-4.7955881542	-0.0313671173	2.0188344196
C	-2.3195379367	-0.2175306265	0.9908056713
N	-1.3062518653	0.650875267	0.6374924043
C	-2.2888313623	-1.5968316503	0.7747161068
C	-1.2684926337	-2.323206903	0.1589360498
C	-1.3603222208	-3.7315139865	-0.2092077866
C	-2.5384225513	-4.638112016	0.0655881783
C	-0.1605092188	-4.0670494534	-0.8020019497
C	0.2406513441	-5.4170859321	-1.381890292
C	0.6535752601	-2.8520862279	-0.789166134
N	-0.0414537229	-1.8139489405	-0.2049606557
C	1.9696701533	-2.7569562652	-1.2418108587
C	2.7760002337	-1.6180361431	-1.211947681
C	4.1848202946	-1.6025315247	-1.6038269711
C	4.9238779615	-2.8638905479	-2.0582007093
C	4.6264801287	-0.301315913	-1.4032599285
C	6.0080468102	0.3392977222	-1.5809022559
C	3.4507827914	0.4569756215	-0.9482417039
N	2.3620056699	-0.3723271485	-0.8032454855
C	3.4055287835	1.84683994	-0.8000993627
C	2.2811915604	2.6242524208	-0.5079357449
C	2.2309766398	4.0794407767	-0.6503556486
C	3.4144101863	4.9796572676	-1.0619549051
C	0.9146292647	4.4457229155	-0.3839222334
C	0.3125446087	5.8563247281	-0.5013515677
C	0.2068017701	3.207017303	-0.0126025439
N	1.0587895858	2.1220834839	-0.1149312369
Fe	0.4814672773	0.1406704538	-0.2005996057
H	-1.6757129553	4.0390248775	0.5584509559
H	-3.1993576486	-2.1502863656	1.0097128181
H	2.4230218996	-3.6651603296	-1.6447312602
H	4.3177274463	2.4033726733	-1.0259868267
H	-4.7449199443	-1.1196267277	1.9762227666
H	-4.9120986105	0.286500787	3.0546501894
H	-5.6475031966	0.3155339281	1.4336563056
H	-5.0141253989	2.5647997746	2.1294506123
H	-3.6234134087	3.6304682773	2.4399031894

H	-2.3536598228	-5.604366535	-0.4041574323
H	-2.6129274078	-4.7674019324	1.1453859111
H	-3.4709827868	-4.2208137477	-0.3153876247
H	1.2848952265	-5.3812259829	-1.6913588336
H	5.9310738936	-2.5901026682	-2.3719992933
H	4.9805490032	-3.5439220206	-1.2080997805
H	4.4075549492	-3.3550684481	-2.8831884773
H	5.9384627767	1.3748627946	-1.2479262159
H	3.0211377829	5.9949967019	-1.1130983293
H	4.218865168	4.9387528722	-0.3272522354
H	3.7996891574	4.6889946128	-2.0396728274
H	-0.7479845841	5.86696803	-0.2494437446
H	0.8548888641	6.5119051993	0.1806652608
O	-0.0998563087	0.3412526633	-1.7401526015
H	-4.3580612369	3.5767370074	0.8196018226
H	0.1087129243	-6.2025194964	-0.6383720546
H	-0.3872547299	-5.6268915754	-2.2472373636
H	6.7559511912	-0.1846577113	-0.985747872
H	6.29772001	0.3138132853	-2.6312978865
H	0.4462021215	6.2066403075	-1.5244076092
C	-6.9074246018	0.144698793	-2.0776128965
C	-5.5396300252	0.8298572512	-1.9576617857
C	-4.3910229539	-0.1891790745	-1.8639535933
O	-4.5719732224	-1.328605814	-1.4306450642
N	-3.1825751406	0.2692508264	-2.308886178
H	-7.6989056426	0.8908940862	-2.1507179345
H	-6.8995842713	-0.4653172094	-2.9809096395
H	-5.3722171045	1.5127362684	-2.8106574209
H	-5.4959645338	1.4582231226	-1.0479794409
H	-2.3222730641	-0.2363705317	-2.08300883
H	-3.0513439142	1.2603824778	-2.4937367958
H	-7.0871379012	-0.4919847111	-1.2108267374

