

How feasible is the reversible S-elimination mechanism for the activation of FeMo-co, the catalytic site of nitrogenase?

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Supplementary Information

Computational methods

Density functional (DF) calculations use the DMol methodology of Delley,¹⁻⁵ with accurate DNP (double numerical plus polarisation) basis sets.⁴ These numerical basis sets avoid the need for basis set superposition corrections, and provide reliable energies at long intermolecular distances.⁶ This advantage of the DMol methodology largely obviates the need for empirical treatment⁷ of the long-range dispersion energies that are involved when the computational model is composed of separate molecular units. The real-space cutoff in the calculation of atomic basis sets was 9 au (4.76Å), which gives results within 0.1% of the limit for larger extensions of the basis sets. The calculations were all-electron, spin-unrestricted, with no imposed symmetry. The gradient-corrected functional PBE,⁸ was used because validation tests demonstrate that it is more accurate than other commonly used functionals (including B3LYP) when deployed with numerical basis sets.⁹ The conductor-like screening model (COSMO)¹⁰⁻¹² was used with a dielectric constant of 5.

For FeMo-co at the resting redox state the core charge is $[\text{Fe}_7\text{MoCS}_9]^{-1}$. H atoms bound to the Fe and/or S atoms of FeMoco are neutral, being formed by separate addition of proton plus electron. The mechanisms for formation of H on S3B and subsequent migration to Fe6, S2B and Fe2 have been described.^{13,14} The electronic state of FeMo-co was controlled via the Fe spin densities, starting with the set of signs +, -, +, -, +, +, - for the spin densities of Fe1, Fe2, Fe3, Fe4, Fe5, Fe6, Fe7 respectively.¹⁵ this is the broken symmetry BS7 scheme of Noodleman,¹⁶ or, without the assumption of C_3 symmetry, the spin coupling scheme BS7-2 as defined by Cao and Ryde.¹⁷ A characteristic of the electronic structure of FeMo-co is diminished spin density on Fe atoms with additional bound ligands, and in some structures reported here the Fe spin densities approached zero. Net spin states S were controlled through occupations of the unrestricted α and β orbitals.

The primary computational model, Chart 2, was constructed from crystal structure PDB 3U7Q¹⁸ of the *Azotobacter vinelandii* protein, and included all amino acids surrounding the reactive face of FeMo-co and S2B, the proposed channel for ingress of N_2 , the Gln191 to His196 helix, and all associated water molecules. The core model contains 486 atoms. Atoms fixed during optimisations are highlighted yellow on Chart 2. The helix Cys62 to Trp72 that includes Val70 and other important residues that enclose the front reaction face was unrestrained except for $\text{C}\alpha$ of Cys62. The sections of protein surrounding the putative N_2 ingress channel were unrestrained except for $\text{C}\alpha$ of Tyr281. The helix from Gln191 to His196 was constrained only at $\text{C}\alpha$ of His196, allowing free movement of the side-chains of key residues His195 and Gln191. Water molecules HOH545 on the protein surface, and HOH531 involved in proton slide to $\text{N}\delta$ of His195 were unconstrained, as were HOH519, HOH506, HOH536 and HOH534 that are part of the water chain to FeMo-co.¹⁴ Equilibrations of the residues surrounding dissociated ligands H_2S or SH^- were made with this S atom fixed.

Investigation involved exploratory mapping of relevant potential energy surfaces, directed by knowledge of the coordination chemistry of FeMo-co, in order to reveal significant reactivity and possible reaction steps. Once the relevant energy minima were established, the energy ridges between them were located and the relevant transition states determined. The general computational procedure, which is pragmatic rather than formulaic, has been described previously.^{19,20,14} This methodology is advantageous for reaction steps with multiple moving atoms and more than one bond breaking/making process, as occurs in the transformation **8** → **9** and the transformations connecting intermediates **13**, **14** and **15** described in this paper. In view of the large size and number of variables in the model, energies are reported as potential energies, to the nearest kcal mol⁻¹.

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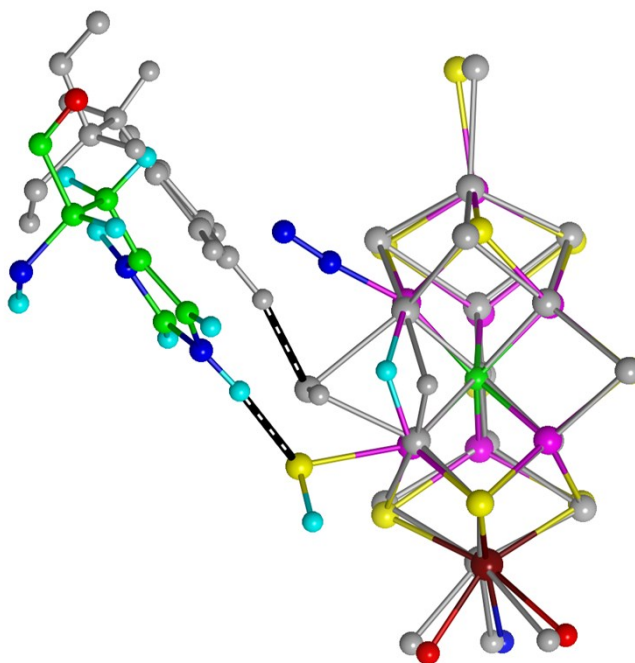


Fig. S1. Superposition of the optimised structures of **4** (coloured) with *exo*- η^1 -N₂-Fe₂, and (in grey) the same structure without *exo*- η^1 -N₂-Fe₂, showing how *exo*- η^1 -N₂-Fe₂ influences the position of His195. Relevant atoms only are drawn.

Coordinates and spin densities for intermediates and transition states

Translation of Fe numbering

Fe1 = Fe143

Fe2 = Fe140

Fe3 = Fe141

Fe4 = Fe142

Fe5 = Fe139

Fe6 = Fe145

Fe7 = Fe144

structure, spin densities	filename, coordinates			
1 (S=3/2)	bm1b2b262n2xsep3c_2_53366.01			
Fe(139) 2.566	C1	-9.238145160	1.514373359	2.82586767
Fe(140) -2.118	C2	-8.066573407	2.398327822	3.26383998
Fe(141) 2.921	C3	-7.254547571	4.700923361	3.56227226
Fe(142) -2.254	C4	-6.607309031	4.592704461	4.93940080
Fe(143) 2.960	C5	-6.848238921	4.086739809	7.30826466
Fe(144) -2.041	C6	-5.818352297	2.955643755	7.41328914
Fe(145) 0.544	C7	-5.142041476	0.748230528	6.59132225
	C8	-3.892663241	1.072061714	5.76723695
	C9	-2.946695300	2.110043696	3.77727675
	C10	-1.954091280	3.056397162	4.46463195
	C11	-1.635670306	4.921462142	6.00240774
	C12	-1.000158505	4.302201309	7.25399192
	C13	-1.377411572	3.135070231	9.37198183
	C14	-0.654363734	1.784702668	9.42095382
	C15	-0.502532880	-0.494288649	8.51069786
	C16	0.459238148	-0.864349491	7.37880848
	C17	1.368900093	-0.208859026	5.17174953
	C18	2.593292298	0.722570481	5.20074220
	C19	0.572705823	-0.142092952	3.84966510
	C20	1.520627558	-0.258653722	2.65208646
	C21	-0.507389300	-1.230300301	3.82853923
	C22	3.430071370	3.042356599	5.15072514
	C23	3.941886251	3.293587890	6.58369311
	C24	3.006296605	4.344552658	4.42897993
	C25	4.078223549	5.431317359	4.57053506
	C26	2.713126345	4.071972887	2.94850317
	C27	3.440476557	3.874434133	8.88704434
	C28	4.371186144	2.825339454	9.46256852
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	C34	2.381390506	-6.174824867	5.81990621
	C35	2.036110407	-4.889697742	5.06654563
	C36	3.703792346	-3.344326032	4.03348027
	C37	4.885854840	-9.416626641	7.60786767
	C38	5.956067695	-8.743199009	6.77578335
	C39	-5.577145160	1.752373359	0.06486767
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C65	7.798279283	-2.852593070	3.52623845
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	H179	3.614121921	3.692720349	2.43964996
	H180	5.033346500	5.097782086	4.13434613
	H181	2.079359478	4.711353998	4.90771993
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	H185	4.031273459	1.601636156	-1.96582581
	H186	4.038833980	3.025490358	-0.88100812
	H187	6.112351878	2.348995588	-0.82265930
	H188	6.649556066	2.848156574	1.59564289
	H189	6.210945020	-0.267159720	-0.07324716
	H190	6.813383748	-2.419131976	0.98967775
	H191	7.940182617	-0.327438823	4.59676369
	H192	-0.079512278	0.828689771	6.37073396
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	H207	-7.489003470	-3.444224455	-4.30722131
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H227	0.377575603	12.491118868	-1.41418184
H228	-0.540261738	10.113939000	1.46066814
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C52	-1.453429207	7.068678514	1.830204104
C53	-0.717273013	5.210650311	0.411210048
C54	-0.859489445	3.848622058	-0.185150184
C55	-1.383858743	2.683637145	0.333092436
C56	-0.605490851	2.324509681	-1.710101924
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C58	-1.847716832	9.881765982	2.389240479
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C60	-1.735834609	11.535352303	-0.394997517
C61	-1.124222142	12.473642001	0.413855606
C62	-1.379271628	13.272059047	-1.637791172
C63	6.223469761	-3.687384844	7.526467379
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C65	4.941537106	-3.467426168	6.677408234
C66	4.800497674	-2.040039796	6.203048071
C67	4.364945027	-1.029191602	7.078672728
C68	5.110805385	-1.678939563	4.879877776
C69	4.244116352	0.294614820	6.652271121
C70	4.988682408	-0.359251940	4.435884314
C71	4.557343877	0.625704412	5.328634553
C72	8.917997641	1.330417854	0.722099554
C73	8.936086145	2.748203614	0.136420060
C74	7.481840115	0.795191031	0.802635182
C75	9.576421117	4.152155151	-1.777636985
C76	8.262109372	4.639602489	-2.387542378
C77	5.939633817	4.087107040	-2.967068328
C78	5.009300643	4.504231798	-1.809280515
C79	5.345577479	2.967502464	-3.845107289
C80	3.999258315	3.274033192	-4.513063394
C81	3.980599778	4.461231817	-5.479186291
C82	3.876884763	6.923131219	-5.358375789
C83	4.320127384	4.208701761	0.519834130
C84	4.796046830	5.436871874	1.310645044
C85	4.211091923	3.046039331	1.524957097
C86	6.733328679	6.428456638	2.409305423
C87	7.293200215	7.800969915	2.066032021
C88	7.618367977	9.521828261	0.347723943
C89	6.812202559	10.777776211	0.738843691
C90	7.921517392	9.473465364	-1.161425315
C91	6.670210726	9.406887158	-2.031926576
C92	4.650212245	11.681457143	1.447753061
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C94	3.238118385	11.148045751	1.807564393
C95	2.657139544	10.338794218	0.673501523
C96	2.085624289	10.977209559	-0.438288949
C97	2.753361067	8.938083813	0.659890371
C98	1.650896472	10.246074774	-1.544943881
C99	2.338396676	8.192035850	-0.446061351
C100	1.794810921	8.856150681	-1.545870665
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	C127	0.075024665	-9.416266464	-4.433086431
	C128	-0.467231631	-7.276217294	-4.238670074
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	C131	-4.346056827	-5.183634213	0.179716701
	C132	-3.169255292	-5.945211406	0.714952365
	C133	-2.510135173	-6.923496106	-0.341986405
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	C136	-3.962928858	-9.965332068	-2.318103177
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	Fe140	2.282612690	-1.404163339	-0.840565451
	Fe141	4.098538189	-3.134836736	0.249534258
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	Fe144	2.364747892	-5.031670510	0.046615756
	Fe145	0.666548708	-3.362659300	-0.835641395
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	H147	-7.766131088	-0.376377520	-3.437764741
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	H149	-9.465146663	1.278657039	-3.532605082
	H150	-10.427625215	0.348342679	-2.386970214
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	H152	-10.710021318	2.368378621	0.705847964
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	H154	-11.273013330	1.695131361	2.863432452
	H155	-9.201120430	0.254005554	1.308952083
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	H159	-7.998720714	-1.710090208	1.709619085
	H160	-4.379909747	3.785345686	4.835723934
	H161	-6.415228142	2.639630873	3.066856258
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	H163	-4.707273191	1.760361022	0.902380479
	H164	-7.143646020	1.466346577	5.378511964
	H165	-6.138313788	4.049629744	4.901424625
	H166	-3.385459668	-2.263632780	2.890925387
	H167	-2.336804641	-1.879649617	1.503028132
	H168	-1.832007243	-3.120666657	2.654299433
	H169	-2.135451138	-0.116792317	3.262287121
	H170	-7.786281246	0.499924940	7.358627829
	H171	-0.473951681	2.607262161	3.964862466
	H172	-2.868632068	1.815586169	7.705868166
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	H174	-0.112532135	-0.567409766	1.907931953
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	H177	-0.109214601	4.316901223	4.289804303
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	H183	-1.931717435	1.131879192	5.231183414
	H184	0.379942258	-0.157933956	3.552410521
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	H186	3.303880892	3.223156544	2.123637888
	H187	5.094867099	2.562226823	3.198871559
	H188	4.205447400	2.521155230	5.579344550
	H189	5.196407623	-0.105035130	3.395272099
	H190	5.438203750	-2.442278770	4.169589845
	H191	4.102370349	-1.280444240	8.109231134
	H192	-3.674146658	-0.750684493	5.225889572
	H193	-5.532901611	-3.273443799	5.822130247
	H194	-5.037589195	-2.919849743	7.492660803
	H195	-5.937465548	-0.922195867	5.481260273
	H196	-6.487965641	1.365191344	8.216647725
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	H201	-1.705413970	-0.380392168	10.001837686
	H202	1.617453976	-11.938988807	6.920946040
	H203	-4.365604902	-3.715613177	-4.073416588
	H204	-5.479615299	-6.526119388	0.975704403
	H205	-3.588875938	-4.476106506	-9.533707176

