

Understanding the tethered unhooking and rehooking of S2B in the reaction domain of FeMo-co, the active site of nitrogenase

Ian Dance

School of Chemistry

UNSW Sydney

Australia

Supplementary Information

Protein model

The quantum computed protein model is an extract from crystal 3U7Q, shown in Chart 3. The six principal chains surrounding FeMo-co are highlighted with different colours, and the connecting hydrogen bonds are marked. Homocitrate, the His442 ligation of Mo, and relevant nearby water molecules are included (486 atoms total). Details, and the rationale for inclusion of amino acids and for truncation of uninvolved sidechains, are provided in the caption for Chart S1.

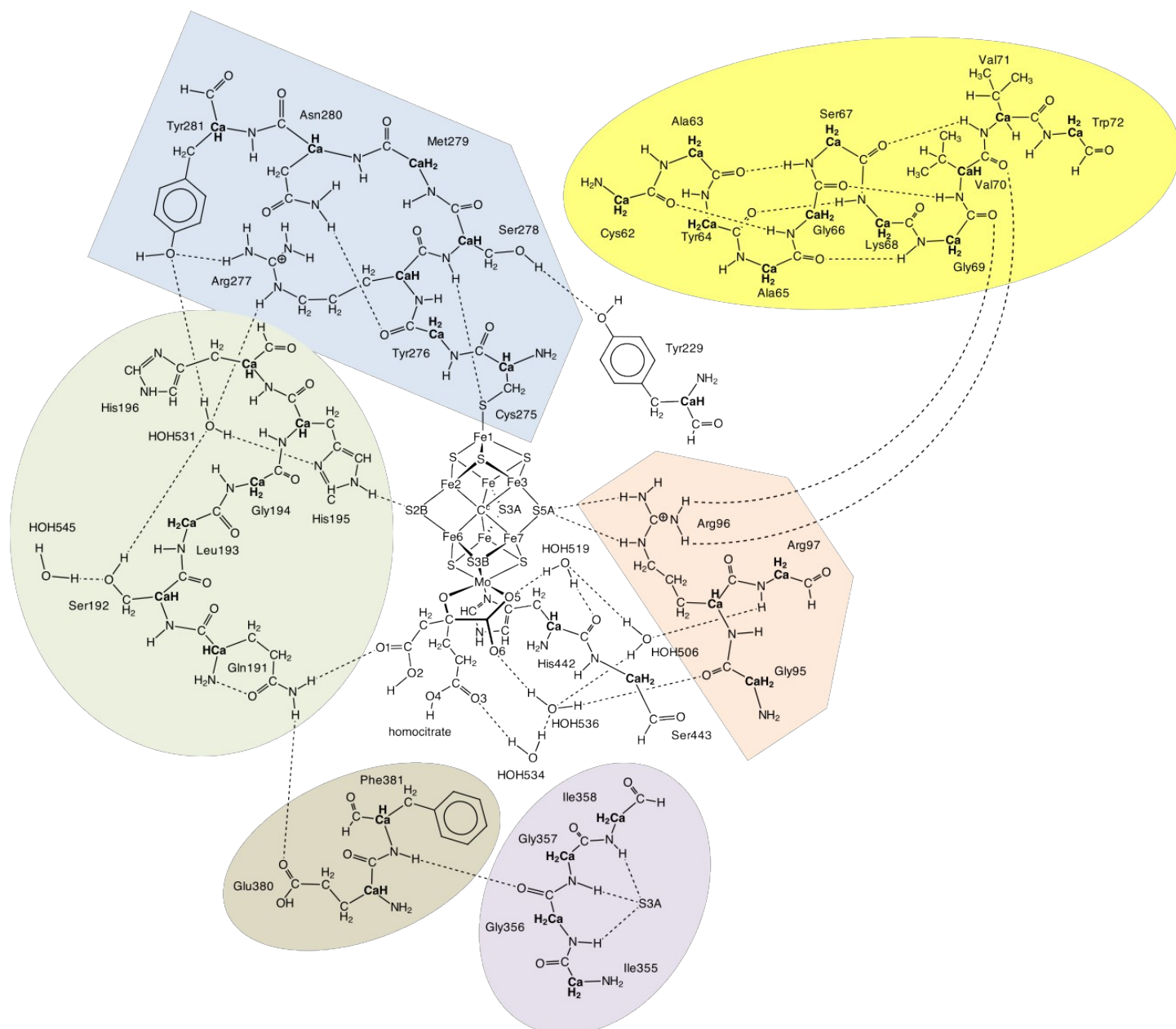


Chart S1. The quantum computed model, with residues and water molecules labelled according to *Azotobacter vinelandii* protein, crystal structure 3U7Q. Ca are labelled as Ca, and hydrogen bonds are broken lines. Non-influential sidechains are truncated to gly. In the ‘front’ chain (yellow highlight) that extends over the Fe2Fe3Fe6Fe7 face of FeMo-co the crucial residues Val70 and Val71 are complete, while 62, 63, 64, 65 67, 68 and 72 are modelled as Gly. In the 191 to 196 chain (highlight green) the significant sidechains of Gln191, Ser193, His195 and His196 are complete. In the 275-281 chain (blue highlight) Cys275, Arg277, Ser278, Asn280, Tyr281 near the N_2 pathway are complete: Tyr229 is included in full because it borders the reaction domain and has an important hydrogen bond with Ser278. In chain 95-97 (salmon highlight) the sidechain of Arg96 is included because it forms crucial hydrogen bonds with S5A, Gly69 and Val70: the sidechain of Arg97 is not nearby and is truncated to gly. In the rear chain (mauve highlight) with hydrogen bonds to S5A, Ile355 and Ile358 are truncated to gly. Glu380 and Phe381 (fawn highlight) are included in full. Ligand His442 is complete and Ser443 is truncated to gly. Homocitrate is complete. HOH531 has hydrogen bonds with two chains, Ser192, His195 and Arg277, Tyr281, and is part of the putative proton transfer from surface water (HOH545) to His195.¹

The four penultimate waters of the proton wire² (HOH519, HOH506, HOH536 and HOH534) are included.

Experimental and computational studies are in general agreement that the redox level of the [CFe₇MoS₉] core of resting FeMo-co cluster is described by net charge -1,³⁻⁶ and so the net charge for the complete model in Chart S1 is -2 (-1 when the His195 side chain is protonated).

Constraints on the computed protein

Some constraints on the protein structure are required during optimization calculations, because the modelled protein is incomplete and the bonding and dispersion influences of the complete protein outside the computational model are absent. The modelled protein must also maintain flexibility sufficient to accommodate the coordination of N₂ and of H₂, and the diffusion of these molecules to and from FeMo-co. The constraints used here involved the C α atoms at the ends of the modelled protein chains, allowing movement of the intermediate residues and all sidechains. The constraints maintained the crystallographic distances between C^c at the centre of FeMo-co and the C α atoms of residues 62, 95, 97, 191, 196, 229, 281, 355, 358, 380, 381, 443, and included C^c -- water distances. As previously explained⁷ trial calculations on the modes of diffusion and coordination of N₂ / H₂ led to the conclusion that the front chain near Val70 should move about 1Å away from FeMo-co. This is consistent with experimental data on mutation of amino acid 70 with smaller and larger side chains.⁸⁻¹⁰ Therefore the C α (Trp72)-C^c distance was constrained to 14.1Å (13.08Å in the resting protein structure), and the C α (Val70)-C^c distance to 8.6Å (7.22Å in the resting protein). The lengths of the hydrogen bonds between the backside water HOH531 and Arg277, Tyr281 and Ser192 (Chart S1) were also constrained.

Density functional procedures

Density functional (DF) calculations use the DMol methodology of Delley,¹¹⁻¹⁶ with accurate DNP (double numerical plus polarisation) basis sets.¹⁴ 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 gradient-corrected functional PBE¹⁷ was used because validation tests demonstrate that it is more accurate than other commonly used functionals when used with DMol.¹⁸ See ref⁷ for results describing the accuracy with which the PBE/DMol method using numerical basis sets reproduces experimental enthalpy data on the binding of N₂. A more extensive study of this set of experimental data using different basis sets and testing many density functionals is available.¹⁹ The calculations were all-electron, spin-unrestricted, with no imposed symmetry. The conductor-like screening model (COSMO)²⁰⁻²² was used with a dielectric constant of 5. Constraints on interatomic distances used the Lagrange Multiplier Algorithm. Control of electronic states was via the input spin populations for Fe1, Fe3, Fe4, Fe5 and Fe7. Output spin populations are calculated by the Mulliken method.²³

Determination of transition states

The following pragmatic procedure is used to map reaction energy surfaces and locate transition states.^{24,25,26} A chemically reasonable geometry between energy minima is evaluated by observing the directions and extent of geometry change during an energy minimisation calculation that is restricted to small (ca 0.03 Å) atom displacements at each cycle. This reveals significant geometrical variables (i.e. which atoms are moving, which bond distances and angles are changing) and also the energy gradients involved. This calculation also indicates the direction of the energy saddle relative the 'reactant' and 'product' minima. Then, as illustrated in Figure 5, a point $\Delta 1$ that is a short distance along this first optimisation is selected, and from this structure an atomic arrangement (2 on Figure 5) on the other side of the saddle is found (by trial and error and chemical experience) and similarly evaluated with small-displacement energy minimisation steps. A point $\Delta 2$ along the second optimisation is selected, and from this the key moving atoms are adjusted to be just back across the suspected saddle-point towards the 'reactant' state. Repetition of this cycle, with subsequent short small-step energy minimisations, always

starting from a point just on the other side of the barrier, allows the barrier to be straddled from opposing trial positions that progressively approach each other in geometry and energy, and converge at the transition state (TS). Confirmation of the TS is obtained by following the complete trajectory of geometries from positions nudged just away from the TS, linking the TS with the connected reactant and product energy minima on the same potential energy surface. The protocol requires human participation, which is itself insightful, and with chemical experience the procedure works efficiently. This method is valuable for the reactions involving FeMo-co where reaction trajectories can be multivariate, because the iterative procedure automatically optimizes all variables, including unrecognised variables that are not part of the principal bond-breaking and bond-making.

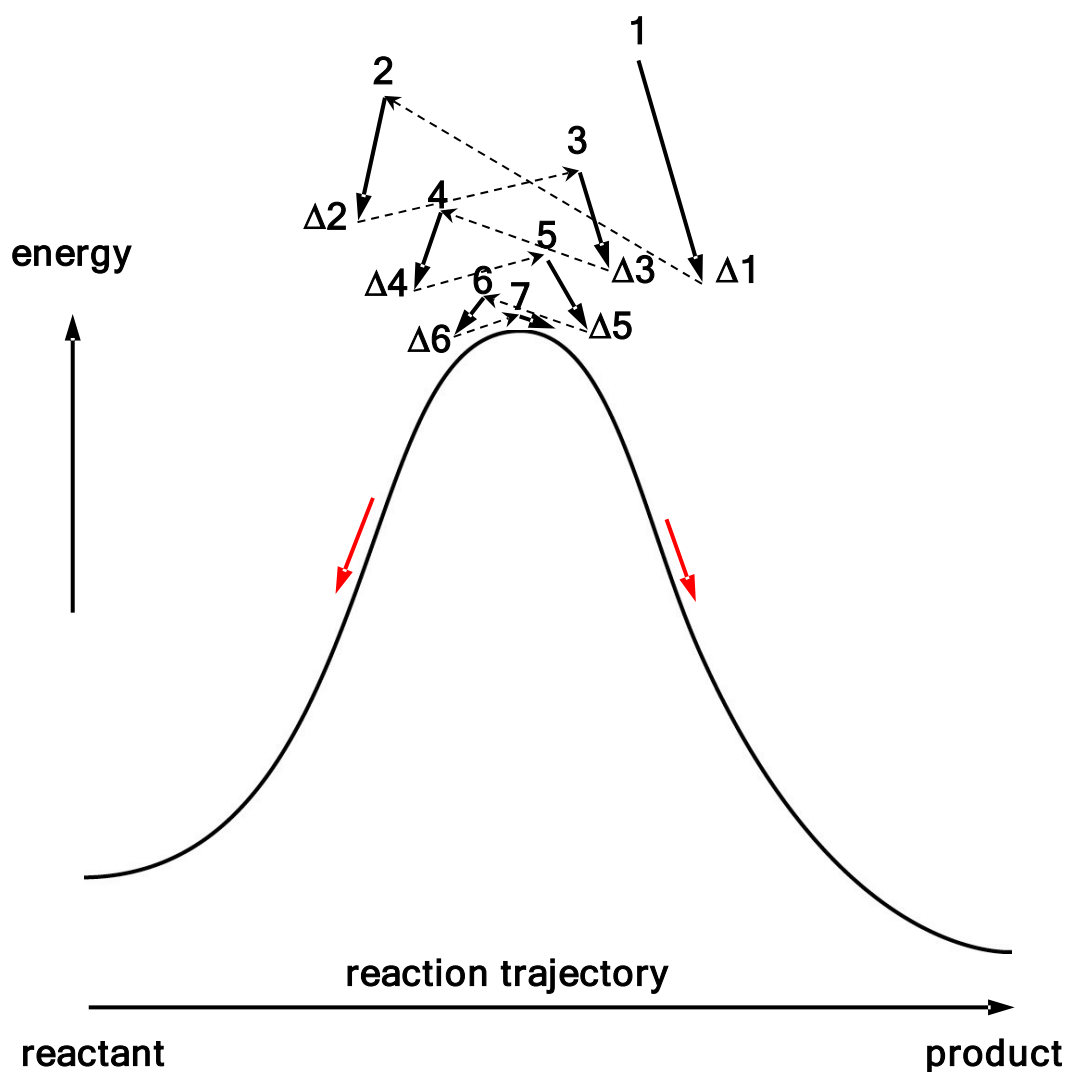


Figure 5. Generalised diagram of the procedure for locating a reaction transition state. The solid arrows represent the course of limited small-step energy reductions from the numbered positions, which are generated (broken arrows) from Δ positions partway along the previous energy reduction, chosen according to geometry and energy gradient. The postulated trials necessarily oscillate across the barrier, and therefore optimise all other variables and decrease the energy and gradient while approaching the top of the barrier. Confirmation that the transition state, reactant and product are on the same potential energy surface is obtained by complete energy minimisations (red arrows).

References

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Table S1. Energies and spin populations.

The entries are identified by the number in Scheme 1, with ‘u’ appended when unhooked, and with a parenthetical letter (ranked by energy) when needed to differentiate electronic and spin states.

Structure	electronic state(S)	relative energy kcal mol ⁻¹	spin populations						
			Fe1	Fe2	Fe3	Fe4	Fe5	Fe6	Fe7
1(a)	35(2)	0.0	3.23	0.09	-2.67	2.80	-2.46	0.25	2.28

1(b)	35(1)	0.3	1.75	-0.01	-2.55	2.69	-2.47	0.18	2.32
1(c)	35(1)	5.3	3.21	-0.12	-2.73	2.80	-2.51	-0.62	1.33
1(d)	35(0)	2.9	1.70	-0.19	-2.68	2.58	-2.51	-0.59	1.50
1(e)	47(1)	5.1	3.12	0.19	1.81	-2.63	2.38	-1.04	-2.21
2(a)	47(2)	0.0	3.19	0.16	2.77	-2.58	2.44	-0.15	-2.33
2(b)	35(1)	0.8	1.83	-0.02	-2.61	2.55	-2.42	0.23	2.35
3(a)	35(1)	0.0	1.75	-0.02	-2.59	2.61	-2.43	0.24	2.33
3(b)	47(2)	0.7	3.19	0.17	2.77	-2.59	2.45	-0.16	-2.33
4u(a)	35(3/2)	0.0	3.10	0.28	-2.65	2.73	-2.48	-0.85	2.33
4u(b)	47(3/2)	1.0	3.03	0.11	1.85	-2.56	2.49	0.06	-2.07
5u(a)	47(3/2)	0.0	2.94	-1.56	2.75	-2.59	2.40	1.02	-2.26
5u(b)	35(3/2)	0.3	2.92	-1.12	-1.97	2.90	-2.28	-0.86	2.37
6⁻²(a)	47(5/2)	9.6	3.17	0.29	2.92	-2.36	2.41	0.49	-2.30
6⁻²(b)	35(3/2)	10.3	3.20	-0.08	-2.81	2.57	-2.39	-0.47	2.28
6⁻²(c)	35(1/2)	9.2	3.20	-0.25	-2.83	2.68	-2.51	-1.62	1.77
6⁻²(d)	47(1/2)	14.5	3.11	0.09	0.96	-2.58	2.49	-1.14	-2.31
6⁻²u(a)	35(1/2)	0.0	2.97	-1.31	-2.54	2.85	-2.35	-1.57	2.37
6⁻²u(b)	35(3/2)	2.2	2.93	-1.23	-2.43	2.94	-2.46	0.36	2.22
6⁻²u(c)	47(3/2)	1.4	2.92	-1.56	2.74	-2.61	2.35	1.09	-2.29
6⁻²u(d)	47(1/2)	4.8	2.87	-1.58	2.65	-2.71	2.53	-0.89	-2.09
6⁻¹	35(1)	2.4	3.17	-0.15	-2.78	2.60	-2.39	-1.32	2.28
6⁻¹u	35(1)	0.0	2.85	-0.96	-2.19	2.87	-2.35	-1.11	2.29
7	35(2)	1.1	3.14	-0.18	-2.50	2.94	-2.45	0.19	2.25
7u(a)	47(1)	0.0	2.87	-2.00	2.58	-2.64	2.17	1.17	-2.32
7u(b)	35(2)	2.1	3.10	0.67	-2.53	2.81	-2.36	-0.55	2.35
8	47(1)	0.0	2.96	-1.79	2.91	-2.56	2.35	-0.14	-2.26
8u(a)	47(1)	3.7	2.84	-0.79	2.89	-2.28	2.47	-1.67	-2.00
8u(b)	47(2)	5.7	2.91	-1.39	2.87	-2.34	2.29	1.66	-2.44
9⁻¹(a)	35(1)	0.0	3.20	-0.11	-2.77	2.70	-2.37	-1.52	2.30
9⁻¹(b)	47(1)	5.5	2.93	-1.44	2.50	-2.75	2.47	-0.05	-2.10
9⁻¹u	35(1)	4.6	2.88	-1.03	-2.23	2.91	-2.37	-0.97	2.24
9⁻²(a)	35(3/2)	0.0	3.20	-0.02	-2.82	2.59	-2.46	-0.61	2.21
9⁻²(b)	47(3/2)	3.9	3.16	0.17	2.84	-2.68	2.45	-1.43	-2.23
10	47(2)	0.0	3.14	0.31	2.50	-2.69	2.48	0.31	-2.31
10u	47(2)	1.4	2.85	-1.30	2.77	-2.45	2.33	1.35	-2.28

11	35(1)	0.0	3.20	-0.13	-2.78	2.69	-2.38	-1.41	2.30
11u	35(1)	6.0	2.93	-1.13	-2.27	2.94	-2.40	-0.87	2.26
12	35(1)	10.8	3.10	-0.42	-2.63	2.44	-2.40	-0.78	2.24
12u	35(1)	0.0	2.88	-0.67	-2.41	2.78	-2.29	-1.31	2.38
13(a)	47(2)	9.8	2.92	-0.94	2.93	-2.23	2.54	0.29	-2.04
13(b)	35(1)	13.2	3.11	-0.53	-2.62	2.45	-2.38	-0.77	2.25
13u(a)	47(1)	0.1	2.75	-1.55	2.79	-2.43	2.33	0.10	-2.25
13u(b)	47(2)	0.0	2.84	-1.56	2.75	-2.43	2.41	2.04	-2.20
14(a)	35(2)	11.7	3.14	0.44	-2.31	2.92	-2.56	0.10	2.16
14(b)	47(2)	9.6	2.94	-0.88	2.94	-2.20	2.49	0.31	-2.09
14u(a)	47(2)	0.0	2.86	-1.63	2.79	-2.49	2.41	1.85	-2.07
14u(b)	35(2)	7.0	3.11	1.56	-2.55	2.73	-2.42	-1.20	2.39
15(a)	47(3/2)	0.0	2.97	-2.14	2.89	-2.41	2.58	0.58	-1.87
15(b)	35(3/2)	4.6	3.17	1.06	-2.65	2.81	-2.65	-0.78	1.63

Atomic coordinates and Fe spin populations

Translation of Fe numbering

Fe1 = Fe143

Fe2 = Fe140

Fe3 = Fe141

Fe4 = Fe142

Fe5 = Fe139

Fe6 = Fe145

Fe7 = Fe144

structure, spin densities	filename, coordinates
1(a)	bm2cnx2b6x2hn2n2x35.car_2
Fe(139) 0.541 2.342	C1 -8.270633891 -4.499431666 0.280032710
Fe(140) 0.435 -1.635	C2 -8.446713775 -5.731825478 -0.614616237
Fe(141) 0.582 2.882	C3 -9.264735974 -2.394606990 1.064881679
Fe(142) 0.555 -2.602	C4 -9.055599227 -2.539216757 2.571013957
Fe(143) 0.563 2.927	C5 -9.422144808 -3.868018793 4.585756382
Fe(144) 0.503 -2.193	C6 -7.971284648 -4.180780944 4.970678326
Fe(145) 0.466 -0.209	C7 -5.824208506 -5.110305924 4.245523595
S=2	C8 -4.962322861 -3.849333197 4.122833912
	C9 -4.529989325 -1.763611539 2.935493864
	C10 -4.724042575 -0.780848475 4.100531885
	C11 -6.221565072 0.151294666 5.775025811
	C12 -5.656454058 -0.361504420 7.106363105
	C13 -5.581510116 -2.212702351 8.709750713
	C14 -4.170284258 -2.774237749 8.914545295
	C15 -2.252249976 -3.930666773 7.902566914
	C16 -1.070220453 -3.156909778 7.311259406
	C17 -0.405013995 -1.196675424 5.948352451
	C18 -0.301850566 0.208105661 6.568962253

C19	-0.664167212	-1.187886922	4.417271866
C20	0.245467223	-0.200702336	3.678895019
C21	-0.514825036	-2.598806645	3.837412189
C22	-1.451571219	2.315511925	7.133387682
C23	-1.587046558	2.258801056	8.668470351
C24	-2.533803938	3.200106978	6.469001376
C25	-2.636492413	4.562182272	7.165417743
C26	-2.241696194	3.382450356	4.974171814
C27	-2.810510162	1.456518901	10.606017837
C28	-1.565338343	1.066806675	11.378957862
C29	3.921018376	-11.075339905	6.483099254
C30	4.691282617	-9.994429945	5.724615843
C31	5.261809371	-7.560527589	5.782566881
C32	6.357626058	-7.158097449	6.789481626
C33	4.223564284	-6.440151595	5.593502721
C34	4.827095522	-5.135349072	5.070120955
C35	3.743379229	-4.158516084	4.618382866
C36	3.968760142	-1.694420106	4.230223527
C37	8.713143871	-6.546949686	7.064025064
C38	9.134219888	-5.098430973	6.942457705
C39	-5.164752224	-2.281497751	-2.024172038
C40	-5.458022771	-0.775814297	-1.915113473
C41	-3.655884658	-2.487717122	-1.751805751
C42	-3.204362622	-3.943305641	-1.513591151
C43	-2.795175353	-4.713593239	-2.768693576
C44	-5.778497068	1.270600330	-3.231082204
C45	-7.123283673	1.870640842	-2.797111482
C46	-5.389656699	1.762604837	-4.639268931
C47	-9.250141603	1.463017157	-1.646536702
C48	-9.017657626	1.698499880	-0.146013759
C49	-7.483026379	1.420398203	1.760052289
C50	-6.361324089	2.421230845	2.043332347
C51	-4.469400264	3.742303536	1.222400856
C52	-4.981580679	5.142938055	1.639632124
C53	-3.640092160	3.989016037	-0.048382041
C54	-2.925161158	2.824736090	-0.654800668
C55	-2.456806426	1.631121617	-0.165273155
C56	-1.811999452	1.787563962	-2.288048073
C57	-6.631192611	6.890393678	1.072577775
C58	-6.928200863	7.267103725	2.522190189
C59	-7.918859295	6.947924959	0.218334578
C60	-8.346764172	8.306159861	-0.255016006
C61	-8.376909004	9.524214239	0.396803819
C62	-9.138433718	9.736324240	-1.673952737
C63	8.157457240	1.194911351	5.258505587
C64	8.957654730	-0.079360242	5.450566687
C65	6.750839405	0.771882806	4.764384306
C66	5.816223104	1.944361941	4.581188034
C67	5.011826532	2.411567628	5.637937162
C68	5.733101816	2.611491433	3.345765956
C69	4.151015468	3.501952775	5.468500030
C70	4.886267618	3.706367711	3.163861469
C71	4.093182058	4.148131776	4.226704909
C72	6.407816434	6.457049799	-1.099846376
C73	5.505486662	7.513198443	-1.749218657
C74	5.571238097	5.251542634	-0.650823501
C75	4.898716303	8.674400378	-3.830606216
C76	3.450581804	8.264351096	-4.108408318
C77	1.800396270	6.425469213	-4.102390000
C78	0.978581316	6.485629332	-2.796370999
C79	1.891641740	5.003558272	-4.685544456

C80	0.576864171	4.274243302	-4.979265871
C81	-0.272617202	4.799858412	-6.151080620
C82	-1.525414096	6.957892188	-6.223874896
C83	0.926412550	6.284070891	-0.367537549
C84	0.828339678	7.710947872	0.205729185
C85	1.533728298	5.369182818	0.707123818
C86	2.048342912	9.787532294	0.628193669
C87	1.560186935	11.121561843	0.071627281
C88	0.420565295	12.327509413	-1.745968797
C89	-0.922304090	12.909947390	-1.256977286
C90	0.424463848	12.162044123	-3.280846506
C91	-0.604122726	11.138415357	-3.748806632
C92	-3.021317405	12.467686535	-0.058310952
C93	-2.975619692	13.637434055	0.918595688
C94	-3.720953461	11.251741701	0.604710638
C95	-3.917474384	10.110434044	-0.367897887
C96	-5.022117976	10.098230616	-1.233193909
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C104	1.825301568	-1.839332908	-7.336668916
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C113	-0.181899749	-6.734912236	-6.105358120
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C116	-3.384181961	-0.639194964	-7.170638887
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	O461	7.992635231	2.161031415	-7.784763770
	O462	-3.690992285	-3.487057371	-9.180702713
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	O471	2.087383756	-11.230724289	-1.609586525
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	O473	4.128912834	-7.742814575	1.913778378
	O474	2.355887405	-6.400041665	-0.895453421
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	O477	-3.243906911	4.769287660	-3.842214679
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	O479	6.406914579	-9.087910227	2.436698993
	S480	4.563174055	4.508092611	-2.015394072
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	C7	-2.198545160	-7.330542918	-4.383802767
	C8	-2.395128412	-6.308579112	-3.259476464
	C9	-2.988635333	-4.026383253	-2.641438595
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C21	-0.190434972	-4.658526518	0.435301349
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C32	6.161553824	-7.070792154	7.054989571
C33	4.115943111	-6.442149371	5.675281423
C34	4.677818429	-5.075248678	5.275978260
C35	3.577623210	-4.158820257	4.744283482
C36	3.647194076	-1.663716054	4.546036666
C37	8.431521796	-6.324511629	7.597346394
C38	8.749005107	-4.844510985	7.557239818
C39	-4.777123571	-2.506381558	-2.637064332
C40	-5.177211569	-1.027966457	-2.491268874
C41	-3.294398476	-2.632542171	-2.213260419
C42	-2.770615808	-4.070154798	-2.007470922
C43	-2.161967224	-4.719142653	-3.249762139
C44	-5.511712014	1.060054589	-3.733108599
C45	-6.932292159	1.541341264	-3.404976405
C46	-5.028300816	1.656900231	-5.068807551
C47	-9.126366329	0.924059882	-2.500829119
C48	-9.060362413	1.099915083	-0.975563371
C49	-7.718480625	0.827531562	1.068596284
C50	-6.690894293	1.871193419	1.514187923
C51	-4.827433010	3.359086635	0.941258405
C52	-5.469757486	4.696635670	1.380200940
C53	-3.922202371	3.736099034	-0.242572627
C54	-3.054764111	2.666936166	-0.821212473
C55	-2.566291882	1.475887123	-0.345963037
C56	-1.698767268	1.801978068	-2.368092996
C57	-7.177724656	6.360638498	0.739462583
C58	-7.649587880	6.646004225	2.163650549
C59	-8.368705544	6.384870544	-0.247465759
C60	-8.841475383	7.736220086	-0.697643863
C61	-9.015087773	8.916946217	-0.000813368
C62	-9.583658672	9.183575532	-2.126119474
C63	7.521371409	1.451116030	6.087010013
C64	8.392980306	0.226258893	6.299468376
C65	6.200057663	0.960342494	5.442399476
C66	5.204912391	2.074585240	5.219752933
C67	4.272365746	2.431860903	6.212430364
C68	5.192328933	2.799885093	4.015102553
C69	3.351882548	3.465527420	6.008820909
C70	4.288879102	3.841333049	3.801217790
C71	3.366783834	4.172283454	4.798857807
C72	6.035127013	6.892190982	-0.194324099