Table S4. Cartesian coordinates of the MauG-**1d** model

C	2.538426388	-2.3725491284	4.8366366637
C	2.0160448847	-1.384493585	3.8069866164
N	2.1940280464	-0.0079374713	3.9259702727
C	1.7199085638	0.596917632	2.7959007137
N	1.2495591055	-0.3043197943	1.9460003126
C	1.4260857132	-1.5343781655	2.563904595
H	2.5900340487	-1.9090113947	5.8219885901
H	1.8882163286	-3.2464654219	4.8797897719
H	2.6008621023	0.4714730993	4.7254081698
H	1.1221900269	-2.4518528161	2.0668459643
H	1.7345388632	1.6714585802	2.6318234461
H	3.5377459231	-2.6785157269	4.5256143054
C	-1.1182131882	3.1050401627	0.4447246767
C	-1.8094178331	1.9298879125	0.7835894897
C	-3.1720983084	1.8597325739	1.3274462216
C	-4.1053831658	2.9890149218	1.7023404829
C	-3.4889869222	0.5279590595	1.4596431194
C	-4.7955881542	-0.0313671173	2.0188344196
C	-2.3308159595	-0.216728753	0.9652443917
N	-1.316607211	0.6505074207	0.6123014977
C	-2.2999661324	-1.5954736	0.7523805582
C	-1.2760278307	-2.321976719	0.1444667833
C	-1.361976215	-3.732191653	-0.2124004891
C	-2.5384225513	-4.638112016	0.0655881783
C	-0.1611258922	-4.0675843311	-0.8018787571
C	0.2406513441	-5.4170859321	-1.381890292
C	0.6509901445	-2.8512724654	-0.7929464937
N	-0.0493226744	-1.8108699996	-0.2167059192
C	1.9690754623	-2.7574269858	-1.2388993113
C	2.7777899751	-1.6194844024	-1.2060301695
C	4.1851432396	-1.6030554769	-1.6015982191
C	4.9238779615	-2.8638905479	-2.0582007093
C	4.6270887916	-0.3015325706	-1.401001494
C	6.0080468102	0.3392977222	-1.5809022559
C	3.4532625382	0.4560604196	-0.9419832882
N	2.3655617107	-0.374524066	-0.7937754629
C	3.4067606784	1.8463258295	-0.7948576334
C	2.2822145935	2.623918865	-0.5042036184
C	2.2313520927	4.0788674225	-0.6490465564
C	3.4144101863	4.9796572676	-1.0619549051
C	0.9146510239	4.445243556	-0.3834829399
C	0.3125446087	5.8563247281	-0.5013515677
C	0.2065334661	3.2066820232	-0.0120547691
N	1.0593516325	2.1220640812	-0.1108556816
Fe	0.4799857291	0.1401153041	-0.2073400859
H	-1.6766659094	4.0391187657	0.5551431112
H	-3.2040038374	-2.1547899542	1.0014378943
H	2.4220985757	-3.6662090317	-1.6411310873
H	4.318485643	2.4034715056	-1.021143028
H	-4.7449199443	-1.1196267277	1.9762227666
H	-4.9120986105	0.286500787	3.0546501894
H	-5.6475031966	0.3155339281	1.4336563056
H	-5.0141253989	2.5647997746	2.1294506123
H	-3.6234134087	3.6304682773	2.4399031894

H	-2.3536598228	-5.604366535	-0.4041574323
H	-2.6129274078	-4.7674019324	1.1453859111
H	-3.4709827868	-4.2208137477	-0.3153876247
H	1.2848952265	-5.3812259829	-1.6913588336
H	5.9310738936	-2.5901026682	-2.3719992933
H	4.9805490032	-3.5439220206	-1.2080997805
H	4.4075549492	-3.3550684481	-2.8831884773
H	5.9384627767	1.3748627946	-1.2479262159
H	3.0211377829	5.9949967019	-1.1130983293
H	4.218865168	4.9387528722	-0.3272522354
H	3.7996891574	4.6889946128	-2.0396728274
H	-0.7479845841	5.86696803	-0.2494437446
H	0.8548888641	6.5119051993	0.1806652608
O	-0.0672636472	0.3471686725	-1.7585333408
H	-4.3580612369	3.5767370074	0.8196018226
H	0.1087129243	-6.2025194964	-0.6383720546
H	-0.3872547299	-5.6268915754	-2.2472373636
H	6.7559511912	-0.1846577113	-0.985747872
H	6.29772001	0.3138132853	-2.6312978865
H	0.4462021215	6.2066403075	-1.5244076092
C	-5.0379107714	-2.6129675581	-4.9632909281
C	-4.332639213	-1.2862522656	-4.6698447906
C	-3.4482926111	-1.3619178063	-3.4103481929
O	-3.7655825148	-2.0586557229	-2.4442850858
N	-2.3268707182	-0.5900714724	-3.4553122228
H	-5.7624889141	-2.5038832744	-5.7871034761
H	-4.313067724	-3.394583668	-5.2452455865
H	-3.7456852962	-0.9528536031	-5.5449129882
H	-5.0868612994	-0.4980251821	-4.4840067933
H	-1.6924805314	-0.4882273558	-2.6528393797
H	-2.1220245208	-0.0140641308	-4.2660324635
H	-5.5704949979	-2.9609941304	-4.0651926269