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H256	3.833928256	7.901674668	-7.158770717
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	H293	9.849828112	2.043016029	-1.568371312
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	H320	-1.474457633	-11.929243868	0.207100200
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	H323	-2.342933071	-11.942103717	-1.085711986
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	H328	-4.114733895	-8.375593194	-0.092746233
	H329	-0.785961158	-8.313252522	-6.054586830
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	H331	-5.186882331	-12.324932011	5.308811527
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Fe(141) 2.752	C3	-8.910186349	-0.377780249	-2.686093324
Fe(142) -2.632	C4	-9.234593804	-1.132630814	-1.400872381
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H177	-3.097692395	2.971042360	4.325125471
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H183	-3.416968977	-0.814394734	4.469203339
H184	-0.535141811	-0.641970485	3.347504370
H185	2.195508048	3.281520889	2.249369131
H186	0.756206909	3.763519508	3.196176658
H187	2.271925642	3.706313529	4.756156560
H188	0.975117765	2.829873143	6.835966071
H189	3.681272029	1.561618272	4.916092226
H190	4.839453569	-0.550316078	5.495304698
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	H195	-5.954476708	-4.401089906	3.400132002
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	H199	-5.714217102	-0.672797461	9.255169794
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	H204	-1.972377646	-8.410801908	-0.854218197
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	H207	0.297576794	-1.881667056	-9.057718991
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	O472	3.130268706	-6.911001836	-0.483451755
	O473	1.809124225	-8.616827360	0.158740519
	O474	1.434747335	-6.009552932	-2.288190074
	O475	4.975586550	-9.726695561	2.767533577
	O476	4.862886770	-7.180091052	1.796444057
	O477	-1.093610721	5.624564007	-2.672912616
	O478	4.479843325	-11.388704597	-1.965307063
	O479	3.481906910	-10.706387971	0.624476694
	O480	-2.301837569	7.870888632	-6.418028492
	S481	5.632360166	3.635043395	1.317058410
	S482	4.165834642	1.430676487	-1.366035493
	S483	2.658505439	-3.145778828	-3.053670061
	S484	3.742906257	0.416975224	2.129276210
	S485	0.042793469	-1.946835616	-1.497324689
	S486	6.151470189	-1.423897983	-3.037584587
	S487	2.067377375	-4.161414023	0.418171430
	S488	6.838677151	-0.052062877	0.472840061
	S489	5.411402547	-4.596106042	-1.056439343
	S490	5.094677252	-3.138120408	2.399106809
4 (S=3/2)	bm2b2b262n2xtl.car_3			
Fe(139) 2.350	C1	-7.216761127	-0.139979386	-6.558754517
Fe(140) -0.917	C2	-7.121873297	0.876058582	-5.416531734
Fe(141) 2.957	C3	-7.333380748	3.239763763	-4.782852006
Fe(142) -2.474	C4	-8.153120884	3.134615946	-3.500071294
Fe(143) 2.791	C5	-10.211373265	2.401618333	-2.416074892
Fe(144) -2.222	C6	-9.610977312	1.445188948	-1.380022574
Fe(145) 0.162	C7	-8.245446700	-0.558497333	-1.014882389
	C8	-6.959519071	0.024904509	-0.421805150
	C9	-4.941702659	1.346958916	-0.781056402
	C10	-5.156095138	2.395367842	0.318586132
	C11	-6.612316957	4.119280719	1.245825835
	C12	-7.247060085	3.499440533	2.500296273
	C13	-9.080103188	2.158469191	3.410430259
	C14	-8.550859261	0.950555176	4.191907506
	C15	-7.367777492	-1.201609101	4.091174113
	C16	-5.862487839	-1.326057102	4.330156123
	C17	-3.639730901	-0.336071548	3.873894952
	C18	-3.148831575	0.758525145	4.831784446
	C19	-2.991722031	-0.307745203	2.472495251

	C20	-1.464138709	-0.213717883	2.570146775
	C21	-3.437041328	-1.542114364	1.684424650
	C22	-3.020983483	3.168280428	5.329886444
	C23	-4.029631998	3.365581040	6.479717967
	C24	-2.814986794	4.458497711	4.496583325
	C25	-2.547381041	5.670027307	5.397491114
	C26	-1.669193072	4.281449890	3.491011823
	C27	-6.346293248	3.632937323	7.165566140
	C28	-6.233022883	2.717662380	8.366650509
	C29	-7.629626009	-10.010208976	4.710833290
	C30	-6.125539432	-9.736998731	4.748077613
	C31	-4.415753018	-8.186056076	5.709160860
	C32	-4.137827888	-8.335620347	7.215898599
	C33	-4.236299969	-6.729910356	5.238554418
	C34	-2.853749867	-6.140498296	5.543958886
	C35	-2.609489392	-4.874899888	4.718710038
	C36	-1.171796675	-2.989095886	5.514230485
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	C38	-1.477623810	-8.212114534	9.373434624
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	C40	-2.467208544	2.286649239	-4.628637402
	C41	-2.508539367	-0.137150923	-3.894512915
	C42	-3.309835543	-1.456784086	-3.809676304
	C43	-2.876245589	-2.542012015	-4.787383570
	C44	-0.863879217	3.925930140	-5.517977562
	C45	-1.661100573	5.200637691	-5.827324129
	C46	0.409661275	3.878148325	-6.381271827
	C47	-3.881833931	6.164401943	-6.252123563
	C48	-4.609630351	6.441912487	-4.929029578
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	C50	-3.989674091	5.946704626	-1.495624804
	C51	-1.743890525	5.694876800	-0.584790682
	C52	-1.391738181	7.194814454	-0.397767482
	C53	-0.418226039	4.946786776	-0.826438427
	C54	-0.474867951	3.470506841	-1.090606306
	C55	-1.118556527	2.403193965	-0.500939578
	C56	0.166681281	1.602242606	-2.116216815
	C57	-1.085761127	9.368020614	-1.572754517
	C58	-2.159118983	10.111415466	-0.774498426
	C59	-1.083777149	9.814269446	-3.046497032
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	C61	-0.336086517	12.275020450	-2.519325258
	C62	0.367385531	12.710605840	-4.575332602
	C63	2.178969912	-1.938312633	9.908216185
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	C65	1.381914543	-1.901364266	8.575020032
	C66	1.528612556	-0.585237686	7.848005622
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	C68	2.474345739	-0.426604201	6.817772441
	C69	0.907449008	1.760461396	7.561973971
	C70	2.643043729	0.798040745	6.166638573
	C71	1.859050595	1.891269329	6.544522012
	C72	7.888489188	1.751617071	4.274483982
	C73	8.231725217	2.965039803	3.401753222
	C74	6.574957499	1.108039283	3.805939187
	C75	9.710070722	3.860021255	1.655527562
	C76	8.771736070	4.180493894	0.493809187
	C77	6.859479464	3.476619989	-0.868634495
	C78	5.553205597	4.080136976	-0.325776362
	C79	6.614709613	2.197042749	-1.694616607
	C80	5.682472130	2.343911021	-2.905340425
	C81	6.139360794	3.318765062	-3.993892091
	C82	6.187030946	5.758656877	-4.364084874
	C83	3.890484569	4.225666029	1.453828356
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	C85	3.250936640	3.272276154	2.476775303
	C86	5.382722858	6.868882449	3.732539391
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	C89	6.549820664	10.841695233	1.540691738
	C90	8.260443701	9.193509373	0.604350118
	C91	7.513475194	8.927102756	-0.696763922
	C92	4.382238873	11.874020614	1.048245483
	C93	4.439904676	12.945864022	2.127547131
	C94	2.911773674	11.426239480	0.836543107
	C95	2.807899858	10.350149976	-0.219815402
	C96	2.829554370	10.682784603	-1.583527954
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	C117	1.598520592	-0.286886873	-6.160289760
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	C121	0.996974049	-1.862854236	-4.397139554
	C122	1.920617359	-1.263776884	-3.532887579
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	C131	-4.434293983	-4.950472896	-0.843274453
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	Fe139	2.753570353	-5.030624746	-0.326252944
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	Fe143	5.144328227	-1.088229861	1.629517317
	Fe144	1.621639049	-4.676969254	2.023789282
	Fe145	0.848744107	-3.276684148	0.020609299
	H146	-6.882696957	-1.813501859	-5.438182039
	H147	-5.568714958	-1.329933715	-6.288953791
	H148	-7.723999113	2.371895041	-6.691786276
	H149	-6.807435180	0.316208323	-7.474453440
	H150	-8.292746696	-0.293429730	-6.756030195
	H151	-6.282991712	3.314443702	-4.470327349
	H152	-9.705133463	2.242979563	-4.506097698
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	H155	-8.795171154	0.316223217	-2.884807070
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	H157	-4.274882451	0.584787314	-0.355297468
	H158	-6.399971502	0.793119628	-2.261551319
	H159	-8.000760751	-1.460143422	-1.592647735
	H160	-5.708689898	4.649177001	1.569416265
	H161	-6.872760772	3.062901821	-0.611240264
	H162	-8.883819040	-0.849318025	-0.172636459
	H163	-4.432731601	1.818362692	-1.634699786
	H164	-8.600973102	2.429096085	1.350195626
	H165	-7.313663233	4.851658081	0.823408435
	H166	-4.530719145	-1.595309689	1.591107878
	H167	-3.005808865	-1.519626143	0.675775058
	H168	-3.073799959	-2.464796750	2.162976796
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	H171	-1.834722021	3.433719759	2.810944134
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	H173	-3.386996782	5.880394499	6.074720113
	H174	-1.013278587	-0.281532390	1.570416342
	H175	-1.039072078	-1.042107771	3.154853004
	H176	1.742042690	-1.187018346	10.593033334
	H177	-1.557280777	5.194512027	2.888323908
	H178	-2.375441584	6.560717953	4.776944133
	H179	-0.716231147	4.110073849	4.017261840

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	H184	-1.136826425	0.730525094	3.032499949
	H185	3.271988224	2.246926132	2.076290396
	H186	2.200696206	3.581371046	2.592097901
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	H190	3.082763594	-1.278223157	6.501105687
	H191	-0.004538382	0.435175957	8.986947758
	H192	-5.566153785	0.379387510	3.253271768
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	H194	-7.861043698	-1.308065938	5.065391223
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	H198	-3.377922975	-1.284570067	4.354797826
	H199	-6.318493183	4.679260039	7.508791158
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	H204	-5.883001974	-6.172771751	-0.473828908
	H205	0.606176524	-6.359869308	-9.048655459
	H206	2.065147730	-6.726038928	-8.091817879
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	H211	-4.377958718	-1.256250511	-3.997865470
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	H218	-3.624841449	0.821827254	-6.868013544
	H219	-2.515236829	0.319207017	-2.896778231
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	H231	0.791591538	13.268825393	-5.405275771
	H232	0.209018682	5.132548152	0.060179043
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	H234	0.500993118	14.175673581	-3.035978705
	H235	-0.478835733	9.084302718	-3.607822811
	H236	-2.521718209	4.750234412	-2.351130463
	H237	-5.609557877	4.808778366	-2.338518532
	H238	-3.335583118	7.077855653	-6.518776157
	H239	0.695385873	0.906476969	-2.759350391
	H240	-4.636542037	5.982319413	-7.028895904
	H241	-0.878719829	0.225399138	-0.935461841
	H242	4.097074394	-1.557217533	10.527354174
	H243	3.758629229	-0.967222613	9.038330485
	H244	5.584171241	2.879693442	1.349518350
	H245	3.186076891	4.365664384	0.622347172
	H246	5.953220667	5.117247650	2.711296293
	H247	1.018996575	3.485161977	-2.657202884
	H248	1.917988588	4.691242469	-4.436190146
	H249	2.437254881	5.300504365	-3.101318908
	H250	0.966990901	2.960842191	-6.152193748
	H251	0.147619088	3.873182804	-7.452401568
	H252	8.896846772	8.345696344	0.895235939
	H253	8.905158147	10.067136387	0.438268464
	H254	8.051013717	6.886021268	-0.699036403
	H255	7.026295654	7.446718380	-2.010525505
	H256	7.175113956	6.433213697	-6.028654677
	H257	5.617737311	3.091055553	-4.937079006
	H258	2.854951883	9.969550739	-3.626380173
	H259	2.725506361	8.686486581	1.179443662

	H260	4.902785594	7.080524604	-3.495077903
	H261	6.210518073	1.411286509	-1.036991907
	H262	7.750333287	2.399482875	0.758929120
	H263	4.655668744	2.599651253	-2.600108090
	H264	-3.283940335	4.106687946	-6.383573021
	H265	10.683987083	3.583110884	1.230623770
	H266	-1.515102024	1.994577400	-6.356811933
	H267	7.597681091	1.845245445	-2.043587689
	H268	2.811666745	6.935946537	-0.551335536
	H269	0.669442630	5.770711850	-6.008119108
	H270	9.841308155	4.795955824	2.215045577
	H271	7.399374840	4.752138165	-5.683403538
	H272	6.026527194	7.774179185	-4.582171602
	H273	-2.810934279	-0.528950561	-6.343761363
	H274	-4.144279915	1.022996182	-4.633541072
	H275	2.840479328	11.731442007	-1.889012615
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	C87	6.051296651	8.110992597	3.371062291
	C88	7.291149847	9.494986440	1.770938097

	C89	6.525536013	10.821839429	1.574749381
	C90	8.223882719	9.190534584	0.583843938
	C91	7.485015376	8.993385122	-0.736168997
	C92	4.375051230	11.877926230	1.060913934
	C93	4.382117264	12.909703220	2.178893612
	C94	2.912714512	11.442503315	0.772868274
	C95	2.838068040	10.366424663	-0.285038593
	C96	2.917894421	10.691326361	-1.648057471
	C97	2.754989093	9.009522945	0.071747046
	C98	2.930829820	9.695347170	-2.626562331
	C99	2.786848727	7.998932386	-0.893858582
	C100	2.877206117	8.354437356	-2.238684397
	C101	5.079051230	-7.974073770	-4.675086066
	C102	4.227331373	-6.787315054	-5.056451367
	C103	3.549742839	-4.491097309	-4.412902403
	C104	4.437609225	-3.314834299	-4.815839788
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	C108	9.658551222	-3.228435842	-1.265841360
	C109	2.591051230	-4.220073770	-8.936086066
	C110	2.412255187	-2.749716028	-9.273476623
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	C112	1.132876752	-6.156662187	-8.091723021
	C113	0.215744441	-6.595030977	-6.967263464
	C114	2.586051230	-0.458073770	-8.488086066
	C115	3.889136003	0.319125936	-8.442112140
	C116	1.474019657	0.107391472	-7.575459853
	C117	1.604462648	-0.319544412	-6.134927564
	C118	2.494136852	0.317956092	-5.252193487
	C119	0.866323360	-1.419569827	-5.666438807
	C120	2.654886779	-0.152597516	-3.943924076
	C121	1.024587545	-1.888570310	-4.359633608
	C122	1.931047462	-1.263846263	-3.497002838
	C123	2.130992918	-10.518177130	1.183410685
	C124	1.807983932	-10.711527838	2.683041336
	C125	0.897333529	-9.833941816	0.551118100
	C126	1.053969705	-9.310604878	-0.845293487
	C127	1.355952009	-10.021633482	-1.989515694
	C128	0.893901828	-7.923190565	-2.528771704
	C129	0.741051230	-12.207073770	4.351913934
	C130	1.746820821	-12.885122944	5.253121256
	C131	-4.477266676	-5.136738104	-0.922445238
	C132	-3.674428872	-5.672483862	0.228145626
	C133	-2.647842869	-6.804426410	-0.176950823
	C134	-3.366931333	-7.921211619	-0.981496088
	C135	-2.436701125	-9.107791065	-1.282720495
	C136	-3.139203276	-10.282669100	-1.897609039
	C137	-2.175579500	-7.433146615	1.168830784
	C138	2.608051230	-3.464073770	0.839913934
	Fe139	2.770095341	-5.021729845	-0.323985068
	Fe140	2.690330033	-1.430747442	0.675027060
	Fe141	3.455164297	-3.015952972	2.679078345
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	H147	-5.503121472	-1.234280975	-6.324160630
	H148	-7.760790588	2.369927745	-6.688727871
	H149	-6.892958019	0.331801833	-7.486824539
	H150	-8.298956613	-0.349881162	-6.679155035
	H151	-6.320709246	3.358911198	-4.482947608
	H152	-9.716897297	2.194004558	-4.485313925
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	H158	-6.348937159	0.815005127	-2.290059670
	H159	-7.867262233	-1.465283443	-1.642022585
	H160	-5.686237436	4.641945635	1.578746408
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	H162	-8.768139672	-0.921919311	-0.206023416
	H163	-4.391166300	1.873894142	-1.680424010
	H164	-8.585783599	2.428862331	1.338026220
	H165	-7.294837756	4.845711344	0.840064700
	H166	-4.571748340	-1.598173258	1.671072746
	H167	-3.174123059	-1.393146458	0.612154476
	H168	-3.017919805	-2.401678212	2.060623960