C73	5.114984109	7.918554901	-0.866767401
C74	5.245510637	5.615722371	0.118709374
C75	4.604408557	9.154622394	-2.929209756
C76	3.226386326	8.663072693	-3.376442689
C77	1.716230091	6.722733501	-3.618252885
C78	0.786341381	6.663155113	-2.386545381
C79	1.956141356	5.343569002	-4.259198008
C80	0.730924531	4.556848489	-4.735297209
C81	-0.034720118	5.114253496	-5.948792349
C82	-1.413144740	7.192437173	-6.023197761
C83	0.534155165	6.332201939	0.012657062
C84	0.270429758	7.714700996	0.637684007
C85	1.112112508	5.413031871	1.101089273
C86	1.286514250	9.844123184	1.283220599
C87	0.758692054	11.173383614	0.751133443
C88	-0.283742569	12.400943629	-1.108293711
C89	-1.703725635	12.863040080	-0.716895771
C90	-0.137735349	12.319619478	-2.642573790
C91	-1.041401706	11.254112860	-3.252481810
C92	-3.874188684	12.219460209	0.225383479
C93	-4.019708146	13.335402841	1.252736033
C94	-4.561291407	10.930905930	0.752552378
C95	-4.576890407	9.831770613	-0.282591735
C96	-5.573121937	9.801015044	-1.271788286
C97	-3.564883120	8.858468760	-0.329562366
C98	-5.548081146	8.848532505	-2.293165656
C99	-3.508755762	7.911610658	-1.358208348
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C101	6.211458908	-4.462478752	-7.455798471
C102	4.719882594	-4.208267029	-7.320805918
C103	3.011266619	-2.619905112	-6.461748607
C104	2.645394960	-1.321828303	-7.192794858
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C106	4.087529862	2.138239965	-7.098311314
C107	6.236128092	2.793579121	-6.113178054
C108	7.450420973	2.540697533	-6.985666334
C109	-0.309709498	-4.090381339	-9.284402140
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C116	-2.615807847	-0.463733428	-7.474364276
C117	-1.612235075	-0.415354264	-6.355362467
C118	-0.935729535	0.774447641	-6.037089905
C119	-1.234066932	-1.602253403	-5.702110526
C120	0.140051792	0.753933419	-5.142588444
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C122	0.554989117	-0.444446720	-4.556222029
C123	8.660216691	-6.598996280	-1.886102511
C124	9.514223038	-6.689577279	-0.610243413
C125	7.219597503	-7.085035112	-1.664509281
C126	6.261220727	-6.845093422	-2.791330981
C127	6.238421513	-7.486703097	-4.013565126
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C137	4.250676040	-6.839672422	0.902560646
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Fe140	2.410928698	0.276106929	-0.492239208
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Fe145	2.594898538	-2.314667037	-0.626733509
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H153	-10.111173142	-2.581856107	-0.202444508
H154	-10.116750757	-5.603405136	3.652877177
H155	-7.527552408	-5.660979286	2.114001895
H156	-9.912288190	-3.877276597	4.041185505
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H159	-5.372042063	-6.374689094	2.644325709
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H162	-5.700532830	-6.169764301	4.382900277
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H166	-1.381371851	-3.614753045	4.043407488
H167	-0.839507977	-2.786739323	2.565294885
H168	0.331889967	-3.145956810	3.847118386
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H174	-0.239346960	-0.331048146	2.604105262
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H184	-0.267193108	0.603563254	4.111467736
H185	1.424780926	4.461266832	0.636759961
H186	0.298137359	5.205859754	1.813790098
H187	2.231582303	5.735417285	2.683876112
H188	1.860607337	5.304817979	5.270639059
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H223	-2.723888471	0.967942800	0.597852627
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H236	-5.721673551	1.855225507	-0.311700550
H237	-7.446012101	-0.137761928	1.520876983
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H239	-1.120418179	1.643443315	-3.272986103
H240	-9.852558328	0.131906283	-2.726083230
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H245	2.095862035	8.388290134	-0.014348554
H246	-2.701815849	3.640254743	-2.743170423
H247	-3.839752243	4.170181083	-4.419652560
H248	-3.693887601	5.501815640	-3.565320096
H249	-3.985286734	1.357358937	-5.242735046
H250	-5.646270632	1.282243927	-5.902131257
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H252	-0.437257940	13.291829507	-3.055686071
H253	0.580560832	9.935033484	-3.557180779
H254	-1.022148311	9.316671758	-3.897253960
H255	-0.879387844	8.691172175	-7.312413083

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H259	-2.924408584	7.564297219	-4.670603676
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H264	5.166162630	9.448780021	-3.825882971
H265	-5.194293863	-0.987774490	-4.492968417
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H267	-2.677643026	7.205787175	-1.413976670
H268	-5.902663552	3.313674428	-4.527866934
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H287	8.640033521	-5.529478234	-2.142038716
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H289	5.879105706	-6.082412290	-8.642015625
H290	5.935688946	4.877340559	0.547794669
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H295	6.537274318	2.789784529	-5.054274293
H296	6.861331915	6.640675010	-0.878083588
H297	3.490028445	-6.354333083	6.578807814
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H299	5.204907713	0.966785375	-5.784344817
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H313	1.417501596	-0.434036056	-3.889601475
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H318	-1.781379594	-2.526782989	-5.897068737
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H323	7.276365569	1.855012686	-7.849455788
H324	6.152857343	-5.182818620	1.701842865
H325	1.899361067	-7.216234473	2.047753862
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H327	2.761831051	-9.100779882	0.609622657
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H329	3.537544038	-5.678016216	-4.104344403
H330	4.760278298	-11.978766724	6.375319640
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H332	7.707654487	-5.885402222	3.380915194
H333	6.902496385	-3.851070346	1.973552336
H334	7.643079883	-6.721506578	5.633393779
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C20	-1.157304857	-2.918906762	1.973516189
C21	-0.184996691	-4.660429399	0.433680528
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	O478	11.529706791	-6.365519652	0.479121817
	O479	9.080554805	-6.584162379	1.966594916
	S480	0.937472464	5.089821915	4.257487923
	S481	1.787007254	3.287174997	1.366718681
	S482	4.997419227	0.021924538	-1.365171344
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	S484	1.765536291	0.400616541	-0.867605353
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	Fe(142)	0.545 -2.627	C3	-9.135868273 -2.835050519 1.087986081
			C4	-8.921492306 -2.973478761 2.594096907
			C5	-9.219277367 -4.323085993 4.605135363

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 Fe(144) 0.492 -2.209
 Fe(145) 0.335 -1.038
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C15	-2.040659192	-4.075149313	7.906289411
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C107	6.314296777	1.525371741	-6.501536817
C108	7.522579178	1.123126049	-7.322434361
C109	-0.368661206	-5.675018601	-8.411868233
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			C13	-6.324662628	-3.271195670	7.863457114
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			C16	-1.620294042	-3.777579002	6.939275749
			C17	-0.949894323	-1.687114336	5.784466280
			C18	-1.035879154	-0.331484608	6.508128595
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			C34	4.659060108	-5.148766589	5.201784715
			C35	3.562127101	-4.224949451	4.672533778
			C36	3.620835562	-1.728590705	4.518095024
			C37	8.377309016	-6.430108007	7.534956169
			C38	8.699351150	-4.951243098	7.523211673
			C39	-4.731589210	-2.510052670	-2.796826726
			C40	-5.217162652	-1.069358827	-2.578300664
			C41	-3.248281453	-2.589081326	-2.372088775
			C42	-2.698944299	-4.015804509	-2.160043280
			C43	-2.084189216	-4.669602998	-3.395177962
			C44	-5.458196910	1.106443125	-3.724340298
			C45	-6.885849468	1.588336273	-3.435824829
			C46	-4.936956778	1.724811731	-5.037656574
			C47	-9.095035044	0.961639616	-2.574958002
			C48	-9.048262929	1.106467025	-1.045239662
			C49	-7.736164078	0.797046471	1.008960643
			C50	-6.769472854	1.873331084	1.511138087
			C51	-4.877151765	3.371860141	1.035241936
			C52	-5.530804582	4.695338929	1.466489436
			C53	-3.920483713	3.718938883	-0.120022321
			C54	-3.179841913	2.550611732	-0.681299972
			C55	-2.919879961	1.277671455	-0.212683618
			C56	-1.925325944	1.406721921	-2.113703577
			C57	-7.219956636	6.359067360	0.802914886
			C58	-7.699917585	6.598445922	2.232709252
			C59	-8.412649160	6.385148051	-0.182932461

C60	-8.895689936	7.740037052	-0.609068131
C61	-9.090759556	8.900134552	0.115668201
C62	-9.621819160	9.220661257	-2.011648200
C63	7.467417372	1.343138097	6.192238009
C64	8.342261202	0.118990220	6.391873675
C65	6.165088576	0.861592073	5.505293206
C66	5.159403102	1.971760606	5.307880763
C67	4.203461710	2.273270570	6.295699685
C68	5.154447800	2.739961907	4.130803107
C69	3.268505501	3.297599686	6.114676160
C70	4.236280662	3.773480992	3.941055557
C71	3.291696960	4.050105325	4.933521770
C72	6.008885277	6.906663158	0.028395154
C73	5.091855352	7.948468535	-0.621991397
C74	5.222179361	5.622275119	0.318117803
C75	4.594502586	9.235466732	-2.656529962
C76	3.222532615	8.749130650	-3.123435460
C77	1.726220261	6.809670010	-3.433741675
C78	0.772812262	6.742642165	-2.220319989
C79	1.983347576	5.441353490	-4.085881414
C80	0.769833679	4.671318173	-4.612774790
C81	0.038239388	5.271436845	-5.826310444
C82	-1.355405844	7.338578188	-5.868615992
C83	0.460913486	6.321878726	0.157642793
C84	0.201726920	7.694665583	0.806413567
C85	1.011670951	5.375748706	1.235434705
C86	1.228026495	9.803917513	1.501776049
C87	0.700823988	11.145139480	1.000312082
C88	-0.348664918	12.416964223	-0.823736124
C89	-1.774405614	12.874417099	-0.444515778
C90	-0.175587505	12.378929990	-2.357458567
C91	-1.062736458	11.322361028	-3.006262513
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C93	-4.117121419	13.307584490	1.524193679
C94	-4.644774138	10.913547987	0.954562635
C95	-4.639297964	9.842200239	-0.111119724
C96	-5.622445065	9.832609606	-1.113509404
C97	-3.622240097	8.874453993	-0.170591260
C98	-5.579968670	8.907184998	-2.158837493
C99	-3.551436060	7.953047067	-1.220425638
C100	-4.531382779	7.987653048	-2.212415566
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C103	3.100261163	-2.456197025	-6.490025088
C104	2.758765386	-1.150486203	-7.217278985
C105	3.078047762	1.275708995	-7.212653343
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C107	6.292910986	2.972346424	-5.982356590
C108	7.520948926	2.747522295	-6.843850433
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H236	-5.688580100	1.871959220	-0.247369726
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H239	-1.323928588	1.197740958	-2.995217116
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H258	-2.860599130	8.819139569	0.612844237
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H269	4.413412286	10.124558682	-2.037033881
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H272	-4.141651699	-3.546371183	-4.471115947
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O472	4.473654911	-7.601035931	1.826877583
O473	2.932280164	-6.176238478	-1.078190016
O474	8.087069527	-6.673694288	3.813268321
O475	6.686291452	-4.701500535	2.345497316
O476	-3.151724799	4.842276603	-3.883368376
O477	7.669196066	-10.684050383	0.553406232
O478	6.784624146	-8.778635117	2.514015389
S479	4.414516216	4.988988420	-1.200681062
S480	2.773523991	1.760299949	-2.406365717
S481	2.811939081	-3.495261578	-2.650803923
S482	3.797845769	1.666263354	1.015003587
S483	1.036180345	-1.065051446	-1.637715845
S484	5.267559995	-0.847938453	-4.208464683

	S485	3.508270323	-3.528899555	0.914803342
	S486	6.260174665	1.625700797	-1.589072582
	S487	6.282060018	-3.337436607	-1.500118218
	S488	6.259173104	-1.063987635	1.500093557
4u(a)	bm2cnx2b262n2x35.car_4			
Fe(139) 0.564 -2.477	C1	-8.257765531	-4.501987211	-0.020558279
Fe(140) 0.346 0.276	C2	-8.432040583	-5.695973584	-0.965671997
Fe(141) 0.543 -2.654	C3	-9.269452140	-2.440548310	0.856141009
Fe(142) 0.568 2.727	C4	-9.079991093	-2.659857428	2.355603080
Fe(143) 0.592 3.099	C5	-9.467427758	-4.089825328	4.295923139
Fe(144) 0.514 2.334	C6	-8.022099772	-4.423690632	4.680022456
Fe(145) 0.394 -0.847	C7	-5.872376577	-5.332835660	3.935719614
S=3/2	C8	-5.000402676	-4.075871146	3.888593939
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	C10	-4.761816105	-1.006820303	4.041195874
	C11	-6.286164865	-0.157724290	5.734253602
	C12	-5.739778776	-0.734107950	7.047609355
	C13	-5.661993763	-2.671796396	8.545069819
	C14	-4.245394614	-3.228689701	8.730072249
	C15	-2.321712924	-4.340448847	7.676826908
	C16	-1.132223170	-3.533974422	7.144927505
	C17	-0.453418507	-1.519128749	5.861386893
	C18	-0.370084774	-0.150852328	6.563893530
	C19	-0.691159451	-1.429739682	4.330921807
	C20	0.239340161	-0.408816757	3.668378014
	C21	-0.538508875	-2.812264894	3.687421145
	C22	-1.528389660	1.924492819	7.213044483
	C23	-1.681038656	1.791497574	8.740908181
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	C26	-2.284990130	3.115449285	5.108400475
	C27	-2.919087571	0.894237875	10.623386510
	C28	-1.678501470	0.460483196	11.379862604
	C29	3.878336469	-11.391934333	5.921176568
	C30	4.659898415	-10.272833181	5.235918090
	C31	5.236508733	-7.853263460	5.438627346
	C32	6.333232764	-7.517809531	6.466999329
	C33	4.207411301	-6.717883523	5.310935650
	C34	4.817037071	-5.398990501	4.832494554
	C35	3.736037840	-4.402556680	4.418614921
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	C38	9.084787786	-5.442189545	6.736212132
	C39	-5.132660857	-2.179231902	-2.205031773
	C40	-5.427339432	-0.682549950	-2.016251117
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	C42	-3.186434440	-3.871276147	-1.747360946
	C43	-2.778941016	-4.587072861	-3.032256852
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	C47	-9.215753323	1.533033853	-1.656172884
	C48	-8.994848652	1.698489978	-0.144053486
	C49	-7.482031100	1.319521810	1.761791751
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	C52	-4.973948225	5.047213994	1.824826024
	C53	-3.607493706	3.938559645	0.104904805
	C54	-2.895398854	2.785564746	-0.535243069
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C65	6.747435893	0.502074102	4.819339674
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C67	4.986979751	2.068823327	5.774336818
C68	5.736323093	2.425358838	3.511238641
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C71	4.081792464	3.895133951	4.473183766
C72	6.423971525	6.510757929	-0.699730488
C73	5.519757102	7.591564253	-1.305135125
C74	5.583861733	5.284883512	-0.323851405
C75	4.917406915	8.846146440	-3.332229328
C76	3.472254758	8.450588268	-3.641903198
C77	1.819208320	6.615185045	-3.731522702
C78	0.982837300	6.609199357	-2.433463544
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C86	2.059775046	9.747324522	1.146091910
C87	1.572244055	11.106329706	0.653470201
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C91	-0.566043425	11.319301704	-3.177100474
C92	-3.029989719	12.454756096	0.558001166
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C94	-3.729680967	11.199002325	1.147118933
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C119	-1.855705603	-1.518040322	-5.550464549
C120	-0.277821539	0.722968349	-5.064945152
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H147	-6.566960307	-5.872423367	-1.780011302
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H149	-8.890736098	-5.346022145	-1.904283949
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H151	-8.436814604	-1.800991793	0.530220699
H152	-10.155389485	-4.409045731	2.280373477
H153	-10.207534509	-1.890719297	0.702490715
H154	-10.104251375	-4.950209033	4.541709648
H155	-7.667406502	-5.154670110	2.795167154
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H158	-5.995669663	-3.398248168	2.206256603
H159	-5.539810970	-6.034278935	3.159143440
H160	-5.842317550	0.837455299	5.604503262
H161	-6.774720297	-1.488571927	4.115075890
H162	-5.712688557	-5.798902207	4.915544954
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H164	-6.515017520	-2.600041292	6.590655602
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H166	-1.230881649	-3.544564988	4.126216172
H167	-0.740600197	-2.760101994	2.606633813
H168	0.488382047	-3.190950063	3.810567678
H169	-1.729204871	-1.090117904	4.183079338
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H172	-3.370210140	0.580984003	8.559893785
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H174	-0.005520210	-0.310062762	2.601137124
H175	1.290199412	-0.724030787	3.729478688
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H177	-3.048673943	3.775406954	4.670739108

H178	-3.469423846	4.810926712	6.881473396
H179	-1.308737901	3.618267766	5.011411045
H180	-1.753348301	4.703630683	7.348357329
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H182	-0.539605440	2.386968048	7.074758609
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H185	1.641851044	4.346391259	0.529905147
H186	0.714645040	5.194744547	1.805072912
H187	2.784045736	5.497983790	2.475266213
H188	2.691712833	5.101058009	5.091173822
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H248	-3.649460139	5.745382637	-3.213326223
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H254	-0.751684407	9.374168819	-3.769660144
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H260	2.488541622	4.560026104	-3.725379543
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H264	5.411410582	9.082379271	-4.284409040
H265	-5.608910975	-0.626373572	-4.006772557
H266	2.515929485	5.344539085	-5.309824111
H267	-2.292123750	7.410272582	-1.243510174
H268	-6.056433164	3.706521341	-3.995685228
H269	4.866734981	9.771003026	-2.741817557
H270	-0.323958342	7.165554683	-7.589168026
H271	-2.711660894	8.879252517	-5.716880557
H272	-4.828124974	-3.307917700	-3.899799902
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H282	1.174636032	13.145358777	-0.788403041
H283	3.143629932	9.835622995	1.302463313
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C107	5.851977999	2.374848137	-6.727525859
C108	6.929355028	2.125764509	-7.764268404
C109	-1.411834406	-4.041243732	-9.204418660
C110	-2.388299098	-2.859953683	-9.147730775
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C112	-0.607410431	-6.031668093	-7.828474924
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C114	-2.709326596	-0.479476948	-8.677621649

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C117	-2.135606599	-0.322164357	-6.196377486
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C128	3.598693068	-6.389441135	-4.205556067
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C131	-0.096099937	-6.947081881	0.586189769
C132	1.329013177	-6.744302045	1.022516132
C133	2.372224164	-7.122794332	-0.105352835
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	C46	-5.542935512	2.955702335	-3.736892833
	C47	-9.254662509	1.367980102	-1.227963917
	C48	-9.068803849	0.995639862	0.251273575
	C49	-7.575475041	0.069678473	1.966426088
	C50	-6.499444753	0.941002505	2.622990226

C51	-4.774925243	2.673804736	2.385383865
C52	-5.402477956	3.765673517	3.276121169
C53	-3.993343355	3.413178200	1.286583370
C54	-3.186353410	2.596098882	0.322846562
C55	-2.684736746	1.313026321	0.388698876
C56	-2.046170790	2.268600275	-1.499232778
C57	-7.161084416	5.486325217	3.349698676
C58	-7.406749850	5.296916886	4.843587040
C59	-8.495686466	5.743945581	2.609667037
C60	-9.026607099	7.146242236	2.664892342
C61	-9.116552529	8.040706657	3.713869429
C62	-9.943715555	8.936428556	1.862833132
C63	8.117317717	-0.184795668	5.472310595
C64	9.024254890	-1.368223319	5.192000798
C65	6.748113481	-0.505044706	4.819655253
C66	5.711549478	0.565291501	5.067325687
C67	4.887342047	0.539955088	6.207006293
C68	5.548182654	1.628083900	4.160814979
C69	3.925887701	1.529944088	6.430043975
C70	4.597672327	2.626353326	4.372964636
C71	3.783576319	2.573708268	5.506467942
C72	5.840300313	6.899212413	1.496859504
C73	4.853065447	8.046903142	1.252276709
C74	5.098291213	5.556048224	1.450293432
C75	4.128944549	9.820143601	-0.287469182
C76	2.717603448	9.422646947	-0.726676262
C77	1.221553651	7.584670185	-1.426035446
C78	0.406694164	7.139849827	-0.193541459
C79	1.419985019	6.458535622	-2.456564562
C80	0.163143026	5.787342503	-3.021544292
C81	-0.734049727	6.642087109	-3.932859728
C82	-2.138495948	8.573765876	-3.225649271
C83	0.360218528	6.044126314	1.983543863
C84	0.176520752	7.144673956	3.045773262
C85	1.016862011	4.830733733	2.655000074
C86	1.242562694	9.015753194	4.206034806
C87	0.646183017	10.419684594	4.157117195
C88	-0.609129739	12.104475814	2.879658012
C89	-1.991948166	12.358508440	3.516497535
C90	-0.602858101	12.514741323	1.391065665
C91	-1.551200372	11.659686832	0.557623038
C92	-4.053153897	11.351502702	4.395051313
C93	-4.099598539	12.066133940	5.739156788
C94	-4.659954740	9.928377947	4.538401831
C95	-4.752887817	9.204449596	3.214573676
C96	-5.847359695	9.419376325	2.361322510
C97	-3.732465674	8.342523882	2.778922056
C98	-5.919550527	8.811889922	1.104981310
C99	-3.774903155	7.745099563	1.514774641
C100	-4.868707935	7.993180242	0.686576748
C101	5.451635901	-1.613896417	-9.048033632
C102	3.978520502	-1.486518284	-8.694358071
C103	2.348147740	-0.330307994	-7.213241087
C104	1.910472601	1.114279065	-7.482002857
C105	2.193796097	3.450289399	-6.807295387
C106	3.314692914	4.432655446	-6.482533566
C107	5.530067072	4.858641019	-5.532810523
C108	6.630982511	5.008444916	-6.563350432
C109	-1.202962187	-0.997900631	-10.042860539
C110	-2.269817178	0.026840262	-9.636908775
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C116	-3.301241159	1.811334018	-7.006199731
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C118	-1.475085707	2.533459903	-5.394476987
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C121	-0.707281728	-0.129013824	-4.995084168
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C124	9.460717108	-5.694989039	-3.614012686
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C132	1.914861336	-6.548157483	-1.147358188
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C137	4.381503964	-6.499612846	-1.638635341
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Fe139	4.369585171	-1.073973334	-3.529383746
Fe140	2.697284348	0.824260812	-0.603336771
Fe141	5.264091762	0.563272850	-0.496683793
Fe142	4.323819341	1.395267001	-2.769257316
Fe143	4.265230229	3.035654931	-0.651272575
Fe144	5.093097776	-1.863030246	-1.167983559
Fe145	2.487060150	-1.572086653	-1.746794545
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H158	-5.648309385	-4.359968247	0.928508752
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H210	-2.922718301	-1.177414120	-3.262746541
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H246	-3.306024103	4.678546229	-1.528684703
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H256	-1.169683889	6.012667359	-4.723352613
H257	-6.786233686	8.976010281	0.460301077
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H266	2.009155835	6.878431089	-3.289041215
H267	-2.946475211	7.125218339	1.166639561
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H269	-1.046482157	9.127037338	-4.878569589
H270	-3.540255418	9.920935414	-2.608204334
H271	-4.619026763	-2.239208120	-4.840803882
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H318	7.533190105	-9.657688307	-2.548003774
H319	7.097135699	-6.919073426	-4.598454668
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H323	6.335262783	-5.096162373	-0.568491039
H324	2.186738288	-7.354003524	-0.449203236
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H327	4.230750790	-4.988387352	-8.036326975
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H333	8.295077596	-7.732802475	2.471155708
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H351	6.903855197	-0.632963725	3.736330984
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H177	-3.514712745	3.578532386	4.519133949
H178	-4.110005511	4.528405232	6.727206391
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H184	-0.236686630	0.409511462	4.073513173
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H186	0.563085707	5.093554653	2.064558026
H187	2.562228283	5.374175023	2.959232639
H188	2.208756691	4.850394402	5.527373769
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H196	-6.675892465	-2.302345183	8.689184973
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	S482	0.789589216	-1.193715357	-1.583334915
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	S484	3.214932446	-3.653345994	0.780755966
	S485	6.328758923	1.244452569	-1.611907560
	S486	6.071169975	-3.768629302	-1.597215555
	S487	6.227362544	-1.469739090	1.396733741
6⁻²(b)	bm1cnx2b262n2x353.car_1			
Fe(139) 0.556 -2.387	C1	-8.257344594	-4.457364908	-0.970126526
Fe(140) 0.345 -0.080	C2	-8.337520441	-5.590249944	-1.998909798
Fe(141) 0.564 -2.806	C3	-9.312219228	-2.413775421	-0.108737221
Fe(142) 0.553 2.572	C4	-9.267549894	-2.694922623	1.391318442
Fe(143) 0.607 3.204	C5	-9.839185886	-4.195925948	3.227603600
Fe(144) 0.498 2.282	C6	-8.438915247	-4.566735668	3.728746839
Fe(145) 0.333 -0.469	C7	-6.229315781	-5.442616124	3.140032750
S=3/2	C8	-5.355971782	-4.186945901	3.233161584
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	C10	-5.118168002	-1.150624764	3.548402746
	C11	-6.790601824	-0.354268861	5.116532556
	C12	-6.373590371	-0.988934755	6.450699369
	C13	-6.440527705	-2.988203425	7.864853106
	C14	-5.052414882	-3.570319416	8.158286204
	C15	-3.036115354	-4.637997822	7.241569261
	C16	-1.804124721	-3.817337481	6.852303787
	C17	-1.004648011	-1.754779820	5.730371248
	C18	-0.975163855	-0.413619301	6.484660682
	C19	-1.100252806	-1.606657679	4.188343956
	C20	-0.113228568	-0.570565899	3.643071998
	C21	-0.897859302	-2.965346327	3.507482907
	C22	-2.182009294	1.637670716	7.117339092
	C23	-2.477280004	1.439979662	8.617737575
	C24	-3.194449646	2.589234017	6.436607631
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	C26	-2.760270280	2.912208676	5.000832124
	C27	-3.889720413	0.466714272	10.335414713
	C28	-2.721735714	0.028693605	11.194998006
	C29	3.275347619	-11.672354077	5.793030273
	C30	4.119213858	-10.530735837	5.224073449
	C31	4.671401407	-8.117177590	5.555213831
	C32	5.660818279	-7.823965971	6.698007616
	C33	3.665960704	-6.966432460	5.360719019
	C34	4.331250226	-5.631520363	5.016476835
	C35	3.301545894	-4.593090940	4.572719885
	C36	3.537145624	-2.109207125	4.411603404
	C37	7.969287137	-7.242194556	7.266050558
	C38	8.409783684	-5.794052174	7.289030531
	C39	-4.932619657	-2.070948552	-2.768949078
	C40	-5.283250189	-0.596370572	-2.518703238
	C41	-3.457004221	-2.293030392	-2.367746337
	C42	-3.030071874	-3.767664950	-2.205782136
	C43	-2.491146025	-4.432482119	-3.470153096
	C44	-5.393391911	1.606698519	-3.631312000
	C45	-6.784652324	2.177935142	-3.327803153
	C46	-4.839778679	2.208967002	-4.938120898
	C47	-9.014701946	1.676156578	-2.435607516
	C48	-8.933556346	1.778297977	-0.904285409