Table S5. Cartesian coordinates of the MauG-**1e** model

C	21.842	25.377	-86.278
C	22.7478382039	26.2570858317	-85.4360237554
N	23.1944113984	25.8866047593	-84.1698848352
C	24.0780834963	26.8263599397	-83.7211198384
N	24.2364050874	27.7844746614	-84.623658782
C	23.4148290285	27.442323985	-85.6882652938
H	21.244	24.726	-85.64
H	21.182	25.991	-86.891
H	22.9062630262	25.0563115178	-83.6578318953
H	23.3634175785	28.070750644	-86.5731726088
H	24.5748135602	26.7797626826	-82.7554083095
H	22.477	24.77	-86.924
C	25.4241905713	30.1490377918	-81.106131503
C	24.3959670603	30.6577272485	-81.9194777228
C	23.2803282214	31.4980330154	-81.4681249945
C	22.923	31.928	-80.063
C	22.5529558204	31.8424729934	-82.5841303609
C	21.278	32.681	-82.598
C	23.2428754913	31.2378403722	-83.7230631047
N	24.3180849044	30.4882356403	-83.2888039306
C	22.9557930372	31.5095860048	-85.062447126
C	23.694458919	31.1037885504	-86.1751069447
C	23.4571708694	31.5596278046	-87.5401915455
C	22.345	32.485	-87.979
C	24.4018067344	30.944084837	-88.3371495364
C	24.6	31.115	-89.84
C	25.2035754237	30.1093319274	-87.4426733066
N	24.760847596	30.2320628157	-86.1412086591
C	26.2402604013	29.2643020782	-87.8403085625
C	27.018960725	28.4586340473	-87.008171577
C	28.0465975195	27.5382892247	-87.4938133388
C	28.342	27.35	-88.985
C	28.5624788917	26.9109702254	-86.3675715359
C	29.613	25.807	-86.216
C	27.8769444735	27.518443277	-85.2160794699
N	26.924913319	28.4194497261	-85.6358610651
C	28.2220787192	27.3062384453	-83.8771506953
C	27.6989866664	27.9619535552	-82.7587095561
C	28.3035336626	27.9197741077	-81.4263100833
C	29.534	27.079	-81.029
C	27.5679802226	28.803678631	-80.6419889473
C	27.86	29.199	-79.183
C	26.4794485211	29.3096345392	-81.4993838498
N	26.5964240593	28.7894956026	-82.7759240925
Fe	25.6900838367	29.5473704943	-84.4698065214
H	25.3910096393	30.4406714946	-80.0521715478
H	22.1270935735	32.1925944414	-85.258178808
H	26.4637561023	29.2203830739	-88.9084370203
H	29.0551608619	26.628781308	-83.6779067735
H	20.958	32.795	-83.634
H	20.506	32.157	-82.035
H	21.444	33.665	-82.159
H	21.986	32.484	-80.096
H	22.797	31.042	-79.441

H	22.474	32.714	-89.037
H	21.403	31.956	-87.834
H	22.333	33.412	-87.405
H	25.375	30.429	-90.181
H	29.185	26.668	-89.095
H	27.456	26.909	-89.442
H	28.573	28.295	-89.477
H	29.674	25.552	-85.158
H	29.734	27.307	-79.982
H	29.332	26.013	-81.136
H	30.402	27.347	-81.632
H	27.139	29.925	-78.807
H	27.813	28.293	-78.578
O	26.7035486714	30.8617723399	-84.4200679076
H	23.706	32.559	-79.642
H	23.669	30.901	-90.364
H	24.906	32.14	-90.047
H	29.326	24.924	-86.787
H	30.584	26.162	-86.561
H	28.863	29.621	-79.127
C	23.559	36.687	-82.742
C	24.3852024153	35.4367075052	-82.4140030219
C	24.6663217813	34.5394606381	-83.6280643275
O	24.0348517696	34.6354778188	-84.6803473753
N	25.6903283362	33.6478927232	-83.4363834781
H	23.486	37.286	-81.834
H	24.07	37.261	-83.515
H	25.3453926694	35.728620202	-81.9490373463
H	23.8634366549	34.8177137053	-81.6594221193
H	25.79484427	32.8386922893	-84.0570426159
H	26.0602744511	33.5068735084	-82.4993248402
H	22.558	36.425	-83.086
C	29.994	35.325	-86.646
O	31.194	35.239	-86.94
N	29.0937794646	34.3328277497	-86.8586164886
C	29.5246358036	33.0333063903	-87.4214888576
C	28.1724106002	32.350651129	-87.7508950658
C	27.1762111032	32.9799129044	-86.764581164
C	27.637853646	34.4342547688	-86.6473940381
C	30.313	33.19	-88.716
O	31.295	32.519	-89.084
H	30.1204889323	32.462298338	-86.6901495051
H	27.8835686648	32.5844398971	-88.7937261031
H	28.2419749212	31.2588139727	-87.6560090031
H	26.1316488823	32.9019698989	-87.0988703304
H	27.2563611952	32.4629578248	-85.7962440314
H	27.4113851849	34.8703647253	-85.6620011567
H	27.1767249207	35.0729379766	-87.4250419745
H	29.616	36.276	-86.302
H	29.873	33.905	-89.396

