

**Methemoglobinemia Caused by 8-Aminoquinoline  
Drugs: DFT Calculations Suggest an Analogy to H<sub>4</sub>B's  
Role in Nitric Oxide Synthase**

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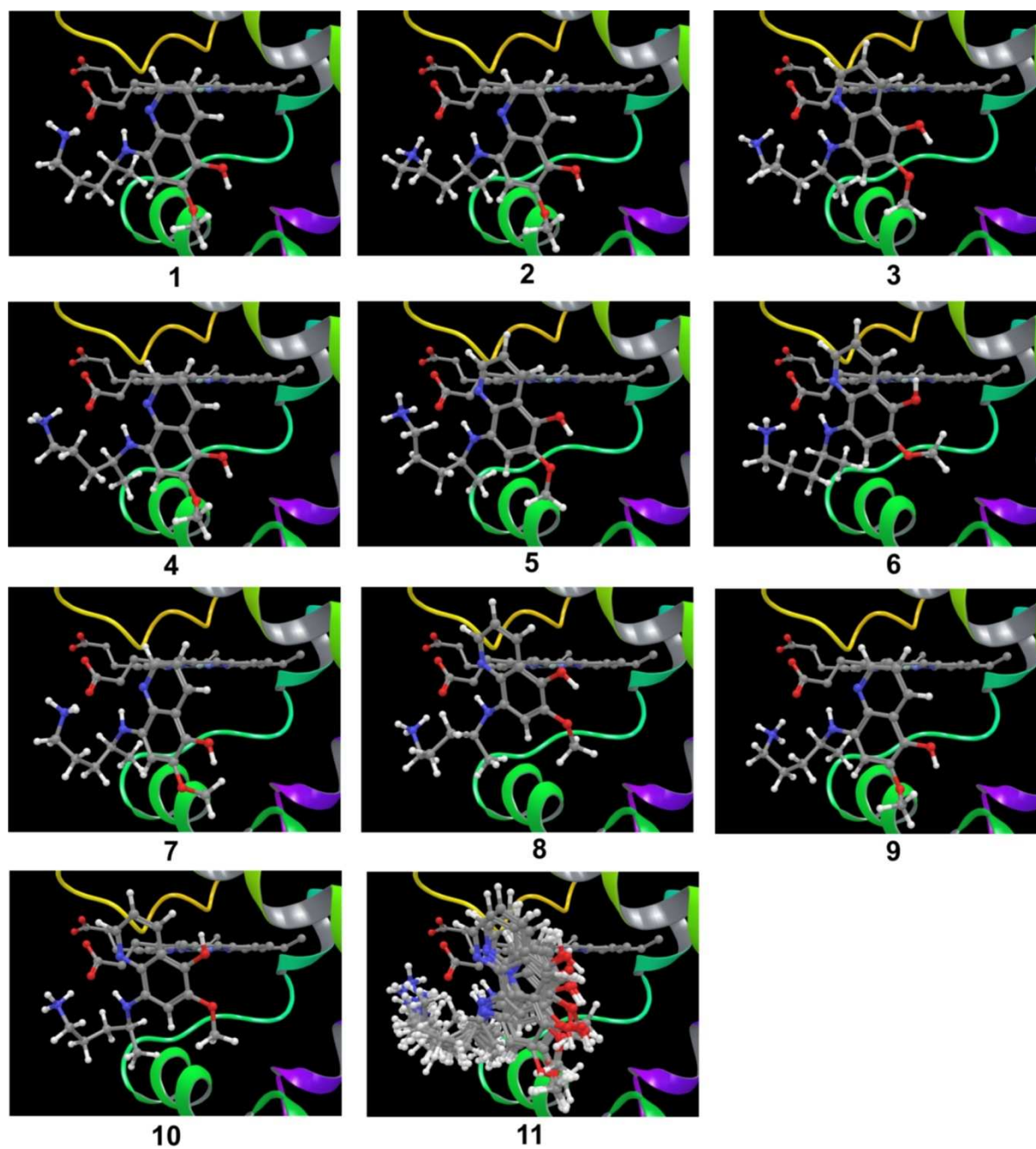
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**Supporting Information**

### **Detailed docking procedure and top 10 binding poses generated by the Glide SP method.**

Docking calculations were performed using the Glide software. The crystal structure (PDB: 2D5X) of carbonmonoxy hemoglobin complexed with the ligand 2-[4-(3,5-dichlorophenylureido)phenoxy]-2-methylpropionic acid (L35) was used. For this tetrameric protein, only the monomer (including heme) with L35 hydrogen bonded with the propionate group of heme was kept for docking, while all the other chains, ligands and water molecules were removed. The location of L35 was defined as the active site for Glide. The extra precision (XP) module of Glide was used and the obtained most preferred binding pose (as ranked by Glide score) was selected to build the chemical model for DFT calculations.



**Figure S1.** The top ten (1–10) binding poses generated by the Glide SP method and a superimposition (11) of the ten binding poses.

### The effect of proton transfer between the $-\text{NH}_3^+$ of 5-HPQ and $-\text{COO}^-$ of heme on the calculated spin densities.

In the gas phase calculations, the  $-\text{NH}_3^+$  of 5-HPQ automatically transfers a proton to the  $-\text{COO}^-$  of heme during geometry optimizations, yielding  $-\text{NH}_2$  and  $-\text{COOH}$ . Hence, this is predicted to be a spontaneous process in the gas phase. The polar environment of the solution phase may be able to stabilize the electrostatic interaction of  $-\text{NH}_3^+\cdots^-\text{OOC}-$ . To investigate the effects of proton transfer, we fixed two of the N–H bonds at 1.0 Å to prevent proton transfer. The geometries of the unprotonated species in the singlet spin state, the singly protonated species in the triplet spin state and the doubly protonated complexes in the triplet spin state were re-optimized and single point calculations were performed with a dielectric constant of 4. The resulting unprotonated, singly protonated and doubly protonated complexes are 34.7, 23.8 and 19.0 kJ mol<sup>-1</sup> higher in energy, respectively, than their counterparts without the N–H bond fixed. The calculated spin densities are listed below.

**Table S1.** Calculated spin densities of the unprotonated complex ( $\text{O}_2$ ) in the singlet spin state, the singly protonated complex ( $\text{OOH}$ ) in the triplet spin state and the doubly protonated complexes ( $\text{HOOH}$ ) in the triplet spin state with two of the N–H bonds fixed at 1.0 Å.

Structure	M	Spin Density				
		Fe	O <sub>inner</sub>	O <sub>outer</sub>	heme	5-HPQ
$\text{O}_2$	1	1.52	-0.66	-0.78	-0.09	0.00
$\text{OOH}$	3	0.82	0.21	0.03	0.40	0.55
$\text{HOOH}$	3	1.06	-0.01	0.00	-0.04	1.01

As can be seen, the calculated spin densities showed that the 5-HPQ donates 0, ~0.6 and ~1.0 electrons to  $\text{O}_2$  in the unprotonated, singly protonated and doubly protonated complexes, respectively, which is similar to the results in Table 1. Thus, even for the system containing the  $-\text{NH}_3^+\cdots^-\text{OOC}-$  interaction, our conclusions do not change.

### The effect of a more polar environment on the calculated spin densities.

We performed single point calculations on the unprotonated species in the singlet spin state, the singly protonated species in the triplet spin state and the doubly protonated complexes in the triplet spin state with a dielectric constant of 80.37, in order to consider the maximum effect that could occur from the binding site being exposed to solvent. The calculated spin densities are listed below.

**Table S2.** Calculated spin densities of the unprotonated complex ( $O_2$ ) in the singlet spin state, the singly protonated complex (OOH) in the triplet spin state and the doubly protonated complexes (HOOH) in the triplet spin state with a dielectric constant of 80.37.

Structure	M	Spin Density				
		Fe	O <sub>inner</sub>	O <sub>outer</sub>	heme	5-HPQ
O <sub>2</sub>	1	1.31	-0.54	-0.70	-0.08	0.00
OOH	3	0.88	0.17	0.02	0.20	0.75
HOOH	3	1.06	0.00	0.00	-0.04	1.01

Upon increasing the polarity of the environment, electron transfers from 5-HPQ to  $O_2$  were again observed in the singly and doubly protonated complexes. A more polar environment has the effect of making 5-HPQ donate more electron density in the singly protonated complex. This is perhaps because of stabilization of the 5-HPQ radical cation in the more polar environment. Nevertheless, the conclusion that 5-HPQ is able to donate an electron to facilitate the conversion of  $O_2$  to  $H_2O_2$  does not change with inclusion of the solvent effects.

It should be noted that neither fixing of the N–H bond lengths nor increasing the polarity of the environment had a significant effect on the spin distribution in the doubly protonated complex. In addition to one electron from iron, the second electron required to convert  $O_2$  to  $H_2O_2$  purely comes from 5-HPQ, thus resulting in essentially the same spin distribution in the three cases shown in Table 1, Table S1 and Table S2.