C49	-7.611979940	1.326827992	1.117090469
C50	-6.545032216	2.299295908	1.629455829
C51	-4.567485718	3.681272195	1.168097147
C52	-5.139878954	5.020676674	1.652477417
C53	-3.617890583	4.023966358	0.006085353
C54	-2.943421762	2.839698079	-0.600679599
C55	-2.752888084	1.541046329	-0.172428661
C56	-1.787990626	1.663082140	-2.087664175
C57	-6.697134133	6.819319872	1.033049885
C58	-7.133854471	7.079548919	2.474334061
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C61	-8.371844654	9.502887077	0.462258235
C62	-8.946686640	9.932337116	-1.635240840
C63	7.603791746	0.612809589	6.115931609
C64	8.381527122	-0.682422279	6.255759064
C65	6.253880359	0.256073534	5.441492409
C66	5.341474299	1.449425958	5.285870464
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C68	5.365023732	2.229223111	4.116564098
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C71	3.649035577	3.686822863	4.991132634
C72	6.469870560	6.495307080	0.168807841
C73	5.650742633	7.627471946	-0.463024895
C74	5.582776413	5.263382664	0.400303385
C75	5.234081791	8.953534243	-2.491433789
C76	3.824845217	8.576456984	-2.955682005
C77	2.187377630	6.753066979	-3.279266710
C78	1.240289218	6.714889916	-2.060305738
C79	2.345837220	5.386625878	-3.970275311
C80	1.074680894	4.705799379	-4.486452731
C81	0.371168458	5.360084919	-5.687133454
C82	-0.850279186	7.541092267	-5.681484183
C83	0.930317145	6.284631035	0.316235684
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C85	1.416263403	5.270532444	1.362208423
C86	1.964806844	9.665413480	1.738702051
C87	1.543501707	11.050454487	1.257088720
C88	0.579313741	12.420867524	-0.541026507
C89	-0.807794054	12.961820846	-0.129572601
C90	0.738318339	12.399814076	-2.076658115
C91	-0.241622004	11.436023472	-2.736566387
C92	-3.014841702	12.421536530	0.797563920
C93	-3.081670967	13.492266832	1.880136567
C94	-3.785132136	11.156169424	1.263684852
C95	-3.878862235	10.113833497	0.172592966
C96	-4.883506017	10.197762466	-0.803079581
C97	-2.930446214	9.083460672	0.062775639
C98	-4.931095710	9.299388371	-1.871653214
C99	-2.947184616	8.191052936	-1.014061605
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C101	5.888879653	-4.555067492	-7.681029576
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C104	2.568937147	-1.177233273	-7.285079870
C105	3.066097824	1.219502998	-7.205774872
C106	4.260819727	2.151918681	-7.032019788
C107	6.435514350	2.613399990	-6.007814992
C108	7.615306745	2.359066530	-6.924742097
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C113	0.445328731	-6.150724723	-6.709106178
C114	-1.920181247	-0.102628159	-8.905749056
C115	-1.201294919	1.130241385	-9.414013671
C116	-2.621705830	0.075135622	-7.537668268
C117	-1.629231723	-0.006392389	-6.412146503
C118	-0.864249557	1.110845152	-6.045149659
C119	-1.352398806	-1.247584412	-5.812831281
C120	0.196806098	0.969564852	-5.146703014
C121	-0.285982434	-1.386884430	-4.921871253
C122	0.510408350	-0.281626341	-4.613782816
C123	8.160114367	-7.091077818	-2.220199257
C124	9.016371978	-7.307599321	-0.960889847
C125	6.689587275	-7.489330547	-2.011591596
C126	5.749001830	-7.135463386	-3.122924279
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H147	-6.401748579	-5.738082806	-2.637450682
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H153	-10.219481940	-1.834274946	-0.326318958
H154	-10.508407315	-5.052429418	3.383092024
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H159	-5.825527859	-6.112955679	2.369349788
H160	-6.324181400	0.638053100	5.074604847
H161	-7.139793772	-1.586016796	3.385492262
H162	-6.165923416	-5.950474365	4.110084447
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H164	-7.092859915	-2.831513224	5.839058336
H165	-7.882137846	-0.226304948	5.113846133
H166	-1.638510960	-3.705581744	3.842896732
H167	-0.990529448	-2.862335303	2.415355276
H168	0.109351535	-3.362065991	3.712167863
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H174	-0.253184782	-0.454103850	2.559958143
H175	0.929017363	-0.882423521	3.800899898
H176	7.388809992	0.984422204	7.136070093
H177	-3.492375175	3.585735957	4.531722338
H178	-4.083532824	4.542703755	6.734552314
H179	-1.781620596	3.419340774	4.999149114
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H181	-4.171197146	2.072844811	6.401992286
H182	-1.183995127	2.099066229	7.092718580
H183	-2.859258283	0.093167990	5.782704892
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H186	0.579732583	5.091308222	2.055710763
H187	2.561299677	5.400346832	2.956694522
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H189	4.545545171	3.917616899	3.039581867
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H206	1.035777343	-5.654961717	-8.720857362
H207	-1.534256693	-4.364064977	-7.644998828
H208	-0.367726713	0.918847462	-10.124568424
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H239	-1.213802109	1.439252560	-2.983740339
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H253	1.266157534	9.996909426	-3.063978625
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H266	3.045973180	5.527849515	-4.810901966
H267	-2.166843622	7.435572481	-1.120677639
H268	-5.618528633	3.900335524	-4.372523595
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H283	3.025462823	9.737534067	2.016292056
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H289	5.422389695	-6.087141223	-8.935272952
H290	6.214089856	4.459872600	0.803669167
H291	6.332483734	7.295713553	2.040496918
H292	6.640767123	7.362535374	-2.245581164

H293	4.798355716	5.511293607	1.129247376
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H295	6.757609390	2.499199425	-4.961181805
H296	7.287061868	6.215908011	-0.514944666
H297	3.052967298	-6.869794674	6.272427022
H298	5.215784400	-8.276468871	4.616676319
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C124	9.016651919	-7.305177942	-0.962614866
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C126	5.746567108	-7.129571151	-3.115693265
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C129	9.617871423	-8.674816232	0.952904479
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C131	-0.098400936	-6.909738122	0.276494806
C132	1.280352561	-6.784180223	0.860997712
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C134	2.214104320	-8.620367764	-0.667351281
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Fe145	2.544820630	-2.350783198	-0.885334045
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O429	-0.671055803	-4.270198898	7.069148238
O430	0.029399995	-0.068041778	7.119887140
O431	-1.805309488	2.003428700	9.487456523
O432	-2.666755320	0.242431772	12.392847856
O433	4.853216590	-10.732576994	4.230123929
O434	5.299800045	-7.883306364	7.885661780
O435	9.522053150	-5.430917024	7.651110829
O436	-5.515853014	-0.154141734	-1.380206358
O437	-2.983428971	-4.227889450	-4.599342402
O438	-6.939758389	3.409353987	-3.261002954
O439	-4.788582415	3.636968440	-4.868470808
O440	-9.880414203	2.293814960	-0.287474498
O441	-6.563515557	2.660959232	2.818659151
O442	-4.593590090	5.698497263	2.538170048
O443	-7.038172768	8.162906383	3.042352582
O444	8.436755271	-1.359176075	7.269156302
O445	2.831028299	4.773408570	4.780343394
O446	4.767819187	8.239295651	0.164496846
O447	3.061111808	9.476502071	-3.365614400
O448	0.051887755	7.064864332	-2.188194487
O449	-0.202222700	7.883582178	1.725830968
O450	2.549922553	5.787305782	2.060917730
O451	1.758506154	12.043170155	1.965882697
O452	-1.116295326	14.145678641	-0.340553030
O453	-1.435983323	11.737147455	-2.901277193
O454	-4.073148634	14.184804966	2.072591854
O455	-3.914597966	7.443532675	-3.074723530
O456	3.531729644	-4.982960849	-7.951787638
O457	1.861419886	-1.076670384	-8.308868721
O458	4.220202730	3.266849364	-7.587841284
O459	8.728952145	2.836905872	-6.744783639
O460	-2.735681772	-2.585216517	-9.809432623
O461	-0.391583522	-6.625671243	-5.945558092
O462	1.721896211	-6.000321522	-6.300129965
O463	-1.503396204	2.279083719	-9.142127512
O464	9.937034070	-6.520723739	-0.663105227
O465	11.945934407	-8.356287446	1.505782588
O466	-0.683766962	-6.050209856	-0.365276529
O467	-0.736419386	-8.111604337	0.470438371
O468	4.285340165	-11.376673769	-1.492674752
O469	2.248065939	-11.025726052	-2.402229573
O470	4.653724059	-6.306540965	0.167943854
O471	3.939690384	-7.917572808	1.571160811
O472	2.422743052	-6.260936695	-1.226222875
O473	7.616369745	-7.361606952	3.544919015
O474	6.351325407	-5.233019561	2.167669406

	O475	-2.811849927	5.143246504	-3.714670002
	O476	6.859628081	-11.256874080	0.204025034
	O477	6.146599407	-9.334176140	2.212908221
	S478	4.743220221	4.655582159	-1.134900406
	S479	2.801355958	1.653290160	-2.433925715
	S480	2.604766911	-3.519861030	-2.867855367
	S481	3.855531538	1.293079993	0.936348282
	S482	0.661032381	-1.271448879	-1.498741867
	S483	5.181282880	-1.096970873	-4.310521351
	S484	3.171932237	-3.695434129	0.779949265
	S485	6.381932645	1.173625371	-1.583444501
	S486	6.052953731	-3.774706939	-1.578912056
	S487	6.230482346	-1.534571066	1.368694929
	6⁻²(d)			
	Fe(139)	0.569	2.486	
	Fe(140)	0.329	0.093	
	Fe(141)	0.489	0.958	
	Fe(142)	0.537	-2.584	
	Fe(143)	0.595	3.105	
	Fe(144)	0.487	-2.312	
	Fe(145)	0.355	-1.140	
	S=1/2			
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	C1	-8.354999421	-4.297789178	0.481378171
	C2	-8.515191197	-5.636565366	-0.248959303
	C3	-9.323150135	-2.073211518	0.885558374
	C4	-9.212495098	-1.999127546	2.407258434
	C5	-9.743560947	-3.034518019	4.560801827
	C6	-8.330447208	-3.317263665	5.084989550
	C7	-6.164648491	-4.374300388	4.613356421
	C8	-5.259636773	-3.161730520	4.375680743
	C9	-4.697401060	-1.260241620	2.957900604
	C10	-4.944344288	-0.146428108	3.985003913
	C11	-6.527434461	1.042090284	5.390862086
	C12	-6.055151464	0.711356686	6.814080970
	C13	-6.087552604	-0.912132204	8.646295662
	C14	-4.689679130	-1.436431494	8.997748254
	C15	-2.735823681	-2.733272700	8.264052490
	C16	-1.508890663	-2.073376864	7.628614440
	C17	-0.723590581	-0.364770246	6.006706127
	C18	-0.649306186	1.111812320	6.439963916
	C19	-0.892797296	-0.572350445	4.478392722
	C20	0.081870790	0.281705786	3.661206383
	C21	-0.756776402	-2.056305442	4.117566196
	C22	-1.790289459	3.283542902	6.620450385
	C23	-2.003740212	3.443153530	8.139208683
	C24	-2.823882543	4.080482188	5.789779813
	C25	-2.935420401	5.527502762	6.285325109
	C26	-2.452011849	4.059107584	4.301553227
	C27	-3.337865879	2.941217249	10.100820453
	C28	-2.139248877	2.685162916	10.991302046
	C29	3.353661971	-10.103221133	8.146971738
	C30	4.208470462	-9.158263058	7.303639535
	C31	4.820571348	-6.749733958	7.040758615
	C32	5.873764052	-6.236144409	8.041397650
	C33	3.831481216	-5.640601386	6.642860302
	C34	4.499602509	-4.447509310	5.957239938
	C35	3.458896635	-3.514549191	5.339750350
	C36	3.736482184	-1.144418934	4.600686387
	C37	8.222957454	-5.599727404	8.338717423
	C38	8.683762879	-4.198443434	7.997283898
	C39	-5.085904275	-2.533938941	-1.995550624
	C40	-5.427245578	-1.037263172	-2.063246177
	C41	-3.596558845	-2.680611201	-1.620388365
	C42	-3.172139268	-4.081561791	-1.137307396
	C43	-2.720034530	-5.050704246	-2.226421687
	C44	-5.536500411	0.868262717	-3.634754347
	C45	-6.895078007	1.541354195	-3.405479428
	C46	-5.029915753	1.140680392	-5.065962739

C47	-9.089091470	1.348626577	-2.330220733
C48	-8.932623882	1.813222362	-0.873314267
C49	-7.528012570	1.805706941	1.144618600
C50	-6.436781885	2.854359453	1.372461547
C51	-4.438618073	4.014285759	0.525359336
C52	-4.937104370	5.456653224	0.690833037
C53	-3.527033555	4.010899367	-0.715078573
C54	-2.958913147	2.671905153	-1.045563238
C55	-2.839800356	1.496045012	-0.331431195
C56	-1.955701732	1.097592776	-2.248118027
C57	-6.473122372	7.119866229	-0.265817544
C58	-6.818965591	7.711748669	1.099577891
C59	-7.736636774	7.071937974	-1.158395861
C60	-8.131110147	8.356961834	-1.823988252
C61	-8.148715305	9.654709929	-1.350829893
C62	-8.847740745	9.590647461	-3.452166665
C63	7.936831724	1.763744718	5.450378669
C64	8.721232838	0.526521781	5.847939306
C65	6.557197843	1.286992385	4.926004633
C66	5.651674463	2.433428466	4.540153866
C67	4.824189922	3.068806253	5.486436056
C68	5.621092239	2.907880663	3.216346062
C69	3.994424335	4.136560918	5.126623519
C70	4.806378961	3.978551150	2.845374639
C71	3.988929545	4.589398635	3.800918940
C72	6.573438931	6.125211605	-1.631690925
C73	5.736667865	7.095849182	-2.473244137
C74	5.673398906	5.031772265	-1.039083209
C75	5.260495845	7.961032796	-4.724866325
C76	3.821389367	7.537091958	-5.024114621
C77	2.126097339	5.747218073	-4.837609144
C78	1.236811836	6.023667736	-3.604770576
C79	2.223210016	4.255675534	-5.205325693
C80	0.920427842	3.505679633	-5.496611258
C81	0.161986654	3.893337510	-6.776528258
C82	-1.010298228	6.054545959	-7.210411578
C83	1.035167478	6.167971336	-1.180098902
C84	0.973531509	7.663669610	-0.813321409
C85	1.537817596	5.394899758	0.047519543
C86	2.246354422	9.743321825	-0.641842198
C87	1.819934691	10.995059675	-1.403292332
C88	0.778365656	11.946020273	-3.421397829
C89	-0.580300316	12.605028489	-3.098589503
C90	0.857856612	11.565049801	-4.915705108
C91	-0.166940943	10.497591385	-5.286017666
C92	-2.744759276	12.374450734	-1.963035495
C93	-2.723073165	13.661314017	-1.146984489
C94	-3.518560864	11.275619616	-1.186145428
C95	-3.687309663	10.017269142	-2.003577727
C96	-4.730702654	9.904666121	-2.935286869
C97	-2.764466570	8.963378290	-1.907034051
C98	-4.841842079	8.783288015	-3.760287907
C99	-2.847313566	7.844117248	-2.739602920
C100	-3.885638508	7.771738674	-3.665845847
C101	5.393417609	-6.389778541	-6.669910549
C102	3.942402193	-5.952209736	-6.551815542
C103	2.442083396	-4.065608748	-5.949486994
C104	2.171715959	-2.906196349	-6.914457175
C105	2.725412540	-0.578366336	-7.442169355
C106	3.949622646	0.324340467	-7.549923575
C107	6.175291919	0.963019684	-6.774057767

C108	7.307342936	0.471755323	-7.653806054
C109	-1.140386282	-5.706587347	-8.333969073
C110	-2.084982380	-4.518603551	-8.557130490
C111	-1.026155568	-6.004670254	-6.821503261
C112	-0.420753102	-7.398140736	-6.567519020
C113	-0.029101135	-7.553952581	-5.115384304
C114	-2.372790690	-2.088262419	-8.553273330
C115	-1.640549507	-1.031799516	-9.357883185
C116	-3.003030099	-1.569665835	-7.236030833
C117	-1.964041429	-1.424991740	-6.158392616
C118	-1.169944398	-0.271077640	-6.069443640
C119	-1.676249153	-2.511894264	-5.314525901
C120	-0.069471991	-0.241123676	-5.207800351
C121	-0.571670290	-2.481675176	-4.460359519
C122	0.253837674	-1.354575296	-4.431953638
C123	7.882322652	-7.643770265	-0.908370455
C124	8.804115951	-7.587602217	0.320161697
C125	6.419070952	-7.930755962	-0.537301173
C126	5.425944985	-7.816949232	-1.652263777
C127	5.277116048	-8.666893849	-2.730506221
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C129	9.486351046	-8.498490742	2.469654879
C130	10.948922620	-8.529736501	2.084778671
C131	-0.227173050	-6.651232243	1.888325567
C132	1.182553044	-6.440130372	2.361158890
C133	2.261906742	-7.077745903	1.394817254
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C135	3.127449035	-9.319805823	0.482394602
C136	3.063731447	-10.816976211	0.573231035
C137	3.639059949	-6.919065668	2.107081198
C138	3.972331053	-1.501530633	-1.107793014
Fe139	4.395494009	-3.103250778	-2.188802133
Fe140	2.443904219	-0.081271825	-0.846539851
Fe141	5.373679207	-0.334483186	-0.424708596
Fe142	4.418671912	-0.583331492	-2.786914614
Fe143	4.437633939	1.871874173	-1.734891543
Fe144	4.868228500	-2.674878937	0.348757886
Fe145	2.453021563	-2.604900465	-0.421641566
H146	-6.897907435	-6.554925331	0.586636168
H147	-6.619705958	-6.001801365	-0.922259434
H148	-10.124606921	-3.634799659	-0.328908470
H149	-8.908953609	-5.450550124	-1.260601610
H150	-9.303924994	-6.197037459	0.282381888
H151	-8.454079618	-1.530355156	0.487680237
H152	-10.336584822	-3.702996699	2.604690480
H153	-10.231720304	-1.536636161	0.580511600
H154	-10.414508550	-3.828160842	4.914831928
H155	-7.889111142	-4.349586284	3.367145340
H156	-10.066221962	-2.084858014	5.007960463
H157	-3.619817985	-1.470979199	2.974065986
H158	-6.125514109	-2.817055312	2.530533400
H159	-5.823083609	-5.213893319	3.992319492
H160	-6.053025799	1.988986820	5.102530355
H161	-6.981771054	-0.530359933	3.992112675
H162	-6.054658423	-4.654755682	5.667947031
H163	-4.959427177	-0.905600659	1.950215756
H164	-6.856943702	-1.193088534	6.675242663
H165	-7.616085654	1.192547376	5.408002440
H166	-1.479401844	-2.678287117	4.666003206
H167	-0.935256023	-2.200110558	3.040853258
H168	0.257790237	-2.426324891	4.334346917

H169	-1.915593645	-0.252093455	4.224242401
H170	-6.808342590	-1.695289420	8.921988529
H171	-2.428203127	3.041209368	3.888472650
H172	-3.702905940	2.236643333	8.118533115
H173	-3.265354331	5.588568744	7.332327809
H174	-0.124307155	0.161817123	2.588756486
H175	1.124818884	-0.026851495	3.821895320
H176	7.765163129	2.359673762	6.367139688
H177	-3.181798516	4.643428998	3.722355106
H178	-3.662900449	6.075402836	5.668008279
H179	-1.459895694	4.514317971	4.149453327
H180	-1.964821204	6.042993977	6.206217826
H181	-3.809082062	3.595389514	5.918319798
H182	-0.790739919	3.706222776	6.440126631
H183	-2.548116965	1.493668892	5.695174835
H184	-0.001823135	1.353607119	3.895913195
H185	1.707677759	4.341976843	-0.236093048
H186	0.739225363	5.428574061	0.804424072
H187	2.789142738	5.822249616	1.505739898
H188	2.620343684	5.929093252	4.114868456
H189	4.776822214	4.314388152	1.808339865
H190	6.220695731	2.412039744	2.449711962
H191	4.820738032	2.727502670	6.525639599
H192	-2.736590693	-0.852961371	6.553070894
H193	-2.760196974	-3.776088624	7.913734365
H194	-2.565978866	-2.748678237	9.348919042
H195	-4.471619198	-2.288044516	7.113862829
H196	-6.261354808	-0.042885333	9.292867577
H197	3.348346508	4.608450194	5.872215113
H198	0.228305390	-0.805255441	6.331816656
H199	-3.732317034	3.948379423	10.314485767
H200	-4.113138861	2.209806201	10.379794685
H201	-1.369150472	2.003500778	10.562459749
H202	9.080980293	-6.286646583	8.271297218
H203	-1.359971841	-6.541988333	-2.585216769
H204	-0.282344158	-8.225653041	3.001588994
H205	-1.167622397	-8.168696411	-6.805894262
H206	0.456056448	-7.554513598	-7.212829035
H207	-2.018201727	-5.957733742	-6.346549097
H208	-0.868508465	-1.439134046	-10.053650393
H209	-1.673358617	-6.549690037	-8.800146407
H210	-2.980562881	-2.372521865	-2.479021051
H211	-4.004628085	-4.571349357	-0.601890128
H212	-0.564302823	-3.168255951	-8.139340304
H213	-3.209716181	-2.398902313	-9.210960465
H214	0.728316400	-4.847060475	-8.604315512
H215	-1.221415164	-5.794187710	-0.995539853
H216	-0.414447166	-5.221704858	-6.348248018
H217	0.634023989	-6.419578127	-9.078084720
H218	-6.332292078	-3.586972594	-3.263824685
H219	-3.374693919	-1.956592333	-0.824704261
H220	1.816736764	-7.105642868	-5.631070391
H221	-2.363460142	-3.971407590	-0.401747470
H222	-3.864557112	3.764323441	1.428902250
H223	-3.157806333	1.301766285	0.690724798
H224	-8.451036449	2.215535553	1.574755694
H225	-7.117270471	0.807767316	-0.698700796
H226	-6.460885691	5.003137904	-0.597504866
H227	-7.859599401	10.088671760	-0.400575334
H228	-7.246527165	6.964607807	1.811610954
H229	-8.575178293	6.658438383	-0.569718049

H230	-5.696344915	7.742180448	-0.739085029
H231	-9.219387867	9.946942256	-4.409385279
H232	-2.724811570	4.743790538	-0.527718870
H233	-4.103797612	4.394520282	-1.574771051
H234	-8.731031103	11.432291865	-2.386555920
H235	-7.545377000	6.352003978	-1.970098838
H236	-5.473578072	2.388164756	-0.391559195
H237	-7.266259704	0.913554859	1.733059742
H238	-9.402232490	2.222912633	-2.914908468
H239	-1.441761405	0.627536215	-3.082521107
H240	-9.902733093	0.611874595	-2.368460905
H241	9.457699771	2.981785280	4.812430779
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C60	-8.263617424	8.413738023	-0.364108087
C61	-8.369037961	9.530736967	0.442995420
C62	-8.896283143	10.036325201	-1.648899707
C63	7.330578720	0.360049804	6.494036733
C64	8.110418569	-0.937569569	6.595701823
C65	6.016564782	0.032811696	5.738279504
C66	5.106873174	1.229341360	5.591743877
C67	4.159265092	1.550439323	6.581731619
C68	5.181517558	2.058702647	4.458866777
C69	3.311089210	2.655400301	6.446963360
C70	4.349518494	3.170653236	4.314791673
C71	3.408142482	3.462753770	5.306111301
C72	6.435080265	6.461459952	0.735975313
C73	5.645203732	7.616240297	0.108820090
C74	5.538658280	5.221878703	0.872432790
C75	5.328143011	9.026409813	-1.878625057
C76	3.946866091	8.668849150	-2.432497590
C77	2.323381693	6.864457889	-2.897948989
C78	1.314367305	6.785079873	-1.731303413
C79	2.513192214	5.523880106	-3.632478065
C80	1.270259697	4.862746012	-4.237579082
C81	0.622688886	5.566282893	-5.441844863
C82	-0.580137072	7.754003917	-5.402509470
C83	0.883015857	6.271797565	0.613873428
C84	0.712590752	7.617926737	1.345416185
C85	1.304839705	5.214065849	1.644029961
C86	1.871396402	9.593575104	2.201902114
C87	1.465626013	10.997418615	1.763015575
C88	0.583873783	12.441143353	-0.024858923
C89	-0.821822589	12.971866878	0.332935519
C90	0.818180274	12.474224114	-1.551370799
C91	-0.124815747	11.531826327	-2.292255721
C92	-3.076381545	12.404479817	1.130822271
C93	-3.194021798	13.424426156	2.256148624
C94	-3.864677611	11.118432586	1.503130513
C95	-3.898472649	10.124123235	0.364856828
C96	-4.851412381	10.253327915	-0.656562610
C97	-2.947866408	9.095123712	0.260464663
C98	-4.846566197	9.401790949	-1.763664569
C99	-2.913236206	8.248233216	-0.851068727
C100	-3.862558476	8.416291085	-1.856856408
C101	6.263909627	-4.281329266	-7.542325874
C102	4.790246087	-3.914787516	-7.460915285
C103	3.154031361	-2.288144260	-6.539065343
C104	2.938468082	-0.909329239	-7.168119138
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C106	4.609972093	2.410304306	-6.730494871