Table S6. Cartesian coordinates of the MauG-**2a** model

C	2.93012400	1.95718600	-0.45413900
C	1.70551300	2.63004100	-0.40915500
C	1.56469000	4.07982600	-0.35545000
C	2.72492600	5.05104300	-0.37445100
C	0.21190600	4.34132400	-0.25680500
C	-0.48293700	5.69004300	-0.16888600
C	-0.45352300	3.04262400	-0.29866000
N	0.47023500	2.02647200	-0.36993000
C	-1.83720900	2.85939400	-0.32446600
C	-2.51443900	1.65092100	-0.47253200
C	-3.96233000	1.53376700	-0.59216000
C	-4.91872000	2.69743700	-0.54910900
C	-4.25395700	0.19421700	-0.73060300
C	-5.57689200	-0.42023500	-1.17551300
C	-2.94709400	-0.49371700	-0.72432100
N	-1.92434900	0.41445400	-0.55379100
C	-2.73368000	-1.87033900	-0.84412100
C	-1.50408500	-2.53086900	-0.71842100
C	-1.34629400	-3.98288000	-0.74251700
C	-2.47814200	-4.90826900	-1.09463000
C	-0.03749700	-4.25946700	-0.39325000
C	0.72419900	-5.58295200	-0.41578900
C	0.60620100	-2.95162000	-0.26863300
N	-0.29771900	-1.93308400	-0.46266800
C	1.97432600	-2.77396700	-0.09722800
C	2.66021100	-1.56250900	-0.18098300
C	4.10888100	-1.45925800	-0.21567600
C	5.03154100	-2.66257900	-0.14793500
C	4.40763800	-0.11322100	-0.35956300
C	5.76949500	0.53215600	-0.62151100
C	3.11465400	0.57657100	-0.39518300
N	2.07761000	-0.32603800	-0.29727600
Fe	0.08955800	0.04744000	-0.53285800
H	3.83098300	2.57217000	-0.50376100
H	-2.45855900	3.75579300	-0.26822300
H	-3.61406800	-2.49948400	-1.00188400
H	2.57940000	-3.67348700	0.04013600
H	-1.55945000	5.54874200	-0.07255300
H	-0.11200300	6.24949500	0.68975000
H	-0.26983800	6.24374200	-1.08369000
H	3.58963600	4.56840100	-0.82897900

H	2.46318900	5.93456400	-0.95593900
H	-5.91830500	2.34698100	-0.80719700
H	-4.91819500	3.07119800	0.47497900
H	-4.62790800	3.49800500	-1.22834200
H	-6.09562800	-1.15307200	-0.57552600
H	-2.09603700	-5.92830100	-1.14001300
H	-3.21977600	-4.83330500	-0.29875000
H	-2.94096600	-4.65110200	-2.04747900
H	1.27170900	-5.89283400	0.46131400
H	6.04879100	-2.28861600	-0.26763000
H	4.93520700	-3.15011900	0.82177600
H	4.81268600	-3.38036000	-0.93798000
H	5.72055000	1.62108900	-0.59561600
H	6.52160800	0.23148900	0.10713700
H	2.96034900	5.35056000	0.64650000
H	-5.19988800	-1.12746000	-1.91376900
H	-6.27803700	0.35065700	-1.49415100
H	1.55894200	-5.38953600	-1.08934700
H	0.04356400	-6.37816000	-0.71910600
H	6.07873900	0.13505800	-1.58807200
O	0.21260400	0.05977700	-2.18934700
C	-1.93895700	-0.69007800	4.74126800
C	-1.01707600	-0.44237100	3.59642700
N	0.31587400	-0.07359300	3.75091200
C	0.84373100	0.15278300	2.51252400
N	-0.07767700	-0.05037500	1.58367000
C	-1.23138500	-0.42067300	2.24368300
H	-2.96079800	-0.79287300	4.37697700
H	-1.83859400	0.16049900	5.41559400
H	0.81586300	0.01259700	4.63208000
H	-2.14645000	-0.64422200	1.70480300
H	1.87344500	0.44838200	2.33194300
H	-1.69021700	-1.61896300	5.25440200

Table S7. Cartesian coordinates of the MauG-**2b** model

C	2.89758300	2.01684300	-0.43598900
C	1.66187800	2.66203000	-0.39511200
C	1.49010900	4.10216200	-0.35238400
C	2.62764400	5.10369300	-0.37940200
C	0.12193700	4.33991200	-0.25441700
C	-0.59197100	5.68105100	-0.17518200
C	-0.52063200	3.03668000	-0.28385600
N	0.42776900	2.02338200	-0.35456200
C	-1.89787200	2.82967600	-0.30499500
C	-2.54790100	1.60752600	-0.44717100
C	-3.98991900	1.45988100	-0.58733500
C	-4.96928500	2.60341800	-0.55428800
C	-4.25561600	0.11226900	-0.72898500
C	-5.56721400	-0.52680900	-1.17847600
C	-2.93785800	-0.55066900	-0.70323200
N	-1.92959500	0.38061600	-0.51251600
C	-2.69960300	-1.91850300	-0.83742800
C	-1.45718500	-2.55389100	-0.72124300
C	-1.27100400	-3.99729800	-0.74532800
C	-2.38276500	-4.95436800	-1.09332600
C	0.05239800	-4.25042800	-0.39531000
C	0.83176600	-5.56683400	-0.41311600
C	0.67261500	-2.93845400	-0.26826500
N	-0.25036300	-1.92470200	-0.47934300
C	2.03415400	-2.73707000	-0.07989400
C	2.69095600	-1.51183700	-0.15087500
C	4.13424100	-1.37994600	-0.20718200
C	5.08208400	-2.56397600	-0.14635700
C	4.40816300	-0.02485400	-0.35454600
C	5.75860700	0.64399600	-0.62218600
C	3.10564100	0.64193300	-0.36888200
N	2.07956600	-0.27972700	-0.25055100
Fe	0.08993200	0.06405300	-0.46000500
H	3.78472300	2.64855600	-0.49586800
H	-2.53580500	3.71358000	-0.25669500
H	-3.56578800	-2.56377900	-1.00148900
H	2.65630600	-3.62377000	0.05728600
H	-1.66559500	5.51915000	-0.07902600
H	-0.23210300	6.24818600	0.68312300
H	-0.38930000	6.23804800	-1.09035400
H	3.50160100	4.63742100	-0.83333100
H	2.34912900	5.98157500	-0.96163800