**Optimized xyz coordinates (in Å) of all structures considered in this study.**

O2 complex

Singlet

C1	21.7809475983	51.7651452776	29.1611303267
N2	23.0893791053	51.3276730686	29.2658998887
C3	21.1382297584	50.8175092227	28.4122764879
C4	23.1917954179	50.1547474807	28.5908030761
N5	22.0290227314	49.8226149539	28.0652528783
Fe6	21.6460405298	48.0216824223	26.8976332899
C7	22.6184599127	49.7039760454	24.0944834417
C8	24.8716599931	46.8971507469	27.3247864416
C9	20.7298879386	46.4780195028	29.8022261079
C10	18.4081850072	49.0152099805	26.3928596554
N11	23.4046076724	48.2730840565	25.9179165153
C12	23.6052855690	48.9977919907	24.7690183727
C13	24.9954147077	48.8979937109	24.3365513115
C14	25.6059953310	48.0866882543	25.2486839589
C15	24.6143177009	47.7063280483	26.2240575877
C16	25.5864407627	49.5692381708	23.1264054436
C17	26.9461128803	48.9926564352	22.7185958157
C18	27.5966849031	49.7458072609	21.5740765659
O19	28.5253226232	49.0149508788	20.9541110893
O20	27.3242011956	50.8994032941	21.2674886662
N21	22.6180527269	46.9223011090	28.2947248866
C22	23.9354949506	46.5403979795	28.2909892543
C23	24.2221251462	45.7313618246	29.4513880090
C24	23.0614374676	45.6320354972	30.1563328232
C25	22.0621516411	46.3714369427	29.4221573469
N26	19.9122388128	47.8008569591	27.9028062772
C27	19.7330877943	47.1302596856	29.0846317814
C28	18.3433606568	47.1743369309	29.4737932106
C29	17.6854352713	47.8696852612	28.5052640531
C30	18.6741748063	48.2583799444	27.5290360347
N31	20.7003649591	49.1488726464	25.5293843164
C32	19.3575454686	49.4289333810	25.4668327837
C33	19.0751810200	50.2442692934	24.3108034540
C34	20.2632328750	50.4527379855	23.6792586957
C35	21.2717292696	49.7575778047	24.4443527997
H36	23.8371603031	51.7941076982	29.7578617584
H37	20.1070986211	50.7756736409	28.0977816224
H38	24.1029311917	49.5818333643	28.5049046652
H39	22.9098174564	50.2409169678	23.1974981522
H40	25.8825927474	46.5153601613	27.4345231737
H41	20.4359520329	45.9856053660	30.7249941149
H42	17.3779230884	49.3115559565	26.2194182210

H43	24.8954349233	49.4831141093	22.2773738262
H44	25.6982201115	50.6482706928	23.2989074005
H45	27.6520266604	49.0310443168	23.5601285121
H46	26.8674613019	47.9344560251	22.4476340786
C47	29.7838930817	46.9865624639	25.3188466062
C48	30.3045498839	48.2570110751	25.1348300687
C49	31.0798676935	48.5856901023	23.9999242889
C50	31.3370157140	47.6352959920	23.0156509111
H51	31.4804128942	49.5863461073	23.8973060065
C52	30.0450246889	45.9863674684	24.3557545585
C53	30.8199494961	46.3043682892	23.1960302035
N54	31.0807460973	45.3925608210	22.2220866539
C55	30.6157013429	44.1665757074	22.3632116428
C56	29.8518737407	43.7468366368	23.4786717583
C57	29.5639685357	44.6561707021	24.4695227935
H58	30.8433709354	43.4644625760	21.5616159763
H59	29.4978599974	42.7215509039	23.5379391190
H60	28.9752538571	44.3795153557	25.3383899946
N61	32.0718245973	47.8797322600	21.8732075891
H62	32.0425181054	47.0795628561	21.2485043616
O63	29.9916022376	49.1408175942	26.1460468259
C64	30.5355605796	50.4497045484	26.1024795396
H65	30.1848118751	50.9520300173	27.0065227360
H66	31.6331994484	50.4285299854	26.1016844754
H67	30.1833497538	51.0026858898	25.2220833441
C68	32.1536142427	49.1940733919	21.2357891593
C69	31.9363289685	49.0083567210	19.7195192210
H70	32.7285423544	48.3482378756	19.3363579399
H71	30.9897418853	48.4731488822	19.5803811345
C72	31.9283481190	50.2932665744	18.8729140713
H73	32.9084016748	50.7849890527	18.9183291974
H74	31.7875587408	50.0094224253	17.8195458978
C75	30.8610904975	51.3305845396	19.2492445201
H76	31.0031414150	52.2279109704	18.6265758633
H77	30.9904226657	51.6490271593	20.2899501861
H78	28.8030440773	51.4438534558	19.4894951207
H79	29.2664770289	50.6024364789	18.1541174735
N80	29.4966552383	50.7855749107	19.1305238994
O81	29.0102220101	46.6841450975	26.4179509862
H82	29.0037154645	47.4836457623	26.9721806500
H83	28.9471900426	49.5871302222	20.2275241943
C84	33.4870684152	49.8831097944	21.5689204733
H85	33.5261558981	50.9085340972	21.1816220283
H86	33.6381048263	49.9253141989	22.6528673418
H87	34.3254202625	49.3200487545	21.1411719122
H88	31.3287654937	49.8057317203	21.6280189009

H89	26.6356601792	47.7534423935	25.2785993909
H90	20.4552738556	51.0132501205	22.7729974732
H91	18.0917428068	50.6019792383	24.0329913151
H92	16.6306651378	48.1063539764	28.4437848715
H93	17.9382782739	46.7183496396	30.3689402250
H94	22.8788291296	45.1006432625	31.0824771084
H95	25.1890038203	45.3012052951	29.6802461079
H96	21.4439349649	52.6831189309	29.6172737462
O97	21.3706126363	46.4190031828	25.8911474035
O98	20.2162374231	46.2166277290	25.4045135506

## O2 complex

### Triplet

C1	21.4692935316	51.7663817350	29.0675809043
N2	22.7953763562	51.4149684694	29.2488578909
C3	20.9254055627	50.7647495551	28.3116217351
C4	23.0069096930	50.2377279075	28.6104719389
N5	21.8944318481	49.8220572326	28.0360589051
Fe6	21.6987584580	48.0235438286	26.9142596105
C7	22.6688973360	49.7702852994	24.1530701158
C8	24.9597961720	47.0904156846	27.4634554973
C9	20.7681898497	46.4816203003	29.8143148894
C10	18.4192135837	48.7696058845	26.2541348610
N11	23.4681557862	48.3867993172	26.0063391252
C12	23.6706522609	49.1261298021	24.8664005789
C13	25.0791462350	49.1047685398	24.4865557794
C14	25.6976137627	48.3194534741	25.4167989503
C15	24.6951457276	47.8826749889	26.3529269595
C16	25.6903566125	49.8175653879	23.3105009987
C17	26.9622275399	49.1384872852	22.7866449881
C18	27.6463786311	49.9307938219	21.6878182412
O19	28.4538300824	49.1709086850	20.9451189710
O20	27.4976756990	51.1331019606	21.5124808669
N21	22.6775352451	47.0118711070	28.3604504025
C22	24.0132370807	46.6967500110	28.4029237504
C23	24.3047592870	45.9233608950	29.5846349243
C24	23.1294950193	45.7785134214	30.2575271074
C25	22.1161289319	46.4502715165	29.4802217053
N26	19.9410143383	47.6978760174	27.8511110209
C27	19.7594931665	47.0454092880	29.0418277216
C28	18.3547144243	46.9963610959	29.3725699752
C29	17.6909571172	47.6155130623	28.3579801392
C30	18.6906751661	48.0531831488	27.4139572279
N31	20.7333864183	49.0705355512	25.4977661761
C32	19.3778983806	49.2455085020	25.3689394167
C33	19.0895689017	50.0356411882	24.1971516548



C34	20.2874267321	50.3383373683	23.6250902389
C35	21.3079118764	49.7228764315	24.4404042182
H36	23.4869944446	51.9389204213	29.7646547925
H37	19.9170519468	50.6509177002	27.9465047009
H38	23.9548930305	49.7221982608	28.5835254244
H39	22.9592964846	50.3304363022	23.2705705784
H40	25.9847264847	46.7607970534	27.6060771732
H41	20.4734158563	45.9912705702	30.7377549251
H42	17.3785637492	48.9851902939	26.0295841413
H43	24.9637200044	49.8867154162	22.4917372242
H44	25.9311395962	50.8569294928	23.5721801226
H45	27.7002471955	49.0154741250	23.5913451768
H46	26.7535805341	48.1280456084	22.4198259611
C47	29.8331199792	47.0722030066	25.4113476566
C48	30.4322364753	48.2964680150	25.1640923522
C49	31.1217282307	48.5575216478	23.9580708551
C50	31.2134866321	47.5830917953	22.9673510644
H51	31.5860375222	49.5236808412	23.8072456366
C52	29.9232101274	46.0495293267	24.4401711372
C53	30.6082055474	46.2992943364	23.2095552933
N54	30.6995546377	45.3669442850	22.2246742058
C55	30.1528505844	44.1830695117	22.4225727960
C56	29.4704687304	43.8292316881	23.6111193809
C57	29.3522801834	44.7621994586	24.6147355074
H58	30.2436987254	43.4631218594	21.6097289019
H59	29.0434316037	42.8359181135	23.7156350818
H60	28.8295069084	44.5366532112	25.5387708200
N61	31.8567354835	47.7595125113	21.7614787810
H62	31.6938829463	46.9740976749	21.1394354810
O63	30.2899239215	49.2057762173	26.1910039650
C64	30.8742021640	50.4903218463	26.0520641647
H65	30.6439321673	51.0275669634	26.9745330149
H66	31.9636667093	50.4254830257	25.9332767823
H67	30.4485946166	51.0352026472	25.1994650450
C68	32.0625208307	49.0648609906	21.1396535578
C69	31.7825565736	48.9322525722	19.6292048039
H70	32.4928662182	48.2060503987	19.2073080112
H71	30.7834204874	48.4972990162	19.5107106255
C72	31.8771485986	50.2333075059	18.8128022736
H73	32.9058175972	50.6156878951	18.8243432492
H74	31.6590815008	49.9975523052	17.7609306044
C75	30.9481176954	51.3685482792	19.2659162193
H76	31.1566519287	52.2629460610	18.6579495531
H77	31.1624796887	51.6415522386	20.3052209130
H78	28.9319449233	51.6881693711	19.6339732580
H79	29.2253941096	50.8736661741	18.2367373831