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	H265	10.652076783	3.747729877	1.109154450
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	H269	0.657135815	5.770853354	-5.964205439
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	N392	-4.437037726	5.513855337	-3.872755113
	N393	-2.687107484	5.481689695	-1.614362450
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	N395	-0.667089117	1.230358597	-1.227533243
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	N402	7.813050289	3.303075389	0.049954196
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	O438	-2.869583959	-2.314997091	-6.034922195
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	O474	-1.213969415	-9.739091160	5.441376814
	O475	0.075974790	-7.735281480	4.080817002
	O476	2.239890368	4.463086178	-3.528768515
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	O478	-2.693185428	-10.413159075	3.186009410
	S479	6.574209355	0.694020651	1.952128867
	S480	4.606235629	-1.231216339	-0.528037271
	S481	1.079821263	-4.647597186	-1.738781983
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	S484	4.863004466	-4.963115307	-1.096943327
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	S486	5.712164348	-3.206105772	2.207939318
	S487	2.249754154	-6.636885811	1.159980111
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Fe(139)	2.354	C1	-7.199621185	-0.135707492	-6.572897169
Fe(140)	-0.911	C2	-7.093566217	0.885728855	-5.435834432
Fe(141)	2.941	C3	-7.286332392	3.254478047	-4.805714748
Fe(142)	-2.462	C4	-8.113460721	3.146759166	-3.526999612
Fe(143)	2.763	C5	-10.166123014	2.393073409	-2.447882036
Fe(144)	-2.324	C6	-9.576200984	1.416349351	-1.425410820
Fe(145)	0.354	C7	-8.171768088	-0.560852582	-1.074009315
		C8	-6.922532027	0.037455765	-0.421333619
		C9	-4.938998310	1.438571936	-0.662315543
		C10	-5.254404098	2.448498857	0.449431027
		C11	-6.754233275	4.180890357	1.274660520
		C12	-7.378067635	3.543837424	2.524022367
		C13	-9.127424408	2.085601239	3.415177761
		C14	-8.532582072	0.907096615	4.195938821
		C15	-7.279286055	-1.205087704	4.074546697
		C16	-5.766835357	-1.320631244	4.272007376
		C17	-3.556252402	-0.318959849	3.782510213
		C18	-3.096466593	0.765756836	4.771067506
		C19	-2.901790732	-0.227195688	2.386700329
		C20	-1.375543649	-0.127013118	2.496474662
		C21	-3.325428428	-1.429120799	1.538505305
		C22	-3.024495326	3.173357839	5.300667988
		C23	-4.058388599	3.367927551	6.428013974
		C24	-2.799718970	4.464761677	4.475560901
		C25	-2.541597190	5.668790620	5.388889595
		C26	-1.639366984	4.283812053	3.488423276
		C27	-6.384072692	3.666533107	7.070622558
		C28	-6.290249148	2.750630635	8.272489844
		C29	-7.605008707	-10.045514676	4.717069955
		C30	-6.102908284	-9.759773768	4.749413466
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		C32	-4.124946172	-8.336268004	7.203966969
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		C34	-2.855898627	-6.132218212	5.537187291
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		C36	-1.186852565	-2.976401629	5.496912627
		C37	-2.535621185	-9.157707492	8.878102831
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		C39	-3.054621185	0.903292508	-4.891897169
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		C41	-2.514206708	-0.159581297	-3.925465661
		C42	-3.383494390	-1.434400530	-3.853266664
		C43	-3.033661301	-2.538157745	-4.844817883
		C44	-0.826216973	3.929485233	-5.464378728
		C45	-1.611955111	5.205553032	-5.787271325
		C46	0.456253233	3.876785177	-6.315037719
		C47	-3.828479794	6.166716996	-6.244221667
		C48	-4.565548308	6.453389956	-4.926173175
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		C50	-3.985108802	5.995903746	-1.476654781
		C51	-1.748332593	5.756926322	-0.526479204
		C52	-1.418727226	7.253873477	-0.365709117
		C53	-0.423377904	5.008478561	-0.774398097
		C54	-0.569769162	3.542501499	-1.033465204
		C55	-1.354553735	2.546821482	-0.480811865
		C56	-0.167803359	1.592207038	-1.999557807
		C57	-1.068621185	9.372292508	-1.586897169
		C58	-2.118778927	10.137554919	-0.779756802
		C59	-1.088212279	9.799963658	-3.067248340
		C60	-0.548680549	11.162421134	-3.386175633
		C61	-0.272140531	12.242225025	-2.571974671
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		C70	2.670706893	0.783982360	6.144771314
		C71	1.882061219	1.875051943	6.517811276
		C72	7.865659346	1.706076194	4.257147825
		C73	8.199303708	2.943575772	3.413169807
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		C75	9.662477154	3.895898634	1.683761634
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	C89	6.566420397	10.843034784	1.528434300
	C90	8.276415253	9.189058172	0.597816195
	C91	7.537382316	8.948834779	-0.713959626
	C92	4.399378815	11.878292508	1.034102831
	C93	4.445551480	12.949148183	2.115894062
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	C95	2.835121725	10.357692536	-0.25108027
	C96	2.863261454	10.689100032	-1.614222863
	C97	2.801557810	8.998634836	0.099900979
	C98	2.887220188	9.697843971	-2.598759563
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	C100	2.893098560	8.353705507	-2.216972766
	C101	5.103378815	-7.973707492	-4.701897169
	C102	4.265321791	-6.770086877	-5.066452520
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	C117	1.580417921	-0.301430665	-6.194496297
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	Fe139	2.840654695	-5.086792923	-0.271241465
	Fe140	2.687645763	-1.443552784	0.555491406
	Fe141	3.439374480	-2.961235672	2.649616079
	Fe142	4.575414120	-3.316805984	0.315451918
	Fe143	5.106046787	-1.048269370	1.586161596
	Fe144	1.673921390	-4.704353068	2.037504096
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	H147	-5.497535238	-1.266983490	-6.401591922
	H148	-7.660505747	2.386158309	-6.720050496
	H149	-6.856301143	0.324913232	-7.511206167
	H150	-8.277951191	-0.331652895	-6.709341886
	H151	-6.238277833	3.329224525	-4.485411405
	H152	-9.661374058	2.250131437	-4.537838879
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	H155	-8.663196212	0.365341379	-2.932908044
	H156	-10.313466734	3.349812664	-1.930861479
	H157	-4.254564319	0.695896063	-0.235483549

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H171	-1.804398467	3.447739713	2.795013678
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H188	1.486470114	3.751880957	6.212388589
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Fe(144) -2.314	C6	-5.430567429	-2.302936201	7.793483284
Fe(145) 2.028	C7	-3.474068737	-3.312089792	6.714405579
	C8	-2.908553752	-2.134552077	5.915684445
	C9	-3.177088185	-0.588920476	4.049372103
	C10	-3.118587461	0.721838626	4.846569636
	C11	-4.129421020	2.121856467	6.562700145
	C12	-3.092950945	2.097423257	7.695621831
	C13	-2.248048955	0.916760494	9.662943642
	C14	-0.766519870	0.554042227	9.504849135
	C15	0.882865012	-0.845590872	8.338007981
	C16	1.655139594	-0.416986457	7.089650859
	C17	1.541039013	0.748943192	4.907894168
	C18	1.761009172	2.269127772	4.969620638
	C19	0.747523648	0.269092051	3.673843248
	C20	1.336059766	0.836621569	2.377024355
	C21	0.708459796	-1.262084409	3.647913111
	C22	0.721206935	4.497869029	5.154147717
	C23	1.016802605	4.957209922	6.596536141
	C24	-0.552242701	5.156989819	4.569633624
	C25	-0.533398550	6.676721554	4.766614860
	C26	-0.711912420	4.815117667	3.083195312
	C27	0.418844185	4.887462945	8.952974522
	C28	1.853772321	4.822507279	9.432333449
	C29	6.527323911	-7.670453616	8.919973021
	C30	6.936076017	-7.001694246	7.606989711
	C31	7.299807226	-4.762483273	6.554866933
	C32	8.560132970	-4.007637591	7.017979530
	C33	6.159286083	-3.794765777	6.184491750
	C34	6.532581666	-2.767010198	5.107962750
	C35	5.274914548	-2.136197988	4.506517113
	C36	5.235673213	0.203978410	3.620015895
	C37	10.830573770	-3.327237705	6.391909836
	C38	10.969821623	-1.993305895	5.688208160
	C39	-5.136426230	-2.728237705	0.409909836
	C40	-5.567757815	-1.309165197	0.015612903
	C41	-3.641037661	-2.931283846	0.394479599
	C42	-3.185864371	-4.164293437	1.210694502
	C43	-3.052541025	-5.460736964	0.419159508
	C44	-6.532464285	0.014124599	-1.826527591
	C45	-7.822953445	0.643161556	-1.286807939
	C46	-6.618963378	-0.123111301	-3.357699850
	C47	-9.545402014	0.548198810	0.466852256
	C48	-9.052993492	1.266359766	1.733239769
	C49	-7.120310008	1.781720470	3.171818264
	C50	-6.114965994	2.882900004	2.830176416
	C51	-4.472204571	3.828706531	1.293902860
	C52	-5.132006404	5.205380720	1.083416751
	C53	-3.703442225	3.471914249	0.007332651
	C54	-3.052611053	2.124903840	0.018997630
	C55	-2.361178865	1.399711837	0.973220090
	C56	-2.415023669	0.167622853	-0.791943969
	C57	-7.140426230	6.355762295	0.205909836
	C58	-7.424264495	7.101762391	1.510345065
	C59	-8.449469500	5.908586457	-0.471891555
	C60	-9.291565569	6.982943498	-1.096214593
	C61	-9.263947769	8.357066631	-0.959703346
	C62	-10.858675935	7.751896706	-2.374724680
	C63	8.983164854	4.347908089	2.689198007
	C64	10.161210587	3.522530041	3.168473890
	C65	7.737465890	3.422312373	2.745141621
	C66	6.483502878	4.121360269	2.275621596

C67	5.772710315	4.979802086	3.133562140
C68	6.005029650	3.957703664	0.961797087
C69	4.633908977	5.661426883	2.698695130
C70	4.866562016	4.631941234	0.512020550
C71	4.186112398	5.487780653	1.383436614
C72	4.933249850	5.832066304	-4.966194051
C73	3.716814297	6.468714176	-5.650436817
C74	4.483703586	4.711815045	-4.016907986
C75	2.464887689	6.729167931	-7.748514985
C76	1.102529584	6.085582998	-7.494094409
C77	-0.154817515	4.252804276	-6.458636361
C78	-0.636452188	4.671605398	-5.057978711
C79	-0.058921144	2.721612045	-6.605863455
C80	-1.358451943	1.943728906	-6.350520344
C81	-2.529833256	2.258862136	-7.284007644
C82	-4.240124306	4.020355991	-7.545673634
C83	-0.100084146	5.266844294	-2.749658910
C84	-0.348701036	6.775208601	-2.575560556
C85	0.938823269	4.843871412	-1.697783582
C86	0.554079863	8.997813842	-3.030354649
C87	-0.132816530	10.077059044	-3.856418667
C88	-1.713547730	10.623520984	-5.651354858
C89	-2.962928577	11.328030176	-5.080178964
C90	-1.987462223	9.990819277	-7.028795110
C91	-3.051232853	8.897653681	-6.995572259
C92	-4.745426230	11.286762295	-3.400090164
C93	-4.605863172	12.728023775	-2.930292684
C94	-5.191557962	10.396034427	-2.208713957
C95	-5.327571943	8.949702246	-2.621308928
C96	-6.477684381	8.499983202	-3.290209074
C97	-4.277396963	8.038064729	-2.421697263
C98	-6.568833753	7.192743611	-3.770701554
C99	-4.344800138	6.731410819	-2.912324005
C100	-5.489021623	6.321809191	-3.595365761
C101	3.377573770	-7.433237705	-6.714090164
C102	2.085000100	-6.900795821	-6.137751574
C103	0.933944375	-4.902854512	-5.236514532
C104	0.261396269	-3.935674238	-6.210364814
C105	0.371956901	-1.738334887	-7.261485889
C106	1.329353766	-0.823215106	-8.014875358
C107	3.584573770	0.084762295	-8.296090164
C108	4.599222361	-0.521665917	-9.241404916
C109	-2.819426230	-7.390237705	-6.507090164
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C112	-1.617276703	-8.900788748	-4.813158997
C113	-0.902232496	-8.914985221	-3.477194341
C114	-4.762426230	-4.145237705	-6.293090164
C115	-4.675153235	-3.119683914	-7.410270868
C116	-4.915911308	-3.530803218	-4.883490911
C117	-3.602531077	-3.081814404	-4.296482428
C118	-3.031582906	-1.838027234	-4.619363367
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C120	-1.762436459	-1.492112304	-4.140280964
C121	-1.608881876	-3.619417633	-3.004622499
C122	-1.040163734	-2.386346244	-3.343101301
C123	7.929571742	-7.329070479	-1.337288797
C124	8.989632099	-6.730696564	-0.388023614
C125	6.613432298	-7.372596324	-0.529999120
C126	5.359301676	-7.647114651	-1.300710217
C127	5.051596366	-8.751543706	-2.069420711
C128	3.271007877	-7.443940973	-1.924890237
C129	10.675573770	-7.253237705	1.342909836
C130	12.081397094	-6.958559746	0.864283988
C131	0.768979092	-5.553863679	3.372678017
C132	2.246867934	-5.324474064	3.351243652
C133	2.985151289	-6.212916345	2.264623581
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Fe139	3.907428002	-3.427665159	-2.621671856
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Fe144	4.906205535	-2.223688933	-0.524884907
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	H147	-5.816609756	-5.935887720	1.857842448
	H148	-9.043400956	-3.808231220	3.629201236
	H149	-8.068900466	-5.647359490	2.547993730
	H150	-7.629575244	-6.149583946	4.176209790
	H151	-7.508419024	-1.466544878	3.410705203
	H152	-8.163579526	-3.318869087	6.415631410
	H153	-9.094503085	-1.591508842	4.206549036
	H154	-7.326151665	-2.988966131	8.554453972
	H155	-5.530012809	-3.700554064	6.295756160
	H156	-7.229364880	-1.242584043	8.214165341
	H157	-2.167917920	-0.766795015	3.657705712
	H158	-4.458876642	-2.247693471	4.550878469
	H159	-3.266851565	-4.249162662	6.180403037
	H160	-3.919570371	3.009658761	5.953607808
	H161	-4.897724391	0.263581197	5.794322982
	H162	-2.941632952	-3.333747916	7.673199405
	H163	-3.853980586	-0.469176083	3.190643016
	H164	-3.704545802	0.201821193	8.274060759
	H165	-5.130739699	2.231024966	7.002416985
	H166	0.312168224	-1.675949173	4.586557303
	H167	0.073950567	-1.610149940	2.821641677
	H168	1.714782107	-1.674228797	3.474009661
	H169	-0.284307679	0.641633332	3.778763953
	H170	-2.697997158	0.171432129	10.334829180
	H171	-0.771174006	3.732428194	2.906134309
	H172	-0.538270731	3.811549660	7.390922420
	H173	-0.498152450	6.962498348	5.827563568
	H174	0.725124108	0.522524903	1.519348846
	H175	2.359825925	0.472723417	2.204639113
	H176	8.828919146	5.174158432	3.408270800
	H177	-1.629731026	5.277467298	2.690715826
	H178	-1.439512577	7.118506884	4.326831038
	H179	0.137711227	5.204857347	2.498609548
	H180	0.339859196	7.126583818	4.267644180
	H181	-1.421688326	4.750629824	5.117787996
	H182	1.596691657	4.821956268	4.573109293
	H183	-0.274897119	2.598478939	4.984753411
	H184	1.364963974	1.937320240	2.385468505
	H185	1.231793501	3.797640989	-1.883156591
	H186	0.445283045	4.897445358	-0.714981430
	H187	2.397310827	5.835943421	-0.835076790
	H188	2.708910103	6.734086323	1.580365361
	H189	4.496941599	4.479139405	-0.503455435
	H190	6.520472806	3.278621255	0.277633392
	H191	6.108365933	5.114815139	4.165115797
	H192	-0.034068266	0.448311200	6.336506899
	H193	0.849513020	-1.945877334	8.332174636
	H194	1.477663401	-0.533453729	9.206749946
	H195	-1.202948940	-0.722834151	7.926374087
	H196	-2.274900843	1.892689431	10.164984636
	H197	4.087481333	6.314263835	3.384178577
	H198	2.541192258	0.303680572	4.878176039
	H199	0.042045832	5.914093194	9.088374783
	H200	-0.169894499	4.220643768	9.602057704
	H201	2.486298299	4.047419555	8.941476637
	H202	11.680924664	-3.973316598	6.127811755
	H203	-1.811639632	-7.062558934	0.136995371
	H204	1.030206014	-6.848763123	4.770447442
	H205	-2.350630388	-9.718580636	-4.817242965
	H206	-0.894985951	-9.073512512	-5.624242977
	H207	-3.210559048	-7.518085050	-4.357360222
	H208	-4.229522305	-3.516487116	-8.353832147
	H209	-3.247809022	-8.352752699	-6.826931897
	H210	-3.302957161	-2.988757226	-0.649917656
	H211	-3.876127418	-4.340883222	2.050410877
	H212	-2.731441206	-4.806539985	-6.422714241
	H213	-5.690982125	-4.708374338	-6.518690435
	H214	-1.290917313	-6.181600304	-7.200977374
	H215	-1.190726740	-5.863833715	1.262029713
	H216	-1.693022176	-6.712791676	-4.779593950
	H217	-1.098910590	-7.767643015	-7.538517009
	H218	-6.729856798	-3.968135709	-0.058715292
	H219	-3.184328620	-2.029159379	0.820633759
	H220	0.611271216	-8.110171735	-4.402386558
	H221	-2.221559609	-3.943079819	1.669737660
	H222	-3.771191178	3.956305727	2.132156138
	H223	-2.127887022	1.684831028	1.996891265
	H224	-7.917675517	2.257562681	3.755036850
	H225	-7.133724337	0.540022046	1.437062262
	H226	-6.803131525	4.247304903	0.398839610