H	-5.96187500	2.23361100	-0.81237400
H	-4.97623500	2.97790000	0.46951200
H	-4.69373000	3.40891200	-1.23405800
H	-6.07193200	-1.26902800	-0.57806600
H	-1.98110500	-5.96689800	-1.13782500
H	-3.12592600	-4.89307100	-0.29770100
H	-2.85018000	-4.70687400	-2.04649500
H	1.38488700	-5.86546300	0.46437000
H	6.09198900	-2.17061400	-0.26606800
H	4.99487000	-3.05254000	0.82370200
H	4.87729300	-3.28643400	-0.93590800
H	5.68872500	1.73180500	-0.59713900
H	6.51615700	0.35840100	0.10689200
H	2.85697700	5.40845900	0.64138100
H	-5.17647400	-1.22721700	-1.91608900
H	-6.28296200	0.23021500	-1.49789200
H	1.66282500	-5.35791600	-1.08660000
H	0.16663200	-6.37521400	-0.71600400
H	6.07570000	0.25218100	-1.58836000
O	0.20982500	0.11746100	-2.25230300
C	-1.92642400	-0.72214500	4.73947700
C	-1.01509400	-0.46457700	3.58715500
N	0.31881000	-0.09321600	3.72418600
C	0.84012700	0.13841500	2.49203700
N	-0.09816100	-0.06387000	1.56984100
C	-1.24882000	-0.44186100	2.23736700
H	-2.94599800	-0.84484600	4.37499400
H	-1.84262400	0.13071800	5.41317700
H	0.82687000	-0.00304000	4.60183000
H	-2.17069600	-0.66574400	1.71334000
H	1.86578100	0.43915000	2.30359900
H	-1.66001400	-1.64568400	5.25339000
H	0.19044300	-0.79795300	-2.60607900

Table S8. Cartesian coordinates of the MauG-**2c** model

C	-3.24582500	1.84481600	0.38811300
C	-2.10459900	2.56485000	0.02645100
C	-1.99738600	4.01845400	0.09051000
C	-3.11511900	4.94313800	0.53555800
C	-0.74125300	4.33664600	-0.38635700
C	-0.12424100	5.71151300	-0.56226700
C	-0.08694400	3.06547700	-0.69188500
N	-0.93675600	2.01873400	-0.44510700
C	1.24896500	2.92986300	-1.08515700
C	1.96256600	1.73939700	-1.22797900
C	3.40145800	1.67046500	-1.47050000
C	4.28683400	2.87127600	-1.68114600
C	3.74951200	0.33913900	-1.51097300
C	5.16417800	-0.24787800	-1.46528700
C	2.48969100	-0.39440300	-1.25795300
N	1.44008200	0.48043000	-1.09331000
C	2.34942800	-1.77993700	-1.15832000
C	1.15190300	-2.47838900	-0.95813500
C	1.05676100	-3.93734200	-0.89362300
C	2.27197100	-4.83846800	-0.90594000
C	-0.28994900	-4.24867400	-0.85540300
C	-0.97363900	-5.59637500	-0.65574500
C	-0.98412700	-2.95984700	-0.77635000
N	-0.09366000	-1.91794600	-0.84907000
C	-2.34430400	-2.82387100	-0.50773900
C	-3.00542900	-1.64013100	-0.16812300
C	-4.35989500	-1.59712600	0.36548400
C	-5.22740300	-2.82924500	0.52832000
C	-4.63050300	-0.27221700	0.66740800
C	-5.85824700	0.30677500	1.39005600
C	-3.41706400	0.46480700	0.28981900
N	-2.45817700	-0.38918700	-0.19849600
Fe	-0.54141200	0.05357200	-0.73621700
H	-4.09333500	2.42099300	0.76705300
H	1.81791800	3.85147200	-1.23301900
H	3.25725600	-2.38134900	-1.26194600
H	-2.93477300	-3.74357200	-0.46872600
H	0.87868100	5.61577600	-0.97832800
H	-0.74321600	6.30047800	-1.23889500
H	-0.06946700	6.20865700	0.40660300
H	-3.79730800	4.40555600	1.19349800
H	-2.71174400	5.80448300	1.06717700