C107	6.748055878	2.847566665	-5.620794950
C108	7.975501307	2.607948080	-6.477099142
C109	-0.111829024	-3.273522734	-9.618011348
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C113	0.778457348	-5.911618033	-6.922417414
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C115	-0.685980090	1.502314295	-9.431772440
C116	-2.190041669	0.393853874	-7.653727931
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C118	-0.519832628	1.306976042	-5.973671873
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C135	3.455176178	-9.033655044	-1.704865067
C136	3.462605487	-10.501282935	-2.023141927
C137	3.707928725	-7.118649781	0.522024585
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Fe139	4.664914081	-2.339455486	-2.490791309
Fe140	2.836434801	0.370736349	-0.567364622
Fe141	5.361586107	-0.040958817	0.206669177
Fe142	4.863732611	0.235318480	-2.354342937
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Fe144	4.914294184	-2.538866430	0.088707594
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H148	-9.876310769	-3.575609322	-2.301882114
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H155	-7.976319982	-5.220219973	1.261515550
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H173	-4.162673053	3.367099731	8.187426101
H174	-0.339439655	-0.574228069	2.490626961
H175	0.758182982	-1.035344049	3.795424808
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H177	-3.735711880	3.405108169	4.474717788
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H184	-0.437892850	0.259820677	4.054971982
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H225	-7.052251141	0.843609882	-1.174151619
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H234	-8.935250921	11.514443981	-0.117866090
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H244	-0.116528369	6.002420785	0.243483396
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H258	-2.215413837	8.930673861	1.056072186
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H265	-4.895198757	-0.233336323	-4.754151879
H266	3.249890543	5.697801714	-4.434579703
H267	-2.133509065	7.491587687	-0.948941469
H268	-5.390704544	4.044947153	-4.477922603
H269	5.181631858	9.894397305	-1.221230452
H270	0.779146067	7.779910332	-6.949832783
H271	-1.853332369	9.343883978	-5.300279580
H272	-4.204714145	-2.964340078	-4.818442856
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H275	-4.610363781	2.047521225	-2.934206486
H276	1.906636975	7.617615369	-3.579453026
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H280	1.263944525	9.356761841	3.088373100
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H320	6.704005386	-8.486516872	-1.856945297
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H362	7.335586118	-5.293863533	7.080466821
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	C6	-8.619620623	-4.697076367	3.138305899
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	C18	-1.287690720	-0.661910511	6.379553903
	C19	-1.283207116	-1.768258738	4.029858382
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	C42	-2.878173495	-3.697005706	-2.505133552
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C93	-3.190573028	13.423788502	2.253715011
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H187	2.387353740	5.245915471	3.282281347
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H189	4.400553033	3.785609585	3.416816521
H190	5.884773995	1.818227302	3.650853681
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H192	-3.300383096	-2.619773732	5.760181638
H193	-3.323827119	-5.790183866	6.283126587
H194	-3.301053468	-5.201804348	7.961886015
H195	-5.017469115	-4.184748858	5.761456603
H196	-7.102446889	-2.643303728	8.263650702
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H198	-0.332728066	-2.466656781	5.858259469
H199	-4.869536282	0.947233758	10.541417334
H200	-5.143978380	-0.758006596	10.093175707
H201	-2.456499102	-0.968589704	10.508606226
H202	8.522943073	-8.130157005	7.189117079
H203	-0.822683773	-5.621728344	-4.371620670
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H206	1.446212274	-5.331127089	-8.886797348
H207	-1.157329782	-4.062077481	-7.869660581
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	C4	-9.249936239	-2.674349760	1.388924332
	C5	-9.846510462	-4.174863863	3.217088976
	C6	-8.453654672	-4.561017328	3.728453040
	C7	-6.244108396	-5.445128944	3.148353979
	C8	-5.366728246	-4.192652285	3.248080308
	C9	-4.791410490	-2.004489898	2.340031097
	C10	-5.125037972	-1.161150167	3.578732559
	C11	-6.813797162	-0.364635743	5.131683649
	C12	-6.401334863	-1.000556531	6.466625385
	C13	-6.453133992	-3.003976758	7.874162146
	C14	-5.057751565	-3.568871015	8.167209299
	C15	-3.033533702	-4.619410306	7.247072807
	C16	-1.803349967	-3.801568725	6.844549147
	C17	-1.002229813	-1.752567212	5.696579849
	C18	-0.975683163	-0.408743450	6.448309824
	C19	-1.090852224	-1.612224634	4.151917324
	C20	-0.098916259	-0.579233547	3.608906946
	C21	-0.887773738	-2.975590038	3.482133198
	C22	-2.197799081	1.631064243	7.092288669
	C23	-2.492833358	1.426779558	8.590706667
	C24	-3.216226667	2.578585161	6.414977654
	C25	-3.391223166	3.870560817	7.222861456
	C26	-2.787710661	2.903529871	4.977539470
	C27	-3.904517923	0.448414029	10.304808033
	C28	-2.729409856	0.037487449	11.168945387
	C29	3.271140260	-11.636630701	5.758991391
	C30	4.127617538	-10.498844466	5.205066114
	C31	4.691338810	-8.092056069	5.551138338
	C32	5.683906994	-7.799682087	6.690919170
	C33	3.683554062	-6.943774691	5.360915437
	C34	4.342854072	-5.611234634	4.998120904
	C35	3.304465774	-4.583318241	4.549994976
	C36	3.531025510	-2.096507720	4.415132713
	C37	7.992819062	-7.208746569	7.250256762
	C38	8.438403620	-5.761989650	7.256991286
	C39	-4.889674330	-2.099853289	-2.789077035
	C40	-5.279411538	-0.637860723	-2.523120805
	C41	-3.416229974	-2.310061677	-2.389671434
	C42	-2.988562772	-3.781014658	-2.217338996
	C43	-2.470890506	-4.467307548	-3.477178458

C44	-5.377154714	1.580127487	-3.616470803
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C47	-9.003606940	1.674292907	-2.440240508
C48	-8.932364486	1.794203113	-0.909372714
C49	-7.637347465	1.353245812	1.130687036
C50	-6.582935506	2.334044640	1.647932310
C51	-4.587799602	3.693481694	1.198438279
C52	-5.127296255	5.054414387	1.661703885
C53	-3.599908305	3.989472458	0.055352863
C54	-2.990876637	2.770020063	-0.550411374
C55	-2.872008079	1.463816766	-0.117421688
C56	-1.908088765	1.524403365	-2.035162915
C57	-6.663846328	6.868080570	1.036339066
C58	-7.098163976	7.129469309	2.476607820
C59	-7.866688261	7.006142681	0.071552545
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C61	-8.348086822	9.550065863	0.481521208
C62	-8.971757413	9.977932187	-1.601743921
C63	7.638514425	0.601108203	6.122021441
C64	8.422271713	-0.693115485	6.229787058
C65	6.289002436	0.248648599	5.442887996
C66	5.372903473	1.439813426	5.292606154
C67	4.473281574	1.801161121	6.313657509
C68	5.390474829	2.221793042	4.124730891
C69	3.617636196	2.899771512	6.174983424
C70	4.550916805	3.327326013	3.976186674
C71	3.661118984	3.662796071	5.001343369
C72	6.461492055	6.481319328	0.182069017
C73	5.638710699	7.609708035	-0.452107885
C74	5.575516948	5.250034943	0.418390173
C75	5.224356710	8.939434920	-2.478871728
C76	3.818058350	8.562853109	-2.951725268
C77	2.174427030	6.743351731	-3.266970252
C78	1.223681674	6.709218053	-2.049795042
C79	2.330830486	5.376988756	-3.959387908
C80	1.059939529	4.694169860	-4.475845915
C81	0.354954117	5.351393053	-5.674237405
C82	-0.845115976	7.542320072	-5.660235195
C83	0.906117467	6.291674729	0.330634478
C84	0.768045430	7.664285519	1.017650442
C85	1.376708683	5.273850730	1.379429898
C86	1.965316420	9.672775374	1.740757984
C87	1.538811582	11.057344924	1.261977415
C88	0.569441551	12.429277993	-0.532781451
C89	-0.815731505	12.978762540	-0.124242262
C90	0.729772208	12.403594288	-2.068493838
C91	-0.246947482	11.434638301	-2.725169138
C92	-3.028145352	12.446686634	0.800594936
C93	-3.099912738	13.507301033	1.893239884
C94	-3.800630810	11.178409320	1.254817378
C95	-3.888228727	10.140522732	0.158692836
C96	-4.885637052	10.231322503	-0.823559314
C97	-2.943917409	9.105826214	0.053158048
C98	-4.932327310	9.333735694	-1.893060970
C99	-2.959415529	8.214360627	-1.024338639
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C101	5.897961097	-4.576086790	-7.657215257
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C107	6.471359998	2.622614046	-6.045867705
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C109	-0.566473972	-3.638144394	-9.462640711
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C116	-2.549929631	0.103839833	-7.549249874
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C120	0.169229698	0.910905570	-4.990352041
C121	-0.399020676	-1.427635116	-4.802243221
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C127	5.658806099	-7.712174616	-4.371320517
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C135	3.372448931	-9.096653365	-1.520701835
C136	3.369903834	-10.575598305	-1.777997866
C137	3.729765175	-7.098628972	0.618152484
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Fe141	5.351857751	-0.069803488	-0.042395295
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Fe144	4.904619582	-2.554241139	-0.062904778
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H184	-0.248891427	0.416755245	4.052393561
H185	1.601334352	4.317128670	0.877012884
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H187	2.551565733	5.362502636	2.954472846
H188	2.207562895	4.834958859	5.531903262
H189	4.553859921	3.901989451	3.049232258
H190	6.038735646	1.937971940	3.292433111
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H208	-0.316474498	0.920338576	-10.161568536
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H211	-3.836465996	-4.385119394	-1.846583846
H212	-0.058220973	-1.200184498	-8.692284902
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H260	2.820343906	4.680565868	-3.260138631
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H265	-5.109715306	-0.411268182	-4.499201963
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H268	-5.600817742	3.873108433	-4.362842450
H269	5.109888170	9.832594168	-1.849174118
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H271	-2.111773283	9.138736334	-5.556173932
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H274	-5.645654172	11.012612129	-0.754273792
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H283	3.029114179	9.746231510	2.005511345
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H289	5.420030300	-6.091337992	-8.924710663
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H293	4.783859885	5.497985374	1.139851916
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H330	3.903394026	-12.541067017	5.738606542
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N394	-2.205344257	0.697737176	-1.044155156
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O423	-8.696088998	-1.885438268	2.171209653
O424	-8.134816668	-4.362404883	4.912185518
O425	-4.560013330	-4.040876405	4.179510328
O426	-4.247534618	-0.524324572	4.183255244
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O428	-4.677979947	-3.678666548	9.341613984
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O433	4.856302428	-10.704440373	4.211056613
O434	5.323576025	-7.865882318	7.879424516
O435	9.547878321	-5.403772368	7.618688745
O436	-5.558628581	-0.209504249	-1.383992221
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O438	-6.922888883	3.393583706	-3.256229556
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O440	-9.877930104	2.314010421	-0.301600503
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O447	3.060545382	9.464432432	-3.368476449
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O449	-0.213262038	7.900863093	1.734960225
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O451	1.757836810	12.049366780	1.968742638
O452	-1.117952005	14.160594822	-0.341268295
O453	-1.440610771	11.732282231	-2.893731591
O454	-4.085789916	14.203472548	2.079648021
O455	-3.920883722	7.462507777	-3.082347876
O456	3.536820469	-4.976241341	-7.959810435
O457	1.885951326	-1.077092518	-8.280705287
O458	4.225562972	3.255735714	-7.582257412
O459	8.758009357	2.842363835	-6.773539438
O460	-2.721598389	-2.579659173	-9.790694008
O461	-0.378333185	-6.657812153	-5.957535886
O462	1.730865123	-6.022711227	-6.318073010
O463	-1.412650614	2.292837138	-9.131400441
O464	9.921148886	-6.501515658	-0.677497309
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O466	-0.751769257	-6.115664741	-0.377717520
O467	-0.741183042	-8.145242025	0.535577044
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	O471	3.913433327	-7.887043652	1.575201023
	O472	2.394424460	-6.250191490	-1.237187822
	O473	7.620272862	-7.338611095	3.528738456
	O474	6.339265210	-5.215684153	2.155850655
	O475	-2.825851311	5.152868998	-3.701519131
	O476	6.854406242	-11.223850443	0.194495979
	O477	6.134226352	-9.304351741	2.201061848
	S478	4.748758977	4.652095599	-1.126744343
	S479	3.078958894	1.603623546	-2.593634901
	S480	2.611325273	-3.556263224	-2.907992689
	S481	3.987410851	1.472720045	0.906839913
	S482	0.252286438	-2.339829514	-1.275919587
	S483	5.263974781	-1.180571255	-4.340911812
	S484	3.089793015	-3.599355128	0.699800718
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	Fe(139)	0.566	2.527	
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	Fe(141)	0.554	2.649	
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	C3	-9.278117603	-2.399054599	-0.110245838
	C4	-9.255100593	-2.678855019	1.389961013
	C5	-9.845521107	-4.178933995	3.220535865
	C6	-8.450759728	-4.561823270	3.729178687
	C7	-6.241333165	-5.444208337	3.146472875
	C8	-5.365192678	-4.190993226	3.245817226
	C9	-4.791375644	-2.003367880	2.335677320
	C10	-5.123740853	-1.158435952	3.573658039
	C11	-6.809897451	-0.362300299	5.129348266
	C12	-6.396567381	-0.997995734	6.463968919
	C13	-6.452099350	-3.000751085	7.872469078
	C14	-5.058586506	-3.570605196	8.166049108
	C15	-3.035338370	-4.625008911	7.246988617
	C16	-1.804760063	-3.805973732	6.848113792
	C17	-1.002601702	-1.753110424	5.705905640
	C18	-0.976346531	-0.410540122	6.458727021
	C19	-1.094770941	-1.611840636	4.164432646
	C20	-0.102773151	-0.579028414	3.619106078
	C21	-0.891009998	-2.974323019	3.490657335
	C22	-2.196231672	1.632743620	7.098606407
	C23	-2.492180919	1.430645295	8.598316909
	C24	-3.213423533	2.581677082	6.420093663
	C25	-3.386835921	3.873986505	7.228389388
	C26	-2.782635119	2.904658553	4.983915665
	C27	-3.902855139	0.452317158	10.312052234
	C28	-2.729784627	0.038896696	11.176053553
	C29	3.273523415	-11.644068949	5.769035918
	C30	4.125418648	-10.506611200	5.210354317
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	C32	5.678144762	-7.807430110	6.693733631
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	C35	3.305130910	-4.588595216	4.554825977
	C36	3.536292248	-2.103442611	4.408272729
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	C39	-4.899751471	-2.095209259	-2.787743148
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C77	2.175148720	6.746126066	-3.269104666
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C79	2.333462110	5.380330735	-3.962028014
C80	1.063685819	4.696503773	-4.479951750
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C82	-0.845197893	7.542660576	-5.665038959
C83	0.908959584	6.291417643	0.328645256
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C85	1.383314719	5.273137417	1.376131117
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C87	1.541129673	11.056587864	1.260537153
C88	0.571899231	12.427510448	-0.534938261
C89	-0.813808070	12.974788024	-0.125230962
C90	0.731912005	12.402652666	-2.070520795
C91	-0.245264212	11.434587486	-2.727829386
C92	-3.025697086	12.441178300	0.799682246
C93	-3.096044152	13.503147807	1.890568896
C94	-3.796383649	11.172165169	1.256521416
C95	-3.885602356	10.134062851	0.161083691
C96	-4.884917439	10.223250151	-0.819242413
C97	-2.940481437	9.100025045	0.054401568
C98	-4.931840645	9.325796863	-1.888496756
C99	-2.956608492	8.208182492	-1.023289179
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C101	5.895961675	-4.572145255	-7.661425832
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C104	2.586531453	-1.185655372	-7.265700203
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C114	-1.881028412	-0.085202084	-8.925692240
C115	-1.145147466	1.139139501	-9.432906579
C116	-2.558249766	0.099475848	-7.545760677
C117	-1.580007206	-0.014921257	-6.405669764
C118	-0.809862128	1.083432997	-5.989786773
C119	-1.361271466	-1.261609699	-5.794326364
C120	0.174385442	0.922332450	-5.009164685
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C128	3.998611374	-6.267226053	-4.141746530
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C132	1.261595521	-6.756305876	0.852127672
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C134	2.204204455	-8.603859825	-0.661679572
C135	3.380425589	-9.092201879	-1.522409348
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C138	4.070785685	-1.123346826	-1.209594414
Fe139	4.581605738	-2.418810864	-2.645873904
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Fe142	4.772057847	0.158816636	-2.592328810
Fe143	4.527381530	2.364297913	-1.132574829
Fe144	4.877816574	-2.569304781	-0.064812540
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	S483	5.344503664	-1.145961473	-4.328274449
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	C20	-0.853266161	-1.446156574	3.259959102
	C21	0.086940630	-3.743565531	2.804770322
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C70	5.044614426	3.984918837	2.584510366
C71	4.274799280	4.463709704	3.650018015
C72	6.239706429	6.396413228	-1.919753773
C73	5.288715478	7.388483975	-2.601083630
C74	5.447187389	5.218030731	-1.335453793
C75	4.552947755	8.380289650	-4.724349014
C76	3.095628704	7.945991549	-4.888405198
C77	1.467200265	6.097897082	-4.663165180
C78	0.709856963	6.267714426	-3.326633997
C79	1.548602618	4.634188425	-5.132588879
C80	0.232802775	3.868807429	-5.303960050
C81	-0.673131651	4.286015975	-6.475139855
C82	-1.903476270	6.454915736	-6.647381905
C83	0.763952278	6.270606576	-0.886511568
C84	0.712145139	7.739788033	-0.422555284
C85	1.404383598	5.435763862	0.230404834
C86	1.954392790	9.842141483	-0.264421624
C87	1.421886585	11.125656395	-0.898278315
C88	0.144291325	12.164108741	-2.726433518
C89	-1.182987566	12.761721457	-2.213668254
C90	0.066140763	11.876102872	-4.242146769
C91	-0.971777294	10.805672242	-4.563399149
C92	-3.214964320	12.382263146	-0.887792813
C93	-3.157663536	13.626765084	-0.009010436
C94	-3.868945758	11.212873028	-0.104457554
C95	-4.094069043	9.997443333	-0.974547844
C96	-5.237404979	9.906658029	-1.782378691
C97	-3.145576959	8.963814583	-1.047442946
C98	-5.422620914	8.832110312	-2.656642922
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C100	-4.437487005	7.846686575	-2.739182692
C101	4.790817981	-5.822170024	-7.589088646

C102	3.352827184	-5.432849374	-7.287448002
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C104	1.510248043	-2.409921980	-7.301606784
C105	1.927210219	-0.028308600	-7.719579070
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C107	5.427195211	1.502236020	-7.327075422
C108	6.441539652	1.148038693	-8.397123655
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C120	-0.617104006	0.078207766	-5.137036924
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C122	-0.245331245	-1.045132289	-4.395491622
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C124	8.959960236	-7.322554414	-1.075143327
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C131	0.073773878	-6.753395060	1.481813059
C132	1.523973754	-6.502930208	1.810529152
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C136	3.305257468	-10.703930162	-0.428925252
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Fe144	4.908128967	-2.526423485	-0.376956241
Fe145	2.362934658	-2.429500993	-0.961572514
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	C14	-3.429090397	-3.239414330	9.093510262
	C15	-1.237393691	-3.864280471	8.172919976
	C16	-0.302435234	-2.832518433	7.534980719
	C17	-0.167381409	-0.878471925	6.011145579
	C18	-0.482346538	0.536766471	6.531738656
	C19	-0.375242996	-1.040576787	4.482407266
	C20	0.253394348	0.111201783	3.691003477
	C21	0.165318525	-2.393648830	4.005359760
	C22	-2.196116402	2.263333108	6.934820983
	C23	-2.353014865	2.270823532	8.468543822
	C24	-3.467679833	2.756251758	6.204154080
	C25	-3.974759935	4.072860456	6.805876091
	C26	-3.204597696	2.923056477	4.701870963
	C27	-3.357441686	1.286854001	10.444201126
	C28	-2.077293156	1.330879879	11.254768561
	C29	6.735917378	-9.066798726	7.263321965
	C30	7.195790049	-7.865375960	6.438632481
	C31	7.060897658	-5.373147021	6.320577547
	C32	7.982422706	-4.613351449	7.293382438
	C33	5.759139023	-4.597467287	6.050244920
	C34	5.984419629	-3.219084050	5.425069543
	C35	4.672734854	-2.635160049	4.903680635
	C36	4.184945797	-0.240762342	4.359115551
	C37	10.062176469	-3.341027840	7.519809637
	C38	10.073842476	-1.846507957	7.287747926

C39	-4.261413821	-3.784302053	-1.893163005
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C43	-1.293429405	-5.495224307	-2.432571753
C44	-5.806572574	-0.627673598	-3.340252231
C45	-7.275007754	-0.401620185	-2.951610012
C46	-5.545685872	-0.142297977	-4.780229305
C47	-9.225566728	-1.317351735	-1.784113228
C48	-9.107646401	-0.913502051	-0.305238410
C49	-7.614881682	-0.611311316	1.627759261
C50	-6.799802211	0.665087395	1.845547682
C51	-5.336566100	2.400647502	0.919529667
C52	-6.212952534	3.643545825	1.216928366
C53	-4.558589463	2.743032533	-0.360853391
C54	-3.535908989	1.762551689	-0.847018153
C55	-2.791563059	0.773368076	-0.251206784
C56	-2.128216511	0.921220557	-2.362040546
C57	-8.296797576	4.809646757	0.570213664
C58	-8.688922007	5.187574199	1.996445054
C59	-9.549400108	4.442148923	-0.261156854
C60	-10.331855778	5.591892671	-0.825721715
C61	-10.738269444	6.780176745	-0.248677187
C62	-11.436007160	6.663651952	-2.348923476
C63	7.414969011	3.766463006	5.162894886
C64	8.534989559	2.782303736	5.446009434
C65	6.197638410	2.931321090	4.690522912
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C67	4.031771285	4.041257384	5.438689881
C68	4.746953430	4.336112037	3.156427042
C69	2.901505837	4.828842705	5.192394471
C70	3.630824148	5.132949185	2.898748936
C71	2.706337215	5.374373774	3.918397844
C72	4.377580696	7.912639213	-1.518341986
C73	3.228910109	8.620745289	-2.247108359
C74	3.898569195	6.556062697	-0.990146479
C75	2.361871505	9.411415244	-4.406529472
C76	1.097958042	8.588713596	-4.663411072
C77	0.024509378	6.367752226	-4.523682501
C78	-0.817187387	6.294352008	-3.230768085
C79	0.519632324	4.990652455	-5.001232417
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C81	-1.465554243	4.104197278	-6.459041420
C82	-3.249505271	5.830902239	-6.697761966
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C84	-1.369502067	7.633043349	-0.317491805
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C87	-1.586451980	11.099333300	-0.719085916
C88	-2.999124866	11.799768876	-2.609649013
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C93	-6.695824485	12.273400380	-0.061974503
C94	-6.719924318	9.753962173	-0.195061229
C95	-6.569188669	8.543144367	-1.087151661
C96	-7.606507223	8.165373153	-1.955030977
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C107	5.146140553	3.111817302	-6.962285007
C108	6.302483862	3.026187247	-7.938243245
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C127	7.427919266	-6.542690384	-3.587498469
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H291	4.096146341	9.002829314	0.182613830
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Fe139	4.951969371	-1.548486553	-2.660346287
Fe140	2.550992266	0.943686075	-0.969805298
Fe141	5.144850469	1.363569897	-0.516381623
Fe142	4.359436446	0.955570902	-2.996307240
Fe143	3.794234585	3.304699417	-1.773284628
Fe144	5.390974166	-1.124587144	-0.107093092
Fe145	3.012003894	-1.696566115	-0.951466717
H146	-4.596789700	-8.322742369	0.441703947
H147	-4.643652455	-7.633359358	-1.038146620
H148	-8.633384978	-6.496394727	-0.047380972
H149	-7.025236284	-7.838326504	-1.158582654
H150	-7.000528186	-8.697299832	0.379869835
H151	-7.590574481	-4.007151958	0.789492861
H152	-8.585399511	-6.752566625	2.854795866
H153	-9.275472878	-4.546147856	0.983144328
H154	-8.475970934	-6.981605114	5.163031832
H155	-6.004477016	-6.701512484	3.443893436
H156	-8.616740613	-5.214458965	5.324625011
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H159	-3.729774200	-6.924799021	3.908341849

H160	-5.997927468	-0.182077887	5.502631402
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H162	-4.013667757	-6.545115958	5.626064672
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H165	-7.234474622	-1.422492306	5.834258289
H166	-0.303946288	-3.230753651	4.530624507
H167	-0.033775771	-2.529013201	2.919490200
H168	1.257657720	-2.458256013	4.136190607
H169	-1.458591609	-1.020296206	4.288657162
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H173	-4.270752483	3.945200808	7.852308698
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H184	-0.111502682	1.093225543	4.003835327
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	O465	13.870031711	-4.369264748	1.705327683
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	O469	5.134239496	-10.214595351	-0.809251804
	O470	6.149514613	-4.575286701	0.745384540
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	O472	4.001477392	-5.471810336	-0.472248597
	O473	9.556299170	-4.259308129	3.915623422
	O474	7.631722966	-2.831873058	2.388977111
	O475	-4.358980921	3.378207553	-4.172787006
	O476	9.784877117	-8.735850540	1.349692408
	O477	8.616138565	-6.766617936	3.084785637
	S478	3.215799716	5.478303067	-2.343712502
	S479	2.308235876	1.966588506	-2.997274024
	S480	3.335703747	-3.109176770	-2.618024038
	S481	3.494240477	2.545302881	0.332834029
	S482	0.798101473	-1.540264058	-0.703261095
	S483	5.196500058	-0.411219571	-4.583531800
	S484	3.887584932	-2.435998424	0.922793731
	S485	5.891473594	2.530341824	-2.264687129
	S486	6.757780430	-2.217865139	-1.491217655
	S487	6.403351060	0.441140527	1.069236714
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Fe(139) 0.539 2.347	C1	-7.368380654	-5.703939765	-1.224620685
Fe(140) 0.449 -1.793	C2	-7.180763582	-6.964520042	-2.076174611
Fe(141) 0.582 2.913	C3	-8.727156107	-3.692028819	-0.838180410
Fe(142) 0.553 -2.563	C4	-8.910501466	-3.771203090	0.675156970
Fe(143) 0.568 2.956	C5	-9.595809409	-5.092281287	2.608960234
Fe(144) 0.499 -2.264	C6	-8.258048907	-5.215818367	3.347582491
Fe(145) 0.467 -0.138	C7	-5.897042115	-5.851987942	3.195975579
S=1	C8	-5.201516731	-4.486789222	3.217126983
	C9	-4.786528812	-2.374841230	2.072359198
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	C13	-7.055677778	-2.877722002	7.445714093
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	C15	-3.389612261	-3.992710690	7.478527828
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	C18	-1.794813168	0.302907441	6.268933787
	C19	-1.431719390	-1.195153850	4.184403921
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C84	-0.510262778	7.744654231	-0.002899773
C85	0.261418282	5.527994504	0.845525754
C86	0.185774738	9.994028921	0.663336614
C87	-0.287159473	11.222221674	-0.110708119
C88	-0.878886546	12.210483917	-2.282241780
C89	-2.379064472	12.574429086	-2.321427462
C90	-0.315661017	12.037099682	-3.709750046
C91	-0.949464839	10.851041343	-4.427322404
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C93	-5.149035235	12.968870791	-1.054620300
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C96	-5.731438321	9.173788206	-3.617099061