N80	29.5273652070	50.9781545394	19.2050747663
O81	29.1456226342	46.8377286705	26.5819193129
H82	29.2570795104	47.6368728725	27.1252764185
H83	28.9017783668	49.7645092171	20.2531796969
C84	33.4731048660	49.5992462173	21.4395213515
H85	33.6104112312	50.6228016088	21.0702647647
H86	33.6637261734	49.6012240419	22.5178818961
H87	34.2305321813	48.9584048348	20.9723076398
H88	31.3212842891	49.7572287178	21.5648275624
H89	26.7414139439	48.0391371689	25.4822953240
H90	20.4798706094	50.9132239336	22.7279893807
H91	18.0957341157	50.3154573111	23.8701521746
H92	16.6255088945	47.7720922191	28.2454778447
H93	17.9461393513	46.5338595195	30.2626979828
H94	22.9458057835	45.2540956325	31.1874400691
H95	25.2850067480	45.5467618044	29.8496338308
H96	21.0526057225	52.6709154891	29.4826634962
O97	21.6169663723	46.4018295276	25.9225083524
O98	20.4560892957	46.1218618085	25.4257555703

#### O2 complex

##### Quintet

C1	21.5858319182	51.9634872133	29.4930177316
N2	22.9265264020	51.6291020406	29.5555156973
C3	21.0104796750	51.0084052801	28.6977665928
C4	23.1057844284	50.5053097352	28.8097311764
N5	21.9678470514	50.1077508743	28.2800259286
Fe6	21.7489595548	48.1789713239	26.9593783656
C7	22.6553721457	49.7696739907	24.0753708817
C8	24.9599310997	47.0286796643	27.3300980029
C9	20.8137131883	46.4647894308	29.7709790897
C10	18.4672116286	49.0177790665	26.3917495596
N11	23.4686956804	48.3938019770	25.9337243733
C12	23.6543481757	49.0952941064	24.7633150955
C13	25.0394339537	48.9911999598	24.3169370024
C14	25.6662759606	48.2058149481	25.2400448451
C15	24.6891069415	47.8393884136	26.2348397872
C16	25.6099890747	49.6196642888	23.0750672951
C17	26.9801869684	49.0532939178	22.6916518624
C18	27.5958974352	49.7325537921	21.4842345405
O19	28.5556970367	48.9911664720	20.9263409105
O20	27.2741210262	50.8424890549	21.0799852351
N21	22.7040880657	46.9982573525	28.2936276414
C22	24.0304165181	46.6392093913	28.2899332977
C23	24.3248058096	45.8007961653	29.4260284519
C24	23.1598093148	45.6559425273	30.1180009160

C25	22.1519988186	46.3996733914	29.4022063999
N26	19.9871827139	47.8136091482	27.8961277874
C27	19.8074059736	47.1116807664	29.0602874293
C28	18.4125730851	47.1144446210	29.4358491783
C29	17.7497358033	47.8217005366	28.4796984698
C30	18.7412613435	48.2539900309	27.5227214587
N31	20.7553672018	49.1961713357	25.5210742235
C32	19.4058326077	49.4540329005	25.4634954693
C33	19.1007141117	50.2521521538	24.3008335579
C34	20.2814919038	50.4726636653	23.6579217078
C35	21.3065493969	49.8054872330	24.4256917522
H36	23.6420227182	52.1248444759	30.0664619595
H37	19.9788426380	50.9005831345	28.3974995441
H38	24.0603528377	50.0148118640	28.6829255457
H39	22.9371510136	50.2903871169	23.1650820447
H40	25.9739977123	46.6518479134	27.4285462950
H41	20.5230464659	45.9393901898	30.6767008784
H42	17.4312830706	49.2956584788	26.2193690443
H43	24.9185383563	49.4757653650	22.2345553060
H44	25.6956513663	50.7081657191	23.1941299178
H45	27.6946035843	49.1717658804	23.5182998036
H46	26.9287503621	47.9758483475	22.5012662226
C47	29.7015541518	46.7798206015	25.2420688972
C48	30.1420872970	48.0843924764	25.0935098939
C49	30.9386358082	48.4821523602	23.9966993976
C50	31.2979367636	47.5661981512	23.0123670811
H51	31.2743564567	49.5090799899	23.9228379770
C52	30.0655485203	45.8140339690	24.2772306688
C53	30.8638399899	46.2011068340	23.1545648593
N54	31.2264931692	45.3228175020	22.1822039413
C55	30.8390016874	44.0667753039	22.2880673707
C56	30.0587379996	43.5802175348	23.3642921758
C57	29.6700359911	44.4533072332	24.3535113449
H58	31.1477918022	43.3933162600	21.4889350925
H59	29.7720308856	42.5328562409	23.3953268453
H60	29.0656232719	44.1254040531	25.1933091009
N61	32.0664308432	47.8740574642	21.9081817672
H62	32.1212592503	47.0787580226	21.2787818689
O63	29.7231261876	48.9314475184	26.0981125865
C64	30.2359021649	50.2533426866	26.1360242833
H65	29.8188294758	50.7124000928	27.0347682343
H66	31.3318661041	50.2565147677	26.1997587978
H67	29.9223354131	50.8320512557	25.2577434637
C68	32.0870681133	49.1955783877	21.2788884179
C69	31.9635423335	48.9993623136	19.7534973320
H70	32.8057324906	48.3746481939	19.4204889685

H71	31.0520460827	48.4206810531	19.5629885049
C72	31.9501094588	50.2781648927	18.8981003383
H73	32.9028861324	50.8131007773	18.9998410139
H74	31.8881351083	49.9817614686	17.8405187410
C75	30.8176625791	51.2712807600	19.1947136127
H76	30.9566489892	52.1653714330	18.5667406167
H77	30.8708213428	51.6090940537	20.2362277509
H78	28.7450906656	51.3047730099	19.2944588172
H79	29.3309746619	50.4337811585	18.0252280902
N80	29.4874398236	50.6652098787	19.0058351208
O81	28.9122664966	46.4129866828	26.3089989742
H82	28.8524185324	47.1966424747	26.8824756525
H83	28.9587765130	49.5188184591	20.1553581019
C84	33.3512892933	49.9724588044	21.6815674688
H85	33.3390386869	51.0006469156	21.2999545023
H86	33.4430531930	50.0182066573	22.7719733372
H87	34.2475958591	49.4712539156	21.2964157299
H88	31.2030183194	49.7467784160	21.6287610158
H89	26.6962855051	47.8736729647	25.2588915532
H90	20.4565260741	51.0273768786	22.7441121799
H91	18.1091958468	50.5888252664	24.0237929916
H92	16.6903041496	48.0351519429	28.4121485886
H93	18.0080043405	46.6267373237	30.3145047982
H94	22.9822446668	45.0897659724	31.0244457417
H95	25.2970879038	45.3780140457	29.6478693674
H96	21.1851256897	52.8238770760	30.0068384367
O97	21.2165682397	46.2292606135	25.5710418988
O98	20.2049243870	45.5550030687	25.4459903190

## O2 complex

### Septet

C1	21.9824422219	51.6550857161	30.0105010890
N2	23.1330775997	51.8363184296	29.2638965428
C3	21.3579318455	50.5687861131	29.4604754819
C4	23.1647628004	50.8730242887	28.3079506757
N5	22.1053426431	50.0928022304	28.4021081175
Fe6	21.6536140613	48.3669644961	27.0673580508
C7	22.6436732876	49.8060353900	24.0787917165
C8	24.7259711678	46.7970966752	27.2545434609
C9	20.5026619324	46.3959334601	29.6585733560
C10	18.4105450459	49.3921299688	26.4714169617
N11	23.4126698199	48.3700934921	25.9039492409
C12	23.6209521220	49.0506360873	24.7328650361
C13	24.9905735321	48.8201744092	24.2615345026
C14	25.5569090159	47.9709894098	25.1704530089
C15	24.5603122962	47.6802626725	26.1830351850

C16	25.5979416967	49.4039249135	23.0152458941
C17	26.9914675696	48.8509640605	22.7040201198
C18	27.6523972399	49.5176627352	21.5124146534
O19	28.6333397195	48.7733852439	20.9978659057
O20	27.3429661559	50.6227851421	21.0843924808
N21	22.4644834078	46.8501315985	28.2329203840
C22	23.7597337221	46.4058346376	28.1944868692
C23	23.9699302683	45.4570349264	29.2653424284
C24	22.7863026523	45.3457479501	29.9388155049
C25	21.8424704872	46.2242915187	29.2846201375
N26	19.7785977257	48.0054762842	27.9578913788
C27	19.5387606438	47.1988615825	29.0352982808
C28	18.1333689051	47.2766469851	29.3909158208
C29	17.5448440013	48.1186778385	28.4935668775
C30	18.5868945964	48.5612677005	27.5851086199
N31	20.6938090771	49.3899840106	25.5349333469
C32	19.3730447063	49.7656725551	25.5234818274
C33	19.1279707542	50.6019534203	24.3701292474
C34	20.3139899010	50.7194124524	23.7019067728
C35	21.2943679058	49.9550004657	24.4407968400
H36	23.8258140240	52.5574965778	29.4018395895
H37	20.4308775662	50.0930631047	29.7418878914
H38	23.9524617830	50.7698233871	27.5759913865
H39	22.9452046299	50.3092886905	23.1636844145
H40	25.7030491462	46.3279857265	27.3451842380
H41	20.1659471048	45.8115549733	30.5116110026
H42	17.4039421507	49.7679270951	26.3037508399
H43	24.9354314514	49.2198845359	22.1582143978
H44	25.6632773579	50.4972741154	23.0935041353
H45	27.6615461705	49.0005828677	23.5618340536
H46	26.9670719296	47.7695275963	22.5326001519
C47	29.7755386167	46.9175179471	25.1251789789
C48	30.1382022141	48.2438991800	24.9607081667
C49	31.0250270586	48.6520802032	23.9407909705
C50	31.5500579100	47.7265128526	23.0445702663
H51	31.2977424673	49.6966340936	23.8533637740
C52	30.3139662625	45.9419645744	24.2569029911
C53	31.2010734475	46.3402157696	23.2070085734
N54	31.7245436248	45.4511660459	22.3210187862
C55	31.4131171902	44.1758793645	22.4463299400
C56	30.5569578397	43.6782119237	23.4579720602
C57	30.0060912473	44.5604827973	24.3578037215
H58	31.8499079855	43.4943866407	21.7167465790
H59	30.3401606095	42.6149753555	23.5093933860
H60	29.3380124637	44.2246307555	25.1445511508
N61	32.4028894455	48.0529849851	22.0060080137