H	5.32504300	2.54555100	-1.74915700
H	3.97675100	3.29737000	-2.63547600
H	4.19285800	3.62409400	-0.89930800
H	5.49787300	-0.92868700	-2.23422600
H	1.94121800	-5.87306200	-0.81241800
H	2.74430000	-4.69462900	-1.87819600
H	2.98977100	-4.61393400	-0.11688500
H	-1.74893100	-5.88061400	-1.35089700
H	-6.17159100	-2.50031700	0.96339300
H	-5.41127100	-3.26188700	-0.45470000
H	-4.77069200	-3.57834700	1.17449400
H	-5.84143900	1.39665300	1.41696900
H	-6.78542400	0.01637800	0.89709200
H	-3.64716100	5.28618800	-0.35141500
H	5.03616000	-1.00605300	-0.69320800
H	5.91214700	0.53114200	-1.32010100
H	-1.57648200	-5.46952200	0.24335100
H	-0.21768600	-6.38022200	-0.61404400
H	-5.86057700	-0.15121300	2.37889400
C	4.82563600	-0.39744900	3.83852600
C	3.43756400	-0.26397000	3.24571600
C	2.95733700	0.94856600	2.72503600
C	1.71628600	1.03331500	2.09504500
C	0.89106400	-0.11547900	1.92525900
O	-0.24323000	-0.08571800	1.26394000
C	1.35235400	-1.32135100	2.52909500
C	2.59434500	-1.38672200	3.15603800
H	5.46548600	0.40764600	3.47782200
H	5.20537200	-1.37210800	3.53179000
H	3.58648600	1.84711600	2.79121600
H	2.93781100	-2.34788800	3.56481700
H	1.37148700	1.98112700	1.67235500
H	0.72232300	-2.21166900	2.43369800
H	4.79544300	-0.32411800	4.92561600
O	-0.91533900	0.14617900	-2.36852900

Table S9. Cartesian coordinates of the MauG-**2d** model

C	-3.25293100	1.84533500	0.42083200
C	-2.11567300	2.56569900	0.05222800
C	-2.01076500	4.01786600	0.10067700
C	-3.12846900	4.94209900	0.54430600
C	-0.75296400	4.33830500	-0.37726100
C	-0.13898300	5.71641100	-0.55313900
C	-0.09291200	3.07080300	-0.67339800
N	-0.94255100	2.01662000	-0.41654100
C	1.24076400	2.93932100	-1.06708900
C	1.95721600	1.75127700	-1.20951600
C	3.39161100	1.68331200	-1.46139800
C	4.27634400	2.88436400	-1.67600200
C	3.74313700	0.35005300	-1.49935800
C	5.15860500	-0.23365800	-1.46385700
C	2.49241800	-0.38812100	-1.23778200
N	1.43824200	0.48731400	-1.06245700
C	2.35517000	-1.77423200	-1.14972600
C	1.15587700	-2.47399900	-0.97271100
C	1.05761200	-3.92837700	-0.89911200
C	2.27368100	-4.82940600	-0.90928100
C	-0.29175200	-4.24169000	-0.86164100
C	-0.97069700	-5.59267800	-0.65941200
C	-0.98942300	-2.95696300	-0.79636100
N	-0.09773200	-1.90967500	-0.89067400
C	-2.34505500	-2.82012100	-0.50817500
C	-3.00003100	-1.64086900	-0.14879300
C	-4.35868600	-1.60039800	0.37297900
C	-5.22858700	-2.83356700	0.52852800
C	-4.63192000	-0.27620300	0.68187100
C	-5.86419300	0.30047400	1.39395700
C	-3.41864800	0.46613300	0.32301100
N	-2.45006900	-0.38545100	-0.15856500
Fe	-0.52979200	0.06632800	-0.64699500
H	-4.10247200	2.41986700	0.79375300
H	1.80353800	3.86165100	-1.22552600
H	3.26347700	-2.37362100	-1.25118900
H	-2.93589800	-3.73826200	-0.46919700
H	0.86401800	5.62271900	-0.96947600
H	-0.75899300	6.30517900	-1.22899000
H	-0.08482300	6.21253200	0.41629000
H	-3.80970500	4.40269800	1.20174400
H	-2.72635300	5.80346600	1.07684200

H	5.31505000	2.56034200	-1.74455900
H	3.96543300	3.31106300	-2.62979200
H	4.18132100	3.63613900	-0.89328700
H	5.49323600	-0.91306400	-2.23363100
H	1.94456400	-5.86462300	-0.81688700
H	2.74562100	-4.68371600	-1.88145000
H	2.99126200	-4.60465100	-0.12008900
H	-1.74566000	-5.87733500	-1.35475800
H	-6.17321500	-2.50661500	0.96413500
H	-5.41194300	-3.26537100	-0.45495500
H	-4.77059500	-3.58269100	1.17376800
H	-5.84908600	1.39034600	1.42211400
H	-6.79099700	0.00919000	0.90081500
H	-3.66119800	5.28533100	-0.34218600
H	5.03190400	-0.99291500	-0.69262600
H	5.90537800	0.54636500	-1.31790600
H	-1.57358600	-5.46779800	0.23993000
H	-0.21351000	-6.37538900	-0.61873300
H	-5.86564000	-0.15864800	2.38227000
C	4.82119100	-0.38982500	3.83983700
C	3.43446700	-0.26022900	3.25291200
C	2.98327600	0.93568100	2.66934700
C	1.76333800	1.00103200	2.00212800
C	0.95075500	-0.15320600	1.89144500
O	-0.17126900	-0.17590000	1.18454100
C	1.35020100	-1.33056000	2.57360600
C	2.57657900	-1.37707100	3.22518100
H	5.45972000	0.41668300	3.47994700
H	5.20240100	-1.36353600	3.53192300
H	3.61992500	1.82703200	2.70955400
H	2.89789500	-2.31303000	3.69760900
H	1.43089200	1.92798400	1.53103200
H	0.70056700	-2.20800700	2.51702100
H	4.79106700	-0.31778500	4.92701600
O	-0.93342500	0.19945900	-2.41191300
H	-0.50000900	-0.54813900	-2.87502300