H227	-8.642139427	9.021766137	-0.371044856
H228	-7.634346616	6.428058819	2.376080067
H229	-9.055925956	5.337859507	0.255107439
H230	-6.567634840	7.018371854	-0.460787921
H231	-11.684205285	7.849588035	-3.075550796
H232	-2.961250285	4.270951779	-0.150705656
H233	-4.397183937	3.520656210	-0.847291954
H234	-10.519518007	9.803590459	-1.915237999
H235	-8.174946572	5.195181368	-1.266853264
H236	-5.378861727	1.893837467	1.160672723
H237	-6.629178425	1.048512485	3.831783592
H238	-10.085420369	1.289963701	-0.135814035
H239	-2.255716643	-0.628595879	-1.515086181
H240	-10.260883235	-0.227299650	0.771085450
H241	-1.221753926	-1.915498974	0.632853543
H242	9.885797905	5.572958246	1.313462886
H243	8.370443210	5.119736601	0.893521480
H244	1.272986544	4.594313481	-4.281414457
H245	-1.048793071	4.762410080	-2.520552429
H246	1.074008042	7.195964731	-3.990937868
H247	-3.442439573	1.603635647	-2.025175467
H248	-5.119490621	1.956085467	-3.782002425
H249	-4.328406535	3.277163207	-3.638056752
H250	-5.689963042	-0.577218142	-3.729319177
H251	-7.466982957	-0.772964582	-3.635820559
H252	-1.034231471	9.624972000	-7.437855786
H253	-2.358278825	10.788318453	-7.687537480
H254	-1.642000373	7.395857512	-7.452131960
H255	-3.305392558	6.884789654	-7.206675787
H256	-5.446490578	3.911054675	-9.200068986
H257	-3.259156672	1.433978298	-7.254318221
H258	-7.472865498	6.855583918	-4.285086449
H259	-3.382212025	8.335636598	-1.869648205
H260	-4.909244256	5.196934827	-6.024915168
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H262	1.977098785	4.511191604	-6.475543930
H263	-1.693950492	2.044440383	-5.306023680
H264	-8.159843245	-0.980502871	-0.116119764
H265	2.693256702	6.621744249	-8.817383244
H266	-6.208507465	-2.155416675	-1.674491988
H267	0.289549988	2.511706762	-7.629022449
H268	-3.508420086	6.044887575	-2.774569867
H269	-7.388783680	1.658903791	-3.403403682
H270	2.342262288	7.799993163	-7.535713923
H271	-4.104349239	2.817203044	-9.206313499
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H278	-2.161184364	2.348572037	-8.320307907
H279	-1.123546670	0.881066992	-6.498705276
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H288	7.823441810	-6.599062594	-2.155188629
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H297	5.592679186	5.397358365	-5.733929261
H298	5.824562769	-3.275158335	7.097510442
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H301	5.166737269	1.964666739	2.583463844
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H303	-1.062474881	-4.311170974	-2.363674835
H304	-0.289153927	-1.074258156	-6.681731115
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Fe(142) -2.606	C4	-7.938283616	-1.044633365	4.817756967
Fe(143) 2.845	C5	-7.847303249	-1.031393612	7.251578602
Fe(144) -2.376	C6	-6.327665821	-0.920295142	7.429910193
Fe(145) 1.889	C7	-4.145106020	-1.914034133	6.929136737
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C126	6.068919864	-7.091828276	1.446388189
C127	5.962255343	-8.389427389	0.987287474
C128	4.092079701	-7.295904526	0.527370201
C129	10.919517622	-5.363761134	4.488909695
C130	12.350534251	-5.056998762	4.101210500
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C132	2.176740173	-4.004959922	4.875656841
C133	3.131007517	-5.049950326	4.165097805
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Fe139	4.529808788	-3.513646591	-1.175092395
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Fe141	5.087872497	0.065368911	-1.129710878
Fe142	4.461978239	-1.636379164	-2.965539844
Fe143	3.953299873	0.916023317	-3.501095493
Fe144	5.181935979	-1.742578940	0.649664057
Fe145	2.717017851	-2.336632973	0.155476813
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	O437	-5.409680202	-0.745312478	0.221637603
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	O459	2.102092909	-2.031015519	-8.304732653
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	S479	3.771689157	2.551561302	-5.076034972
	S480	2.562961776	-0.776535225	-3.842831512
	S481	2.656569176	-4.502500409	-0.359001668
	S482	3.562706269	1.658536212	-1.368004426
	S483	-0.768482378	-3.108761134	0.865909695
	S484	4.950915472	-3.753437924	-3.366359666
	S485	3.540272383	-1.938177640	2.171447407
	S486	5.999050221	-0.046279554	-3.218349701
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Fe(139) 2.425	C1	-8.644243852	-3.971563525	-2.116036885
Fe(140) -1.695	C2	-8.157275039	-3.667928080	-0.696369152
Fe(141) 2.360	C3	-8.728338680	-2.621350084	1.456728489
Fe(142) -2.607	C4	-8.232366993	-3.691542370	2.424483599
Fe(143) 2.828	C5	-8.299894239	-6.016042456	3.158749172
Fe(144) -2.344	C6	-6.831416854	-6.391929670	2.925983650
Fe(145) 2.016	C7	-4.993490747	-6.497381706	1.309604490
	C8	-4.074415949	-5.364676218	1.775920330
	C9	-3.746574675	-2.961581773	2.055968500
	C10	-3.526489098	-2.949238867	3.574357498
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	C12	-3.639662317	-4.562543733	6.285311390
	C13	-3.309928874	-6.983517144	6.244875045
	C14	-1.890764128	-7.312161289	5.762627909
	C15	-0.363141066	-7.446629767	3.844023238
	C16	0.637583006	-6.350003617	3.479896931
	C17	0.996957478	-3.925642815	3.167893343
	C18	1.493069246	-3.185810353	4.419051419
	C19	0.289875387	-3.042115544	2.118523625
	C20	1.132667193	-1.810650472	1.771439578
	C21	-0.020444374	-3.882762642	0.877068830
	C22	0.868270488	-1.964450951	6.472221836
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	C33	4.319406750	-8.479634933	-0.341766142
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C49	-6.980534437	-0.029769891	3.930096688
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C51	-3.731426645	1.965688162	4.379542519
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C53	-2.881253308	2.686037266	3.311232808
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C56	-2.347972218	1.403785607	-0.051743754
C57	-5.647243852	4.796436475	6.065963115
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C95	-2.943151234	8.056504140	6.467354448
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C55	-0.949888488	2.892664386	0.407546768
C56	-2.223545576	1.470016700	-0.723373109
C57	-2.589201629	9.046824847	-1.661067210
C58	-1.643788535	10.136337982	-1.156248485
C59	-4.060496667	9.492435485	-1.508109869
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C62	-6.055656861	11.400240719	-3.798001461
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C65	8.856458109	-1.451284538	-1.461830660
C66	7.947082531	-0.338009762	-1.929014566
C67	8.217826896	1.001915319	-1.599078584
C68	6.809765419	-0.605317928	-2.711759411
C69	7.387911383	2.038894359	-2.030450600
C70	5.964459362	0.420094499	-3.144690823
C71	6.259838487	1.741959215	-2.804571992
C72	3.715161897	-0.457008952	-8.178009274
C73	2.766740825	0.531783714	-8.868399614
C74	3.422069682	-0.512871638	-6.672616928
C75	0.915899825	0.800887126	-10.466546822
C76	-0.260642335	1.305393435	-9.630790887
C77	-1.501044486	1.133932838	-7.522375096
C78	-1.007715043	2.208228482	-6.535139454
C79	-2.148632470	-0.075740429	-6.822047228
C80	-3.359937368	0.233483389	-5.935702474
C81	-4.568403764	0.864795196	-6.630630290
C82	-5.262148131	3.105800954	-7.406414593
C83	0.816019699	3.124067448	-5.191082766
C84	1.355053819	4.392532845	-5.872499298
C85	1.957533602	2.545705338	-4.340339645
C86	2.743066098	5.203228397	-7.707204562
C87	2.22281566	6.164465926	-8.766894889
C88	0.300986198	6.956229354	-10.073509410
C89	-0.085549540	8.396658720	-9.671757950
C90	-0.866116617	6.219175767	-10.759626584
C91	-2.083988016	6.039075496	-9.857413849
C92	-0.566201629	9.949824847	-7.837067210
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C94	-0.651785784	9.916503432	-6.287953582
C95	-1.604399521	8.849288569	-5.804506665
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C103	-4.169672210	-5.768624813	-1.648736045
C104	-4.734990626	-4.963803232	-2.824126733
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C107	-1.515201629	-4.808175153	-7.447067210
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	C116	-7.729364693	-1.012488210	-0.730108226
	C117	-6.261734759	-1.182426131	-0.985397540
	C118	-5.654661300	-0.578834319	-2.096091935
	C119	-5.514660175	-2.076368478	-0.200275099
	C120	-4.353270948	-0.929756158	-2.461253708
	C121	-4.215173893	-2.425841247	-0.566423293
	C122	-3.648627822	-1.883749249	-1.724702575
	C123	2.149351923	-10.770418951	1.204467732
	C124	3.681877833	-10.646162405	1.359027694
	C125	1.539917037	-9.718418688	2.153872964
	C126	0.088356526	-9.391372105	1.977735510
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	C131	0.137424934	-3.596430497	5.813924591
	C132	1.249073769	-4.306788309	5.099549401
	C133	0.867103034	-5.766817263	4.610353362
	C134	0.260472079	-6.583253616	5.785845167
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	Fe145	0.501714498	-3.446709648	0.512027641
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	H148	-6.516731936	4.021185325	7.123049036
	H149	-7.109054374	1.763383867	7.061034720
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	H159	-1.046776666	0.911856631	8.228732954
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	H163	-1.528203432	2.984552683	3.870956220
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	H165	0.689719073	6.936292895	5.531601921
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	H167	0.985434470	-0.629837821	3.348937660
	H168	2.590617104	-1.325494653	3.584179722
	H169	1.988888421	1.626310817	2.945716940
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	H182	5.486982933	3.862840595	0.722991119
	H183	3.428853686	3.550555720	2.798085603
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	H188	5.741198942	3.601753044	-2.995240213
	H189	5.070861338	0.188683407	-3.724711112
	H190	6.567615162	-1.636191194	-2.984987655
	H191	9.085537673	1.242426440	-0.980630506
	H192	3.392714790	2.263063360	4.990789319
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	H166	1.364921053	0.057343669	4.959488379
	H167	0.601913782	-0.526305229	3.458203046
	H168	2.211263605	-1.103815228	3.891941918
	H169	1.493413177	1.795278199	3.142361108
	H170	1.763124979	5.353866388	9.147358428
	H171	2.045608287	4.162100189	0.790018940
	H172	4.051969494	5.788880971	4.502135074
	H173	4.755619614	7.492115052	1.578412825
	H174	1.494848912	0.174126790	1.212318798
	H175	3.150404593	-0.280893498	1.571532120
	H176	10.921786584	0.130905964	-0.807256356
	H177	1.944592884	5.706506571	-0.091125682
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	H179	3.283044954	4.579635818	-0.415456690