C97	-4.008878192	8.453458423	-2.092291805
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C104	4.579969412	-1.604656585	-6.078291664
C105	4.706098019	0.839609635	-6.219547909
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C113	3.014033270	-6.770295439	-5.379226092
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C115	1.399489001	-0.155207156	-9.512869725
C116	-0.355922312	-1.182609032	-7.925577358
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C118	0.701770649	0.205114452	-6.071151448
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C124	9.790154764	-5.782353658	2.399913246
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C127	7.535932155	-7.176753414	-1.581439623
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C136	4.988494865	-10.025318353	0.786076580
C137	4.310560284	-6.261509762	2.609536815
C138	4.354130891	-0.563517934	0.003816265
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N406	-0.561992734	11.060492054	-1.439008344
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N419	0.151876326	1.494824602	-0.349495093
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O421	-6.393471153	-5.520852677	-1.227948519
O422	-8.632672461	-2.981834914	0.203657236
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O426	-7.669756602	-0.430186877	5.666638115
O427	-6.512557330	-3.171585580	8.353063039
O428	-2.038079986	-3.362234603	7.325781434
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O436	-1.024696562	-5.280711830	-4.465266828
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O438	-3.701252950	2.140415281	-6.343183622
O439	-9.624088175	0.711880742	-3.145456950
O440	-7.426877313	1.881427587	0.690569755
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O447	-0.276887785	6.704881890	-3.148397200
O448	-1.665505526	7.900314108	0.416598483
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O451	-2.750754530	13.666105322	-2.775123252
O452	-2.074072708	10.929211906	-4.946739658
O453	-6.214294639	13.540655636	-1.224012623
O454	-3.878377245	6.328280042	-5.086435727
O455	6.154992369	-5.250673643	-5.938799173
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O461	4.098829230	-6.355808692	-4.694524082
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	O465	0.176942343	-6.140325072	0.406640805
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	O467	5.856848657	-10.622948250	1.418213915
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	O470	4.321768537	-6.884433917	3.697767521
	O471	3.433203938	-5.867430416	0.373496201
	O472	7.287051984	-5.516910098	6.379549941
	O473	6.146976568	-3.811646708	4.422895906
	O474	-2.396702725	4.156285936	-5.023329742
	O475	7.878477902	-9.858744096	3.625162569
	O476	6.446642128	-7.840487053	5.069309066
	S477	4.364501320	5.236295839	-0.667346408
	S478	3.701316209	1.847682380	-2.149592659
	S479	3.719326785	-3.342332668	-1.605041563
	S480	3.261750055	2.249011836	1.422471283
	S481	0.756744804	-1.976899644	-0.049261251
	S482	6.427915452	-0.807774064	-2.638393577
	S483	3.261607238	-2.951652357	1.974570511
	S484	6.571638886	2.016939849	-0.031201789
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	C4	-9.324732473	-2.693703597	-0.070447935
	C5	-10.170372318	-4.365420291	1.495359288
	C6	-8.859598281	-4.834132159	2.138325043
	C7	-6.597198752	-5.692894469	1.760983850
	C8	-5.739461899	-4.474271493	2.113703309
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	C10	-5.544290403	-1.499205712	2.804016884
	C11	-7.432235049	-0.850516495	4.191053467
	C12	-7.189174216	-1.629792992	5.491039732
	C13	-7.397897145	-3.773361797	6.653577825
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	C15	-3.905886596	-5.315905082	6.313668471
	C16	-2.640156571	-4.468390505	6.147446301
	C17	-1.708895406	-2.329153682	5.301983734
	C18	-1.786738549	-1.065496147	6.178101969
	C19	-1.600351341	-2.033819893	3.782338852
	C20	-0.546553578	-0.963496372	3.477813657
	C21	-1.309174103	-3.323743766	3.007211867
	C22	-3.101717797	0.899847413	6.866082412
	C23	-3.578296805	0.544936922	8.288786611
	C24	-4.036623966	1.914994366	6.165576267
	C25	-4.322200432	3.117497927	7.073403385
	C26	-3.430409539	2.381970242	4.835898998
	C27	-5.184095769	-0.599318895	9.704544621
	C28	-4.126515069	-1.107232677	10.662946098
	C29	2.605638321	-12.194097954	4.911689348
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	C32	4.864285722	-8.491930252	6.495044388
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C42	-2.629545283	-3.515977548	-2.966443409
C43	-1.952570698	-4.076266601	-4.213246952
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C45	-6.290498212	2.507296435	-3.880256914
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C48	-8.754300688	1.973838782	-1.842005209
C49	-7.748953777	1.333231514	0.301065225
C50	-6.778648578	2.242119941	1.060610354
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C81	1.022452077	5.891230145	-4.966813888
C82	-0.156950943	8.090107515	-4.869556488
C83	0.821614238	6.216161345	1.106986825
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C85	1.153339344	5.081504265	2.085912038
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C88	0.593821136	12.408901789	0.860703646
C89	-0.833827571	12.923658974	1.145609173
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C91	0.054887677	11.657949965	-1.507921523
C92	-3.144030765	12.319137925	1.718670101
C93	-3.354879102	13.258162836	2.898942047
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C103	3.669299719	-1.885260661	-6.410069415
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C113	1.313295913	-5.449143075	-7.237844558
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C118	-0.068119127	1.716912136	-5.924422940
C119	-0.615631622	-0.630312102	-6.082077159
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C124	9.088809354	-7.226190716	-0.628882617
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C126	6.088530570	-6.819956835	-3.120105310
C127	6.161320557	-7.283379798	-4.418550503
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H147	-5.985240695	-5.416493203	-3.976003936
H148	-9.629036030	-3.321752152	-3.310999462
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H151	-8.214763536	-1.656100223	-1.542319807
H152	-10.356192960	-4.371132645	-0.650250330
H153	-9.976225487	-1.627112284	-1.811053575
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H161	-7.519724594	-1.862522525	2.294276430
H162	-6.668839590	-6.306412927	2.666604277
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H164	-7.787721034	-3.395632906	4.588861719
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H166	-2.089019702	-4.081113982	3.172310696
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H190	5.583026015	1.471427416	4.154828161
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	C26	-2.280059466	2.933303355	5.203875568
	C27	-2.924313346	0.506761672	10.640118189
	C28	-1.680047999	0.071541798	11.390133656
	C29	3.888579211	-11.606537668	5.521061541
	C30	4.670122191	-10.461932019	4.877417786
	C31	5.238921464	-8.046517671	5.165321772
	C32	6.333707771	-7.739224273	6.205795572
	C33	4.208952089	-6.906689146	5.073647581
	C34	4.825956948	-5.570735527	4.654621298

C35	3.752747431	-4.548360261	4.290402301
C36	3.966622893	-2.062437227	4.110635512
C37	8.687578559	-7.134285136	6.528236421
C38	9.086927126	-5.673941654	6.527495343
C39	-5.137713482	-2.100404611	-2.277252579
C40	-5.424128477	-0.608524371	-2.037165227
C41	-3.639783025	-2.348523085	-1.990797060
C42	-3.215237121	-3.828318383	-1.882314557
C43	-2.773861842	-4.475917937	-3.193109712
C44	-5.730543194	1.545257272	-3.175799942
C45	-7.082344051	2.096423191	-2.702602924
C46	-5.338919592	2.151461630	-4.538207869
C47	-9.214046145	1.578133732	-1.611078244
C48	-8.994493376	1.704883611	-0.094505711
C49	-7.488124912	1.266567951	1.804998542
C50	-6.347184883	2.216738588	2.174279856
C51	-4.459242426	3.606698760	1.464348565
C52	-4.962234298	4.974803176	1.981308136
C53	-3.615497941	3.921221555	0.220361467
C54	-2.873917038	2.785424097	-0.414386239
C55	-2.415836219	1.574565915	0.042366282
C56	-1.688998481	1.810512184	-2.039521493
C57	-6.636018699	6.755380893	1.610239266
C58	-6.913641029	6.996362174	3.091495896
C59	-7.932994655	6.889883388	0.776734203
C60	-8.353955946	8.289654899	0.432688431
C61	-8.379984618	9.439142921	1.198707678
C62	-9.108658532	9.859246270	-0.851512171
C63	8.137407538	0.701757995	5.394565053
C64	8.945974409	-0.579689155	5.469725171
C65	6.743870555	0.322549878	4.828945058
C66	5.807510968	1.505101759	4.748038121
C67	4.984903715	1.860955723	5.832926648
C68	5.749395720	2.299205952	3.589492258
C69	4.131810428	2.967800752	5.765882296
C70	4.911674280	3.412106733	3.511659197
C71	4.101309936	3.743828582	4.600642653
C72	6.413849161	6.516766926	-0.474064479
C73	5.516993209	7.626509557	-1.036518751
C74	5.572659204	5.277105442	-0.139921389
C75	4.911403098	8.950493597	-3.017024579
C76	3.465838655	8.568669735	-3.340380719
C77	1.809247468	6.740169225	-3.491046946
C78	0.972522642	6.687990830	-2.194843671
C79	1.907512357	5.377342026	-4.198588613
C80	0.598465199	4.676223192	-4.574891591
C81	-0.238254251	5.299824725	-5.705894261
C82	-1.457576292	7.473429921	-5.596891097
C83	0.889971693	6.298883188	0.211394108
C84	0.812336125	7.675586035	0.902106688
C85	1.464331559	5.287195022	1.211240495
C86	2.055648839	9.699422404	1.487971995
C87	1.559658465	11.073234660	1.045321728
C88	0.439278938	12.427195360	-0.673644948
C89	-0.908198411	12.962471108	-0.146408074
C90	0.456766408	12.397344361	-2.218573979
C91	-0.564180102	11.416522159	-2.780761280
C92	-3.026729335	12.414223880	0.969327669
C93	-2.985263133	13.499622733	2.040517945
C94	-3.732418529	11.149387813	1.528897522
C95	-3.919952667	10.091100950	0.466850373

C96	-5.021854056	10.140468703	-0.400937061
C97	-2.969332453	9.075769668	0.275306141
C98	-5.163385717	9.221096826	-1.443153699
C99	-3.079236757	8.163966758	-0.779140730
C100	-4.176676907	8.254077547	-1.632586845
C101	5.179865313	-4.575971575	-8.156060783
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C103	2.222566380	-2.551218184	-6.815183700
C104	1.897566268	-1.208538490	-7.481291394
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C106	3.583763432	2.130363391	-7.415606845
C107	5.852784568	2.594079074	-6.618455262
C108	6.924851250	2.363500443	-7.665271195
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C112	-0.608505498	-5.753945115	-8.022737125
C113	-0.145348231	-6.204976229	-6.656047450
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C115	-2.055996176	1.036010718	-9.277259814
C116	-3.322944353	-0.004240328	-7.278720962
C117	-2.243650270	-0.051902678	-6.234928368
C118	-1.482816385	1.088486869	-5.938754575
C119	-1.869326360	-1.283961150	-5.666964445
C120	-0.326975268	0.979611624	-5.158681192
C121	-0.719886184	-1.386809901	-4.882622470
C122	0.078286019	-0.259777266	-4.658229230
C123	7.954784637	-7.043267138	-2.904866455
C124	8.939938296	-7.243548256	-1.738636705
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C131	-0.058726607	-6.913495135	0.335939014
C132	1.367762264	-6.794899541	0.803290333
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C135	3.272147423	-9.098106041	-1.782048012
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C137	3.818698511	-7.108386280	0.322534518
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Fe139	4.213918205	-2.437271967	-2.998123978
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Fe141	5.328565119	-0.028994395	-0.542286429
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Fe143	4.394963397	2.342524421	-1.347514627
Fe144	4.931812303	-2.537955208	-0.515198305
Fe145	2.422543087	-2.324614376	-1.080733211
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H151	-8.423304997	-1.824430823	0.464917477
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H153	-10.195586066	-1.906159507	0.634750626
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H155	-7.662993332	-5.236313231	2.611582879
H156	-9.777258548	-3.408526301	4.803487280

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H159	-5.540730596	-6.147566803	2.955267358
H160	-5.852649238	0.634672580	5.633254037
H161	-6.772742919	-1.626749201	4.049998265
H162	-5.718849857	-5.964999625	4.717264865
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H174	0.014462814	-0.431816458	2.576106348
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H182	-0.544463499	2.129683180	7.147300384
H183	-2.318058918	0.103701997	6.007159872
H184	0.191903779	0.422530757	4.121768015
H185	1.625728162	4.326536270	0.692850745
H186	0.707406793	5.138405474	1.997041864
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H188	2.703470141	4.921760478	5.249572582
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H213	-3.571964675	-0.373515453	-9.379724491
H214	0.425556919	-2.783851800	-9.494176756
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H222	-3.835037116	3.191451397	2.268800784
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H226	-6.653466100	4.749015027	0.847219630
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H236	-5.568957112	2.209830634	0.261520987
H237	-7.248492472	0.267410901	2.199783436
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H239	-1.185321916	1.613939882	-2.982672416
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H246	-2.605808194	3.715904182	-2.352149348
H247	-3.961964168	4.546113916	-3.896958524
H248	-3.649862122	5.816135349	-2.993910848
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H253	0.917349838	9.976610070	-3.206925562
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H262	-0.033751631	4.522095678	-3.686571274
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H264	5.405328425	9.224335794	-3.959304698
H265	-5.601543665	-0.486681991	-4.024792939
H266	2.509817638	5.527432638	-5.110148138
H267	-2.295698557	7.424466887	-0.956016917
H268	-6.072310445	3.838506833	-3.893518141
H269	4.862177125	9.852131050	-2.390504941
H270	-0.331926455	7.430213786	-7.318913321
H271	-2.712123692	9.071513606	-5.384139110
H272	-4.816572134	-3.155756212	-4.015779245
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H291	6.441467462	7.352381012	1.385895631
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H293	4.864670448	5.521315059	0.664488585
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H317	0.282651950	1.856214626	-4.936201779
H318	-2.483410241	-2.168375133	-5.848188709
H319	6.738715540	-10.585676307	0.370080084
H320	6.457916592	-8.490194268	-2.334233078
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H323	6.612010073	1.727321508	-8.528671753
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	O472	2.299601327	-6.241313265	-1.367754151
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	O477	6.397697662	-9.276168735	1.686092873
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	S480	2.257925272	-3.555321014	-2.979954657
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	O466	-0.630182503	-6.066623267	-0.695341410
	O467	-0.646497917	-8.143056380	0.101186993
	O468	4.423445515	-11.203632828	-2.066795624
	O469	2.383463860	-10.824289174	-2.959319371
	O470	4.684118710	-6.157730309	-0.146256856
	O471	4.042572818	-7.874462225	1.162029898
	O472	2.456531065	-6.119335774	-1.537027731
	O473	7.748019506	-7.423291957	3.128341162
	O474	6.410954831	-5.242622891	1.897770727
	O475	-2.946663854	5.226854162	-3.428206807
	O476	7.053285863	-11.138410747	-0.396232304
	O477	6.281015061	-9.342612104	1.713185338
	S478	4.617311392	4.751582812	-0.846964691
	S479	2.886011511	1.776066610	-2.416400475
	S480	2.547721534	-3.302377456	-2.998285687
	S481	3.978622442	1.392686474	1.022559607
	S482	0.702362110	-1.055224437	-1.423590169
	S483	5.231261210	-0.835075511	-4.405633124
	S484	3.169920652	-3.577775384	0.534523114
	S485	6.342022227	1.417157403	-1.586938470
	S486	6.047445374	-3.603803530	-1.833580892
	S487	6.217950725	-1.472676328	1.239980173
	9⁻¹u			
	Fe(139)	0.551	-2.369	
	Fe(140)	0.352	-1.031	
	Fe(141)	0.508	-2.233	
	Fe(142)	0.580	2.911	
	Fe(143)	0.560	2.879	
	Fe(144)	0.508	2.240	
	Fe(145)	0.401	-0.967	
	S=1			
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	C1	-7.656556218	-5.367799035	-0.812050413
	C2	-7.666581480	-6.457065055	-1.891590169
	C3	-8.919823738	-3.535141830	0.232477550
	C4	-8.748156882	-3.895913755	1.707023221
	C5	-9.043370006	-5.558118097	3.471365200
	C6	-7.584668352	-5.797766187	3.876473480
	C7	-5.328551597	-6.382414949	3.125748415
	C8	-4.601591759	-5.040683623	3.258633941
	C9	-4.349297174	-2.750276356	2.469139007
	C10	-4.703361639	-2.020013827	3.773712487
	C11	-6.386127970	-1.523048882	5.456829022
	C12	-5.813782221	-2.174688823	6.723428189
	C13	-5.537584425	-4.247335787	7.999623793
	C14	-4.065683488	-4.634341111	8.190445399
	C15	-1.986650142	-5.376810190	7.106469940
	C16	-0.890708123	-4.394904328	6.683443191
	C17	-0.409844895	-2.209566477	5.616334844
	C18	-0.495450568	-0.917893669	6.449564828
	C19	-0.603680436	-1.982679827	4.093008063
	C20	0.241702582	-0.816233315	3.569627246
	C21	-0.295526496	-3.265147911	3.311955778
	C22	-1.923035406	0.911085221	7.289059879
	C23	-2.106109493	0.589129008	8.785513639
	C24	-3.091153859	1.750930547	6.716148516
	C25	-3.396091681	2.958924346	7.609666471
	C26	-2.778434814	2.211251825	5.286081258
	C27	-3.288163176	-0.661290046	10.498607611
	C28	-2.034348278	-0.986507586	11.284324031
	C29	5.027957654	-11.461154305	4.786710886
	C30	5.708231284	-10.195349030	4.269758651
	C31	6.010736513	-7.767438720	4.761161294
	C32	7.037543874	-7.415009247	5.854616740

C33	4.856827668	-6.748688330	4.720819808
C34	5.318544541	-5.320171913	4.423362374
C35	4.136820768	-4.412054514	4.094429541
C36	4.059379788	-1.908754359	4.104959465
C37	9.293764717	-6.557988710	6.292478709
C38	9.504778861	-5.063305041	6.415654369
C39	-4.770059778	-2.487268001	-2.626199252
C40	-5.249830085	-1.065669694	-2.293717654
C41	-3.260055840	-2.559808922	-2.316384598
C42	-2.644272661	-3.972544461	-2.271551451
C43	-2.129979206	-4.510107717	-3.604004431
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C45	-7.200246472	1.470996266	-2.833294462
C46	-5.413250623	1.870495288	-4.580362474
C47	-9.281920767	0.636005643	-1.848340433
C48	-9.116163718	0.688265811	-0.320983572
C49	-7.631981302	0.266124749	1.596976976
C50	-6.638076786	1.325151978	2.079975363
C51	-4.877521394	2.941998902	1.534021910
C52	-5.532107694	4.231440864	2.098294318
C53	-4.008284421	3.388081579	0.350187446
C54	-3.122024796	2.368164698	-0.301775190
C55	-2.523626520	1.195383564	0.097439308
C56	-1.790316347	1.634802114	-1.941905770
C57	-7.410081341	5.823324541	1.839251268
C58	-7.731152057	5.899698071	3.330328313
C59	-8.708082461	5.874160459	1.000620530
C60	-9.278938476	7.241763590	0.755180669
C61	-9.477316070	8.306087148	1.614607996
C62	-10.168556534	8.822336714	-0.426528266
C63	7.886449350	1.191703095	5.716169150
C64	8.812663223	-0.011500663	5.699857214
C65	6.543140301	0.717949914	5.105184626
C66	5.484664897	1.796104924	5.075514636
C67	4.568987298	1.958582416	6.131796190
C68	5.386419657	2.673018675	3.980133004
C69	3.584412577	2.952781350	6.093157488
C70	4.418162118	3.676974557	3.932824953
C71	3.512761948	3.810794517	4.989071836
C72	5.624725774	7.227510212	0.251788451
C73	4.618444842	8.261946787	-0.266473818
C74	4.931500355	5.872173786	0.449902817
C75	3.915214166	9.656222920	-2.163195133
C76	2.536159501	9.133638498	-2.567838707
C77	1.111419108	7.146529028	-2.918127011
C78	0.249209355	6.909142158	-1.659387479
C79	1.387034604	5.858260415	-3.712949088
C80	0.177902447	5.041294497	-4.178989188
C81	-0.699956200	5.650974098	-5.286776280
C82	-2.158934654	7.659633165	-5.052846979
C83	0.138730493	6.327561143	0.707451673
C84	-0.113523088	7.628668082	1.494850308
C85	0.795397428	5.311791285	1.652055685
C86	0.871767540	9.729087900	2.269026231
C87	0.247968437	11.074813730	1.909459409
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C90	-0.908995940	12.500116333	-1.284873712
C91	-1.806266329	11.461998209	-1.948861983
C92	-4.477435244	11.887391924	1.751821623
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C94	-5.045671890	10.512754003	2.196767607
C95	-5.077925742	9.519861406	1.057694628
C96	-6.154660794	9.510878780	0.156506700
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C98	-6.159581457	8.668685781	-0.957097710
C99	-3.988191629	7.800937682	-0.295071777
C100	-5.063383461	7.833824190	-1.180705588
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C104	2.251250194	-0.418386194	-7.469018492
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C106	3.514981580	3.085603122	-7.102288925
C107	5.711714106	3.732798033	-6.230321000
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C109	-0.698809935	-3.147228787	-9.634152489
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C112	0.287119225	-5.155872259	-8.422050767
C113	0.753453286	-5.665609726	-7.078177795
C114	-2.395473106	0.178917968	-8.803650873
C115	-1.852656685	1.503769358	-9.301510089
C116	-3.009871165	0.216913467	-7.383485459
C117	-1.962045136	0.178226966	-6.302164542
C118	-1.289566306	1.343429979	-5.899610636
C119	-1.565814941	-1.053263775	-5.749172181
C120	-0.222822418	1.266435124	-4.996918552
C121	-0.508751928	-1.125517009	-4.838092557
C122	0.183986488	0.034514623	-4.475957677
C123	8.769371644	-5.849494202	-3.120312932
C124	9.727564386	-6.017290596	-1.926938059
C125	7.351525569	-6.351986579	-2.801102042
C126	6.305083023	-6.095604794	-3.844623393
C127	6.248885386	-6.613467199	-5.123304239
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C132	2.062668420	-6.577722535	0.352251849
C133	3.165247101	-6.728749733	-0.766826284
C134	3.132476004	-8.173729314	-1.346240907
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Fe139	4.555809601	-1.682181504	-3.047324609
Fe140	2.768239075	0.797827782	-0.677049672
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Fe145	2.612140432	-1.795791521	-1.240104993
H146	-5.916369156	-7.354405157	-1.352832323
H147	-5.764226292	-6.353057496	-2.633240754
H148	-9.555407456	-4.803565261	-1.364536072
H149	-8.122498646	-6.049414819	-2.808045714
H150	-8.353560287	-7.246309770	-1.539974509
H151	-8.156170859	-2.776134565	0.013153416
H152	-9.640683414	-5.722078673	1.409391980
H153	-9.909261736	-3.076722249	0.097944585
H154	-9.603100824	-6.493560096	3.601978527

H155	-7.093152488	-6.242045654	1.933659004
H156	-9.450489363	-4.813413216	4.167312010
H157	-3.253942783	-2.810364548	2.426909598
H158	-5.586328901	-4.287857311	1.602469978
H159	-4.895808992	-6.956657406	2.295420566
H160	-6.068026556	-0.472883202	5.458934486
H161	-6.663999679	-2.679471098	3.663204596
H162	-5.155533511	-6.931803801	4.058468134
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H164	-6.334853231	-4.054388516	6.029866704
H165	-7.483184174	-1.554929569	5.510333880
H166	-0.935449578	-4.101203589	3.629207955
H167	-0.449688295	-3.097114348	2.235681680
H168	0.756540090	-3.562465047	3.451290856
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H172	-3.625517785	-0.784316277	8.398679817
H173	-3.678391050	2.666414849	8.631408058
H174	0.027026992	-0.649236440	2.504378225
H175	1.315672422	-1.036227226	3.644919275
H176	7.703040446	1.457450771	6.775519314
H177	-3.614719802	2.810440526	4.896735344
H178	-4.226004084	3.539266232	7.181272017
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H181	-3.987230987	1.104122966	6.689929981
H182	-0.998496373	1.504637987	7.245377937
H183	-2.480114562	-0.649295721	5.919851023
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H185	1.073467824	4.416993707	1.069815980
H186	0.039334251	5.022093210	2.397980334
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H188	1.958195213	4.762411486	5.654631590
H189	4.341892335	4.332201915	3.064452755
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H193	-1.889466463	-6.262715782	6.460591916
H194	-1.767908866	-5.682494803	8.137676726
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H196	-5.814841046	-3.640950800	8.871397112
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H198	0.601797442	-2.596573171	5.796585215
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H200	-3.933805483	-1.553410744	10.534545688
H201	-1.205252341	-1.431388978	10.685548718
H202	10.237241318	-7.033816758	5.985072268
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H204	0.943670628	-8.699791449	0.508040563
H205	-0.373523435	-5.911544207	-8.870902132
H206	1.149795874	-5.010979731	-9.089150697
H207	-1.455102926	-4.037237927	-7.788307976
H208	-1.123089145	1.408489587	-10.140320557
H209	-1.135726336	-3.895566880	-10.313258879
H210	-2.717955080	-1.936551817	-3.044338421
H211	-3.384985678	-4.699084565	-1.890727237
H212	-0.447103286	-0.715073943	-8.732968461
H213	-3.222043242	-0.048962484	-9.508152627
H214	1.035928006	-2.006190444	-9.663018808
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H238	-9.751603953	1.579998054	-2.153110098
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H244	-0.855162551	5.943794854	0.436310325
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H256	-1.081505329	4.850446579	-5.938055923
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H263	-7.733930202	-0.491280200	-2.823262937
H264	4.397858109	10.058094966	-3.064381096
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H266	1.993199229	6.140688446	-4.589484001
H267	-3.123829357	7.164974472	-0.493368508
H268	-6.360851764	3.405734340	-3.844754524
H269	3.739061646	10.493498492	-1.473298941
H270	-0.984280080	7.889453930	-6.729658061
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H275	-5.140665016	1.520192535	-2.477684303
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H277	-0.088918734	6.307206464	-5.919204754
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H284	-2.645069221	10.830639991	1.391275123
H285	6.415637438	-2.380342235	-8.233750505
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H291	5.485951086	7.894967976	2.175844714
H292	5.552873550	8.280947058	-2.098707409
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H296	6.432194371	7.103889922	-0.486821543
H297	4.317002439	-6.786220834	5.681992130
H298	6.501962520	-7.792764525	3.780653292
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H302	-0.214916227	-2.075875704	-4.385863306
H303	1.551910581	2.391103774	-6.721815806
H304	3.451861500	-4.326028599	4.947393527
H305	3.282506251	0.496750505	-5.970949520
H306	3.553596482	-4.842164766	3.263123595
H307	4.160371870	-7.085971504	3.936192128
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H311	4.949157206	-9.276031647	5.874519048
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N390	-8.045260030	0.447553983	-2.585678689
N391	-7.922361353	0.249462661	0.174230598
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N393	-2.647912862	2.611597734	-1.588672718
N394	-1.712465349	0.760945538	-0.935990154
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O424	-7.213369866	-5.618379926	5.048120635
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O426	-3.867445231	-1.320125024	4.368679383
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O428	-3.606934572	-4.748661442	9.334817900
O429	0.300466127	-4.705353432	6.832938414
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O435	10.577532872	-4.560438363	6.710546691
O436	-5.387752880	-0.648908658	-1.122461650
O437	-2.720120908	-4.291712924	-4.687582619
O438	-7.504520289	2.668707948	-2.652827918
O439	-5.549189970	3.289461671	-4.405242143
O440	-10.052500029	1.093076860	0.378430813
O441	-6.561111513	1.606957881	3.278167904
O442	-4.940403368	4.938128780	2.920109035
O443	-7.745936297	6.933096208	3.977165092
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O447	1.640392525	9.952140845	-2.860213122
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O449	-1.059101734	7.690641828	2.292663049
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O452	-2.862551572	13.899443638	0.631279938
O453	-3.029987614	11.635201714	-2.059248498
O454	-5.656285859	13.469604280	3.147128589
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O456	3.602080321	-4.046597094	-8.398819370
O457	1.484121779	-0.359935245	-8.453969712
O458	3.268184352	4.235864941	-7.501323889
O459	7.891405759	4.322029249	-7.072861908