H62	32.5969317280	47.2316447118	21.4399327826
O63	29.5414142303	49.1019516927	25.8612184091
C64	29.9582697090	50.4576749661	25.8906502066
H65	29.4044868923	50.9251893584	26.7074742708
H66	31.0354263928	50.5414269668	26.0853424309
H67	29.7183992684	50.9729879502	24.9517995540
C68	32.3178541574	49.3181969667	21.2698612204
C69	32.1603450337	48.9978915872	19.7674035337
H70	33.0379532531	48.4173294044	19.4457873622
H71	31.2923009279	48.3374271032	19.6565817412
C72	32.0122916853	50.2036605092	18.8226152216
H73	32.9225819457	50.8164053739	18.8425827389
H74	31.9325220045	49.8247304047	17.7929143358
C75	30.8173524876	51.1271491138	19.0981174195
H76	30.8623606950	51.9802892734	18.4027857006
H77	30.8841801975	51.5446058050	20.1094425983
H78	28.7564138734	51.0174486689	19.2901285080
H79	29.3532388370	50.1096621042	18.0533115261
N80	29.5311785317	50.4123915418	19.0107623730
O81	28.8925125901	46.5361914144	26.1097751668
H82	28.6956594401	47.3378863228	26.6250144609
H83	29.0545138403	49.2871527270	20.2300753234
C84	33.5333574656	50.2083415178	21.5726756345
H85	33.4460614849	51.1956263680	21.1026776025
H86	33.6395012141	50.3547794681	22.6529165676
H87	34.4548487801	49.7356393157	21.2112078635
H88	31.4078338364	49.8327075285	21.6055380740
H89	26.5524686500	47.5449769012	25.1577628777
H90	20.5111931705	51.2660691577	22.7874428176
H91	18.1702576819	51.0350741617	24.1072108062
H92	16.5014721908	48.4033230120	28.4324813604
H93	17.6645812370	46.7386896294	30.2063142270
H94	22.5647027295	44.7213995779	30.7961675695
H95	24.9010856911	44.9408822623	29.4663013475
H96	21.7279348735	52.2996341751	30.8376494420
O97	20.3927360103	45.8178552916	25.7137516410
O98	19.3287004634	45.3370167064	26.0462459951

#### OOH complex

##### Singlet

C1	21.1053762736	52.0974926859	28.5627759377
N2	22.4189836451	51.8064131576	28.8749032549
C3	20.6366748230	51.0017097065	27.8918332260
C4	22.7004489090	50.5703552047	28.3956054706
N5	21.6410739392	50.0588186304	27.7950658691
Fe6	21.5314724916	48.1554502831	26.9053439123

C7	22.4723093928	49.7012525432	23.9829256546
C8	24.8018440275	47.4630771420	27.5753321203
C9	20.6326977270	46.9535454757	29.9741320499
C10	18.2578714132	48.6542256394	26.1167117910
N11	23.2959180769	48.5387800447	25.9693859719
C12	23.4921272934	49.1726054417	24.7807248051
C13	24.9085005166	49.1860059783	24.4212762166
C14	25.5419886753	48.5169477709	25.4268205426
C15	24.5382916762	48.1222957124	26.3882527521
C16	25.4900357961	49.8239976280	23.1900095572
C17	26.9537559685	49.4454098240	22.9483844453
C18	27.5940671770	50.2292256715	21.8153733788
O19	28.6405025122	49.5873313561	21.2871557705
O20	27.2225036296	51.3345991148	21.4544482805
N21	22.5222680875	47.3911492579	28.4785063532
C22	23.8558484492	47.1360709170	28.5560891731
C23	24.1812547939	46.5151874876	29.8228672125
C24	23.0153269025	46.4028050272	30.5128053175
C25	21.9775922744	46.9396058708	29.6612683434
N26	19.7940782944	47.8822110141	27.8670632508
C27	19.6108093529	47.3709002002	29.1139519734
C28	18.2007057260	47.2816597364	29.4252296301
C29	17.5321490638	47.7310202257	28.3307645894
C30	18.5347539327	48.1084638557	27.3577273726
N31	20.5605430559	49.0175942372	25.3582148628
C32	19.2117535266	49.0937344966	25.1905174773
C33	18.8911984601	49.7446806964	23.9375844907
C34	20.0754531088	50.0691189987	23.3554076403
C35	21.1174403195	49.6025202714	24.2446284477
H36	23.0585993370	52.4036225118	29.3787942347
H37	19.6575430731	50.8245423708	27.4774231559
H38	23.6586431827	50.0854302788	28.4991620745
H39	22.7603457324	50.1924302150	23.0593139401
H40	25.8338977407	47.1927208146	27.7780558702
H41	20.3382126063	46.5670465949	30.9449311225
H42	17.2132032680	48.7799490552	25.8491175794
H43	24.8981277725	49.5444269057	22.3081886985
H44	25.4192441197	50.9181112112	23.2520110043
H45	27.5499867944	49.6554580044	23.8480133923
H46	27.0662994843	48.3741402620	22.7529868716
C47	29.8470141457	46.1238070162	25.0968710080
C48	30.0462448429	47.5161627370	25.0448561444
C49	30.6824119686	48.1278767906	23.9626381974
C50	31.1314800674	47.3533321036	22.8782881550
H51	30.8180760357	49.2008084783	23.9504175459
C52	30.2971635110	45.3061763404	24.0285239363

C53	30.9438790781	45.9113822179	22.9163782687
N54	31.4012892612	45.2033151268	21.8616609911
C55	31.2401861199	43.8890266469	21.8684300335
C56	30.6135801319	43.1899640182	22.9233989905
C57	30.1399920899	43.8984615550	24.0068649984
H58	31.6212404823	43.3500952762	21.0032963186
H59	30.5105306114	42.1107584664	22.8709854925
H60	29.6500937802	43.4028735228	24.8383896667
N61	31.7258424525	47.8517468046	21.7767004115
H62	31.9889761797	47.1347703110	21.1034534399
O63	29.5526420776	48.1689449564	26.1380930747
C64	29.8777035255	49.5467610372	26.3290941970
H65	29.4590230658	49.8190811660	27.2983902289
H66	30.9638703865	49.6922514355	26.3405808503
H67	29.4266497534	50.1693176265	25.5481166393
C68	31.9839571546	49.2546531229	21.4486814909
C69	31.9257047417	49.3845368847	19.9130852139
H70	32.7221802227	48.7601323312	19.4825998430
H71	30.9744753839	48.9572398963	19.5755274881
C72	32.0775119322	50.8094840493	19.3518605635
H73	33.0675013266	51.2138382583	19.5959250702
H74	32.0487445655	50.7405976800	18.2554872472
C75	31.0238705920	51.8282233733	19.8096151945
H76	31.2392861650	52.7945649649	19.3306805275
H77	31.0933998054	51.9941989428	20.8917206658
H78	28.9610868714	52.0564819507	19.8301291414
H79	29.5144616633	51.2245269288	18.5296339465
N80	29.6505223175	51.3646000344	19.5309824992
H81	29.0414551292	50.1788817806	20.5525807754
C82	33.3183001433	49.7201541655	22.0543958371
H83	33.4751361290	50.7909435030	21.8869121536
H84	33.3408091082	49.5405720535	23.1344560733
H85	34.1579059137	49.1768251408	21.6057882220
H86	31.1602731287	49.8353953795	21.8773894718
H87	26.5974979687	48.2983973204	25.5301771041
H88	20.2484592919	50.5675442662	22.4104544313
H89	17.8878615206	49.9256575018	23.5733997147
H90	16.4636670257	47.8127868452	28.1791362870
H91	17.7961061736	46.9124828297	30.3590497172
H92	22.8516953532	45.9850119285	31.4981059397
H93	25.1751862004	46.2107519389	30.1262401827
H94	20.6400069999	53.0303636156	28.8402575108
O95	21.4240086556	46.5964756759	26.0573471688
O96	21.1052543008	45.4868762758	26.9161017264
H97	20.7872934528	44.8573411813	26.2440673929
O98	29.2382354981	45.5504844341	26.1571808615



H99	29.0434323095	46.2554721876	26.8018395669
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OOH complex

Triplet

C1	21.0463455698	51.6854276056	28.7411049171
N2	22.3468079453	51.3661065953	29.0794029483
C3	20.6143071329	50.6636517643	27.9413089436
C4	22.6568764273	50.1863541208	28.4893392157
N5	21.6277587743	49.7370944518	27.7935590473
Fe6	21.5679924382	47.9303795347	26.7184092416
C7	22.5686412396	49.7684520646	23.9908871864
C8	24.8253201042	47.1947777475	27.3991340222
C9	20.6037052165	46.4347210357	29.6340057807
C10	18.3129540168	48.4674194305	25.8897428716
N11	23.3526231101	48.4209716301	25.8709400294
C12	23.5747979716	49.1785777568	24.7544675869
C13	24.9975843884	49.2367027079	24.4391304211
C14	25.6083358864	48.4707139314	25.3901974877
C15	24.5838109495	47.9756237091	26.2755627427
C16	25.6162954351	49.9892863102	23.2927957885
C17	27.0709700729	49.5857932835	23.0263160747
C18	27.7271782204	50.4162293634	21.9359732479
O19	28.6816092995	49.7359754987	21.2945610647
O20	27.4377043332	51.5758524765	21.6908459671
N21	22.5272513972	47.0247092839	28.2375160400
C22	23.8654139392	46.7668833894	28.3204746942
C23	24.1627354276	46.0276874972	29.5253196724
C24	22.9792185204	45.8465818638	30.1734949898
C25	21.9620726099	46.4593073312	29.3544963464
N26	19.8073370136	47.5489411851	27.6040777331
C27	19.5975375779	46.9192517181	28.7973303389
C28	18.1838195260	46.7888840122	29.0580249332
C29	17.5394677358	47.3329246980	27.9893969964
C30	18.5624163815	47.8076742872	27.0875448261
N31	20.6281656551	48.9317077276	25.2355015001
C32	19.2777728718	49.0055403039	25.0367076318
C33	18.9840031466	49.7687112084	23.8461154743
C34	20.1813076348	50.1651603783	23.3343329134
C35	21.2017355909	49.6292115834	24.2042732694
H36	22.9605117771	51.9098505179	29.6688869861
H37	19.6553097460	50.5283305537	27.4682248076
H38	23.6126980121	49.6952757298	28.5851286642
H39	22.8708169416	50.3524176993	23.1268956413
H40	25.8564864203	46.9126500244	27.5924904401
H41	20.2933192031	45.9545844344	30.5576177537
H42	17.2731448677	48.6037314530	25.6075947357