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H187	4.235943173	2.756259900	-3.947039498
H188	5.816700804	3.975279864	-2.331209172
H189	5.467446687	0.514531599	-3.080308494
H190	6.976821077	-1.196307759	-2.128028690
H191	9.028540452	1.865823201	0.129309487
H192	2.589821332	2.547123617	5.330692495
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	O470	-0.471348488	-3.557281881	7.216142705
	O471	-0.080857659	-9.783032704	7.062231625
	O472	-1.959328776	-8.539760675	6.894504916
	O473	2.401599352	-6.612549856	3.384797082
	O474	2.888603699	-6.351957187	5.568331770
	O475	-0.048554385	-5.673597612	3.621737411
	O476	6.654933441	-7.883914575	4.658537198
	O477	5.148236441	-6.816407595	2.661229357
	O478	-3.990659017	2.825459244	-3.901623310
	O479	2.573413568	-10.614803935	5.986422816
	O480	4.425915070	-8.456427301	6.228316822
	O481	-8.307580961	3.236253343	-5.173097535
	S482	2.475423991	-0.856149004	-6.010338380
	S483	0.018014167	-2.271923835	-3.551810321
	S484	-0.959940288	-5.039496359	0.707630471
	S485	3.267120564	-1.369299073	-2.129128365
	S486	-0.770469839	-1.875637868	-0.164045183
	S487	-0.186322244	-6.182990323	-3.004517507
	S488	2.289139243	-3.937709052	2.007576208
	S489	2.877081068	-4.241937143	-4.281086197
	S490	2.063326580	-6.968437509	-0.053380510
	S491	4.802567728	-4.470036481	-0.682956948
8 (S=1)	bm1b2b6x262n2xassta.car_6			
Fe(139) 2.410	C1	-7.117476639	1.140751707	6.635356434
Fe(140) 0.040	C2	-6.097557041	2.229651457	6.288830798
Fe(141) 2.682	C3	-5.775924756	4.595213110	5.690383360
	C4	-4.589835956	4.939286984	6.586406046
	C5	-3.664054501	5.071144545	8.837516274

Fe(142) -2.600	C6	-2.457668246	4.141953977	8.653777682
Fe(143) 1.900	C7	-1.705755846	1.891569186	8.031624091
Fe(144) -2.382	C8	-1.057182873	2.129580066	6.665888277
Fe(145) -0.136	C9	-1.353233214	2.716153753	4.321531291
	C10	-0.403042846	3.920487664	4.273070486
	C11	0.112001702	6.153160393	5.105323744
	C12	1.347662251	5.994229084	6.000436014
	C13	2.213993393	5.348282440	8.197339928
	C14	3.198381499	4.175717344	8.108801739
	C15	3.503516071	1.788229406	7.607780867
	C16	3.918005586	1.256261055	6.232563761
	C17	3.473484965	1.314461853	3.798859058
	C18	4.283380353	2.337801340	2.981494698
	C19	2.150882088	0.875940711	3.129748474
	C20	2.387974131	0.476816013	1.671808571
	C21	1.511597490	-0.270532620	3.921768108
	C22	4.429701903	4.647083454	2.117637836
	C23	5.431573730	5.379228660	3.034320200
	C24	3.423788640	5.605608975	1.437227135
	C25	4.129243304	6.832243678	0.846058737
	C26	2.635009880	4.867405276	0.349552458
	C27	5.858028686	6.587024973	5.097322135
	C28	7.116551049	5.812604318	5.433016288
	C29	5.309996258	-6.087894193	10.692557102
	C30	5.470212838	-6.353434307	9.195175068
	C31	6.331071446	-5.337352399	7.081040968
	C32	7.863581134	-5.305683050	6.941502541
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	C35	5.107625096	-3.104098472	4.131130458
	C36	5.735216569	-1.737742506	2.136544419
	C37	9.787523361	-6.301248293	5.798356434
	C38	10.178761849	-5.779792742	4.432787895
	C39	-5.247476639	1.035751707	2.444356434
	C40	-5.118822167	2.291202516	1.563466296
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	C42	-3.715838429	-0.900522514	3.321283560
	C43	-4.363735129	-2.262513172	3.091772291
	C44	-5.719828346	3.184953957	-0.662070970
	C45	-5.899075833	4.663915888	-0.320133925
	C46	-6.670704056	2.751351311	-1.802453285
	C47	-7.038206822	6.298543298	1.111437181
	C48	-5.873546216	6.932611400	1.883214667
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	C50	-2.479716334	6.672859483	1.941652204
	C51	-1.458317231	5.958210080	-0.169499479
	C52	-1.538385130	7.296370686	-0.917598933
	C53	-1.602140808	4.865062920	-1.239001947
	C54	-1.610870219	3.459989155	-0.739099516
	C55	-0.981877967	2.887204211	0.343512710
	C56	-2.122928402	1.350759054	-0.779618054
	C57	-3.000476639	8.816751707	-2.134643566
	C58	-2.172838802	9.993031579	-1.612571013
	C59	-4.502978034	9.173683681	-2.135702324
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	C62	-6.389227275	10.877410506	-4.665201963
	C63	10.614315570	-0.750754616	-1.057382318
	C64	11.511123938	-1.774971583	-0.390932956
	C65	9.246270435	-0.797140414	-0.322205790
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	C68	7.246781250	-0.182254002	-1.767692460
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	C71	6.432861435	2.085461349	-1.907014893
	C72	4.888236871	-0.243068986	-7.586999668
	C73	3.965185663	0.653406309	-8.419614783
	C74	4.391159306	-0.321207672	-6.138870446
	C75	2.355018529	0.772034434	-10.269766169
	C76	1.041186300	1.200961844	-9.617363179
	C77	-0.475306873	0.947068148	-7.707245235
	C78	-0.212748818	2.063559051	-6.680454075
	C79	-1.116721824	-0.306141657	-7.082558552
	C80	-2.449861892	-0.082305226	-6.362206246
	C81	-3.606704915	0.441506748	-7.216933526
	C82	-4.400717734	2.628082922	-8.058849740
	C83	1.308987233	3.155597225	-5.114821682
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	C85	2.306250080	2.688444397	-4.047447041

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	C89	0.554355729	8.283390218	-9.761985199
	C90	0.116138245	6.040636714	-10.906704573
	C91	-1.190977373	5.758600469	-10.172425042
	C92	-0.294476639	9.800751707	-8.030643566
	C93	0.581484560	10.997372877	-8.374631627
	C94	-0.564022191	9.775488443	-6.503090723
	C95	-1.460633936	8.623418804	-6.116735853
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	C106	-2.366763987	-4.214681881	-6.476457000
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	C115	-8.062899977	-2.433796080	-4.064340352
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	C117	-6.154642477	-1.336305468	-1.895207722
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	C119	-5.303882381	-2.164241020	-1.151762439
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	C122	-3.429834345	-1.497876054	-2.538899363
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	Fe140	1.169724999	-1.963971830	-1.621169507
	Fe141	3.331075767	-3.701411506	-2.042029027
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	Fe144	2.718508220	-4.831216239	0.106452228
	Fe145	0.532574791	-3.416154072	0.533292604
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	H147	-6.547960539	-0.440762536	5.469453398
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	H159	-2.144251247	0.884517574	8.049667045
	H160	0.467267953	6.402444363	4.099013476
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	H262	1.388902900	-0.057006857	-8.013054478
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	H267	-1.265310730	-1.031771631	-7.898498044
	H268	-1.296736594	5.364843116	-5.059538630
	H269	-7.575525427	3.309235461	-4.379290566
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	H275	-3.301810976	9.645674031	-6.625440637
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	C85	-0.447963081	5.148585216	1.113131003
	C86	-1.927850915	9.078344882	2.304655326
	C87	-3.015733444	10.144524557	2.313200839
	C88	-5.092801067	10.991290184	1.319744003
	C89	-6.237689788	10.894417398	2.350425102
	C90	-5.625439300	11.060326955	-0.124514955
	C91	-6.397637178	9.814304355	-0.546320160
	C92	-7.420448065	9.481295316	3.966452138
	C93	-7.448283681	10.480741105	5.114156398
	C94	-7.320257952	8.039250278	4.529361303
	C95	-7.349623337	7.016055122	3.419965258
	C96	-8.567300723	6.630299897	2.837326606
	C97	-6.161236850	6.490575042	2.888096152
	C98	-8.600116208	5.772585405	1.736535558
	C99	-6.175605947	5.643112355	1.776710032
	C100	-7.400032854	5.295784965	1.205121229
	C101	2.675551935	-1.915704684	-10.020547862
	C102	1.489223693	-2.152013498	-9.114061316
	C103	0.232532456	-1.291559948	-7.160945481
	C104	-0.826668767	-0.204015972	-7.356910483
	C105	-1.361153585	2.155129704	-7.060175636
	C106	-0.804141009	3.554909363	-7.279949543
	C107	1.090551935	5.099295316	-7.311547862
	C108	1.829321089	5.331082325	-8.612393620
	C109	-3.130448065	-3.822704684	-8.949547862
	C110	-4.414338083	-3.391092166	-8.262398565
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	C112	-1.262458136	-5.537512533	-8.545111078
	C113	-0.193607175	-5.973453811	-7.562362920
	C114	-5.481448065	-1.831704684	-6.747547862
	C115	-5.883379867	-0.427856635	-7.164888799
	C116	-5.418491022	-2.044329099	-5.219429278
	C117	-4.152495675	-1.449970407	-4.675243739
	C118	-4.064055535	-0.080287721	-4.382832263
	C119	-2.988956578	-2.235131598	-4.633007726
	C120	-2.818007539	0.503244369	-4.132628540
	C121	-1.747442599	-1.651742101	-4.384890075
	C122	-1.657886928	-0.272352662	-4.165418323
	C123	8.524755304	-3.044153710	-6.284715358
	C124	9.659925497	-2.688073454	-5.299694967
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	C131	2.918798495	-6.143043100	-0.323421281
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	C133	4.767373643	-5.358503250	-1.952434779
	C134	4.934865443	-6.823807453	-2.442545190
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	C137	6.197146229	-4.741270413	-1.852667187
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	Fe143	2.074979340	3.946603492	-2.621932006
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	Fe145	2.612209505	-1.205234721	-2.110770771
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	H148	-6.834027063	-7.595834872	2.279186271
	H149	-5.897459038	-8.299305412	0.265156736
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H158	-2.533771620	-5.544427183	3.210151128
H159	-0.566200665	-7.596857727	3.397466876
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H164	-1.259531836	-4.979627232	7.495954219
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H174	1.271728550	-0.266259951	1.411271449
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H177	-1.690325662	2.412475813	5.326014123
H178	-1.424854735	3.152131118	7.662828790
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H181	-0.721328317	0.847111201	7.025665605
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H188	1.840729393	5.562399454	4.593533475
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H198	3.818180115	-1.486193879	3.962880499
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H202	13.497758070	-2.873975182	1.416011244
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H212	-3.466965322	-1.720180297	-7.467210924
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	H252	-4.781394563	11.266623230	-0.798188254
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	H264	-7.868240581	-2.947661614	0.453615220
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	H370	-10.231017297	1.172164566	-3.591186896
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Fe(140) -0.619	C2	-8.376371518	2.519747172	2.337321583
Fe(141) 2.781	C3	-7.575951474	4.301041539	3.829789844
Fe(142) -2.507	C4	-7.251295320	3.482150177	5.077147257
Fe(143) 2.429	C5	-8.070056570	2.083348263	6.898027229
Fe(144) -2.337	C6	-7.197067967	0.845497064	6.668123443
Fe(145) -0.452	C7	-6.570868273	-0.934732762	5.103235962
	C8	-5.143302128	-0.535123960	4.716671768
	C9	-3.712089280	1.042391032	3.523438734
	C10	-2.795248698	1.481909314	4.670107367
	C11	-2.652555146	2.332531896	6.959669435
	C12	-2.389601913	1.132347934	7.882741365
	C13	-3.377569111	-0.645160422	9.249353367
	C14	-2.828716806	-2.015787437	8.835706074
	C15	-2.737511939	-3.760427974	7.108006692
	C16	-1.522172566	-3.823163798	6.179013953
	C17	-0.026854101	-2.496064943	4.717825046
	C18	1.254751268	-1.914071153	5.343523305
	C19	-0.505837310	-1.728128010	3.466204450
	C20	0.655624042	-1.491244881	2.501212662
	C21	-1.648177850	-2.480653147	2.776608680
	C22	2.287634973	-0.016602228	6.548993307
	C23	2.434541117	-0.484962641	8.011674448
	C24	2.194561324	1.522903741	6.422093862
	C25	3.323142068	2.210194039	7.199723739
	C26	2.226817469	1.950242457	4.949356219
	C27	1.397945197	-0.850925385	10.178696056
	C28	2.048486942	-2.206770984	10.369292642
	C29	-4.737063512	-11.806221470	4.276481376
	C30	-3.574743696	-11.475071623	3.338616453
	C31	-1.355449522	-10.329383722	3.264828657
	C32	-0.201695534	-11.119716363	3.909073105
	C33	-1.141229611	-8.809439813	3.395136551
	C34	0.192083013	-8.321848192	2.818100779
	C35	0.204465183	-6.800113512	2.687563552
	C36	2.209844871	-5.309302265	2.649992468
	C37	1.830361514	-12.407519072	3.449899745
	C38	3.148999566	-11.695067656	3.242685109
	C39	-5.202638486	2.693480928	-0.239100255
	C40	-4.283303434	3.888974265	0.040729227
	C41	-4.339494073	1.442792782	-0.509651135
	C42	-5.061263288	0.081746944	-0.427324397
	C43	-5.704922865	-0.396782198	-1.727380183