	O460	-2.974009412	-2.335257915	-9.825452145
	O461	0.037985622	-6.292833916	-6.303034158
	O462	2.017079280	-5.354055269	-6.726023939
	O463	-2.197852217	2.599299871	-8.882297996
	O464	10.520193377	-5.113838764	-1.601401629
	O465	12.938931341	-6.834978651	0.316240227
	O466	-0.076113657	-6.125440593	-0.707693254
	O467	0.251664276	-8.193250020	0.041461050
	O468	5.462222081	-10.612814860	-2.407635615
	O469	3.363070666	-10.454090514	-3.226344992
	O470	5.254900216	-5.557074289	-0.464253582
	O471	4.905105636	-7.376180042	0.817210198
	O472	2.972803777	-5.769611916	-1.746143424
	O473	8.655852025	-6.542964058	2.604203124
	O474	7.001077042	-4.508806781	1.503268405
	O475	-3.700969336	4.894047099	-3.173581812
	O476	8.186912868	-10.270935948	-0.935769270
	O477	7.333874642	-8.592909099	1.233414323
	S478	4.119729016	5.251522476	-1.095326590
	S479	2.627525184	2.212702325	-2.479455504
	S480	2.714564537	-2.946960912	-3.209370361
	S481	4.019974036	1.883664636	0.833464155
	S482	0.417371551	-1.602243701	-1.374859595
	S483	5.037983828	-0.236509723	-4.677911601
	S484	3.473076137	-3.124160642	0.299275416
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	Fe(142)	0.561	2.588	
	Fe(143)	0.603	3.195	
	Fe(144)	0.500	2.206	
	Fe(145)	0.386	-0.605	
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	C2	-7.686944088	-6.469232258	-1.891081058
	C3	-8.929983562	-3.544746426	0.237879091
	C4	-8.755830959	-3.904846665	1.711865792
	C5	-9.038550420	-5.571969275	3.473980920
	C6	-7.577649809	-5.803611625	3.876956324
	C7	-5.318432418	-6.373151031	3.123418735
	C8	-4.597255307	-5.028347826	3.254993547
	C9	-4.348588590	-2.739660465	2.458910566
	C10	-4.703383565	-2.006987493	3.761884267
	C11	-6.380660580	-1.516245763	5.451510581
	C12	-5.808056180	-2.167051793	6.718828322
	C13	-5.532656854	-4.240733066	7.995082416
	C14	-4.064159725	-4.642290224	8.184214158
	C15	-1.990364447	-5.397269239	7.097795393
	C16	-0.894827013	-4.403612240	6.700631184
	C17	-0.416704316	-2.211844422	5.642999655
	C18	-0.512166041	-0.928184288	6.488490573
	C19	-0.609129526	-1.980521382	4.120461742
	C20	0.233201861	-0.809750021	3.602721201
	C21	-0.294115835	-3.258735758	3.334069786
	C22	-1.926558052	0.915763745	7.307071516
	C23	-2.112539068	0.598772032	8.804808025
	C24	-3.085327206	1.766709451	6.732451976
	C25	-3.384639585	2.975790728	7.627230160
	C26	-2.763312917	2.230336067	5.305394391
	C27	-3.287100171	-0.649486140	10.524624739
	C28	-2.027091374	-0.981144451	11.297942042
	C29	5.038500810	-11.477318004	4.810366459
	C30	5.719899689	-10.210740536	4.289351175
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C49	-7.629268879	0.270193579	1.602688259
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C71	3.509835647	3.810272138	4.988111124
C72	5.620302079	7.228375390	0.244981989
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C74	4.903843049	5.887179006	0.449296795
C75	3.918631907	9.660550265	-2.167786140
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C77	1.115883114	7.147945116	-2.917402816
C78	0.254550393	6.912541734	-1.657592169
C79	1.393132505	5.858850140	-3.710722369
C80	0.184868549	5.045542646	-4.182394054
C81	-0.681043313	5.654716515	-5.298426447
C82	-2.148176396	7.662102719	-5.073277610
C83	0.145421967	6.321844298	0.702629635
C84	-0.111318038	7.625301732	1.483481539
C85	0.807780077	5.315528606	1.654324412
C86	0.877607380	9.723274749	2.258840024
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C88	-0.982438281	12.409578320	0.248310983
C89	-2.401854247	12.747361681	0.750222737
C90	-0.905020749	12.495562378	-1.292263152
C91	-1.796071947	11.454106427	-1.959826374
C92	-4.469922497	11.883218445	1.757944713

C93	-4.597062898	12.883662776	2.899932347
C94	-5.035934339	10.506854941	2.199654543
C95	-5.071568046	9.516969162	1.057684422
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C99	-3.979539936	7.807550620	-0.304738003
C100	-5.057448396	7.840410988	-1.187416783
C101	5.904375519	-3.336186124	-8.261222414
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C103	2.698548407	-1.769682190	-6.872865025
C104	2.234263355	-0.428951065	-7.455815253
C105	2.440337224	2.006221404	-7.253934118
C106	3.533888788	3.060710678	-7.106155128
C107	5.703586609	3.727544081	-6.195269405
C108	6.822255739	3.710819759	-7.216341902
C109	-0.704556883	-3.139767564	-9.643636595
C110	-1.805349720	-2.080900549	-9.515100752
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C112	0.293431085	-5.146455380	-8.436057893
C113	0.768353057	-5.656236329	-7.094442863
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C115	-1.873091904	1.501150754	-9.274825940
C116	-3.066169765	0.195926588	-7.387734143
C117	-2.023680820	0.181427167	-6.304714336
C118	-1.386076839	1.366332301	-5.905301251
C119	-1.557525077	-1.043689274	-5.793585455
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C124	9.757455912	-6.029273842	-1.937686920
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C128	4.441306897	-5.474986254	-4.723399203
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C131	0.728735720	-6.881984519	-0.155395895
C132	2.114880287	-6.609713626	0.354503239
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Fe144	5.175149781	-1.930914508	-0.521121244
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N409	-3.080463671	11.740353144	1.351152567
N410	6.128105807	-3.979892281	-9.560483047
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N412	2.754730673	0.651215510	-6.844818024
N413	4.677353429	2.733097801	-6.452553689
N414	0.492207236	-2.591582037	-10.296324759
N415	-1.434851111	-0.878594863	-8.994945307
N416	9.367321071	-6.448504872	-4.348653227
N417	5.185876665	-5.400243703	-3.626413188
N418	5.070703517	-6.210668378	-5.675316647
N419	9.747069665	-7.220201784	-1.275344216
N420	0.360940126	1.787576908	1.034135739
N421	1.118647592	1.314518612	0.331341160
O422	-6.710975951	-5.197498680	-0.050158876
O423	-8.234125223	-3.101045876	2.500882776
O424	-7.207377126	-5.625890887	5.049349300
O425	-3.757234530	-4.830094148	4.146639658
O426	-3.870979840	-1.299504021	4.351487617
O427	-5.359761423	-1.471840313	7.646797157
O428	-3.604267233	-4.755913725	9.328617671
O429	0.295459460	-4.708391479	6.865440312
O430	0.470791579	-0.505166966	7.116002629
O431	-1.467927599	1.201846281	9.679126994
O432	-1.929824585	-0.852422073	12.509474674
O433	6.415404399	-10.270685779	3.253197841
O434	6.750258354	-7.598967745	7.050468076
O435	10.572505213	-4.590664499	6.728521668
O436	-5.418665782	-0.666416873	-1.115350037
O437	-2.753088460	-4.318567948	-4.678430042
O438	-7.497547427	2.674863053	-2.636681993
O439	-5.543076992	3.291407821	-4.395000915
O440	-10.058598343	1.076318591	0.386869535
O441	-6.562748189	1.604931346	3.289214845
O442	-4.977160410	4.930323836	2.970357396
O443	-7.778779579	6.936108118	3.979310421
O444	8.936306176	-0.768730603	6.660009700
O445	2.558644099	4.808794633	4.895678875
O446	3.710578027	8.728925284	0.448468303
O447	1.649649875	9.955375536	-2.882182600
O448	-0.973970956	7.108432777	-1.705131089
O449	-1.061053039	7.696615222	2.276329679
O450	1.918669063	5.933384594	2.310166695
O451	0.380347435	12.031240322	2.670574246
O452	-2.864177680	13.889210596	0.617996857
O453	-3.021142269	11.623710861	-2.068504447
O454	-5.639986431	13.458428693	3.168174928
O455	-4.993454308	7.025455533	-2.330808043
O456	3.600169331	-4.027345988	-8.425828570
O457	1.452740455	-0.371841583	-8.433992534
O458	3.321666986	4.193848365	-7.572871916

	O459	7.871237273	4.320068190	-7.072146857
	O460	-2.978494882	-2.328750399	-9.844936161
	O461	0.052103154	-6.278942271	-6.314703246
	O462	2.035402294	-5.356896534	-6.753091444
	O463	-2.281544367	2.593444866	-8.906497974
	O464	10.592149951	-5.152520268	-1.645327168
	O465	12.951951028	-6.854010858	0.300419839
	O466	-0.003167448	-6.075308728	-0.711478041
	O467	0.256564762	-8.163438597	0.009253246
	O468	5.494708912	-10.656322962	-2.432309281
	O469	3.398190045	-10.486643180	-3.254737058
	O470	5.336589085	-5.647913256	-0.438089934
	O471	4.942915358	-7.456480427	0.850887958
	O472	3.066316141	-5.853466167	-1.755454939
	O473	8.670771803	-6.539816141	2.616634113
	O474	7.040280705	-4.512744754	1.483673570
	O475	-3.689380445	4.908650709	-3.188379464
	O476	8.174553319	-10.292621855	-0.920213160
	O477	7.357372420	-8.599871717	1.246578369
	S478	4.037232652	5.288084708	-1.071932461
	S479	2.454423431	2.215976433	-2.441176321
	S480	2.703531765	-3.040802853	-3.144870631
	S481	3.836841646	1.752551869	0.836037422
	S482	0.690923989	-0.885869079	-1.604160826
	S483	4.927416483	-0.177025049	-4.645396319
	S484	3.518785328	-3.225167565	0.292454221
	S485	6.135137680	2.052006236	-1.880351149
	S486	6.294626524	-2.871514143	-2.197808292
	S487	6.474166561	-0.856805354	0.919669881
	9⁻²(b)			
	Fe(139)	0.561	2.450	
	Fe(140)	0.349	0.169	
	Fe(141)	0.576	2.842	
	Fe(142)	0.560	-2.675	
	Fe(143)	0.605	3.158	
	Fe(144)	0.505	-2.232	
	Fe(145)	0.384	-1.434	
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	C1	-8.262326669	-4.505173337	-0.173509450
	C2	-8.434852314	-5.659910488	-1.166845080
	C3	-9.260183486	-2.467570619	0.769120485
	C4	-9.072196187	-2.738172094	2.259911602
	C5	-9.470535092	-4.234300606	4.149462774
	C6	-8.027983884	-4.588495314	4.526262281
	C7	-5.876228200	-5.469048676	3.752369657
	C8	-5.001737063	-4.212902719	3.749571660
	C9	-4.539846887	-2.030444997	2.770094946
	C10	-4.756057346	-1.162416724	4.019510606
	C11	-6.292971647	-0.368232291	5.726770332
	C12	-5.748432788	-0.987389596	7.021820455
	C13	-5.666888148	-2.975149500	8.450086185
	C14	-4.248621652	-3.533974547	8.616636333
	C15	-2.322249879	-4.608489517	7.531432589
	C16	-1.135617869	-3.774645365	7.036737131
	C17	-0.456960096	-1.732278460	5.802596121
	C18	-0.378672585	-0.389323919	6.551299953
	C19	-0.679850387	-1.593637962	4.272233375
	C20	0.264144047	-0.565886782	3.640679036
	C21	-0.536652368	-2.955673874	3.582022792
	C22	-1.536863195	1.661935073	7.267325458
	C23	-1.694852609	1.480364142	8.790660920
	C24	-2.606678794	2.605834053	6.666506148
	C25	-2.722606020	3.898850094	7.483289449
	C26	-2.279924035	2.930297782	5.203468030
	C27	-2.930352388	0.507778902	10.641262354
	C28	-1.685786935	0.072993406	11.390152173
	C29	3.887559430	-11.603783900	5.521232253
	C30	4.674294910	-10.460805813	4.881372547

C31	5.241892873	-8.045235134	5.164601481
C32	6.338466802	-7.741472068	6.202997452
C33	4.212014465	-6.905426693	5.071949051
C34	4.830903077	-5.570217214	4.651655487
C35	3.763089293	-4.541287331	4.285520574
C36	3.969783435	-2.057489080	4.098624651
C37	8.689819173	-7.134587403	6.525957117
C38	9.088631532	-5.674028513	6.526130856
C39	-5.137618618	-2.100629959	-2.279218626
C40	-5.430915732	-0.610777734	-2.038902183
C41	-3.639598001	-2.347783129	-1.989871943
C42	-3.216764122	-3.828283395	-1.882082324
C43	-2.776944866	-4.478761814	-3.191911668
C44	-5.728069698	1.544811975	-3.177438135
C45	-7.080257138	2.096537406	-2.705617846
C46	-5.338290486	2.150888714	-4.540328391
C47	-9.211324530	1.576906197	-1.612623267
C48	-8.991448692	1.704237339	-0.096566911
C49	-7.487191390	1.266251551	1.802044699
C50	-6.347295044	2.216986449	2.173675674
C51	-4.456706142	3.606670243	1.463316911
C52	-4.963375616	4.976890956	1.981426318
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C56	-1.682171232	1.798622748	-2.039185186
C57	-6.640732128	6.756090518	1.611694859
C58	-6.914747937	6.996426112	3.094684928
C59	-7.937376482	6.890493753	0.778634545
C60	-8.357897591	8.290295832	0.435928703
C61	-8.381711414	9.438957103	1.202860042
C62	-9.110111461	9.863364591	-0.846759699
C63	8.142193489	0.698786784	5.396735037
C64	8.949098144	-0.582816078	5.468164648
C65	6.748318946	0.323364949	4.826457743
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C67	4.992541450	1.861912471	5.832559591
C68	5.754253976	2.299063617	3.587814628
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C71	4.110631678	3.745366277	4.601209295
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C73	5.520980820	7.635618822	-1.031293823
C74	5.568260183	5.294446004	-0.132333143
C75	4.911242784	8.951768829	-3.014092398
C76	3.466233116	8.565652580	-3.335864170
C77	1.810280021	6.739358455	-3.488468090
C78	0.974853676	6.691355838	-2.190668003
C79	1.907427673	5.375762867	-4.195443853
C80	0.598410629	4.674443104	-4.570753287
C81	-0.235989305	5.297504870	-5.702940343
C82	-1.454415847	7.473897632	-5.593745331
C83	0.890050083	6.298575709	0.212365013
C84	0.811331821	7.676496694	0.899241248
C85	1.464854369	5.291350045	1.216664770
C86	2.056517154	9.698287857	1.485896822
C87	1.560423140	11.072491516	1.045378835
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C89	-0.907691493	12.963027989	-0.145973504
C90	0.457158063	12.395436097	-2.218210923
C91	-0.563631039	11.415218312	-2.781903239

C92	-3.029199426	12.419350330	0.967865746
C93	-2.985932128	13.502212167	2.039655527
C94	-3.734300887	11.151916059	1.526167862
C95	-3.920097411	10.093081734	0.464333719
C96	-5.023002327	10.140796039	-0.402148524
C97	-2.969039449	9.077876406	0.273206597
C98	-5.164703238	9.220718897	-1.443490675
C99	-3.079042201	8.165453984	-0.780566044
C100	-4.177236921	8.254541300	-1.633480770
C101	5.177069320	-4.574802697	-8.150902607
C102	3.726575617	-4.219256840	-7.867852930
C103	2.218662824	-2.552401420	-6.810905950
C104	1.894792319	-1.210598019	-7.478522161
C105	2.378784415	1.192728090	-7.472295809
C106	3.586467492	2.123888225	-7.418494922
C107	5.853075315	2.589185856	-6.621779899
C108	6.924376740	2.362411699	-7.668498789
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C113	-0.143250437	-6.207788984	-6.658308342
C114	-2.715636789	-0.192675492	-8.693289559
C115	-2.049873851	1.035493911	-9.278962742
C116	-3.316346104	-0.004494455	-7.280868925
C117	-2.236982910	-0.053380789	-6.236173707
C118	-1.476826342	1.086460882	-5.938114336
C119	-1.862488527	-1.286484698	-5.667462423
C120	-0.324675620	0.977890062	-5.151171097
C121	-0.718887196	-1.387441533	-4.874358249
C122	0.076449283	-0.259428642	-4.641108290
C123	7.952441969	-7.043110629	-2.906592529
C124	8.938591169	-7.244192388	-1.743281117
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C126	5.462817120	-7.083904481	-3.560749971
C127	5.298561912	-7.658572103	-4.804850876
C128	3.610630672	-6.282940459	-4.398049477
C129	9.735286891	-8.590877442	0.119393983
C130	11.180508107	-8.532360408	-0.323647311
C131	-0.057142544	-6.911723758	0.343658437
C132	1.365486128	-6.793144867	0.808718899
C133	2.409402592	-7.158333751	-0.328368852
C134	2.172454022	-8.621426160	-0.800919183
C135	3.264677727	-9.101882800	-1.772160241
C136	3.246823944	-10.581750217	-2.016337178
C137	3.821786271	-7.118385002	0.334469727
C138	3.941800825	-1.123089292	-1.562170769
Fe139	4.215019411	-2.402476939	-3.022020068
Fe140	2.463949159	0.229105577	-0.800118756
Fe141	5.309796421	-0.044735422	-0.547789009
Fe142	4.329973832	0.188513383	-2.968950471
Fe143	4.346924208	2.373139243	-1.453268646
Fe144	4.890115795	-2.562616778	-0.518436506
Fe145	2.408044863	-2.301041886	-1.068130468
H146	-6.761594734	-6.695277056	-0.633766354
H147	-6.570972503	-5.807616031	-1.990347084
H148	-10.101967077	-3.757896903	-0.712048000
H149	-8.890877016	-5.274144614	-2.092655263
H150	-9.180440356	-6.343328464	-0.724274176
H151	-8.421712929	-1.825345818	0.463893175
H152	-10.152363514	-4.478502013	2.121251844

H153	-10.193120690	-1.904229316	0.632875016
H154	-10.113156389	-5.099473981	4.359346845
H155	-7.663817425	-5.231460709	2.611660475
H156	-9.779277466	-3.407311353	4.802148904
H157	-3.460872895	-2.220774722	2.701773298
H158	-5.981521967	-3.478033478	2.082600798
H159	-5.543389839	-6.146366295	2.954410431
H160	-5.853812090	0.632934711	5.632620399
H161	-6.774545292	-1.627064753	4.050173111
H162	-5.721115732	-5.966565924	4.716999228
H163	-4.846772827	-1.469639554	1.875583282
H164	-6.515146912	-2.838848712	6.495734317
H165	-7.383327113	-0.266476112	5.818404748
H166	-1.240577710	-3.696062160	3.988112966
H167	-0.727121482	-2.856661569	2.502518936
H168	0.485864111	-3.348031896	3.698215085
H169	-1.713522784	-1.239255278	4.127791377
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H171	-2.237022881	2.029904413	4.574588601
H172	-3.365698877	0.253060123	8.565341655
H173	-3.021202930	3.712534954	8.525251933
H174	0.018528316	-0.430514964	2.578085484
H175	1.309728063	-0.900084673	3.681726169
H176	7.997856647	1.061980567	6.432294339
H177	-3.045795621	3.599168701	4.783898034
H178	-3.473279007	4.560248993	7.026004356
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H182	-0.546764174	2.127095241	7.147985903
H183	-2.318963915	0.103970914	6.005291218
H184	0.197511581	0.420559732	4.124509859
H185	1.639790301	4.329940735	0.704206444
H186	0.701395861	5.138700190	1.995985188
H187	2.799150936	5.389276468	2.657601110
H188	2.701036056	4.912111872	5.245470830
H189	4.854534335	3.991437104	2.589393851
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H194	-2.111458392	-4.889748134	8.571391143
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H196	-5.818968662	-2.270244728	9.277489673
H197	3.489357433	3.217593007	6.609815927
H198	0.515360515	-2.210310186	5.980535877
H199	-3.320540455	1.429425830	11.103670090
H200	-3.682662741	-0.285307486	10.773841279
H201	-0.932395726	-0.472108597	10.775448031
H202	9.557130984	-7.749588042	6.241607476
H203	-1.407742962	-5.802026547	-3.952515947
H204	-0.071481582	-8.688779920	1.093111455
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H206	0.236543287	-5.753582829	-8.727186575
H207	-2.203018480	-4.418304837	-7.426548981
H208	-1.323725846	0.815557826	-10.096993230
H209	-1.952795651	-4.462501194	-9.963830215
H210	-3.038342283	-1.842731557	-2.762704995
H211	-4.052202362	-4.432882627	-1.487040291
H212	-0.867673253	-1.284605587	-8.605993050
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H214	0.424724717	-2.779284006	-9.493696832
H215	-1.232271861	-5.481445491	-2.230142028
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H217	0.335579137	-4.213022575	-10.298941386
H218	-6.427682953	-2.920293155	-3.668906098
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C40	-5.211179000	-0.129371498	-2.645320858
C41	-3.263824275	-1.606386320	-3.099617670
C42	-2.694421122	-2.987702427	-3.486020475
C43	-2.115241889	-3.091276805	-4.894595038
C44	-5.516344276	2.325299339	-2.806225645
C45	-6.895674950	2.508861746	-2.163604426
C46	-5.185767271	3.388604172	-3.891653121
C47	-9.141182028	1.566478701	-1.877205820
C48	-9.064953791	1.088064524	-0.418214230
C49	-7.701631132	0.007756626	1.319397817
C50	-6.691320492	0.805508922	2.149875220
C51	-4.924072911	2.506019995	2.234876120
C52	-5.619007412	3.511606958	3.177428896
C53	-4.047878260	3.347592743	1.293891241
C54	-3.166004890	2.617599644	0.327806846
C55	-2.643020067	1.342010105	0.351586294
C56	-1.865120148	2.433326275	-1.406630724
C57	-7.369868630	5.238868744	3.268672019
C58	-7.760184074	4.899096536	4.704530188
C59	-8.621483430	5.591327790	2.429749715
C60	-9.152698256	6.986719106	2.578421757
C61	-9.365288857	7.759310710	3.705458396
C62	-9.959735273	8.872430189	1.883020048
C63	7.599831369	-0.855803040	6.077111744
C64	8.515268796	-2.020970464	5.753103092
C65	6.285399465	-1.086567335	5.287324474
C66	5.245645983	-0.023433942	5.554835067
C67	4.314083871	-0.157043033	6.601443535
C68	5.182890988	1.135923044	4.763151137
C69	3.349703640	0.826059168	6.845779803
C70	4.234440232	2.130075862	5.002125870
C71	3.314756925	1.971591273	6.041888168
C72	5.758501776	6.631991402	2.662408528
C73	4.803979114	7.816521051	2.456836763
C74	5.014963166	5.313179156	2.415286363
C75	4.223777229	9.745131920	1.045643605
C76	2.847838107	9.422613332	0.454245463
C77	1.401657073	7.687561717	-0.549212520
C78	0.481453395	7.118898347	0.553993036
C79	1.681642114	6.681231318	-1.678732710
C80	0.475916883	6.072626611	-2.404259550
C81	-0.342202556	7.015230445	-3.303809085
C82	-1.798752987	8.883979285	-2.531761594
C83	0.247639037	5.807027648	2.596389519
C84	-0.017362863	6.805188271	3.738158271
C85	0.845510853	4.529960597	3.201748097
C86	0.972937642	8.529673097	5.160778422
C87	0.380857182	9.934889152	5.217798568
C88	-0.743985919	11.762258267	4.018238266
C89	-2.172796488	11.966640782	4.568188028
C90	-0.617915911	12.318761495	2.584000220

C91	-1.502751444	11.562251096	1.599064950
C92	-4.303953368	10.903815956	5.152340185
C93	-4.475160682	11.501106787	6.542608030
C94	-4.933148661	9.483651691	5.107384871
C95	-4.918799667	8.896822631	3.714659836
C96	-5.943565586	9.199922746	2.803817453
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C99	-3.794370088	7.625201872	1.957035704
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C102	4.692375676	-0.689870263	-8.456866417
C103	2.950913869	0.353592586	-7.021561745
C104	2.550428243	1.826653112	-7.175871891
C105	2.786146943	4.071678370	-6.223617419
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C108	7.195849839	5.524290432	-5.431117467
C109	-0.377766030	0.012083116	-10.168250544
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C118	-1.074285582	3.135113108	-5.262704672
C119	-1.340636980	0.814160375	-5.902259997
C120	0.021720964	2.781032439	-4.472774544
C121	-0.245997919	0.465214453	-5.110387305
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C124	9.700229672	-5.472331229	-3.354238284
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C126	6.388288856	-4.867724588	-5.371567515
C127	6.368413514	-4.951041691	-6.749592041
C128	4.549396872	-3.899784928	-6.048781550
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C138	4.118200235	-0.217880701	-1.463458509
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Fe140	2.516835911	0.681011980	-0.323892736
Fe141	5.236444926	0.525804490	0.015140825
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Fe145	2.726991468	-1.540857079	-1.615155967
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H152	-9.821252330	-5.577943426	-0.767863955
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H157	-3.435202141	-3.250821459	1.292827487
H158	-5.754983569	-4.364756234	0.003072061
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H160	-6.271572262	-1.904397017	4.834678252
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H162	-5.445989009	-7.643198122	1.525559785
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H166	-1.179520380	-4.989820450	2.199094180
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H183	-2.754084204	-2.306359297	5.349856301
H184	-0.187816394	-1.139532460	3.991320176
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H212	-0.128457117	2.027800905	-8.530358586