H43	25.0298601569	49.8245671403	22.3790547804
H44	25.5792801332	51.0718220318	23.4731276333
H45	27.6740243068	49.7246254465	23.9349565146
H46	27.1475417827	48.5256368844	22.7649082605
C47	29.9549723398	47.1275584126	25.6873430128
C48	30.6410903277	48.3212034412	25.3960139858
C49	31.1559844367	48.5801360560	24.1218556996
C50	30.9962263919	47.6374150938	23.0907831837
H51	31.6773083391	49.5080663817	23.9293963729
C52	29.7886530256	46.1445531176	24.6796595058
C53	30.3122134402	46.3870644185	23.3793084690
N54	30.1971505340	45.5006795989	22.3670091967
C55	29.5717388628	44.3569658704	22.5986903721
C56	29.0166538188	44.0176960432	23.8524116267
C57	29.1243887800	44.9115102331	24.8957150575
H58	29.4981891785	43.6664311338	21.7608917381
H59	28.5145605899	43.0639856249	23.9814079258
H60	28.7145874308	44.6896736829	25.8754752755
N61	31.4297798136	47.8078135907	21.8267902541
H62	31.2181486997	47.0208988304	21.2174217424
O63	30.7392600739	49.1562882044	26.4677987787
C64	31.5496367606	50.3274140830	26.3668167796
H65	31.5380945356	50.7825636838	27.3576885269
H66	32.5783882497	50.0666243665	26.0927312893
H67	31.1346200536	51.0298255191	25.6348875944
C68	32.0069091957	49.0195009075	21.2464735550
C69	31.6481833986	49.0371673239	19.7471904655
H70	32.1801426522	48.2119904566	19.2523127034
H71	30.5783159135	48.8211368050	19.6538228589
C72	31.9719808274	50.3458518477	19.0052370698
H73	33.0514171514	50.5409791686	19.0230204760
H74	31.7142054042	50.2060753277	17.9462765899
C75	31.2538572785	51.5995435131	19.5270708284
H76	31.5876030837	52.4666972975	18.9385369620
H77	31.5378820775	51.8017804786	20.5666814833
H78	29.3168097694	52.2638419958	19.8769538367
H79	29.4561874214	51.3291166612	18.5415548463
N80	29.7862862704	51.4394822899	19.5005637210
H81	29.0925301407	50.3401356708	20.5793979800
C82	33.5209141582	49.0880671433	21.5066021777
H83	33.9417893665	50.0308543828	21.1414296086
H84	33.7422436251	49.0114778308	22.5762949326
H85	34.0348213743	48.2639099562	20.9988782800
H86	31.5098750118	49.8668745229	21.7339721752
H87	26.6616630736	48.2465703747	25.4991901912
H88	20.3724554276	50.7563687666	22.4481891710

H89	17.9894805767	49.9724810196	23.4699430490
H90	16.4744418098	47.4179600909	27.8164366687
H91	17.7563135310	46.3309786918	29.9409864610
H92	22.7942886127	45.3348220149	31.1090782263
H93	25.1501994531	45.6979685521	29.8229922524
H94	20.5632776160	52.5839610802	29.0919799644
O95	21.5031495077	46.4606153423	25.7205343355
O96	21.1817327369	45.2685710901	26.4600783458
H97	20.7893007105	44.7401220824	25.7418375631
O98	29.4450083708	46.9062533219	26.9226332949
H99	29.7125504430	47.6561115901	27.4862590188

OOH complex

Quintet

C1	21.2326093032	51.8718711371	28.4528800507
N2	21.9348757441	51.2082264520	29.4393285372
C3	21.0404784030	50.9526488534	27.4588236527
C4	22.1410834919	49.9351989585	29.0247071534
N5	21.6112979326	49.7486194669	27.8277463020
Fe6	21.6243696006	47.8776572008	26.7171706265
C7	22.5242687394	49.6277710698	23.9012417068
C8	24.9551782223	47.3818490761	27.4468763801
C9	20.7372367384	46.2414187651	29.5872044363
C10	18.2990451886	48.4339532504	26.0014317287
N11	23.4406310623	48.4657796215	25.8512180285
C12	23.5871143549	49.1500881446	24.6783260678
C13	25.0090692214	49.2754356749	24.3523909606
C14	25.6720110924	48.6278655352	25.3583204378
C15	24.6833787470	48.1223136898	26.2868346913
C16	25.5822508257	49.9795392293	23.1537546113
C17	27.0815821442	49.7310238321	22.9774554415
C18	27.7004000207	50.5414162498	21.8523761683
O19	28.8678290552	50.0211184511	21.4554314243
O20	27.2177678586	51.5573447112	21.3850820146
N21	22.6768773583	47.0009476156	28.2735872756
C22	24.0300890214	46.8529477647	28.3628332361
C23	24.3488466171	46.0769520704	29.5438270465
C24	23.1633171122	45.7619887563	30.1439482600
C25	22.1132862157	46.3402310105	29.3316419351
N26	19.8097623614	47.4103781366	27.6365800243
C27	19.6713313858	46.7379865986	28.8186770578
C28	18.2642027499	46.6238863900	29.1387299077
C29	17.5770352451	47.2406900669	28.1312382045
C30	18.5615423691	47.7329584323	27.1908564292
N31	20.5864938454	48.8630776146	25.2101814290
C32	19.2263992786	48.9477909780	25.0838063061

C33	18.9051247535	49.6724229979	23.8709115079
C34	20.0909196921	50.0073511323	23.2840572591
C35	21.1437658947	49.4909920427	24.1359662156
H36	22.2377829143	51.5970174802	30.3210391700
H37	20.5352692457	51.0690411209	26.5142518613
H38	22.6649636297	49.1903647770	29.6021637618
H39	22.7925272535	50.1592373398	22.9920592167
H40	26.0042843791	47.1805746170	27.6511559130
H41	20.4604692825	45.7030522510	30.4903545446
H42	17.2514899785	48.6036766773	25.7672467099
H43	25.0573698583	49.6599641587	22.2434539677
H44	25.4074622540	51.0613210201	23.2222672828
H45	27.6214258015	50.0072043461	23.8940595482
H46	27.2933551243	48.6691787061	22.8104401813
C47	29.8534346355	47.1684335986	25.7381398036
C48	30.6250934855	48.3122284615	25.4582386250
C49	31.1496548549	48.5494375040	24.1850119593
C50	30.9181365625	47.6339143824	23.1429487906
H51	31.7345036490	49.4401680731	23.9985384727
C52	29.6155761874	46.2105980344	24.7208631778
C53	30.1465531103	46.4325009041	23.4197647559
N54	29.9556550252	45.5737047997	22.3953896336
C55	29.2486850339	44.4760950767	22.6166783302
C56	28.6823538517	44.1590197626	23.8710586388
C57	28.8643447936	45.0268353324	24.9260497942
H58	29.1146675137	43.8071427339	21.7689247073
H59	28.1115939203	43.2435637887	23.9909300407
H60	28.4455046130	44.8222739419	25.9055750164
N61	31.3634717949	47.7859678946	21.8801452635
H62	31.0844582938	47.0246803156	21.2645642005
O63	30.7853430568	49.1238363755	26.5395258436
C64	31.6254695465	50.2733239529	26.4303231256
H65	31.6335525137	50.7300070328	27.4204690763
H66	32.6447826832	49.9853260089	26.1484362201
H67	31.2226097784	50.9846234520	25.7001033220
C68	31.9887563224	48.9713523212	21.2895540406
C69	31.5888604381	49.0067427280	19.8000193372
H70	32.0177900200	48.1221580166	19.3071270725
H71	30.4996684461	48.9036005614	19.7437380098
C72	32.0274473834	50.2549904347	19.0130620385
H73	33.1217193175	50.3274146714	18.9883290363
H74	31.7178284058	50.1158811063	17.9677529530
C75	31.4722502127	51.5975665744	19.5086867654
H76	31.8658817904	52.3971134529	18.8638842599
H77	31.8288711760	51.8102636664	20.5238843209
H78	29.6354190646	52.5042125895	19.8373409091

H79	29.6118958296	51.4187140678	18.6229177833
N80	29.9958196196	51.5934862741	19.5522722455
H81	29.2565346102	50.6074851500	20.7162552402
C82	33.5107057278	48.9538666194	21.5042385144
H83	33.9702891775	49.8780280315	21.1382670768
H84	33.7579256341	48.8520785677	22.5661051014
H85	33.9656268837	48.1104682392	20.9723515867
H86	31.5531371734	49.8416872439	21.7946918106
H87	26.7392384443	48.4868509269	25.4684764819
H88	20.2461849081	50.5530603473	22.3621049260
H89	17.9038672140	49.8900772866	23.5205867313
H90	16.5049589979	47.3532735578	28.0304810612
H91	17.8602468808	46.1383648006	30.0183763959
H92	23.0068080012	45.1840012106	31.0463551718
H93	25.3475387024	45.8060687590	29.8631104485
H94	20.9419047440	52.9065244710	28.5482672599
O95	21.6036326596	46.3598822537	25.6860072694
O96	21.3895704249	45.1667650325	26.4000085022
H97	20.4146169168	45.1003712259	26.3917698748
O98	29.3327240634	46.9724484914	26.9725461055
H99	29.6443233741	47.7026946700	27.5395915441