Table S10. Cartesian coordinates of the MauG-**2e** model

C	-2.5909207826	-0.8214881409	-2.8386582647
C	-2.039696145	-1.8721783834	-2.1156386026
C	-2.30162174	-3.2753128333	-2.384718185
C	-1.609515689	-3.9917001956	-1.4316583726
C	-0.9170649841	-3.0173141979	-0.6073317065
N	-1.1968671438	-1.7318629778	-1.0326309509
C	-0.0532705976	-3.3474130857	0.4284580785
C	0.709100152	-2.4437052368	1.161233409
C	1.6613770833	-2.8252799043	2.184831392
C	2.2398509849	-1.6558757042	2.6388467009
C	1.616828496	-0.5750491246	1.9012227309
N	0.6915036165	-1.070957886	0.999494625
C	1.8678363155	0.7734642039	2.1274832661
C	1.204071273	1.8258328293	1.5073120671
C	1.4230523727	3.2266095363	1.8175916809
C	0.5524607917	3.9430409253	1.022793905
C	-0.1720006733	2.9696169621	0.2248959731
N	0.2328467981	1.6886102015	0.5362177926
C	-1.1089363049	3.2988007829	-0.7482937572
C	-1.7589234183	2.3951582386	-1.5787588108
C	-2.6439579432	2.7793066514	-2.6617499296
C	-3.0389881745	1.61005104	-3.2799782398
C	-2.4054931154	0.5260642405	-2.553717426
N	-1.628535489	1.018292102	-1.5208899677
Fe	-0.4355362677	-0.0247369845	-0.2940298352
H	-3.2337820046	-1.0739595694	-3.6842396026
H	0.0672434947	-4.4075282855	0.6609776704
H	2.6244006888	1.0254780008	2.8732763928
H	-1.3199507686	4.3592823647	-0.9008950894
C	6.49939	-0.002895	-0.493862
C	5.0362696904	-0.018031997	-0.8722269185
C	4.3217559194	-1.2284408014	-0.9825943813
C	2.9543380468	-1.2402203322	-1.2305454276
C	2.2522100656	-0.0173941086	-1.3676340445
O	0.9295628679	-0.0090624287	-1.5267486444
C	2.9749328374	1.2013831756	-1.3485898413
C	4.3419392207	1.1886221646	-1.1012918351
H	6.742407	-0.915937	0.049268
H	6.689118	0.881565	0.114398
H	4.8501154968	-2.1780295767	-0.8464479019
H	4.8873152597	2.1375734108	-1.0577193754
H	2.3968614255	-2.1777065712	-1.2925695697
H	2.4322223417	2.1377860937	-1.4976147004
H	7.115621	0.012346	-1.392795
C	-3.290787	-0.119766	4.596071
C	-2.9130844099	-0.0475497711	3.1494264092
N	-3.8505463503	-0.0056902731	2.1210445437
C	-3.2012128716	0.0156681863	0.929689758
N	-1.8874059488	-0.0128662538	1.1399995748
C	-1.6970636627	-0.0495623821	2.5113531399
H	-2.389867	-0.188558	5.205205
H	-3.935883	-0.987087	4.73705
H	-4.8619012179	0.0076265067	2.2365907291
H	-0.7055311681	-0.0777850358	2.9499622792
H	-3.6914105815	0.0481243835	-0.0382216025

H	-3.805172	0.794253	4.892688
C	1.9284444869	-4.2346700442	2.6185189142
H	1.0132722587	-4.7236290119	2.9954827924
H	2.3102896658	-4.8516770104	1.7862218737
H	2.6756291199	-4.2736673111	3.424471824
C	3.2931237271	-1.4751023715	3.6892731175
H	4.1796438728	-0.9546505918	3.2878159637
H	2.9220019811	-0.8794169063	4.5419226985
H	3.6331669935	-2.4412683807	4.0897217902
C	2.4158108371	3.7317283448	2.8200770065
H	2.2063721004	3.3451275309	3.832882871
H	3.4446987146	3.4277511232	2.5594257893
H	2.4043209019	4.8297413311	2.880770807
C	0.3562456129	5.4265512718	0.9422594973
H	0.6095460796	5.8178077908	-0.0588646151
H	-0.690252541	5.709808007	1.1500157241
H	0.9887811867	5.9566269723	1.669238673
C	-3.0009493184	4.1919884422	-3.0110139174
H	-3.4412565001	4.726078915	-2.151040032
H	-2.1144209166	4.7653872736	-3.3345848091
H	-3.7324253372	4.2316449037	-3.8311415144
C	-3.9283946903	1.4302384656	-4.4720707978
H	-3.3880543745	0.9550044042	-5.3096110033
H	-4.8000215891	0.792865442	-4.2413445765
H	-4.314317856	2.3931572398	-4.8369748598
C	-3.1610164294	-3.7804882373	-3.5030535132
H	-4.1976647131	-3.4085470218	-3.4226141125
H	-2.7730655561	-3.4608630029	-4.486090053
H	-3.20681325	-4.8791807665	-3.5113310574
C	-1.5280690951	-5.4765551747	-1.2474217674
H	-0.4995407293	-5.8492095347	-1.3980523648
H	-1.8423258784	-5.7794937352	-0.2334067315
H	-2.1747859608	-6.0065816728	-1.9618223203