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H246	-3.125712866	4.847336909	-1.335782703
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H262	-0.191213316	5.556048302	-1.696850682
H263	-7.633144804	0.948945258	-3.269662272
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H266	2.323411706	7.190461863	-2.417343193
H267	-2.939502585	7.039820149	1.613915984
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H269	-0.603382382	9.576454898	-4.051078689
H270	-3.228187817	10.187418216	-1.884009858
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	O476	6.924912469	-8.061283248	3.966721718
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	S478	2.888841703	1.234371792	-3.016274792
	S479	2.740236850	-3.821511492	-2.144946971
	S480	3.975757846	1.943088985	0.354432223
	S481	0.378987588	-2.114213778	-0.555228042
	S482	5.220799113	-1.732246843	-4.178785684
	S483	3.326917754	-3.064267071	1.336100532
	S484	6.366712846	1.235167455	-2.143169793
	S485	6.206815318	-3.565244281	-0.933942998
	S486	6.347270480	-0.753659063	1.449238921
11	bmlcnx262n2x351.car_1			
Fe(139) 0.553 -2.379	C1	-8.187182156	-4.447705328	-1.394492609
Fe(140) 0.322 -0.129	C2	-8.224678753	-5.572270052	-2.436264405
Fe(141) 0.562 -2.775	C3	-9.282597593	-2.410242301	-0.562393953
Fe(142) 0.572 2.694	C4	-9.313765632	-2.709149438	0.933942740
Fe(143) 0.606 3.204	C5	-9.977698756	-4.226220849	2.723430959
Fe(144) 0.507 2.295	C6	-8.604862798	-4.609013321	3.288686031
Fe(145) 0.376 -1.409	C7	-6.369489195	-5.478539783	2.796394523
S=1	C8	-5.500754081	-4.224075467	2.942478959
	C9	-4.893584674	-2.027540417	2.078281568
	C10	-5.276584029	-1.193077384	3.308283574
	C11	-7.028595068	-0.410969877	4.797275553
	C12	-6.677374689	-1.060520548	6.143377634
	C13	-6.800849101	-3.075355072	7.530929507
	C14	-5.424895254	-3.653793180	7.882419424
	C15	-3.364940870	-4.706086658	7.047824411
	C16	-2.114984411	-3.883400436	6.721822594
	C17	-1.261592664	-1.812609297	5.650115805
	C18	-1.274795277	-0.480240633	6.422237048
	C19	-1.286228603	-1.653580175	4.106765543
	C20	-0.274637620	-0.613479597	3.616024183
	C21	-1.054205941	-3.007401695	3.425008111
	C22	-2.513911073	1.563475966	7.014610071
	C23	-2.876978998	1.344763016	8.496838881
	C24	-3.498236587	2.518669359	6.297957604
	C25	-3.711727538	3.802296731	7.109546432
	C26	-2.999305090	2.855728921	4.887130179
	C27	-4.369310582	0.353564218	10.134243533
	C28	-3.239911668	-0.083655283	11.045010280
	C29	3.011232830	-11.721297979	5.810124988

C30	3.885603451	-10.575776277	5.299807245
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C33	3.427222106	-7.017687409	5.454050111
C34	4.105139191	-5.679141798	5.152609291
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C39	-4.783916296	-2.056801400	-3.021412681
C40	-5.161645325	-0.589811980	-2.767194584
C41	-3.328618782	-2.276259555	-2.557147909
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C44	-5.214250595	1.629861194	-3.854690072
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C48	-8.885511768	1.787512670	-1.299615299
C49	-7.664685700	1.320037463	0.780877282
C50	-6.628778549	2.292704986	1.351172914
C51	-4.625632670	3.668518201	0.999362094
C52	-5.209702210	5.009728132	1.465418400
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C54	-2.932922862	2.814396440	-0.694943736
C55	-2.799897856	1.505711784	-0.275417149
C56	-1.732823284	1.624114776	-2.135753410
C57	-6.729502403	6.819728430	0.789638051
C58	-7.232891011	7.064129263	2.211069279
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C62	-8.879251790	9.955723900	-1.939622788
C63	7.321784379	0.550821063	6.466132248
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C67	4.156051706	1.750734630	6.520040792
C68	5.171634449	2.183173052	4.377712615
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C71	3.411086174	3.625419285	5.185300139
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C73	5.652963644	7.622220658	-0.130144837
C74	5.544344281	5.251741187	0.713413199
C75	5.331305088	8.974853580	-2.156196378
C76	3.948992308	8.599883808	-2.695106863
C77	2.328779940	6.780579323	-3.107172851
C78	1.324462923	6.735441227	-1.933900914
C79	2.517883160	5.418639308	-3.799345475
C80	1.272770394	4.744437548	-4.383047855
C81	0.627108080	5.410519324	-5.609076040
C82	-0.588759911	7.593892125	-5.634420570
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C93	-3.179910494	13.470961602	1.869873609
C94	-3.850062449	11.140889137	1.195659626
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C121	-0.063992804	-1.339224172	-4.946841494
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H159	-5.927999519	-6.140709656	2.038980601
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H161	-7.286644045	-1.620222605	3.035366568
H162	-6.350178630	-5.993927345	3.764342403
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H166	-1.806518868	-3.749445378	3.728097670
H167	-1.106844780	-2.894202802	2.331382009
H168	-0.055650914	-3.405135572	3.666164625
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H176	7.057712669	0.904795132	7.480828446
H177	-3.710887900	3.531935721	4.391078364
H178	-4.402147820	4.469423458	6.573569801
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H181	-4.470917531	1.999834632	6.214065483
H182	-1.518224011	2.030134273	7.038229390
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H184	-0.434910337	0.374354026	4.074480895
H185	1.600554931	4.306368447	0.974947246
H186	0.472639996	5.072176733	2.135366218
H187	2.409644113	5.363844756	3.125402449
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H189	4.392414230	3.876100219	3.278050483
H190	5.861202359	1.906380353	3.576942791
H191	4.070278086	1.154356120	7.432055953
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H193	-3.314409250	-5.619309234	6.436313534
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H244	-0.096246213	5.988389004	0.066191922
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H253	1.398366835	10.025827747	-2.905290602
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H266	3.256018963	5.565791689	-4.605610199
H267	-2.122429265	7.447294122	-1.156061412
H268	-5.402869120	3.932993509	-4.590655876
H269	5.185166404	9.859883163	-1.521896939
H270	0.757335702	7.577256362	-7.191599061
H271	-1.873205085	9.178436907	-5.572241417
H272	-4.234345757	-3.081347625	-4.717666446
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H282	1.285312130	13.153089891	0.056952961
H283	2.925281937	9.714622125	2.242297684
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H293	4.727109563	5.494492347	1.407985917
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H295	6.987516143	2.560504419	-4.629247412
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C127	5.620187627	-8.576581822	-2.328423208
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O426	-6.096476125	1.472488843	7.095889635
O427	-4.969877261	-1.375023652	9.811794410
O428	-0.911731660	-2.501656441	7.842488643
O429	-0.140987763	1.568947034	6.924211849
O430	-2.004863984	4.136098270	8.705709124
O431	-2.967982580	3.133675026	11.904869331
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O434	9.257900409	-3.616587037	8.928068844
O435	-5.527584104	-0.456062114	-1.447744498
O436	-2.968368712	-5.206563501	-3.568045729
O437	-6.772900562	2.639666467	-4.123370119
O438	-4.594835711	2.452701855	-5.687536988
O439	-9.827878213	2.303167959	-1.089294032
O440	-6.605150266	3.349590778	1.962292108
O441	-4.524520327	6.212131398	1.033240872
O442	-6.944285544	8.770958062	0.887786084
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O444	2.814829865	5.686863275	3.645059954
O445	4.888892342	7.963746705	-1.592708552
O446	3.306090806	8.395418066	-5.364499702
O447	0.222068152	6.389896367	-3.748066777
O448	-0.092649726	8.086736295	-0.115925497
O449	2.579765306	6.050627866	0.749156729
O450	1.931275089	12.147899748	-0.800996153
O451	-0.853816777	13.699316255	-3.625595557
O452	-1.153912621	10.762322608	-5.551912253
O453	-3.848110524	14.352694659	-1.358367744
O454	-3.709399011	6.595321114	-4.817095993
O455	3.626575847	-6.721657263	-6.511645575
O456	2.060664462	-2.997444948	-7.762062433

	O457	4.465191579	1.358000245	-8.011720003
	O458	8.959483758	1.098538419	-7.014787251
	O459	-2.546327964	-4.737578777	-9.007864658
	O460	-0.360857363	-7.847120269	-4.271434415
	O461	1.762416410	-7.333210096	-4.725712464
	O462	-1.155729683	0.141055107	-9.442944730
	O463	9.813245453	-6.612442138	1.105089372
	O464	11.744740707	-7.947716311	3.694424774
	O465	-0.861637025	-6.047352714	1.024623422
	O466	-0.894179357	-7.800004115	2.392730599
	O467	4.090651123	-11.453588531	1.270650606
	O468	2.077180936	-11.281274761	0.265309482
	O469	4.485633885	-6.080084961	1.754925387
	O470	3.739098174	-7.372877680	3.444893735
	O471	2.325250299	-6.387484401	0.298030578
	O472	7.404994308	-6.431330867	5.322693701
	O473	6.190691949	-4.661434599	3.470307199
	O474	-2.644760192	4.190836794	-4.860680006
	O475	6.639929870	-10.975554326	2.956397011
	O476	5.912274811	-8.631659691	4.451060580
	S477	4.877709403	4.183567225	-2.053980460
	S478	3.142246444	0.978801351	-2.794360446
	S479	2.640827882	-4.130782502	-1.952167297
	S480	3.965164804	1.545570971	0.686560727
	S481	0.352859064	-2.408529780	-0.661033735
	S482	5.404071141	-2.197063733	-3.818266615
	S483	3.031385888	-3.352131742	1.569706840
	S484	6.582676624	0.679238295	-1.529053102
	S485	6.011687502	-4.108359124	-0.504338027
	S486	6.101033284	-1.218255589	1.884553125
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	Fe(139)	0.556	-2.402	
	Fe(140)	0.280	-0.423	
	Fe(141)	0.552	-2.625	
	Fe(142)	0.549	2.441	
	Fe(143)	0.590	3.103	
	Fe(144)	0.506	2.240	
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	C1	-7.791051514	-5.134675787	1.168980207
	C2	-7.856804699	-6.520676800	0.514222627
	C3	-8.984036306	-3.034373358	1.609806480
	C4	-8.761072045	-2.898172075	3.115025593
	C5	-9.012732291	-3.895439353	5.331588750
	C6	-7.539006778	-3.997649117	5.741423153
	C7	-5.316580106	-4.850089649	5.152354430
	C8	-4.565270377	-3.560691986	4.808522775
	C9	-4.319363408	-1.664365721	3.296602411
	C10	-4.608108772	-0.538532653	4.301161718
	C11	-6.202512375	0.526335332	5.793030913
	C12	-5.603587143	0.307732520	7.188609953
	C13	-5.334000751	-1.237381053	9.069020489
	C14	-3.866286606	-1.592225197	9.335005682
	C15	-1.850596170	-2.726688089	8.493163987
	C16	-0.747724931	-1.971018095	7.747334244
	C17	-0.272949437	-0.222177143	6.050383953
	C18	-0.315965870	1.266717162	6.438729309
	C19	-0.526140734	-0.484692643	4.540155671
	C20	0.306114918	0.441291010	3.647244587
	C21	-0.259433283	-1.955822283	4.200364823
	C22	-1.663945065	3.317397372	6.650182796
	C23	-1.795450297	3.503557450	8.175410970
	C24	-2.826642856	3.972147251	5.866797035
	C25	-3.066503504	5.412007665	6.336207856
	C26	-2.547809124	3.941366116	4.358133716
	C27	-2.925645257	2.913893232	10.240370818
	C28	-1.640885024	2.803950305	11.037012662
	C29	4.979481920	-9.412385697	8.172999232

C30	5.656359673	-8.409521135	7.238119389
C31	5.984918921	-5.957491963	6.877659488
C32	7.048833254	-5.308769065	7.784409685
C33	4.856958256	-4.966572530	6.538064590
C34	5.341502055	-3.737616496	5.765939241
C35	4.166839530	-2.947119123	5.193767567
C36	4.121538318	-0.573929302	4.399840428
C37	9.323193507	-4.411829351	7.902698713
C38	9.615156340	-2.974193270	7.531740981
C39	-4.911319549	-3.063456175	-1.537839798
C40	-5.337301839	-1.591983243	-1.675436761
C41	-3.393403829	-3.087531986	-1.248382833
C42	-2.815891370	-4.434896763	-0.769113961
C43	-2.338541038	-5.371404773	-1.876223739
C44	-5.859083058	0.164539852	-3.307828831
C45	-7.256028546	0.692994886	-2.953418127
C46	-5.533420745	0.446913340	-4.787585743
C47	-9.326722081	0.276167046	-1.712008168
C48	-9.108262089	0.815017023	-0.289220483
C49	-7.570576342	0.986911708	1.625567775
C50	-6.525093934	2.098545728	1.728787682
C51	-4.777999961	3.445328797	0.663893588
C52	-5.418805513	4.844267469	0.848658266
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C54	-3.088419472	2.405263687	-1.032211538
C55	-2.417597220	1.420425174	-0.346669601
C56	-1.853070741	1.243952930	-2.485868418
C57	-7.226593592	6.319139830	0.026775609
C58	-7.537773449	6.915715819	1.397395995
C59	-8.521205998	6.111460432	-0.794779327
C60	-9.089475542	7.327906694	-1.465882788
C61	-9.236408883	8.625025913	-1.012892468
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C63	8.039619111	2.804843087	4.824459046
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C65	6.683159223	2.169858713	4.416409058
C66	5.633095751	3.194265212	4.056480675
C67	4.784256899	3.742650446	5.035333811
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C76	2.624528670	7.730603423	-5.497082725
C77	1.153956713	5.774904198	-5.137645406
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C79	1.387044081	4.292725558	-5.483901740
C80	0.152230242	3.397607389	-5.633945327
C81	-0.746639963	3.640864182	-6.858966430
C82	-2.165187167	5.657171196	-7.269495379
C83	0.290059676	6.189372017	-1.420094286
C84	0.079859382	7.679605115	-1.084018424
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C86	1.115935992	9.895865958	-1.051528587
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C90	-0.740103961	11.419245799	-5.273243534

C91	-1.661436775	10.236203956	-5.547052112
C92	-4.187344108	11.922164346	-2.080005269
C93	-4.271744014	13.234361267	-1.309184488
C94	-4.784299416	10.771847059	-1.224853449
C95	-4.864576949	9.473883246	-1.993759701
C96	-5.961772109	9.205733071	-2.826621331
C97	-3.821960476	8.532890768	-1.944958342
C98	-6.009564232	8.050530061	-3.609375246
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C113	0.436718804	-7.656681248	-4.877551240
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C118	-1.485571625	-0.636738526	-5.936411923
C119	-1.747859390	-2.863445728	-5.032531313
C120	-0.373565032	-0.443251603	-5.110129526
C121	-0.637090119	-2.665872671	-4.205159079
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C124	9.588796455	-6.590643112	-0.078383441
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C126	6.135958591	-7.231140991	-1.817233042
C127	6.029440007	-8.130939419	-2.857827380
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C132	2.029491825	-6.202903200	2.411254659
C133	3.101587511	-6.743118138	1.384288235
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C135	4.164799757	-8.918727906	0.504475837
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Fe139	4.546336578	-2.686374138	-2.418722061
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Fe143	3.915008565	2.332879927	-1.960578050
Fe144	5.137144983	-2.106649098	0.037806686
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H147	-5.991740734	-6.695969447	-0.303851757
H148	-9.719024265	-4.744455150	0.556407730
H149	-8.356321150	-6.430202065	-0.463693410
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H151	-8.215213924	-2.415071960	1.126473453

H152	-9.685380803	-4.699687950	3.451695111
H153	-9.968212549	-2.610615899	1.367741539
H154	-9.562366114	-4.738780693	5.769577183
H155	-7.128178752	-5.088944299	4.051478271
H156	-9.400345194	-2.965804173	5.769161502
H157	-3.227290424	-1.758196657	3.232273565
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H160	-5.848166130	1.501158479	5.436937696
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H162	-5.109313880	-5.070762785	6.206209850
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H164	-6.188708662	-1.678693524	7.163951758
H165	-7.296992553	0.565537153	5.880903060
H166	-0.875695043	-2.633078642	4.809132969
H167	-0.493100461	-2.148271248	3.142016335
H168	0.799925127	-2.214587572	4.357849716
H169	-1.591400237	-0.274020647	4.353116994
H170	-5.944869132	-2.083767494	9.416298645
H171	-2.430514466	2.917363555	3.976227458
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H173	-3.340840835	5.464028469	7.399477174
H174	0.039330348	0.285888271	2.591152030
H175	1.379209759	0.227412566	3.736288515
H176	7.869790283	3.417464857	5.731124660
H177	-3.376112237	4.415915845	3.811817887
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H183	-2.295429802	1.427210159	5.840915919
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H185	1.234515806	4.479583136	-0.487880279
H186	0.225122013	5.491527487	0.599575197
H187	2.249439877	6.141637265	1.136960472
H188	2.215677890	6.329168633	3.753906586
H189	4.401737974	4.912921204	1.351444250
H190	6.093531647	3.195306747	1.940114404
H191	4.875784299	3.417890532	6.075492308
H192	-2.175669360	-0.887421956	6.780645894
H193	-1.801664656	-3.774953177	8.163219234
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H195	-3.702938794	-2.504096184	7.474481716
H196	-5.562330061	-0.367459290	9.698201644
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H199	-3.406524382	3.878609753	10.469712755
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H202	10.236751418	-5.012693095	7.781263684
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H206	0.793059084	-7.692828290	-7.003399359
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H208	-1.466236714	-1.857969160	-9.949719459
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H210	-2.859711311	-2.750860701	-2.151178561
H211	-3.569831605	-4.983635874	-0.177558271
H212	-0.764411055	-3.484115549	-8.021263477

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H214	0.665973280	-5.033487685	-8.514400921
H215	-0.695321649	-5.944170356	-0.741849984
H216	-0.256633648	-5.427504829	-6.175388433
H217	0.699691051	-6.623199874	-8.941458198
H218	-6.138103231	-4.314130290	-2.635110034
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H221	-1.981637809	-4.237585129	-0.081290122
H222	-4.114290881	3.295616764	1.527547726
H223	-2.406917084	1.163892961	0.706937352
H224	-8.487156927	1.376860116	2.087478132
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H226	-7.035793338	4.197891596	-0.226954613
H227	-8.957863217	9.112936684	-0.085090375
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H236	-5.742485337	1.696419481	-0.141216167
H237	-7.235595983	0.140459142	2.243992861
H238	-9.796630047	1.080392943	-2.291232205
H239	-1.391577412	0.884834521	-3.401169624
H240	-10.038126090	-0.558779512	-1.660206140
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C58	-7.567223745	6.629732654	2.210251236
C59	-8.007239683	6.825645286	-0.270938981
C60	-8.370589499	8.261332791	-0.525691326
C61	-8.624621233	9.298863147	0.350838401
C62	-8.839265050	9.987449472	-1.744055877
C63	6.643569136	-0.057242659	7.205759915
C64	7.425033084	-1.353237032	7.317575869
C65	5.433278155	-0.345188018	6.278546744
C66	4.514468976	0.843467763	6.126905158
C67	3.451752119	1.057930906	7.024718971
C68	4.699577710	1.778106766	5.092556272
C69	2.601237215	2.161482590	6.896736439
C70	3.866482428	2.890102805	4.958318841
C71	2.815065439	3.079174861	5.860501155
C72	6.202963288	6.443500315	1.857160553
C73	5.446180471	7.627467281	1.244450609
C74	5.320406999	5.189854146	1.820395076
C75	5.304470535	9.201664773	-0.636841709
C76	3.987151736	8.878557072	-1.345251583
C77	2.442501971	7.107088023	-2.110886787
C78	1.329416420	6.908292958	-1.061302261
C79	2.725678399	5.841053493	-2.942922730
C80	1.546748646	5.191456710	-3.676095311
C81	0.972524632	5.945003212	-4.888336540
C82	-0.242870908	8.124135636	-4.789568666
C83	0.686507774	6.206839220	1.181770090
C84	0.427816924	7.486778335	2.005228490
C85	1.018957371	5.064627984	2.153788424
C86	1.466177885	9.408126737	3.108514224
C87	1.070081244	10.836272133	2.745997978
C88	0.347117700	12.416769853	1.003823770
C89	-1.099927200	12.895424469	1.253967071

C90	0.731756022	12.583243660	-0.484244511
C91	-0.109413840	11.693025985	-1.389757572
C92	-3.406702642	12.231803135	1.781209365
C93	-3.652236373	13.165961513	2.959508804
C94	-4.197325741	10.911640852	1.979888474
C95	-4.106894646	10.006454949	0.772567514
C96	-4.971240451	10.192719332	-0.318604647
C97	-3.125837841	9.006378821	0.678657722
C98	-4.851477969	9.421849580	-1.477499416
C99	-2.974029088	8.242481947	-0.483959725
C100	-3.838977330	8.464664019	-1.553294372
C101	7.048775768	-3.592505077	-7.205991320
C102	5.570472959	-3.245237465	-7.227125917
C103	3.837205072	-1.717427478	-6.311079834
C104	3.643000748	-0.305050984	-6.871056613
C105	4.061882383	2.076451899	-6.481536557
C106	5.196429175	2.999178089	-6.047565993
C107	7.204298942	3.373013197	-4.695981743
C108	8.516528997	3.266549805	-5.447053228
C109	0.893174465	-2.500757589	-9.797318640
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C113	1.556355754	-5.308291716	-7.218317630
C114	-0.565942463	0.954871797	-9.045758377
C115	0.188569749	2.240677380	-9.319550132
C116	-1.422103439	0.961648284	-7.756768377
C117	-0.616833676	0.700358035	-6.507840382
C118	0.098328044	1.728698203	-5.872092303
C119	-0.506173698	-0.604724129	-5.997172598
C120	0.920402250	1.445748072	-4.775749170
C121	0.312582181	-0.885892859	-4.898547586
C122	1.040720578	0.139895792	-4.288185355
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C124	9.203003098	-7.044077594	-0.445745286
C125	7.033600931	-7.050061984	-1.798078855
C126	6.262506482	-6.605265307	-3.005390596
C127	6.422623961	-7.040351619	-4.305840139
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C132	1.220692490	-6.810083531	0.209772186
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C134	2.447647123	-8.440463671	-1.339912058
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C136	3.811649394	-10.271195419	-2.477554825
C137	3.716981260	-7.060229107	0.322590243
C138	4.254959669	-0.936616930	-0.725831986
Fe139	4.913558106	-2.067311221	-2.194257309
Fe140	3.006792333	0.473587893	-0.316558307
Fe141	5.212617777	0.035500489	0.799815554
Fe142	5.084360644	0.503477986	-1.804210662
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Fe144	4.841088676	-2.478225241	0.379514971
Fe145	2.606271365	-2.057712319	-0.905075672
H146	-6.256962157	-6.463102932	-3.031387593
H147	-5.789759325	-5.426985718	-4.204867005
H148	-9.545658774	-3.503210364	-3.534594303
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H152	-10.284291194	-4.560403573	-0.911023161
H153	-9.990069305	-1.828203145	-2.032520340
H154	-10.769425913	-5.453236027	1.181593406
H155	-7.974151473	-5.422541951	0.055210621
H156	-10.560912439	-3.833677943	1.892757710
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H158	-6.228824127	-3.637125316	0.160520415
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H162	-6.566823027	-6.444180536	2.445547216
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H164	-7.797548918	-3.547341442	4.371859873
H165	-8.539639190	-0.898725173	3.834639388
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H167	-1.247745384	-3.116950301	1.863231643
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H173	-4.990588163	2.675277316	7.966154666
H174	-0.584679450	-0.708746243	2.409195769
H175	0.432809830	-1.330272266	3.708228329
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H177	-4.201886537	3.021433185	4.337874422
H178	-5.108973091	3.706374821	6.520768003
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H182	-2.247270677	1.261062177	7.007091755
H183	-3.658175672	-0.612443011	5.254169135
H184	-0.774767092	-0.068128809	4.051790653
H185	1.336167615	4.183002717	1.568469465
H186	0.092810379	4.814623302	2.695084878
H187	1.936429299	4.976978773	3.892995879
H188	1.281494893	4.175916898	6.321137901
H189	4.007534816	3.590792265	4.134182768
H190	5.489161404	1.618322538	4.354936263
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H193	-3.795725630	-6.287412634	5.435173247
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H207	-0.300395351	-3.414139423	-8.205598854
H208	1.038729654	2.126610789	-10.033991006
H209	0.524777210	-3.143791788	-10.611759582
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H224	-8.692045244	1.386040921	0.490517844
H225	-6.898270142	0.841829930	-1.833633752
H226	-6.724631773	4.678526064	-0.163636454
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H232	-2.980669171	4.614233232	0.450162302
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H234	-9.143395905	11.321220815	-0.113232112
H235	-7.606080588	6.437978866	-1.221533527
H236	-5.482976763	2.227634054	-0.776102981
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H238	-8.868554717	2.919753144	-3.808125165
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H250	-4.668863220	2.568806798	-6.327062103
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H254	-0.097441043	9.851603937	-2.273683316
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H257	-5.542046605	9.569218737	-2.311361265
H258	-2.456256095	8.801908335	1.520148671
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H260	3.162790097	5.076713352	-2.280025281
H261	4.304424369	6.858202127	-1.088526924
H262	0.733038581	4.952312201	-2.972664255
H263	-7.016899392	0.637777565	-4.257562038
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H265	-4.473992831	0.086304022	-5.254669439
H266	3.508436396	6.101079011	-3.675441740
H267	-2.161870192	7.517988776	-0.567982942
H268	-5.029284884	4.376916102	-4.710846817
H269	5.086078478	10.016622962	0.068071698
H270	1.261402813	8.267883050	-6.188170748
H271	-1.518368252	9.714684054	-4.677944352
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H274	-5.754760954	10.951575138	-0.265437192
H275	-4.326433346	2.288795565	-3.288505913
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H278	1.921230262	4.226848392	-4.045146135
H279	-0.962342473	6.363522432	-4.082786283
H280	0.795112132	9.094172958	3.921980048
H281	0.680498756	10.294480059	0.803385882
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H300	3.137271107	-0.582487770	4.555925866
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H339	1.618622554	-8.453514615	-2.061474895
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H343	1.268723461	-5.772053698	0.563156929
H344	6.842184955	-8.346545654	3.102827551
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H350	6.869613319	4.420371658	-4.767950985
H351	4.881366741	-1.193059716	6.711954024
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H354	9.311214142	-8.320507179	-2.779385585
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H362	6.635015020	-5.766044966	7.429261648
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H366	-4.364891578	7.907258900	-3.345827858
H367	2.084766568	-0.808569264	0.101651422
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	C5	-9.913591633	-3.388025942	3.894963010
	C6	-8.525171313	-3.622377119	4.499474053
	C7	-6.299916719	-4.596182787	4.171570995
	C8	-5.428963309	-3.348356202	3.991748805
	C9	-4.856716551	-1.424419065	2.607788953
	C10	-5.194785374	-0.315238801	3.615689705
	C11	-6.899625383	0.826291521	4.917295304
	C12	-6.519577868	0.506857360	6.368924893
	C13	-6.624986515	-1.128322491	8.190393385
	C14	-5.242822716	-1.614869157	8.641945402
	C15	-3.196077100	-2.835793086	8.031191040
	C16	-1.952258411	-2.128709725	7.486079025
	C17	-1.119651470	-0.380389401	5.931946227
	C18	-1.110217912	1.095687784	6.370319602
	C19	-1.181350092	-0.578944282	4.392433693
	C20	-0.181315158	0.317406384	3.653957436
	C21	-0.962131929	-2.054667660	4.037388489
	C22	-2.332397424	3.232071753	6.483897412
	C23	-2.661922045	3.379072078	7.981140933
	C24	-3.333010309	3.992602530	5.579855929
	C25	-3.538105895	5.431273589	6.069632065
	C26	-2.863310918	3.988389002	4.119293035
	C27	-4.118750652	2.813844015	9.836361289