OOH complex

Septet

C1	20.4480586219	52.2225464225	28.4987166959
N2	21.6625801163	51.8974678302	29.0713542306
C3	20.1055834755	51.1402981646	27.7344693791
C4	22.0042813622	50.6553824775	28.6434169415
N5	21.0832589479	50.1695694602	27.8327860730
Fe6	21.1325154364	48.0454476858	26.8072513819
C7	22.2886527899	49.6746729996	23.9880998650
C8	24.3715371888	47.6373684059	27.8729269183
C9	19.9903492139	46.8089815478	29.8120437970
C10	17.9029497967	48.6433218215	25.8273560487
N11	23.0121490040	48.5783114790	26.0528226901
C12	23.2733620169	49.2179697822	24.8733275132
C13	24.7179705285	49.3329355136	24.6828119831
C14	25.2820519096	48.7332017086	25.7771332025
C15	24.2103201587	48.2727407052	26.6307450957
C16	25.3969392158	50.0011444633	23.5196498337
C17	26.8952155840	49.6891179182	23.4167940899
C18	27.5801790636	50.5015906552	22.3307544674
O19	28.5952017967	49.8468428685	21.7604209823
O20	27.2539566888	51.6399955503	22.0319759937
N21	22.0299352388	47.3683577114	28.5627282929
C22	23.3734071762	47.2220822281	28.7691901545

C23	23.5934501275	46.5985217385	30.0566633218
C24	22.3618604368	46.3770306976	30.6045023562
C25	21.3842332632	46.8598647652	29.6535360646
N26	19.2599839940	47.7855540168	27.6846979191
C27	19.0066671773	47.2305447407	28.9053821196
C28	17.5746077672	47.1438987105	29.1036564917
C29	16.9880913576	47.6509816180	27.9802163410
C30	18.0595435005	48.0523701428	27.0923794035
N31	20.2510454380	48.9921862209	25.1783174925
C32	18.9036462694	49.0868878063	24.9490815608
C33	18.6826843108	49.7502569433	23.6824440132
C34	19.9137080655	50.0513947851	23.1730939823
C35	20.8931053450	49.5699367197	24.1232557787
H36	22.1988375330	52.4766737454	29.7013961114
H37	19.2276169099	50.9920854467	27.1251528777
H38	22.9104730397	50.1490712169	28.9408723972
H39	22.6382689112	50.1669098242	23.0848202814
H40	25.3969763356	47.4570317274	28.1860955444
H41	19.6305606434	46.3795245078	30.7435166620
H42	16.8785989378	48.7935613190	25.4958940400
H43	24.9073969583	49.7024399528	22.5831983692
H44	25.2749377142	51.0907346044	23.5791173511
H45	27.3944910858	49.9443520075	24.3621497376
H46	27.0739744094	48.6235108073	23.2433906876
C47	31.6146751695	46.1173521902	25.2954939759
C48	32.0055721570	47.4570689628	25.1133305445
C49	32.0582434804	48.0409887523	23.8436889580
C50	31.7235117318	47.2866448320	22.7060464797
H51	32.3565002816	49.0752873458	23.7367554036
C52	31.2663000879	45.3254150109	24.1724345763
C53	31.3220213227	45.8994131399	22.8724970133
N54	31.0126073933	45.2085549747	21.7536219708
C55	30.6407295583	43.9439588041	21.8770626806
C56	30.5516731053	43.2799857065	23.1205820181
C57	30.8652780655	43.9701332010	24.2714264392
H58	30.3987613096	43.4179360529	20.9556758614
H59	30.2405700330	42.2407086435	23.1575880725
H60	30.8125662029	43.4990613190	25.2473695640
N61	31.7422917115	47.7581780168	21.4424637538
H62	31.4684238715	47.0643249795	20.7504728909
O63	32.3154134328	48.0847394102	26.2812721680
C64	32.8403093976	49.4110620676	26.2428947492
H65	33.0548812439	49.6754701214	27.2788438812
H66	33.7641401384	49.4481074351	25.6539716970
H67	32.1059050029	50.1119563083	25.8292756856
C68	32.0835298464	49.1083957766	20.9953963256

C69	31.4526038006	49.3004293526	19.6022684164
H70	31.8976489994	48.5597974923	18.9221513989
H71	30.3859293718	49.0594255035	19.6766385072
C72	31.6254809134	50.6942136430	18.9751357943
H73	32.6888445574	50.9200151692	18.8300294642
H74	31.1899295869	50.6640250435	17.9665443865
C75	30.9889944341	51.8564158995	19.7497477355
H76	31.1919761793	52.7927890716	19.2092976013
H77	31.4505183347	51.9600613797	20.7393908262
H78	29.1116563961	52.4114665988	20.4605380241
H79	29.0618670581	51.5712713132	19.0642547887
N80	29.5463078467	51.6351412525	19.9602170079
H81	28.9955600823	50.4577508870	21.0461442228
C82	33.6072060043	49.3219124321	20.9995012781
H83	33.8601898627	50.3628496189	20.7731051427
H84	34.0388767635	49.0757416289	21.9748509138
H85	34.0858516416	48.6806252847	20.2506699921
H86	31.6110474291	49.8088415576	21.6969778135
H87	26.3348390400	48.6098838423	25.9962891304
H88	20.1426083597	50.5532450166	22.2416929237
H89	17.7131878567	49.9609323761	23.2486855471
H90	15.9312551521	47.7485963637	27.7673835582
H91	17.0891434361	46.7460952335	29.9860584622
H92	22.1311317750	45.9238550943	31.5602114343
H93	24.5617079600	46.3611948542	30.4797126942
H94	19.9578358899	53.1655327778	28.6852354881
O95	21.1173343120	46.3181530767	25.9525600217
O96	20.7649119132	45.2120681611	26.7443552040
H97	20.7522016156	44.5027772905	26.0755927217
O98	31.5712897142	45.5694099742	26.5294446175
H99	31.8683728101	46.2470341542	27.1648389601

#### HOOH complex

##### Singlet

C1	21.1826810720	51.7994912163	29.1421248099
N2	22.3630561402	51.1532355162	29.4602031158
C3	20.5305105476	50.9739964514	28.2734338545
C4	22.4051461665	49.9810706021	28.7988882335
N5	21.3031583378	49.8451441859	28.0687422507
Fe6	20.8826339261	48.3084563561	26.9478933838
C7	22.1808111375	49.8945701863	24.2491300944
C8	23.9348769132	46.8279731793	27.5575129481
C9	19.5957256883	46.7789061548	29.7216809441
C10	17.7568036873	49.5624310038	26.2013352400
N11	22.6887551240	48.3498557566	26.0841818275
C12	23.0443852934	49.1029902067	24.9873847916

C13	24.4536272841	48.9200565599	24.6766648422
C14	24.9228859106	48.0345978744	25.6035126908
C15	23.8321197571	47.6876321779	26.4729770471
C16	25.1775155741	49.5922283176	23.5458406329
C17	26.6458130094	49.1784601345	23.4041086919
C18	27.3428566240	49.9703845432	22.3078559325
O19	28.4551457850	49.3789447157	21.8626034071
O20	26.9318911351	51.0418047170	21.8917867591
N21	21.6066683935	47.0156323056	28.3162879120
C22	22.8932527122	46.5242299853	28.4253124110
C23	23.0104862053	45.6939341085	29.5923843172
C24	21.7945570183	45.7015310175	30.2079106757
C25	20.9242965447	46.5265328940	29.4140379314
N26	19.0363553566	48.1491923786	27.7534403129
C27	18.7239796167	47.5395367200	28.9564570215
C28	17.3501450587	47.7858793926	29.2927715717
C29	16.8237722276	48.5553472393	28.2967016348
C30	17.8751958152	48.7937101238	27.3513506416
N31	20.1172776710	49.4582114737	25.5145460572
C32	18.8067337236	49.8607254600	25.3460672772
C33	18.6883460689	50.6931438608	24.1781975472
C34	19.9362325628	50.8067619473	23.6484175983
C35	20.8202597491	50.0349320832	24.4839377996
H36	23.0751712769	51.4947823668	30.0917696632
H37	19.5783022367	51.1059598137	27.7875472273
H38	23.2124918504	49.2691714955	28.8610870925
H39	22.5883777332	50.4289158168	23.3980476722
H40	24.9001904591	46.3714418802	27.7515843959
H41	19.2031900305	46.3386942845	30.6325647964
H42	16.7811532675	49.9764965565	25.9682803407
H43	24.6572814186	49.3831993375	22.6015627418
H44	25.1341742449	50.6825220522	23.6607498450
H45	27.1899534197	49.3619310433	24.3419217887
H46	26.7482076756	48.1088510868	23.1905318737
C47	32.7637201438	46.2105776200	25.1555522529
C48	32.7346898827	47.6266010758	24.9654723416
C49	32.5525705528	48.1810422757	23.7082976567
C50	32.3929271507	47.3370320788	22.5825697119
H51	32.5330763707	49.2553344704	23.5830912156
C52	32.6017104285	45.3290583073	24.0474159110
C53	32.4152905254	45.8820207994	22.7585958942
N54	32.2603295988	45.1335903045	21.6537778243
C55	32.2845715829	43.8115055335	21.7831461340
C56	32.4657890054	43.1594575660	23.0201242566
C57	32.6260432999	43.9190387272	24.1622827902
H58	32.1574552339	43.2347609136	20.8701786794