Table S11. Cartesian coordinates of the MauG-**2f** model

Fe	0.2924288404	0.0110685337	-0.0010955582
N	-0.5386420481	-1.224219848	1.3227423977
N	1.0911984061	-1.5806776294	-0.9543318482
N	1.2183903816	1.2548626456	-1.2877526794
N	-0.405150389	1.5866106827	0.9955325304
C	-1.142316986	-0.8705214923	2.517840389
C	-1.6212829081	-2.049314233	3.1943139743
H	-2.1381062858	-2.0473348221	4.1538570278
C	-1.3253270774	-3.1200405746	2.3943269052
H	-1.5430732922	-4.173389496	2.5696638374
C	-0.6303002316	-2.6069524169	1.2421505218
C	-0.0513176589	-3.395458153	0.2531537494
C	0.7796657556	-2.9111463696	-0.7544181965
C	1.4966463842	-3.7344323827	-1.6972768158
H	1.4248610701	-4.8202368188	-1.7565084879
C	2.257782089	-2.8915549292	-2.4600547422
H	2.9316173844	-3.1452183434	-3.2782098908
C	1.9835413039	-1.5485295398	-2.0057854582
C	2.486317992	-0.3980021757	-2.6062437254
C	2.0911482131	0.8996841261	-2.2953195454
C	2.4750930134	2.0696485234	-3.0493339307
H	3.1583042794	2.0649942336	-3.898395632
C	1.8008835811	3.1311246149	-2.5104710603
H	1.8247639131	4.1752424479	-2.8215062688
C	1.0284041746	2.6178209474	-1.4063287819
C	0.2602686549	3.3968489532	-0.5446402389
C	-0.3687022972	2.9160649592	0.5984924772
C	-0.9936719502	3.74342356	1.5978689601
H	-1.1067116161	4.8249200033	1.5260044893
C	-1.3754178301	2.9179628826	2.6206668799
H	-1.8725038373	3.1856305956	3.5528494842
C	-1.0205704695	1.5751337921	2.2355559497
C	-1.329786344	0.4331053804	2.96892565
H	-0.2124257637	-4.4748033915	0.3055120982
H	3.1869460209	-0.5266844671	-3.4347269422
H	0.1990059998	4.4689663227	-0.74547514
H	-1.8186960929	0.5690423214	3.9365632549
C	2.5433406268	-0.972438369	1.7190174658
H	2.2230349517	-2.0068448419	1.6464324176
N	1.9466055022	0.0774253888	1.1500152769
C	2.6788502358	1.2014240227	1.4952937293
C	3.7329671284	0.8192627999	2.2850567208
N	3.6276943502	-0.555015862	2.4129379522
H	2.401093065	2.1934745798	1.1555384183
H	4.2572095802	-1.1576132472	2.9389425086
C	-2.4316779738	-0.078215805	-1.2610858411
C	-2.9816384305	-0.2964159288	-2.5628585164
C	-3.3127875488	0.1212757496	-0.1607331387
C	-4.3566985867	-0.3157373981	-2.7441251473
H	-2.2901742084	-0.4455226379	-3.3956228471
C	-4.6872960441	0.0985958998	-0.3675454877
H	-2.9045144334	0.2949497439	0.8344902901
C	-5.2197589213	-0.1196829976	-1.6503383324
H	-4.7689340266	-0.4842214946	-3.7429653685
H	-5.3606924027	0.2539520876	0.4802600877

O	-1.1168459914	-0.0701646765	-1.1795677672
H	-6.3028702709	-0.1353761449	-1.7977048907
H	4.5291751971	1.3885828601	2.7552422352

Table S12. AIM results of some hydrogen bonds (HBs) in proteins

Models	HB distance	$\rho(\mathbf{r})$ (au)	$G(\mathbf{r})$ (au)	$-V(\mathbf{r})$ (au)	$\nabla^2\rho(\mathbf{r})$ (au)	$H(\mathbf{r})$ (au)
protein backbone HBs[a]		0.012~0.025	0.004~0.026	0.003~0.024	0.020~0.109	0.001~0.003
MauG **1c:** H_{Gln103}…O	2.322	0.012	0.010	0.009	0.043	0.001
MauG **1d:** H_{Gln103}…O	2.034	0.020	0.018	0.017	0.074	0.001
MauG **1e:** H_{Gln103}…O	2.206	0.015	0.012	0.011	0.052	0.001
MauG **1e:** H_{Pro107}…O	2.182	0.017	0.014	0.013	0.059	0.001

[a] Reference S12.