	C44	-3.310573266	5.903433100	-0.965259759
	C45	-3.671972224	7.072904243	-0.040132210
	C46	-3.043804731	6.420027541	-2.391264361
	C47	-5.217610062	7.907571031	1.679079342
	C48	-4.755572939	7.435206721	3.065530614
	C49	-3.691168730	5.627744771	4.360480874
	C50	-2.170686921	5.461854023	4.375470764
	C51	-0.077582060	5.169994222	3.149586484
	C52	0.623114154	6.437013463	3.676912004
	C53	0.457975178	4.974330786	1.723148324
	C54	-0.100822384	3.809107679	0.983488633
	C55	-0.605029799	2.603055721	1.401534591
	C56	-0.637597725	2.635686106	-0.829393064
	C57	0.620361514	8.889480928	3.541899745
	C58	0.745743317	9.054078218	5.059829822
	C59	-0.304648819	9.966578299	2.937510835
	C60	0.260287924	11.353208656	2.825760472
	C61	1.245633192	11.995058431	3.551035445
	C62	0.433056083	13.343051378	1.991508132
	C63	7.650558395	-5.976323124	3.540870684
	C64	7.518816344	-7.486461872	3.571651205
	C65	6.223228663	-5.404121395	3.325030104
	C66	6.203132538	-3.893941070	3.284147505
	C67	6.226894268	-3.139413688	4.470505960
	C68	6.171187305	-3.196918231	2.062264101
	C69	6.220113742	-1.742850414	4.443348198
	C70	6.161443289	-1.799183841	2.018242275
	C71	6.186818593	-1.075043970	3.212354373
	C72	8.660144073	0.440671079	-2.466644242
	C73	8.680960992	1.953409231	-2.713956982
	C74	7.303669637	-0.001610168	-1.903378111
	C75	8.866531048	3.739722981	-4.389487531
	C76	7.537151474	4.485002018	-4.291129899
	C77	5.100688901	4.302637336	-4.050354218
	C78	4.689589394	4.446904455	-2.571819066
	C79	4.065811633	3.523870613	-4.885917712
	C80	2.648134619	4.106603333	-4.919091055
	C81	2.503752149	5.513335412	-5.502175758
	C82	2.896355645	7.841391238	-4.787603661
	C83	4.780755385	3.582289530	-0.288319699
	C84	5.690640374	4.511116539	0.530579998
	C85	4.822362035	2.196731047	0.387351627
	C86	8.020931957	5.022472226	1.037898574
	C87	8.670761382	6.385564963	0.844695720
	C88	8.767922472	8.461126396	-0.465045438
	C89	8.394470653	9.643654958	0.455087506
	C90	8.544142986	8.789126167	-1.952717531
	C91	7.090311589	9.098795156	-2.295008592
	C92	6.814361514	10.516480928	2.114899745
	C93	7.850352897	10.993183813	3.124013688
	C94	5.544909504	10.031268575	2.864333313
	C95	4.480873877	9.579179195	1.892786111
	C96	3.662973751	10.517417953	1.241784320
	C97	4.346388890	8.224726168	1.544628361
	C98	2.759651720	10.122875981	0.252383953
	C99	3.460405397	7.814747584	0.543252905
	C100	2.683743916	8.774133199	-0.104170073
	C101	-1.783638486	-4.328519072	-9.427100255
	C102	-2.331406806	-3.189055410	-8.596151070
	C103	-1.791429819	-1.479547733	-6.884714725
	C104	-1.128181611	-0.161731974	-7.297714153
	C105	0.947067368	1.100951059	-7.420895089
	C106	2.430463912	0.996389921	-7.751635773
	C107	4.524361514	-0.272519072	-7.746100255
	C108	4.891769163	-1.084091750	-8.970350701
	C109	-5.394638486	0.651480928	-8.653100255
	C110	-5.353388288	2.083505462	-8.144149800
	C111	-5.682458322	-0.278565668	-7.442270336
	C112	-6.357286869	-1.594484325	-7.871295935
	C113	-6.343100474	-2.608148049	-6.745090035
	C114	-4.108638486	3.770480928	-6.927100255
	C115	-2.980510489	4.554786268	-7.572479952
	C116	-4.133590799	3.824014046	-5.382798507
	C117	-3.097308909	2.906947807	-4.795834830
	C118	-1.752044891	3.302078243	-4.711699074
	C119	-3.438314604	1.583677867	-4.468762876
	C120	-0.761782761	2.366532080	-4.394539529
	C121	-2.448572860	0.652398198	-4.146392071
	C122	-1.103240873	1.034847265	-4.148062585
	C123	-0.566987104	-9.700750498	-5.071301383

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C125	-1.663204820	-8.947704262	-4.287733780
C126	-2.364426467	-7.822359050	-4.985989951
C127	-3.143872479	-7.863587412	-6.124165608
C128	-3.221118067	-5.826530160	-5.255750650
C129	0.222361514	-12.660519072	-2.738100255
C130	1.223842331	-13.659408506	-3.273303797
C131	-4.847866854	-4.737358255	0.648774114
C132	-3.699511935	-5.694072023	0.519952693
C133	-3.648825520	-6.427655868	-0.884952387
C134	-5.011108347	-7.116701412	-1.179895607
C135	-4.965033594	-7.920819619	-2.490943851
C136	-6.213558291	-8.713220820	-2.744182461
C137	-2.583873542	-7.557741095	-0.739403366
C138	1.427361514	-3.131519072	-2.710100255
Fe139	0.297551312	-3.842889916	-4.120588302
Fe140	1.687724477	-1.378290772	-1.552990579
Fe141	3.334793955	-3.596309358	-2.268586430
Fe142	2.297376910	-2.264272087	-4.223102059
Fe143	4.167088088	-1.013313875	-2.825633633
Fe144	1.295569367	-5.053616671	-2.067087279
Fe145	-0.401101703	-3.097465872	-1.627463554
H146	-8.753002009	0.193070695	1.032435493
H147	-8.398157328	1.236756569	-0.177864483
H148	-9.365646636	4.291138190	2.662230773
H149	-9.773513482	2.943500671	0.744539157
H150	-10.345434786	1.809567250	1.962965859
H151	-6.626218356	4.440126290	3.294841728
H152	-9.231845821	2.971273284	5.314563996
H153	-7.937485625	5.287947319	4.148936634
H154	-9.044253601	1.764834135	7.291002971
H155	-8.020765551	0.609528677	4.807167093
H156	-7.568726463	2.691966481	7.662478580
H157	-3.170032022	0.247150480	2.992298672
H158	-5.854828066	1.049654893	3.586356335
H159	-7.049087861	-1.437871171	4.251684797
H160	-1.678641651	2.747521014	6.676211650
H161	-4.414495840	2.163836978	5.740217967
H162	-6.492359224	-1.651440432	5.929900090
H163	-3.852805740	1.889510188	2.835564886
H164	-4.397386149	0.610170524	7.860856487
H165	-3.205753540	3.096773878	7.523852425
H166	-2.489476825	-2.663626277	3.459240448
H167	-2.023637439	-1.899527476	1.920324061
H168	-1.299932869	-3.443052477	2.372087497
H169	-0.888137602	-0.747087682	3.800086218
H170	-4.388404022	-0.805576358	9.651400289
H171	1.393233643	1.528544644	4.370815806
H172	0.430148296	-0.090854239	8.434894360
H173	3.287680425	1.990822103	8.276844721
H174	0.296813256	-0.977021148	1.601602123
H175	1.103021332	-2.435480316	2.158939502
H176	8.005248260	-5.645958975	4.535363170
H177	2.170226073	3.046583156	4.880179063
H178	3.252475756	3.300252286	7.071883337
H179	3.169209234	1.632645205	4.473881051
H180	4.306218059	1.887405434	6.821205927
H181	1.231365770	1.840244081	6.861467297
H182	3.204007490	-0.366094438	6.052725023
H183	0.287041204	-0.149850650	5.790426615
H184	1.450497906	-0.871820027	2.941605073
H185	4.378596291	1.454259078	-0.294101954
H186	4.199359935	2.255734509	1.292091889
H187	6.139610990	1.292611406	1.527091764
H188	6.273962975	0.693382327	4.013735442
H189	6.106997001	-1.279184281	1.060192756
H190	6.138396952	-3.751209083	1.120178151
H191	6.236947219	-3.648180895	5.438043767
H192	-1.624040909	-1.802502066	5.969176392
H193	-3.577471976	-4.219246756	6.565936747
H194	-2.515033481	-4.386733923	7.981149384
H195	-3.688429622	-1.857204064	6.946544539
H196	-2.736707940	-0.291858337	10.067611567
H197	6.223874256	-1.174307947	5.377503380
H198	0.230341530	-3.522980685	4.430566421
H199	1.934213844	-0.104967990	10.787918503
H200	0.369501166	-0.932595846	10.564980171
H201	1.916482117	-2.915875556	9.518634143
H202	1.862906833	-13.386516010	2.947276862
H203	-6.060606129	-2.091604970	-2.803348279

H204	-5.819421369	-6.148908016	1.531647459
H205	-7.404596473	-1.397824724	-8.140278515
H206	-5.843725776	-2.008344143	-8.750445495
H207	-6.339762928	0.233768103	-6.721318048
H208	-2.752181006	4.237851756	-8.617893874
H209	-6.286252291	0.627729767	-9.299129130
H210	-3.851950497	1.555060704	-1.491623321
H211	-5.855950230	0.117901780	0.338065995
H212	-3.400379894	1.822312923	-7.474678640
H213	-5.019546169	4.293347320	-7.287432682
H214	-3.382621310	0.276036515	-8.943546871
H215	-5.161920616	-2.369913386	-1.322340396
H216	-4.734774246	-0.473828068	-6.919697366
H217	-4.376886167	-0.621278778	-9.884105075
H218	-6.978234982	3.389781951	-1.043235575
H219	-3.545187510	1.442255852	0.248304722
H220	-4.595119615	-3.151958330	-7.404131332
H221	-4.347248193	-0.681113170	-0.085337388
H222	0.233869346	4.342231112	3.803638943
H223	-0.760372873	2.193690459	2.397613738
H224	-3.936911629	6.317878216	5.177059382
H225	-4.204968782	5.596697506	2.288792869
H226	-0.876045400	7.540554461	2.815499781
H227	1.871960143	11.672605289	4.375933912
H228	-0.075652189	8.561258206	5.634285318
H229	-1.253921498	9.984137889	3.503668647
H230	1.626795066	8.959172189	3.098994654
H231	0.301473221	14.241499455	1.395186076
H232	1.553216572	4.871164528	1.799994275
H233	0.275737524	5.890589320	1.139494889
H234	1.978097479	13.990268976	3.306611469
H235	-0.562605120	9.642095483	1.915981046
H236	-2.071735018	5.031203524	2.346640384
H237	-4.156939779	4.659499149	4.602797168
H238	-4.760120023	8.890501380	1.507114435
H239	-0.770600653	2.316620295	-1.861027946
H240	-6.306699048	8.044653838	1.707475260
H241	-1.234055410	0.936961264	0.187674375
H242	9.502501648	-5.749961969	2.687083282
H243	8.428691431	-4.596373456	2.244995856
H244	5.506573251	2.610558458	-2.074295316
H245	3.760014603	3.979922159	-0.202311776
H246	7.280017031	3.992491209	-0.647118430
H247	0.146852736	4.616786578	-1.027271371
H248	-0.395484742	6.450136169	-2.154173337
H249	1.057339742	6.587041236	-1.599528859
H250	-2.778297276	5.571153651	-3.036329155
H251	-3.945789609	6.906730093	-2.798400387
H252	8.935824008	7.956052587	-2.554665722
H253	9.134107947	9.686260431	-2.186301915
H254	6.908655379	7.358073311	-3.473178799
H255	5.484926889	8.378338121	-3.327349523
H256	2.639948223	9.301071302	-6.203629235
H257	1.454010390	5.686274926	-5.789446406
H258	2.127070941	10.863982257	-0.244466953
H259	4.938291621	7.457868059	2.051245528
H260	2.915256122	8.473704410	-2.848888037
H261	4.005689085	2.487998134	-4.515400003
H262	6.516491172	2.699923441	-4.123797187
H263	2.182635340	4.081596097	-3.921319578
H264	-5.500504095	6.263595761	0.329885846
H265	9.218454887	3.818308823	-5.426966187
H266	-4.864099888	4.549193904	-1.749598524
H267	4.455994860	3.473061700	-5.914833241
H268	3.399248184	6.763957535	0.256946860
H269	-2.060830121	7.903252383	-1.601755049
H270	9.578362214	4.281519215	-3.750687541
H271	2.605090761	7.682119192	-6.815954907
H272	3.122362201	9.707591943	-4.012288765
H273	-6.287197335	2.125296411	-1.897229016
H274	-5.747208590	2.522441810	0.707663796
H275	3.735049283	11.575432443	1.503454253
H276	-2.353492322	5.533923442	-0.561352440
H277	5.182983926	5.330058295	-4.428184992
H278	3.123725473	5.600868866	-6.410937432
H279	2.052088746	3.443950131	-5.560682281
H280	3.248019627	6.211122063	-3.592536358
H281	7.590899576	5.016796781	2.050370431
H282	7.405062133	6.797133543	-0.706222756
H283	9.848442850	8.327449265	-0.307623222

H284	8.829410179	4.278527045	1.010705111
H285	6.800950403	8.594458108	1.173856336
H286	-0.714552236	-4.171052660	-9.631033154
H287	-1.853950566	-5.229381615	-8.780922997
H288	0.167603245	-8.973135986	-5.449965766
H289	-2.323821791	-5.351497140	-11.107783568
H290	-3.518158064	-4.419148741	-10.482053505
H291	7.298312136	-1.096476380	-1.828255020
H292	9.632739539	0.596886412	-0.678936673
H293	8.866648565	1.630649847	-4.740650401
H294	7.160973285	0.440171058	-0.906876147
H295	10.636586637	0.260655127	-1.926946863
H296	5.009518254	-0.706805425	-6.857984729
H297	8.832785896	-0.080283253	-3.421389826
H298	-1.217278596	-8.527065973	4.458750033
H299	-1.430631696	-10.588519238	2.202447875
H300	2.626980094	-0.957884802	-7.065722676
H301	3.732353850	-4.008501932	2.247011249
H302	0.464844625	1.578473592	-8.284346957
H303	-2.719920698	-0.373976561	-3.889883123
H304	0.866579925	1.821477754	-6.589186321
H305	0.030828381	-6.323647866	3.662066443
H306	0.629774644	-0.889895898	-6.565803544
H307	-0.618408641	-6.475355399	2.030314465
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Fe(143) 2.966	C5	-8.101279255	2.057603516	6.876311653
Fe(144) -2.241	C6	-7.208214527	0.833045851	6.651067197
Fe(145) -0.427	C7	-6.536485234	-0.932507341	5.090815705
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	C124	0.247412242	-10.538455831	-4.018249554
	C125	-1.630317862	-8.958869088	-4.291602939
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	C127	-3.090371090	-7.871505626	-6.144326287
	C128	-3.181972297	-5.838609464	-5.267776305
	C129	0.222316973	-12.661280164	-2.737120654
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	C131	-4.867836193	-4.748767532	0.632393139
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	Fe142	2.286957825	-2.251018492	-4.237432838
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	Fe145	-0.448130301	-3.100875199	-1.685757424
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	H186	4.177246335	2.189366298	1.227339708
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	O449	7.473882162	5.787468570	-4.415865021
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	O458	-3.552899010	-2.905664661	-8.647549394
	O459	-1.764575161	0.796368112	-7.863473781
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	O461	6.027187856	-1.552100853	-9.129482857
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	O472	-1.561133033	-7.479491756	-1.528799165
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	O477	0.418973931	5.916628163	-1.964340461
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	O479	-2.429465217	-11.137395977	-0.283702075
	S480	5.942293107	0.530482987	-3.071054991
	S481	2.220346698	-0.094378300	-3.499138445
	S482	-1.792097266	-3.387939926	-3.497817053
	S483	3.773671150	-1.914640530	-0.784730715
	S484	-0.915752055	-0.850224820	-1.683575479
	S485	1.200146829	-3.012251910	-6.023905739
	S486	-0.326806730	-4.944627854	-0.513531996
	S487	4.433966642	-2.840783262	-4.154630616
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Fe(139) 2.467	C1	-6.949080873	3.196569824	6.099934622
Fe(140) -1.429	C2	-6.945136035	3.527023297	4.604598882
Fe(141) 2.724	C3	-8.302945848	3.709786865	2.563796234
Fe(142) -2.618	C4	-7.779313513	5.027091373	1.998069635
Fe(143) 2.901	C5	-7.498181236	7.430840577	2.272962590
Fe(144) -2.189	C6	-5.972962769	7.519912541	2.153985663
Fe(145) -0.247	C7	-3.819883967	6.786978954	3.068051009
	C8	-3.305768160	5.845543524	1.975724915
	C9	-3.561143277	3.736928408	0.787748895
	C10	-3.696784524	4.280031117	-0.640380070
	C11	-4.930932254	5.735300580	-2.163037054
	C12	-4.024494590	6.953549343	-2.391762997
	C13	-3.295122289	9.140077970	-1.573664109
	C14	-1.776560489	9.162639349	-1.364666262
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	C16	0.980562794	7.180607775	-0.429685590
	C17	0.982910689	4.878196248	-1.343642172
	C18	1.015823260	4.764265437	-2.877442063
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C27	-0.872903134	8.393165680	-5.597866718
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C29	6.219912255	10.244220515	5.960459262
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C57	-7.803080873	-1.126430176	-5.452065378
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C59	-9.074977676	-1.744823106	-4.837141122
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	C47	-9.611476299	-0.431783478	0.499962816
	C48	-9.338865013	0.874041895	-0.260073362
	C49	-7.634145585	2.517380185	-0.946911534
	C50	-6.729642950	2.249733128	-2.150420255
	C51	-5.059003641	0.860012813	-3.256991709
	C52	-5.839080905	0.575967110	-4.560968232
	C53	-4.164796244	-0.368349426	-3.022072215
	C54	-3.343923825	-0.390891991	-1.774367746
	C55	-2.640091622	0.562242615	-1.075921683
	C56	-2.337028802	-1.393159896	-0.061720641
	C57	-7.809366053	-0.552773006	-5.530777096
	C58	-8.157138312	0.679862100	-6.368493359
	C59	-9.085244468	-1.218557672	-4.976430397
	C60	-9.895878064	-2.022240170	-5.952813505
	C61	-10.052787893	-1.896104282	-7.320786701
	C62	-11.252914226	-3.595109705	-6.557641264
	C63	8.285408616	3.585623985	-5.403850680
	C64	9.495720480	4.209171236	-4.736371013
	C65	7.158896777	3.537060881	-4.335474541
	C66	5.880504832	2.933488682	-4.870516281
	C67	5.020878994	3.677854687	-5.697654252
	C68	5.523325566	1.606512358	-4.572331737
	C69	3.844987676	3.123193130	-6.208043559
	C70	4.347546216	1.037907987	-5.072231685
	C71	3.514400161	1.799720029	-5.894073739
	C72	4.786766476	-4.426186897	-6.346182447
	C73	3.611481166	-5.255765510	-6.879647918
	C74	4.319495677	-3.510808830	-5.205662149
	C75	2.616993458	-7.498152392	-7.050425444
	C76	1.297032544	-7.387798300	-6.288208327
	C77	0.125994325	-6.501626568	-4.322832556
	C78	-0.552047195	-5.159787192	-4.657578103
	C79	0.409074356	-6.661733330	-2.816804035
	C80	-0.814978834	-6.586725932	-1.895799806
	C81	-1.899428495	-7.640946907	-2.125938555
	C82	-3.787432521	-8.020232601	-3.668750986
	C83	-0.351118983	-2.816467817	-5.307625997
	C84	-0.801949566	-2.697039177	-6.774766818
	C85	0.601934177	-1.645460556	-5.018926549
	C86	-0.132846842	-3.068885278	-9.091769433
	C87	-0.889133852	-3.951598818	-10.076911075