H59	32.4803858600	42.0753608260	23.0628599013
H60	32.7715187893	43.4585489869	25.1338082531
N61	32.2196378200	47.7712300023	21.3352669707
H62	32.1331207813	47.0108374688	20.6573220545
O63	32.9025244784	48.3019494221	26.1187544995
C64	32.9555313845	49.7375844773	26.1042879013
H65	33.1166113349	50.0344430214	27.1400140602
H66	33.7890386119	50.0818394462	25.4836060331
H67	32.0093768251	50.1508377278	25.7394456194
C68	32.2088156229	49.1557770439	20.8295908940
C69	31.4593415961	49.1326611924	19.4827453559
H70	31.9965217765	48.4536743702	18.8050172281
H71	30.4673762608	48.6969965443	19.6512096516
C72	31.3142966801	50.4930118816	18.7792170736
H73	32.3005777441	50.9049458321	18.5355949886
H74	30.8245571346	50.3125002980	17.8128556188
C75	30.5188842004	51.5601351356	19.5420649708
H76	30.4944036655	52.4760736040	18.9350048699
H77	31.0204691013	51.8229158121	20.4820787150
H78	28.6131705513	51.8149440739	20.3349734388
H79	28.6528208161	50.8437756744	19.0324850965
N80	29.1648498614	51.0836072261	19.8829961927
O81	32.9442009770	45.7002951125	26.3717096757
H82	33.0628569971	46.4322031301	27.0100409788
H83	28.8156533985	49.9572880546	21.0976317121
C84	33.6465628208	49.6913750623	20.7256473803
H85	33.6418239619	50.7481797709	20.4433465334
H86	34.1777354964	49.6011009769	21.6787895625
H87	34.2126825806	49.1372838957	19.9689989718
H88	31.6363414321	49.7519839430	21.5503469824
H89	25.9233906549	47.6337476324	25.6998834336
H90	20.2455617068	51.3530157746	22.7670922516
H91	17.7631102901	51.1295548650	23.8247102164
H92	15.8145964819	48.9346415929	28.2037835238
H93	16.8563097105	47.4080308801	30.1788857560
H94	21.4981267989	45.1929257526	31.1164865117
H95	23.9132166919	45.1798172874	29.8964533307
H96	20.9217799986	52.7624063182	29.5526667501
O97	20.5205659911	46.6486772823	25.7733638506
O98	19.1425548797	46.2548893641	25.5578601175
H99	20.8894694106	45.8828313086	26.2580477909
H100	18.7124097723	46.7450322527	26.2945876009

HOOH complex

Triplet

C1	21.0540755358	51.6572035247	29.3587930264
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N2	22.2221099267	50.9636584860	29.6177594321
C3	20.3712962453	50.9063222170	28.4469527868
C4	22.2272562041	49.8366386862	28.8809547000
N5	21.1133532493	49.7750499593	28.1590059150
Fe6	20.6389454810	48.3269609154	26.9461236392
C7	22.0110738081	50.0052472304	24.3417667553
C8	23.6223655546	46.6841966921	27.4727783395
C9	19.2781549251	46.6959290446	29.6259689308
C10	17.5725601227	49.7584169418	26.2737762149
N11	22.4466438167	48.3397709933	26.0876311355
C12	22.8371790894	49.1352212980	25.0330632178
C13	24.2372817631	48.9062183681	24.7114422666
C14	24.6647552368	47.9512067742	25.5880709746
C15	23.5588822997	47.6066795465	26.4381146210
C16	24.9982531108	49.6022929111	23.6199810393
C17	26.4374116423	49.1052977315	23.4558168744
C18	27.1912916872	49.8962548116	22.3986124222
O19	28.2900574720	49.2687723830	21.9717085239
O20	26.8355630979	50.9925055252	21.9962541526
N21	21.3021447741	46.9277287088	28.2390118472
C22	22.5665200236	46.3774862264	28.3219269037
C23	22.6453760745	45.4795181391	29.4411980653
C24	21.4287325615	45.5036362792	30.0547583612
C25	20.5964372059	46.4070970610	29.3069615921
N26	18.7837353820	48.1978746589	27.7375781024
C27	18.4418685436	47.5341023755	28.9035689412
C28	17.0789339372	47.8189752701	29.2519411670
C29	16.5892256126	48.6673910135	28.3024164444
C30	17.6528959945	48.9151827666	27.3736624794
N31	19.9279855100	49.5911488642	25.5827017724
C32	18.6376871424	50.0626622163	25.4398425436
C33	18.5598161320	50.9689775239	24.3249443611
C34	19.8119677768	51.0548496536	23.8000027127
C35	20.6580583675	50.1939820795	24.5864129354
H36	22.9506660551	51.2465064886	30.2595091457
H37	19.4169206358	51.0920899015	27.9828622611
H38	23.0175486558	49.1031353005	28.8853004285
H39	22.4435930494	50.5674969547	23.5215363474
H40	24.5668020754	46.1765365920	27.6407486803
H41	18.8642332725	46.2218805840	30.5100156630
H42	16.6168720317	50.2287327735	26.0661652030
H43	24.4674536688	49.4812748552	22.6660767948
H44	25.0189297934	50.6845059096	23.8002466405
H45	26.9926989941	49.2089185510	24.3990925805
H46	26.4719032616	48.0419843378	23.1936185805
C47	33.6188333841	46.3483404237	25.0541867042

C48	33.6460426641	47.7473051172	24.7625276384
C49	33.2474159364	48.2335974986	23.5268706425
C50	32.8050317693	47.3355406574	22.5257084937
H51	33.2758871565	49.2958770833	23.3242582764
C52	33.1763097651	45.4143534474	24.0729855323
C53	32.7678779629	45.8973601589	22.8075092392
N54	32.3416692732	45.0946676395	21.8180438900
C55	32.3042913868	43.7859230624	22.0440548701
C56	32.6896803931	43.2018027603	23.2680411147
C57	33.1296098067	44.0173760886	24.2919800689
H58	31.9559620879	43.1641509289	21.2228235852
H59	32.6404585086	42.1250607177	23.3926679433
H60	33.4389971915	43.6099429417	25.2487247537
N61	32.4059521615	47.7012608948	21.3079239815
H62	32.1342978211	46.9078205866	20.7232732872
O63	34.0911793493	48.4767985791	25.8018570554
C64	34.2256519447	49.9018096241	25.6722671588
H65	34.6135154579	50.2465478984	26.6300563224
H66	34.9329035035	50.1460055512	24.8731522128
H67	33.2507156012	50.3602137730	25.4767500032
C68	32.3835678431	49.0457836257	20.7037871106
C69	31.3799113877	48.9926952969	19.5338535234
H70	31.7488013488	48.2553250894	18.8066045029
H71	30.4236236442	48.6153868067	19.9153290280
C72	31.1498808181	50.3227858441	18.7955684289
H73	32.0983758001	50.7185313804	18.4142115878
H74	30.5443116873	50.1067195512	17.9051124810
C75	30.4511692211	51.4245189639	19.6035090496
H76	30.4154698215	52.3358054605	18.9896460830
H77	31.0274799053	51.6772304333	20.5025738530
H78	28.6197922008	51.7492884652	20.5345434895
H79	28.5263968204	50.7922222893	19.2288831084
N80	29.1084182911	50.9997570129	20.0421408860
O81	34.0084645037	45.9036019621	26.2461127106
H82	34.2974625982	46.6626584493	26.7918782040
H83	28.7083408216	49.8512609136	21.2459371711
C84	33.8030689841	49.4576246868	20.2783801547
H85	33.8107205361	50.4903208596	19.9179880037
H86	34.5073406816	49.3893207411	21.1138964528
H87	34.1687571113	48.8108412341	19.4735050275
H88	32.0111423341	49.7340071097	21.4724465445
H89	25.6461423787	47.5014505458	25.6619788486
H90	20.1475312199	51.6378234396	22.9524632309
H91	17.6562358245	51.4683349278	23.9999090650
H92	15.5976513581	49.0948031956	28.2315213411
H93	16.5669833145	47.4118004618	30.1140410798

H94	21.1081339202	44.9579985316	30.9331443957
H95	23.5248624300	44.9117508046	29.7165824566
H96	20.8219671361	52.5968731233	29.8351949242
O97	20.2166546498	46.7581352734	25.6706657476
O98	18.8248090319	46.4170441467	25.4534988413
H99	20.5683261793	45.9535254034	26.1024317723
H100	18.4187055097	46.8835209604	26.2189113925

HOOH complex

Quintet

C1	20.3911082070	52.2734179417	29.0865096212
N2	20.6756283188	51.4154709906	30.1310832217
C3	20.2824186975	51.4808486972	27.9791262601
C4	20.7317927022	50.1567269247	29.6473941126
N5	20.4969668126	50.1628687859	28.3409669774
Fe6	20.4055421950	48.4455607439	27.0530438146
C7	21.9196212860	49.8753257512	24.3419508090
C8	23.4520314606	47.2427920089	28.1277699710
C9	18.8343926364	46.6309999338	29.5579922539
C10	17.3104128177	49.3839359826	25.8415549440
N11	22.3289446308	48.5380962072	26.3610011168
C12	22.7563315051	49.2157974250	25.2385217489
C13	24.2063808731	49.1367290621	25.1367459005
C14	24.6163012113	48.3968898398	26.2149239041
C15	23.4513036068	48.0223601877	26.9718615440
C16	25.0296559455	49.7737108572	24.0538894261
C17	26.5112478321	49.3830745713	24.0691769401
C18	27.3034294765	50.1453142857	23.0176251009
O19	28.4912054168	49.5887822421	22.7608226458
O20	26.9047522737	51.1662134692	22.4811637879
N21	21.0258369434	47.1471537715	28.5464040167
C22	22.3319736642	46.8287736861	28.8552008852
C23	22.3549589457	45.9995141071	30.0312892739
C24	21.0568742502	45.8209193392	30.4255807757
C25	20.2259664777	46.5389463105	29.4952020345
N26	18.4252742387	47.9940927287	27.5440263949
C27	18.0015632885	47.3271774045	28.6796259237
C28	16.5795471032	47.4827442312	28.8211963884
C29	16.1516411177	48.2638330073	27.7819620200
C30	17.3063555638	48.5923647677	26.9923530492
N31	19.7381243168	49.4471238893	25.4112600694
C32	18.4278731002	49.7543315384	25.0948094126
C33	18.3998998802	50.5117997946	23.8721018581
C34	19.6936277331	50.6426835848	23.4483657900
C35	20.5273609059	49.9716807828	24.4096134732
H36	20.8137428435	51.6810111191	31.0972332894