C88	-2.314708994	-5.916490467	-10.434260566
C89	-3.700807213	-5.482701316	-10.961381071
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C98	-6.930349935	-4.459966694	-6.401594930
C99	-4.731372826	-3.448033713	-6.204476177
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C108	5.379331923	-8.818242340	0.117728327
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C120	-1.477714526	-4.533398794	1.382069926
C121	-0.919390647	-3.316053500	3.394693920
C122	-0.604832258	-3.695378956	2.084214924
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C135	4.254995387	2.160421728	8.191579187
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Fe141	5.130189320	-1.408368265	-0.383001185
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Fe143	3.758567658	-3.336176782	-1.825695497
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H160	-4.675895616	5.310122947	-2.486629154
H161	-5.392647717	5.292184859	0.363513233
H162	-3.335429245	7.503955905	3.579811959
H163	-4.142933887	2.766493505	1.143454982
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H165	-5.932056942	6.279391326	-1.678859748
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	H168	1.674681137	3.686676778	1.505445693
	H169	-0.644824026	3.670972406	-0.517336480
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	H171	-1.497266771	2.756081295	-3.633085336
	H172	-1.604241497	7.233625886	-3.702426925
	H173	-1.805172315	5.777169102	-6.765480010
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	H176	7.959657669	4.262763150	-6.215464275
	H177	-2.549755667	2.524788996	-5.052501142
	H178	-2.710397507	4.247796855	-6.849222319
	H179	-0.781871977	2.442969116	-5.231299642
	H180	-0.947085199	4.253596377	-7.095930146
	H181	-2.407092574	4.950213047	-4.479687837
	H182	0.600667265	4.573176686	-4.953448085
	H183	-0.997346880	4.875548637	-2.510142575
	H184	0.902347351	2.390493726	-2.008034780
	H185	1.062472556	-1.789353362	-4.028299757
	H186	-0.012383587	-0.731365320	-4.989422245
	H187	1.888428305	-0.626490188	-6.095462608
	H188	1.903131202	1.796146877	-6.981656795
	H189	4.070509139	0.017502427	-4.802599058
	H190	6.161395677	1.003634554	-3.920744440
	H191	5.263788833	4.715650545	-5.937998888
	H192	-0.647351788	6.233867129	-0.403548112
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	H194	0.636836191	9.265495713	0.435544120
	H195	-1.862894649	7.722143721	0.882827711
	H196	-3.395662150	9.733728360	-1.696086880
	H197	3.182029380	3.721796094	-6.838369864
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	H199	-1.218483345	9.024429944	-5.808337846
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	H201	1.268520800	8.950287329	-4.003522492
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	H203	-0.839109494	-0.073900884	7.018490523
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	H205	-0.855310188	-4.977177051	10.028485794
	H206	0.580113547	-5.640223067	9.199594403
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	H208	-3.000804883	-8.652319559	4.024970750
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	H210	-2.885492504	-0.886718124	3.191247407
	H211	-3.456021875	1.678624023	4.760815647
	H212	-1.614474127	-6.557013748	5.101982949
	H213	-4.539011809	-6.951363042	5.358310615
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	H216	-0.552093587	-4.784121590	6.974347411
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	H218	-6.166932784	-0.664873730	4.771343600
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	H230	-7.248864605	-1.261924451	-6.159891108
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	H233	-4.792479842	-1.271803385	-3.027642437
	H234	-11.239603891	-3.101288742	-8.629169060
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	H236	-5.773029122	0.647081715	-1.237871245
	H237	-7.130161721	3.234496810	-0.279058341
	H238	-10.169769577	-1.088914311	-0.178640146
	H239	-1.967689526	-2.155187340	0.620610668
	H240	-10.258570336	-0.202555573	1.357127836
	H241	-1.330066866	0.263833856	0.658591237
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	H244	1.254424150	-4.168908113	-4.765643518
	H245	-1.251687493	-2.683842457	-4.691585817
	H246	0.719197326	-3.933305630	-7.366426009
	H247	-3.514471688	-2.530973730	-1.432732325

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	H251	-7.071125833	-4.277903492	1.539425319
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	H256	-4.815003515	-9.784751531	-3.462995665
	H257	-2.518907153	-7.737992679	-1.220084123
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	H263	-1.273181881	-5.585284268	-1.917784405
	H264	-8.048929232	-0.905292833	1.890781698
	H265	2.977699576	-8.530337631	-6.946812250
	H266	-5.818318152	-2.203016849	2.834919129
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	H268	-3.829018799	-3.256215189	-5.623548120
	H269	-7.194046581	-4.048774925	-0.887482177
	H270	2.376412577	-7.329579521	-8.109869983
	H271	-3.334712997	-9.694753463	-2.565090686
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	H276	-5.645023899	-2.117581039	-0.108907755
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	H278	-1.427474335	-8.620448849	-2.318042580
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	H281	-0.569975952	-2.062164397	-9.174714908
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	H283	-1.693627682	-5.986309461	-11.338992827
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	H285	-3.817769261	-4.035179748	-9.529318507
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	H316	5.221774911	11.268175230	6.341743021
	H317	5.824204492	3.077181718	0.831392032
	H318	-1.248343402	-4.814686799	0.353016781
	H319	-2.322630206	-3.491953997	5.026072449
	H320	7.913238954	3.585724386	8.121729381
	H321	7.331363901	1.074981443	7.358031135
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	H323	7.090524658	3.011630246	9.312450153
	H324	5.206595472	-9.208965312	1.149746167
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	H168	1.991045449	-2.162924971	3.467375179
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	O461	3.003125742	-2.194017533	-10.537110652
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	O464	-3.378534931	-8.337966461	-2.783062017
	O465	-7.098569902	-0.302137934	-6.100907977
	O466	6.009376663	-8.663406263	-1.483457112
	O467	9.817938995	-10.915954599	-0.810484888
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	O472	2.927678276	-6.679420412	1.049959554
	O473	3.097710963	-7.363842366	3.187260183
	O474	0.340430210	-6.215479611	1.187108927
	O475	7.259739439	-8.125851468	2.322251515

	O476	5.781633296	-6.613577194	0.594284151
	O477	-3.926509042	3.570038870	-2.851970621
	O478	3.521353780	-11.579893796	1.883549900
	O479	4.899062239	-9.429541929	3.153103611
	S480	3.440768759	1.888410889	-5.638016131
	S481	0.972757110	-0.838903538	-4.702159883
	S482	-0.192667078	-4.778360615	-1.701796005
	S483	3.449473260	0.277817323	-2.259961493
	S484	-0.806089833	-2.227900899	0.386510340
	S485	1.556359984	-4.578563269	-5.205267049
	S486	2.313406942	-3.632752572	0.699539470
	S487	4.356059070	-1.866645906	-4.971130988
	S488	3.297759101	-5.876387304	-2.057534565
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Fe(139) 2.497	C1	-8.794051125	1.048020450	4.147973415
Fe(140) -1.471	C2	-7.679676479	2.089238961	4.293289220
Fe(141) 2.673	C3	-7.121958182	4.482266717	4.303806343
Fe(142) -2.610	C4	-6.219083215	4.551392816	5.530422120
Fe(143) 2.918	C5	-5.977754721	4.273010509	7.939972489
Fe(144) -2.187	C6	-4.829658253	3.257871623	7.952193491
Fe(145) -0.167	C7	-4.080247701	1.034322911	7.238564093
	C8	-3.045348800	1.349290832	6.150883826
	C9	-2.607480239	2.225988912	3.917967050
	C10	-1.614396254	3.332005356	4.299822247
	C11	-1.203685187	5.345447312	5.609203426
	C12	-0.277908433	4.896010382	6.750012522
	C13	-0.119699094	3.991925258	9.016444353
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	C15	0.904955024	0.358181987	8.363763546
	C16	1.707535020	-0.045663920	7.124272091
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	C42	-4.845050998	-0.888656028	1.893867497
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Fe(142) -2.607	C4	-7.181685008	-6.103678437	-0.354655975
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C79	-0.229877392	7.160124272	1.231798589
C80	-1.497930293	6.740218630	0.477691297
C81	-2.692166560	7.690677391	0.585105259
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	H187	2.294946151	2.215957975	5.456647168
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	H190	6.664573993	0.671903598	3.361834644
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	H196	-1.895873206	-9.505569727	4.183924399
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Fe(141) 2.791	C3	-6.802868074	4.106871701	4.758122280
Fe(142) -2.607	C4	-5.852742292	4.237465064	5.944943633
Fe(143) 2.776	C5	-5.477727661	3.958546286	8.338737263
Fe(144) -2.345	C6	-4.314569107	2.959726608	8.287068393
Fe(145) -0.376	C7	-3.551665590	0.774103448	7.485196256
	C8	-2.529718610	1.177260101	6.417108170
	C9	-2.128615686	2.189227537	4.232203555
	C10	-1.184769950	3.317846021	4.665077734
	C11	-0.878247292	5.349820137	5.965017262
	C12	0.140599643	4.904610493	7.025067465
	C13	0.480857195	3.815761220	9.186763234
	C14	1.427759947	2.615344392	9.067083502
	C15	1.727243811	0.318596921	8.239821439
	C16	2.418347695	-0.001839088	6.912372689
	C17	2.596793755	0.566841111	4.511847276
	C18	3.643951148	1.635277408	4.152300116
	C19	1.456830113	0.430971670	3.480034700
	C20	2.011565640	0.248952534	2.061575462
	C21	0.533259252	-0.724688064	3.873744325
	C22	4.072491310	4.044235524	3.790954198
	C23	4.845502684	4.490006765	5.048648168
	C24	3.288078602	5.199958576	3.123748221
	C25	4.150791607	6.459319845	2.980488880
	C26	2.746224847	4.764192091	1.756649420
	C27	4.791268641	5.168841354	7.381173804