H37	20.0661667244	51.7566526207	26.9591528138
H38	20.9353504573	49.2838529055	30.2478436816
H39	22.3911109277	50.3605701901	23.4936855992
H40	24.4187780712	46.9064128552	28.4903854401
H41	18.3502706750	46.1225282077	30.3861323595
H42	16.3467387709	49.7391670359	25.4892556726
H43	24.6053296932	49.5205208648	23.0735567407
H44	24.9573873793	50.8669711376	24.1215767512
H45	26.9648466975	49.6124944089	25.0437398895
H46	26.6504115517	48.3076980659	23.9112164417
C47	34.6282005503	46.0137485023	24.4016718654
C48	34.7712769912	47.4029522719	24.0952116271
C49	34.1080748249	47.9751539051	23.0200085429
C50	33.2717735902	47.1774756207	22.2026636539
H51	34.2308352662	49.0276876955	22.8020127957
C52	33.7964048588	45.1788607635	23.5999405345
C53	33.1160039755	45.7503187623	22.4992661611
N54	32.3160379830	45.0435888354	21.6832259545
C55	32.1607600961	43.7466020078	21.9260814594
C56	32.7918217460	43.0798241501	22.9958629610
C57	33.6159118570	43.7966285228	23.8411339926
H58	31.5095372797	43.2028497636	21.2459055894
H59	32.6280144038	42.0173775356	23.1429831726
H60	34.1232848329	43.3230462588	24.6749581543
N61	32.5883443046	47.6300974551	21.1515167382
H62	32.0533359754	46.8973104035	20.6803503368
O63	35.5963649243	48.0321236831	24.9510942479
C64	35.8839834274	49.4293805463	24.7747804636
H65	36.5737574412	49.6884726915	25.5770298879
H66	36.3595035313	49.5996916778	23.8035410882
H67	34.9669856767	50.0207711491	24.8643787084
C68	32.5642511169	48.9838490040	20.5706125918
C69	31.2362654939	49.1111148941	19.7942894885
H70	31.2428602757	48.3573557335	18.9939294347
H71	30.4117920645	48.8530412420	20.4699642995
C72	30.9671445051	50.4874552588	19.1620452783
H73	31.8102512089	50.7896285624	18.5300347747
H74	30.1144789267	50.3796718622	18.4782090510
C75	30.6592851986	51.6258423624	20.1440426873
H76	30.6132179307	52.5671582026	19.5776639261
H77	31.4680507641	51.7422678902	20.8766315720
H78	29.1722187781	52.1734924146	21.4766731164
H79	28.6251386612	51.2950912117	20.2452242316
N80	29.4118625083	51.3722988723	20.8921023189
O81	35.2724653560	45.4851684795	25.4381190326
H82	35.8055662799	46.1809926301	25.8732207431

H83	28.9549026588	50.1748698457	22.0719450480
C84	33.8142061800	49.2052997055	19.7020806253
H85	33.8547279622	50.2371766232	19.3417223052
H86	34.7314515206	49.0122025994	20.2681185105
H87	33.8053764408	48.5382871670	18.8331786924
H88	32.5658721881	49.6913091862	21.4086802300
H89	25.6279196792	48.1167058472	26.4780758675
H90	20.0533877458	51.1447484421	22.5597215030
H91	17.5030942590	50.8852265116	23.3943901229
H92	15.1424017325	48.5923674258	27.5703000497
H93	15.9843081437	47.0541292022	29.6174259952
H94	20.6915415583	45.2499383888	31.2694016838
H95	23.2492710544	45.6016121236	30.4938131897
H96	20.2934638741	53.3389813093	29.2250452469
O97	20.3395578306	46.4862777538	25.7406423611
O98	19.0268344916	45.8918705237	25.5627609902
H99	20.7913149594	45.8039038716	26.2730436836
H100	18.5110295077	46.4532140165	26.1820550368

#### HOOH complex

##### Septet

C1	20.5359742539	52.1822516531	29.3253609408
N2	21.1152170782	51.3006628927	30.2172889958
C3	20.2323869291	51.4398622562	28.2194891871
C4	21.1467161371	50.0766842975	29.6490657519
N5	20.6178614946	50.1285368925	28.4328801047
Fe6	20.3694043551	48.4765769279	27.0814886323
C7	21.8924117178	49.9214262823	24.3859495756
C8	23.3590854085	47.0197957883	27.9970850057
C9	18.7629239904	46.6977668607	29.5835662283
C10	17.3042276482	49.6579516063	26.0027827778
N11	22.2726737532	48.4688389673	26.3296119480
C12	22.7100326091	49.1698643700	25.2255204323
C13	24.1470842172	48.9982327898	25.0694568462
C14	24.5387306729	48.1791588148	26.0957566987
C15	23.3750837475	47.8484533910	26.8756761218
C16	24.9759857732	49.6292094536	23.9872679263
C17	26.4298102057	49.1455942176	23.9353680369
C18	27.2329894613	49.9048395911	22.8896581811
O19	28.3132159077	49.2348759069	22.4797284934
O20	26.9271356512	51.0150259911	22.4837735542
N21	20.9488779614	47.0839972970	28.5041342378
C22	22.2376871479	46.6586138836	28.7510213118
C23	22.2404489454	45.7910884805	29.8999443049
C24	20.9480453754	45.6985874218	30.3403682168
C25	20.1406841016	46.5076129050	29.4658058582

N26	18.3793942149	48.1475094255	27.6255682540
C27	17.9506248796	47.4754347215	28.7558815163
C28	16.5470462396	47.7171767781	28.9504890450
C29	16.1366589958	48.5534796379	27.9477979591
C30	17.2841946054	48.8314879568	27.1288383742
N31	19.7180231145	49.5844921991	25.5015588015
C32	18.4214162193	49.9837330329	25.2350157279
C33	18.4083298042	50.7903401995	24.0436099570
C34	19.6964793332	50.8603341827	23.5895521392
C35	20.5116645519	50.1015260335	24.4998557232
H36	21.4522699027	51.5283029150	31.1432870147
H37	19.7683895579	51.7475380298	27.2957890324
H38	21.5445193201	49.1950229296	30.1269170571
H39	22.3697609331	50.4131076730	23.5446907680
H40	24.3108604224	46.6004302077	28.3094393286
H41	18.2728206110	46.1989933252	30.4140794777
H42	16.3553806129	50.0849516775	25.6923750899
H43	24.5056129952	49.4437496695	23.0125320207
H44	24.9775714011	50.7208529408	24.1018693927
H45	26.9248476149	49.3067122204	24.9036500103
H46	26.4947602931	48.0722305603	23.7276579646
C47	34.6128534489	46.1296364690	24.5153448947
C48	34.6639776603	47.5323136750	24.2435361990
C49	34.0670339953	48.0687894976	23.1127446345
C50	33.3922154846	47.2203077700	22.2024898796
H51	34.1189476467	49.1324631790	22.9221545083
C52	33.9443931823	45.2441064118	23.6205468788
C53	33.3332500762	45.7788908272	22.4622565382
N54	32.6853566276	45.0246242572	21.5587659601
C55	32.6193089691	43.7142304063	21.7676533995
C56	33.1928758642	43.0807217173	22.8888866045
C57	33.8607675011	43.8466240271	23.8241876298
H58	32.0905175930	43.1319712336	21.0168486737
H59	33.1071841331	42.0053425161	23.0050278904
H60	34.3188110153	43.4000876590	24.7003983792
N61	32.7809345716	47.6368589414	21.0936270737
H62	32.3634901103	46.8722701683	20.5585358644
O63	35.3372499166	48.2120242612	25.1892320433
C64	35.5178714271	49.6320673918	25.0596303283
H65	36.0952219746	49.9335096317	25.9327624634
H66	36.0746562499	49.8622788119	24.1456087414
H67	34.5482682411	50.1406236198	25.0587683858
C68	32.6887598624	48.9990539046	20.5394998075
C69	31.4382953326	49.0286329803	19.6353691981
H70	31.6042224618	48.3196584896	18.8118036267
H71	30.5824267341	48.6559152197	20.2111788454

C72	31.0864240724	50.4011610501	19.0362337041
H73	31.9598891342	50.8375396918	18.5379728076
H74	30.3485761154	50.2387046434	18.2389614054
C75	30.5159182689	51.4328241665	20.0192097094
H76	30.4322460240	52.3963130715	19.4960435439
H77	31.2004944735	51.5942789084	20.8617558366
H78	28.7930076877	51.7319419582	21.1375438877
H79	28.5566739042	50.8410957083	19.8120459507
N80	29.2197257257	50.9944993916	20.5740453058
O81	35.1910776806	45.6360115614	25.6066839190
H82	35.6144111197	46.3655318314	26.1029058108
H83	28.7776269963	49.8003654003	21.7755721156
C84	33.9922050102	49.3579690391	19.8059801811
H85	33.9693968278	50.3975265655	19.4667589354
H86	34.8628541604	49.2381256208	20.4591097755
H87	34.1338358280	48.7143566386	18.9309890884
H88	32.5421533411	49.6789628189	21.3873665621
H89	25.5360579885	47.8168724967	26.3084733406
H90	20.0636835923	51.3759542348	22.7117869879
H91	17.5240938036	51.2360185308	23.6060546270
H92	15.1442666935	48.9511657309	27.7795059764
H93	15.9515252082	47.3043259303	29.7547794650
H94	20.5719848132	45.1292346081	31.1810041964
H95	23.1180105558	45.3109374537	30.3140403400
H96	20.3961991083	53.2272205427	29.5548235912
O97	20.1172263921	46.5813039285	25.7055965311
O98	18.7530547308	46.1293048259	25.5043870940
H99	20.5016659433	45.8330180780	26.2010669304
H100	18.2977256062	46.6841136937	26.1749368431