C28	5.997874903	4.336942576	7.761115407
C29	2.269410328	-7.996772863	10.423358931
C30	2.700372930	-8.021881538	8.955464582
C31	4.161219628	-6.833009858	7.306604302
C32	5.685858939	-6.922430083	7.503056750
C33	3.743685235	-5.481678064	6.692572601
C34	4.448686794	-5.148196741	5.372140745
C35	3.749748522	-3.987151203	4.660280221
C36	4.968903303	-2.384862737	3.162133355
C37	7.763931423	-7.934348753	6.684974380
C38	8.495856530	-7.219969654	5.570008763
C39	-5.650068577	1.081651247	1.213974380
C40	-5.217809833	2.379301979	0.522592414
C41	-4.532477764	0.027109057	1.243765773
C42	-4.693768334	-1.027265094	2.358672725
C43	-5.510086331	-2.260229694	1.996427753
C44	-5.415272561	3.657924972	-1.571979397
C45	-5.979766666	5.024125404	-1.165456686
C46	-5.786846604	3.358475748	-3.034972471
C47	-7.229377796	6.288179411	0.528531649
C48	-6.215603314	6.821296776	1.552184565
C49	-4.159866713	6.352375315	2.828236280
C50	-2.777201447	6.556844186	2.208484917
C51	-1.144631111	5.993179348	0.484650780
C52	-0.933506426	7.409535466	-0.080086321
C53	-0.924770764	5.000469462	-0.676465593
C54	-1.216990763	3.569247325	-0.347493906
C55	-0.952725328	2.770652624	0.751659317
C56	-1.986295810	1.518402519	-0.659469586
C57	-2.009068577	9.275651247	-1.275025620
C58	-1.388756726	10.290562690	-0.313277558
C59	-3.458018489	9.674498209	-1.625979494
C60	-3.620372588	10.789436675	-2.618755004
C61	-2.821254141	11.879974530	-2.901735809
C62	-4.627819546	11.893605902	-4.184807110
C63	10.539024551	-1.594286292	1.198692938
C64	11.197071249	-2.834977747	1.771280249
C65	9.009526336	-1.756673912	1.402124477
C66	8.223904453	-0.564862286	0.903043528
C67	8.217043269	0.640840309	1.628588817
C68	7.470032739	-0.624259964	-0.282906323
C69	7.482089129	1.745966118	1.194815736
C70	6.726835500	0.473142217	-0.729118977
C71	6.736456080	1.657375637	0.012870293
C72	6.584767593	0.539584369	-6.153868513
C73	5.932037676	1.653971345	-6.981700684
C74	5.687641608	0.164978992	-4.964689749
C75	4.849176351	2.240873604	-9.109800505
C76	3.420830164	2.638569442	-8.737618101
C77	1.465923352	2.192934371	-7.315000119
C78	1.509393035	3.081205659	-6.057983860
C79	0.632730913	0.911287778	-7.106879429
C80	-0.820928213	1.110836902	-6.659577427
C81	-1.734335849	1.864288052	-7.629441660
C82	-2.138207600	4.210191074	-8.300192650
C83	2.645259831	3.753441276	-4.001447232
C84	3.396958419	5.080914740	-4.223347781
C85	3.311847853	3.020286079	-2.830370660
C86	5.323145652	6.144954026	-5.287279107
C87	5.206801074	7.253795627	-6.328412272
C88	3.905742802	8.260585398	-8.154263130
C89	3.333101434	9.640341751	-7.766739789
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C91	1.657730665	7.358769324	-8.985130173
C92	2.109931423	10.953651247	-6.099025620
C93	3.049335375	12.150285768	-6.051408517
C94	1.477566074	10.734293695	-4.700032326
C95	0.480044843	9.602470164	-4.723794314
C96	-0.811121011	9.801101043	-5.237932305
C97	0.839435807	8.309659414	-4.309377309
C98	-1.707852398	8.738603957	-5.370397931
C99	-0.040935371	7.233013921	-4.450123674
C100	-1.305004738	7.452839226	-4.995724122
C101	-2.885068577	-9.060348753	-4.695025620
C102	-3.522049682	-7.748912928	-4.293182964
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C104	-3.249477813	-4.340743818	-5.061455173
C105	-2.022935638	-2.840423564	-6.551329973
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C113	-6.702646183	-7.275394294	-1.174993714
C114	-7.372068577	-1.506348753	-4.904025620
C115	-6.905529380	-0.989658700	-6.253149828
C116	-6.916124241	-0.647518837	-3.703760053
C117	-5.470905313	-0.875635780	-3.348361334
C118	-4.437446652	-0.187304263	-4.003997315
C119	-5.132758797	-1.848909465	-2.393736551
C120	-3.099792931	-0.480495334	-3.725444124
C121	-3.796363811	-2.154248881	-2.125362245
C122	-2.775262221	-1.479171952	-2.800659940
C123	1.289947603	-10.950196138	0.837361740
C124	2.772486855	-10.900513781	1.289675957
C125	0.670376070	-9.615267969	1.282575860
C126	-0.661732637	-9.254677396	0.705804075
C127	-1.714899427	-10.070734085	0.346497130
C128	-2.318321317	-7.952444763	0.108701334
C129	4.459931423	-11.826348753	2.827974380
C130	5.530979706	-12.496071963	1.992539919
C131	-1.965442611	-3.931474728	4.836926106
C132	-0.703809550	-4.692371558	4.583292222
C133	-0.930852372	-6.007455648	3.722952788
C134	-1.967951882	-6.917295215	4.436438813
C135	-2.108100154	-8.288140325	3.755519370
C136	-2.913262076	-9.266771884	4.559816588
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C138	1.565931423	-3.815348753	-1.609025620
Fe139	0.513926780	-5.464333307	-1.844483414
Fe140	1.300011303	-1.832498685	-1.948822447
Fe141	3.516423140	-3.417569890	-1.885543367
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Fe143	3.023661886	-1.739918307	-4.016398058
Fe144	2.384973469	-4.844479181	-0.133537939
Fe145	0.185011624	-3.345926601	-0.234121952
H146	-7.304165064	-0.962692320	5.075045164
H147	-7.763617397	-0.751974600	3.516138649
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H149	-9.248921426	1.010252665	4.073010628
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H151	-6.166589558	3.987497834	3.870278122
H152	-7.299280919	3.585628924	7.248743763
H153	-7.359654942	5.047493805	4.655550056
H154	-6.090098737	3.747631187	9.225309879
H155	-5.470774445	1.659812802	7.197017623
H156	-5.037807829	4.958341330	8.452601009
H157	-1.499680937	1.360361343	3.886118145
H158	-4.037321892	1.805052764	5.153567031
H159	-4.030477074	-0.170410516	7.190960675
H160	-0.311667706	5.803627601	5.142206620
H161	-2.712204806	4.250313291	5.702398492
H162	-2.997189448	0.607385811	8.416677915
H163	-2.735178869	2.527134630	3.379542394
H164	-1.340005916	3.905686420	8.070815695
H165	-1.531062730	6.115501558	6.406608268
H166	0.208715664	-0.650103539	4.919769752
H167	-0.368231047	-0.716611369	3.248673730
H168	1.031029434	-1.693413023	3.718358706
H169	0.873355693	1.365445045	3.505384930
H170	-0.189752170	3.623059127	10.036396791
H171	2.100191252	3.877401488	1.820991249
H172	3.107654083	4.637703799	6.195924845
H173	4.490424927	6.848244217	3.950978415
H174	1.188200087	0.245446442	1.333501828
H175	2.552522081	-0.703989556	1.951872190
H176	10.878049040	-0.729505128	1.799279845
H177	2.162932063	5.580200578	1.305903851
H178	3.568460934	7.248811411	2.483631067
H179	3.574911786	4.531202104	1.067385828
H180	5.041811190	6.256563786	2.366132774
H181	2.432657704	5.445269059	3.780077227
H182	4.853145642	3.692998428	3.101285481
H183	2.186331259	3.092697425	4.176665344
H184	2.696638436	1.062502833	1.773496045
H185	2.858999096	2.020297071	-2.722858805
H186	3.090531573	3.602928876	-1.921160785
H187	5.145949257	2.804142522	-2.178597873

H188	6.163715330	3.509237417	0.071652002
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H190	7.441062350	-1.551945020	-0.860489236
H191	8.781842935	0.714152979	2.560982453
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H196	1.108991784	4.680610158	9.435271721
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H209	-8.715796014	-5.752030120	-4.412683584
H210	-4.476286121	-0.459179609	0.257247781
H211	-5.178004692	-0.566229340	3.237762187
H212	-6.158180127	-3.272337258	-4.952477089
H213	-8.477536241	-1.434424259	-4.960099729
H214	-5.960032643	-5.326853963	-5.370364782
H215	-4.137905898	-3.476376209	2.968988478
H216	-6.156517598	-5.227827707	-2.849307610
H217	-6.799228265	-6.726192963	-5.345965868
H218	-7.702556097	0.981088661	0.997751567
H219	-3.574313896	0.541301471	1.397819861
H220	-5.156450072	-7.651902863	-2.299494392
H221	-3.702008900	-1.346558170	2.700944887
H222	-0.376911203	5.854108059	1.259811378
H223	-0.454206842	3.053979159	1.677406277
H224	-4.444400696	7.305292299	3.290311003
H225	-5.170399715	5.033768327	1.488767602
H226	-2.933051335	7.490601291	-0.514818668
H227	-1.868174473	12.207564020	-2.502044630
H228	-1.654875433	10.115188101	0.756917279
H229	-4.004896649	9.903405628	-0.693445149
H230	-1.392470255	9.236955981	-2.187498779
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H232	0.119016257	5.132381709	-1.006445186
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H234	-3.154608935	13.423026615	-4.345768633
H235	-3.948555298	8.787815287	-2.058598409
H236	-3.000714502	4.996085978	0.858202627
H237	-4.069745082	5.611583200	3.639057191
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H239	-2.449397997	0.677655923	-1.166443819
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H243	10.227054766	-0.828801062	-0.674395897
H244	3.136642652	2.083195817	-5.286232303
H245	1.625037475	4.022630627	-3.695429882
H246	4.527140495	4.236790495	-5.713041240
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H250	-5.373655103	2.380808319	-3.316827835
H251	-6.883471937	3.325555946	-3.150399976
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H254	1.937997954	5.266735739	-9.020600448
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H256	-3.423805063	4.534659762	-9.865586672
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H260	-1.809109564	5.808083413	-7.081601577
H261	1.134009344	0.271718277	-6.362832280
H262	3.303640232	1.096247655	-7.368122704
H263	-0.872739898	1.591188847	-5.669366156
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H265	4.828548432	1.812985418	-10.120696111
H266	-6.407727700	1.789447070	-0.970359571
H267	0.641968738	0.362590699	-8.061992285

	H268	0.259091121	6.226401722	-4.156907254
	H269	-5.319504943	5.203235321	-3.450465236
	H270	5.428343996	3.173742176	-9.150928240
	H271	-2.947606229	2.882329291	-9.643828667
	H272	-2.451747215	6.193538922	-8.624585438
	H273	-6.920591080	-0.462172204	0.746253131
	H274	-5.815807085	1.390119262	2.264019594
	H275	-1.123787170	10.801131160	-5.549548368
	H276	-4.321931396	3.786655719	-1.516973583
	H277	0.993315867	2.816372196	-8.086129469
	H278	-1.548560366	1.513631072	-8.658995441
	H279	-1.251690056	0.107890068	-6.540373858
	H280	-0.780097410	3.650762829	-6.874319670
	H281	5.351606245	6.639809668	-4.304930522
	H282	3.376938214	6.559685386	-6.927424311
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	H286	-2.059350534	-8.884299638	-5.399936826
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	H288	1.325216067	-10.979180468	-0.265157029
	H289	-3.489865597	-10.892029298	-5.354940155
	H290	-4.687075058	-9.999175740	-4.681499957
	H291	6.133990509	-0.692990978	-4.447609079
	H292	7.813948317	1.836944411	-5.166169364
	H293	5.590679577	0.326529512	-8.515052296
	H294	5.624065449	1.016251481	-4.272267648
	H295	8.541719284	1.096282987	-6.430576424
	H296	2.246942639	-3.480092447	-7.555108684
	H297	6.719966884	-0.350074918	-6.788817838
	H298	3.934030619	-4.683053984	7.428562660
	H299	3.822345710	-7.645840313	6.654010589
	H300	0.201625012	-4.280603058	-6.489777847
	H301	5.844091818	-1.289067639	1.673543543
	H302	-2.961273667	-2.904011152	-7.115953023
	H303	-3.548233730	-2.921302776	-1.389375464
	H304	-1.999167704	-1.839220209	-6.090549603
	H305	3.662522699	-3.115601999	5.324914836
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	H307	2.720896051	-4.278820542	4.394533941
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Fe(144) -2.175	C6	-5.292420823	-1.966885381	8.123321613
Fe(145) -0.364	C7	-3.495963085	-3.259277574	7.074256000
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	C128	2.296406128	-7.692736423	-2.453221623
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	C131	0.211590583	-5.955643931	3.057134263
	C132	1.668063738	-5.625151089	2.831967216
	C133	2.367587872	-6.539546925	1.758729500
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	N422	-0.122244095	1.308239056	-1.271951543
	N423	0.741945739	0.648880712	-1.584944494
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	O425	-6.362839937	-0.052787922	5.971814467
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	O427	-1.625440134	-1.812777365	6.538640729
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	O441	-6.917012364	1.936866429	-3.487052165
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	O445	-6.127644630	9.193794858	1.847868558
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	O449	0.667256958	7.142709643	-7.575608596
	O450	-1.443539857	5.220136024	-4.613650992
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	O452	2.610630604	5.488427717	-1.588308754
	O453	1.208695372	11.468165991	-3.245767689
	O454	-2.235367551	12.921970187	-5.042223857
	O455	-3.425021689	9.869523618	-6.277359758
	O456	-4.341056473	14.055577243	-2.258976878
	O457	-5.079155595	5.681949436	-3.730216069
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	O459	-1.542993507	-3.837132583	-7.014990651
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	O462	-6.106915438	-6.075077760	-6.206635624
	O463	-2.363962467	-9.570696085	-3.020494979
	O464	-0.609435716	-8.686822110	-4.084380498
	O465	-5.593616086	-1.179132340	-7.135728628
	O466	8.363503229	-6.744595577	-1.158420641
	O467	12.329437699	-8.006831273	0.381449473
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	O473	4.461684456	-6.695002173	3.015965751
	O474	1.975521733	-6.182809550	0.478242427
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	S480	3.633347856	3.342773279	-4.808146530
	S481	1.806505043	0.080488245	-4.392310194
	S482	1.447482677	-4.443002249	-2.172952490
	S483	3.606916368	1.377533230	-1.582373696
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	S485	3.416435136	-3.263523911	-5.266834552
	S486	3.271658087	-3.135866552	0.744445260
	S487	5.361775320	-0.103211182	-4.239879715
	S488	5.170994276	-4.598312984	-2.118309617
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16 (S=1) Fe(139) 2.549 Fe(140) -1.231	bm22b26262n2xshdisd_1_53149.07			
	C1	-7.601316973	-6.096171779	0.781660532
	C2	-7.691323849	-4.606911083	1.130440926
	C3	-9.006447714	-2.546577423	0.871487431

Fe(141) 2.807	C4	-8.940455886	-1.987610701	2.288813507
Fe(142) -2.571	C5	-9.474737754	-2.274180307	4.649755304
Fe(143) 2.811	C6	-8.063818891	-2.150949182	5.236467380
Fe(144) -2.341	C7	-5.788826207	-3.064103178	5.259116715
Fe(145) -0.486	C8	-4.978188804	-1.981702681	4.538837846
	C9	-4.504638335	-0.809470180	2.453056884
	C10	-4.815510064	0.621291203	2.914570290
	C11	-6.453419590	2.143221196	3.882330097
	C12	-5.957603667	2.369128544	5.318734198
	C13	-6.008956367	1.594238344	7.637593560
	C14	-4.590299396	1.366399467	8.169833922
	C15	-2.538281121	0.021411552	8.040172749
	C16	-1.334573750	0.441393673	7.197258947
	C17	-0.604529054	1.417141741	5.042526337
	C18	-0.531897450	2.942693657	4.927934497
	C19	-0.769691821	0.673219433	3.703977795
	C20	0.254398906	1.146128553	2.666758020
	C21	-0.651735436	-0.830814875	3.966976470
	C22	-1.732528405	5.013631658	4.327779512
	C23	-2.032842188	5.632701258	5.708686525
	C24	-2.761752615	5.424330639	3.246858617
	C25	-3.020169452	6.934341555	3.263621880
	C26	-2.298058267	4.973504285	1.856702193
	C27	-3.436357746	5.663392160	7.690719793
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	C43	-2.543809476	-5.717647037	-0.217739547
	C44	-5.243260375	-0.891589633	-4.273177223
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	C46	-4.696547400	-1.156467969	-5.688754344
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	Fe141	5.206039639	0.309118180	0.345769067
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	H151	-8.225421639	-2.030180473	0.296908406
	H152	-9.910257410	-3.638803977	3.039656380
	H153	-9.979958781	-2.276502251	0.440434027
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