C28	-2.986241505	2.587279808	10.818728868
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C30	4.002602296	-9.003763660	7.580396035
C31	4.556401961	-6.575729244	7.362142829
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C33	3.550714620	-5.510391309	6.890940508
C34	4.214146704	-4.280657453	6.266948497
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C37	7.817970294	-5.311447870	8.891438903
C38	8.243363364	-3.889815501	8.592956083
C39	-4.857955297	-2.608923215	-2.330485332
C40	-5.171187432	-1.103922672	-2.412752996
C41	-3.398817390	-2.755341257	-1.841891261
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C43	-2.444487875	-5.103799640	-2.406021750
C44	-5.211375408	0.826775411	-3.964699475
C45	-6.563792364	1.472355113	-3.636251615
C46	-4.764998220	1.044238097	-5.436203901
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C48	-8.886308089	1.478872947	-1.517724494
C49	-7.647765092	1.485464623	0.606542612
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C51	-4.600918505	3.791842935	0.144362579
C52	-5.196589773	5.203358245	0.310043303
C53	-3.643862583	3.887029391	-1.054227984
C54	-2.816645413	2.683715006	-1.384287086
C55	-2.388727375	1.624133790	-0.611774308
C56	-1.547874373	1.452762767	-2.650285254
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C58	-7.189306809	7.392152000	0.614281309
C59	-7.910038198	6.752473222	-1.718652847
C60	-8.294627843	8.033743764	-2.398390564
C61	-8.398406340	9.324036108	-1.914854065
C62	-8.918580247	9.262112362	-4.068538226
C63	7.463563692	2.062806339	5.966603085
C64	8.254546165	0.850966150	6.422054566
C65	6.142187351	1.534009824	5.351000950
C66	5.222633902	2.643817643	4.898967693
C67	4.299890646	3.230347866	5.783789991
C68	5.271020419	3.131596438	3.579881237
C69	3.455015486	4.266517391	5.372470417
C70	4.444312949	4.173880678	3.158914116
C71	3.534601165	4.738720011	4.056627255
C72	6.433649529	6.359071807	-1.204319645
C73	5.629698435	7.313285838	-2.097730569
C74	5.531290596	5.224980940	-0.696075714
C75	5.280241792	8.159867341	-4.382812584
C76	3.880464255	7.692272438	-4.787621481
C77	2.231992772	5.847836260	-4.707747253
C78	1.256746221	6.102095717	-3.535898445
C79	2.402409502	4.355917563	-5.048026562
C80	1.142783507	3.553447365	-5.384448179
C81	0.438900291	3.888152308	-6.710401899
C82	-0.794033178	5.995663514	-7.219210015
C83	0.885573192	6.201775409	-1.128659170
C84	0.749967006	7.691386459	-0.757409250
C85	1.333427724	5.432801639	0.122616202
C86	1.931000402	9.818130442	-0.510029844
C87	1.515351830	11.052359896	-1.305105200
C88	0.578438008	11.967584135	-3.385692815

C89	-0.816818752	12.581279336	-3.144426674
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C91	-0.191409627	10.493853998	-5.309476436
C92	-3.054482589	12.254980343	-2.190819614
C93	-3.138856964	13.537995004	-1.373614218
C94	-3.841545042	11.126141120	-1.474797629
C95	-3.893335596	9.854279143	-2.290407854
C96	-4.873094728	9.677180471	-3.278377778
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C98	-4.890343600	8.535849743	-4.082885078
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C138	4.093279942	-1.363764210	-0.836977007
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Fe141	5.162801067	0.031456941	0.107221449
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H167	-1.026644223	-2.201035695	2.948245805
H168	0.037630418	-2.391287974	4.354788015
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H175	0.856546358	0.029013130	3.871648100
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H177	-3.594734449	4.514640150	3.488272659
H178	-4.236007603	5.956034296	5.401116105
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H184	-0.306357205	1.381051163	3.907014154
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H186	0.486120272	5.432324331	0.825148517
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H289	6.153845494	4.530884839	-0.116169054
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H291	6.685396395	6.680751064	-3.745429313
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C130	11.164320674	-8.469462100	-0.105523635
C131	-0.042486168	-7.005117147	1.069722301
C132	1.391494967	-6.636423280	1.350094571
C133	2.390077399	-7.088371495	0.209971910
C134	2.168095835	-8.600588985	-0.086816518
C135	3.209163344	-9.185469265	-1.054715625
C136	3.171572083	-10.685691205	-1.142020771
C137	3.826473286	-6.957032253	0.804576545
C138	3.874713726	-1.240767523	-1.717870148
Fe139	4.121530580	-2.706702184	-2.990565422
Fe140	2.708837873	0.284955274	-1.496008130
Fe141	5.168145896	0.023691779	-0.739783447
Fe142	4.544697883	-0.162739968	-3.257925770
Fe143	4.355417160	2.234959229	-2.153078764
Fe144	4.760878876	-2.500480006	-0.443910349
Fe145	2.319139920	-2.348314759	-1.174426533
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H188	2.913715977	5.345768635	4.565118698
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O440	-5.922868567	2.730066745	3.484339557
O441	-4.290851892	5.910280677	2.509739653
O442	-6.601709830	8.397597048	3.155600455
O443	9.455608094	-0.600299932	5.978260871
O444	3.389447609	5.156556582	3.735572391
O445	4.582970469	8.156255077	-1.404720670
O446	2.374611331	9.071200099	-4.731139236
O447	-0.375518538	6.911968552	-2.914346323
O448	-0.053186293	8.052816030	0.917692427
O449	2.668455943	5.886920920	1.012632504
O450	1.833441649	12.185023255	0.414187795
O451	-1.381355912	14.045247602	-1.653199284
O452	-2.053776572	11.360201266	-3.831541813
O453	-3.989658901	14.330476819	1.103466953
O454	-4.471047071	6.990153540	-3.161862754

	O455	2.367476486	-5.805090051	-7.774608146
	O456	0.682320607	-1.968733489	-8.299604378
	O457	2.976106851	2.461046643	-8.379020981
	O458	7.578965490	2.164119815	-8.360337343
	O459	-4.121592750	-3.628623994	-8.989851192
	O460	-1.214858315	-7.202813435	-5.055355115
	O461	0.809536586	-6.607973999	-5.780193401
	O462	-2.713009579	1.283871221	-8.954899639
	O463	9.779638231	-6.536131430	-1.443656807
	O464	12.112101395	-8.162185353	0.604247431
	O465	-0.815983099	-6.402346479	0.343982680
	O466	-0.503938222	-8.142990333	1.694217974
	O467	4.099797975	-11.442636310	-0.863355792
	O468	1.974966124	-11.162014645	-1.574580541
	O469	4.603327624	-6.125613841	0.194353626
	O470	4.174890592	-7.668250034	1.776674123
	O471	2.230918164	-6.303839584	-0.915603445
	O472	8.151607903	-6.934286824	3.086307095
	O473	6.623238788	-4.955040980	1.737951540
	O474	-3.551655575	4.588877486	-3.714582445
	O475	6.917041139	-11.158770685	0.359117471
	O476	6.502102568	-9.022902323	2.222602109
	S477	4.491137115	4.501744981	-2.364340580
	S478	2.830026113	1.304955035	-3.479319564
	S479	2.151815250	-3.743098123	-2.900751918
	S480	3.682966864	1.609683815	-0.066669496
	S481	-0.006973393	-2.351087569	-0.793104492
	S482	4.737463189	-1.678365635	-4.883618179
	S483	3.028836018	-3.416403836	0.608465664
	S484	6.276330925	1.030928306	-2.494566325
	S485	5.734594886	-3.875510802	-1.909183726
	S486	6.183165105	-1.293977400	0.752424051
	13u(b)			
	Fe(139)	0.563	2.411	
	Fe(140)	0.315	-1.561	
	Fe(141)	0.559	2.751	
	Fe(142)	0.526	-2.430	
	Fe(143)	0.552	2.838	
	Fe(144)	0.509	-2.197	
	Fe(145)	0.479	2.041	
	S=2			
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	C1	-8.200539513	-4.461423698	0.760378057
	C2	-8.430868289	-5.701477891	-0.112762899
	C3	-9.137375336	-2.324252553	1.543058286
	C4	-8.900615788	-2.465767828	3.044283533
	C5	-9.208866059	-3.794007006	5.067372702
	C6	-7.748518759	-4.118659332	5.401579162
	C7	-5.629793418	-5.042700002	4.588063238
	C8	-4.759369553	-3.790253405	4.439298834
	C9	-4.343710616	-1.701202055	3.255176774
	C10	-4.503178295	-0.737376578	4.440714231
	C11	-5.976416063	0.224932883	6.115754765
	C12	-5.377846188	-0.282502823	7.433424495
	C13	-5.195816931	-2.148850819	9.007965929
	C14	-3.754756750	-2.651230724	9.155881293
	C15	-1.849967277	-3.763886341	8.071342099
	C16	-0.707584023	-3.004912904	7.392715949
	C17	-0.108712651	-1.117117358	5.898959030
	C18	0.023443734	0.295017284	6.496900944
	C19	-0.433994043	-1.130035406	4.382370937
	C20	0.454551479	-0.162753330	3.591197501
	C21	-0.324484898	-2.553686283	3.824707299
	C22	-1.124355939	2.396277741	7.100532004
	C23	-1.214649797	2.337812461	8.638603926
	C24	-2.239771748	3.265186310	6.469822147
	C25	-2.339634809	4.626072262	7.169985353
	C26	-1.999886046	3.448637233	4.966454052
	C27	-2.369428549	1.527044285	10.612262990

C28	-1.079026965	1.220924759	11.343945211
C29	4.272374037	-10.945090170	6.389929122
C30	5.026609798	-9.876957934	5.598860019
C31	5.587175089	-7.438909380	5.589829432
C32	6.732497925	-7.021268830	6.532618188
C33	4.536560242	-6.324007666	5.437137518
C34	5.096701881	-5.012042675	4.880032259
C35	3.965188729	-4.089793810	4.426820695
C36	4.113834252	-1.608476048	4.147528891
C37	9.093916783	-6.383252046	6.672944476
C38	9.468259847	-4.923857658	6.511185780
C39	-5.226117373	-2.282043926	-1.817566592
C40	-5.495457978	-0.780434290	-1.639509565
C41	-3.728587328	-2.532950948	-1.552945087
C42	-3.321802818	-4.000007596	-1.303233880
C43	-2.969222065	-4.804093716	-2.549940204
C44	-5.664747666	1.358306957	-2.877635001
C45	-6.856128149	1.976804367	-2.144848984
C46	-5.610987847	1.777131172	-4.370123911
C47	-9.131265996	1.626574026	-1.293834477
C48	-8.888195544	1.785578122	0.213871251
C49	-7.359425935	1.407950339	2.097290421
C50	-6.183109069	2.361249030	2.327596069
C51	-4.405714566	3.752877422	1.374307520
C52	-4.919903540	5.154385913	1.763921522
C53	-3.618736345	3.929140077	0.064363461
C54	-2.871455928	2.749627239	-0.481889854
C55	-2.326785471	1.633641707	0.121053294
C56	-1.866073332	1.617101956	-2.042080206
C57	-6.571235212	6.892286826	1.242934939
C58	-6.714361471	7.272509592	2.715254213
C59	-7.944826445	6.956886413	0.534469471
C60	-8.395544234	8.319491794	0.096832457
C61	-8.370454689	9.533328325	0.757135576
C62	-9.251821555	9.771274762	-1.262553829
C63	8.458131508	1.251256772	4.769888478
C64	9.294380125	-0.006975714	4.915898609
C65	7.044661823	0.804769663	4.316872439
C66	6.077745417	1.958162883	4.185711559
C67	5.340738819	2.423371227	5.290655711
C68	5.885922053	2.597862544	2.947535081
C69	4.437051674	3.484054578	5.166228953
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C73	5.387796150	7.506341130	-2.095724201
C74	5.513901872	5.246317977	-1.018582091
C75	4.656729641	8.631218464	-4.158962542
C76	3.201466594	8.209425207	-4.374651358
C77	1.551231488	6.372791236	-4.267072446
C78	0.800204437	6.512264406	-2.926038831
C79	1.599134976	4.921203293	-4.776778235
C80	0.260896026	4.187399105	-4.929178340
C81	-0.659690617	4.653157700	-6.072185076
C82	-1.874213787	6.829978997	-6.111583895
C83	0.817607941	6.305309017	-0.499592051
C84	0.793812824	7.737510198	0.069286360
C85	1.416246454	5.369143802	0.557557448
C86	2.068194175	9.802752581	0.374569261
C87	1.537381890	11.129391581	-0.161455319
C88	0.288753211	12.311591260	-1.921543632

C89	-1.030059835	12.888137638	-1.365824100
C90	0.202229595	12.131850861	-3.453257552
C91	-0.843748127	11.092153211	-3.844740685
C92	-3.085722426	12.440515172	-0.104907185
C93	-3.024180784	13.629005444	0.846036676
C94	-3.761306972	11.233488590	0.599411533
C95	-3.990563282	10.073845716	-0.342331735
C96	-5.134099560	10.030470524	-1.153041847
C97	-3.043063827	9.045714584	-0.475644869
C98	-5.325920896	9.003712675	-2.081005072
C99	-3.206905969	8.023805734	-1.414142893
C100	-4.350405616	8.014348241	-2.209326644
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C103	1.899337713	-3.220728144	-6.592149216
C104	1.517632490	-1.955875793	-7.366293849
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C107	5.473184047	1.947326375	-7.224373221
C108	6.480316608	1.640940828	-8.313458674
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C111	-1.663776786	-5.105779667	-7.404132935
C112	-1.034032998	-6.511013532	-7.365698589
C113	-0.506911961	-6.820872745	-5.983969888
C114	-3.206181759	-1.050020330	-8.494052201
C115	-2.588609260	0.108519134	-9.254554620
C116	-3.633901027	-0.725845183	-7.042166240
C117	-2.490884513	-0.754526894	-6.056995493
C118	-1.626714876	0.344693611	-5.910262209
C119	-2.233054301	-1.912077264	-5.302157561
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C121	-1.131333861	-1.982960723	-4.442388883
C122	-0.267414940	-0.891261389	-4.318321807
C123	7.792808563	-7.252666470	-2.641789291
C124	8.837339420	-7.348717612	-1.518170137
C125	6.369544446	-7.571384695	-2.153014081
C126	5.273116717	-7.350839519	-3.151363206
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C128	3.386766753	-6.629659951	-3.986221797
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C131	-0.041736686	-7.000658326	1.074123445
C132	1.391558220	-6.631667590	1.356050443
C133	2.387268653	-7.094679102	0.216033515
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C135	3.201760441	-9.182293638	-1.051645311
C136	3.167637169	-10.681154413	-1.144215104
C137	3.827831075	-6.965572219	0.802212371
C138	3.874648269	-1.246429938	-1.721809579
Fe139	4.187057492	-2.700518288	-3.000160683
Fe140	2.658641017	0.331664398	-1.504499733
Fe141	5.114130082	0.007661253	-0.751329423
Fe142	4.467868653	-0.140100328	-3.270791753
Fe143	4.337826181	2.261693219	-2.159125619
Fe144	4.795291459	-2.503539809	-0.493740820
Fe145	2.278115909	-2.315679859	-1.121203996
H146	-6.743012880	-6.696003648	0.447964524
H147	-6.613102382	-5.962348677	-1.004494683
H148	-10.037682878	-3.725470783	0.206318478
H149	-8.916699147	-5.392962935	-1.052007994

H150	-9.168830951	-6.329011410	0.417548527
H151	-8.309267097	-1.715938357	1.152688622
H152	-9.988587372	-4.207324610	3.102846471
H153	-10.071209088	-1.767013654	1.389142642
H154	-9.837359434	-4.637474441	5.383776665
H155	-7.459523445	-4.868528185	3.511130875
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H157	-3.270020131	-1.901633455	3.150220431
H158	-5.806385083	-3.206285726	2.756140627
H159	-5.332410915	-5.783768140	3.833935216
H160	-5.546322528	1.215263688	5.918489488
H161	-6.528147174	-1.153906927	4.560359520
H162	-5.427623299	-5.457297104	5.583066873
H163	-4.693292139	-1.218561489	2.330628838
H164	-6.133983953	-2.181355805	7.092133259
H165	-7.062204590	0.333305946	6.242819791
H166	-0.982961929	-3.253835739	4.358824005
H167	-0.603495387	-2.570722956	2.760244933
H168	0.709138454	-2.926991843	3.898017593
H169	-1.477564372	-0.793601164	4.274291777
H170	-5.864526790	-2.994994579	9.224087983
H171	-1.986735414	2.489347712	4.430504077
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H173	-2.607559300	4.529248521	8.232663167
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H176	8.361894482	1.705426271	5.775306745
H177	-2.795055884	4.068869503	4.528511435
H178	-3.108731848	5.241584205	6.680609906
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H181	-3.199582653	2.735662067	6.611090216
H182	-0.147811399	2.861347016	6.898603325
H183	-1.956712826	0.710752800	6.057286570
H184	0.386185105	0.869477068	3.965417787
H185	1.534149577	4.361620218	0.118797291
H186	0.695126458	5.311858877	1.388397948
H187	2.817003209	5.574269010	1.924197265
H188	2.908536879	5.333717335	4.556829174
H189	4.837986278	4.134660860	1.839068179
H190	6.417498024	2.235545739	2.065061806
H191	5.466999462	1.945638347	6.266398180
H192	-2.055729096	-1.708985426	6.573245369
H193	-1.895128483	-4.755466313	7.595730528
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H196	-5.340720551	-1.390193362	9.787373521
H197	3.856120843	3.820879857	6.029458007
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H202	9.956108437	-7.010773790	6.400432991
H203	-1.583200481	-6.132118244	-3.268462538
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H206	-0.221365030	-6.582711091	-8.103357354
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H209	-2.485613817	-5.437722787	-9.366086257
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H214	-0.090360535	-3.725093132	-9.175920963
H215	-1.274967725	-5.575896725	-1.626809279
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H217	-0.219738210	-5.223539807	-9.838770846
H218	-6.594652411	-3.050206728	-3.156718325
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H220	1.279005679	-6.275349327	-6.609314879
H221	-2.457453793	-4.004365606	-0.624460630
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H223	-2.333742351	1.288888372	1.149327571
H224	-8.214812177	1.814256355	2.651542832
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H226	-6.553669813	4.863086755	0.547099055
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H231	-9.705374024	10.258518117	-2.121730512
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H233	-4.318554585	4.273133228	-0.714339213
H234	-9.034352712	11.438816945	0.044316017
H235	-7.880708914	6.344849189	-0.378106621
H236	-5.800471621	2.528864624	0.296977672
H237	-7.103493452	0.447424615	2.566321479
H238	-9.520124176	2.594031300	-1.642076798
H239	-1.468755980	1.275615368	-2.992268154
H240	-9.927016748	0.882425303	-1.435426248
H241	9.892824743	2.588394326	4.178599734
H242	8.425813018	2.866898752	3.512009911
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H244	-0.236267930	6.023003944	-0.642009433
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H246	-3.142458940	3.955979971	-3.026875195
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H248	-3.882831314	5.364417495	-3.208910307
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H253	0.632344827	9.639981794	-4.259299292
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C75	5.053584165	8.110887566	-4.690546641
C76	3.598345912	7.707060056	-4.943098299
C77	1.892485196	5.928291882	-4.718207642
C78	1.063718363	6.166334313	-3.435583658
C79	1.961148796	4.446816458	-5.134303274
C80	0.640506587	3.711253328	-5.378491245
C81	-0.181608740	4.133958666	-6.605685788
C82	-1.345106626	6.323001432	-6.905452452
C83	0.978877602	6.219493164	-1.000419563
C84	0.956256742	7.701774471	-0.581462936
C85	1.530741784	5.396798554	0.172931704
C86	2.276607398	9.752432470	-0.396626854
C87	1.817489679	11.033475181	-1.087432301
C88	0.690536127	12.060573379	-3.018391499

C89	-0.641965116	12.708826035	-2.584784016
C90	0.680337086	11.735846965	-4.528238692
C91	-0.364015644	10.679625450	-4.874203794
C92	-2.745607181	12.428163648	-1.351766265
C93	-2.682815982	13.682320110	-0.489513003
C94	-3.480625667	11.297965632	-0.583359185
C95	-3.706296293	10.078153820	-1.447212957
C96	-4.803933461	10.019005153	-2.319027089
C97	-2.798633944	9.005521648	-1.446706808
C98	-4.984541752	8.935541852	-3.183099100
C99	-2.948126617	7.925297885	-2.321943968
C100	-4.042331407	7.904894640	-3.184927082
C101	5.003571603	-6.178072568	-7.204995538
C102	3.568119590	-5.733158406	-6.977336214
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C104	1.810402752	-2.664566557	-7.125852302
C105	2.334029688	-0.312984786	-7.572848352
C106	3.558796143	0.582116097	-7.741125419
C107	5.832497385	1.183507929	-7.064752053
C108	6.907801295	0.703527906	-8.019149677
C109	-1.606739287	-5.406384814	-8.480690145
C110	-2.548787139	-4.202729713	-8.605086836
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C113	-0.336122945	-7.369101084	-5.390089351
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C116	-3.374727778	-1.308131678	-7.148148267
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C119	-1.970692344	-2.324122362	-5.319345141
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C122	-0.018682575	-1.192425983	-4.451952365
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C125	6.323464411	-7.909310056	-1.161301189
C126	5.272729222	-7.743032120	-2.217747065
C127	5.057363106	-8.548741720	-3.318809883
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C129	9.551230861	-8.656586344	1.642485538
C130	10.993618269	-8.670781660	1.187671454
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C135	3.065480223	-9.297231225	-0.026203752
C136	3.003436838	-10.797363141	0.017769859
C137	3.702055107	-6.949484855	1.641727150
C138	3.918935885	-1.499356042	-1.392528136
Fe139	4.288471332	-3.043412004	-2.567685112
Fe140	2.404426825	-0.095287201	-1.055255905
Fe141	5.027528270	-0.129713687	-0.505769180
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Fe144	4.862528368	-2.640318626	-0.059298824
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	C16	-1.303809849	-2.986743276	7.329151634
	C17	-0.581332830	-1.090857763	5.902724880
	C18	-0.492699767	0.324973474	6.500936874
	C19	-0.778365502	-1.115723282	4.362303976
	C20	0.187908100	-0.168789112	3.642631253
	C21	-0.645049656	-2.546346476	3.827109954
	C22	-1.654436613	2.440997856	6.994901058
	C23	-1.835065236	2.404692157	8.526301285
	C24	-2.720467884	3.315838392	6.292545786
	C25	-2.841446484	4.687537382	6.966970930
	C26	-2.391183407	3.478568703	4.803435471
	C27	-3.122914514	1.632201630	10.433159055

C28	-1.894931174	1.297640324	11.254670785
C29	3.659201546	-10.965342903	6.777295342
C30	4.479690450	-9.914340740	6.029892303
C31	5.068457974	-7.486325632	6.044369440
C32	6.142802659	-7.079726378	7.070029735
C33	4.055050050	-6.351033954	5.808495232
C34	4.686707365	-5.063428661	5.273787671
C35	3.617720388	-4.078702445	4.807247950
C36	3.825170914	-1.620490993	4.396779243
C37	8.491179343	-6.461269711	7.383441719
C38	8.950798657	-5.030572889	7.205331722
C39	-5.109383975	-2.339176358	-2.171559741
C40	-5.459166644	-0.849001436	-2.046438320
C41	-3.609360319	-2.522610217	-1.867387882
C42	-3.176023761	-3.969413561	-1.558058129
C43	-2.758820901	-4.803429498	-2.764264675
C44	-5.617220881	1.235025273	-3.359837620
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C46	-5.146910595	1.686329726	-4.756417931
C47	-9.142806795	1.535977208	-1.935171707
C48	-8.949406637	1.829430789	-0.438591070
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C50	-6.440000333	2.618784201	1.864927209
C51	-4.459507230	3.875923413	1.132573877
C52	-4.942789797	5.295267284	1.464218391
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C54	-2.966301174	2.717954821	-0.575000855
C55	-2.766195078	1.494306617	0.033837899
C56	-1.952183241	1.290999244	-1.945322473
C57	-6.493082474	7.066648026	0.750063946
C58	-6.786847548	7.490423188	2.188363302
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C60	-8.217546572	8.467635406	-0.589794837
C61	-8.255182503	9.689902431	0.053121519
C62	-9.021344761	9.882431577	-2.017694666
C63	8.081716603	1.164991780	5.403776841
C64	8.881760923	-0.106490283	5.612848537
C65	6.692391905	0.741330912	4.862390771
C66	5.766502022	1.916607045	4.648899413
C67	4.967921451	2.416572546	5.695340505
C68	5.681109958	2.549614356	3.395707650
C69	4.109090928	3.503258164	5.498543261
C70	4.834669751	3.640232933	3.186036634
C71	4.044740287	4.113000516	4.238712801
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C74	5.575337039	5.189914099	-0.587560684
C75	5.072870543	8.550216721	-3.837121117
C76	3.627990908	8.156078752	-4.154628706
C77	1.948147484	6.338822626	-4.148390874
C78	1.085434297	6.456940764	-2.871209430
C79	2.047949854	4.898873123	-4.682345351
C80	0.741005841	4.174276557	-5.016039438
C81	-0.049616700	4.681780384	-6.234591276
C82	-1.231169724	6.878998463	-6.370485173
C83	0.933800176	6.289692194	-0.442937104
C84	0.875857741	7.727674972	0.108389091
C85	1.463019503	5.368609828	0.665378778
C86	2.152432219	9.778468310	0.502914714
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C88	0.601549522	12.289616299	-1.949091333

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C93	-2.863738443	13.669818651	0.595321684
C94	-3.623449973	11.284927328	0.290639993
C95	-3.804627057	10.139404554	-0.678580749
C96	-4.878822574	10.138441264	-1.582284699
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C98	-5.019321545	9.132077399	-2.540172884
C99	-2.989589797	8.082154427	-1.713980577
C100	-4.058154917	8.121606803	-2.608326611
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C103	2.344207323	-3.279379635	-6.454033210
C104	2.036531994	-2.013511410	-7.261611933
C105	2.537136936	0.374489364	-7.493456999
C106	3.755486047	1.290208624	-7.554409412
C107	6.004761672	1.852075356	-6.765137727
C108	7.111777761	1.470535129	-7.727177741
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Fe144	4.879127323	-2.593311696	-0.140732111
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H183	-2.425447268	0.762102424	5.893196513
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H188	2.676831816	5.386001626	4.764898575
H189	4.762554214	4.104193125	2.201781197
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H319	6.576902458	-10.535807684	1.604832790
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H321	5.475263726	-8.526385071	2.462597431
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Fe145	2.650098186	-2.152047702	-1.087263220
H146	-6.391810702	-6.831795035	-1.482987029
H147	-6.172901863	-5.862241767	-2.779292937
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H150	-8.820025094	-6.588034082	-1.698227324
H151	-8.328504037	-2.110875865	-0.199793457
H152	-10.095203232	-4.913016667	1.170189724
H153	-10.102576670	-2.263840204	-0.168776093
H154	-10.194207275	-5.653432291	3.374625665
H155	-7.621041195	-5.618378483	1.772444059
H156	-9.910868345	-3.984656928	3.925769918
H157	-3.538101708	-2.507678404	2.353440942
H158	-5.960215775	-3.796031425	1.471451904
H159	-5.502182518	-6.497645194	2.190239608
H160	-6.209281909	0.075399099	5.289840030
H161	-6.956280537	-2.096032228	3.500118163
H162	-5.798112761	-6.452118375	3.946640522
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H164	-6.810459853	-3.464421936	5.873709160
H165	-7.722716244	-0.869962804	5.314222803
H166	-1.317520149	-3.964132942	3.654439734
H167	-0.818782407	-3.013356435	2.237834283
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H169	-1.935924798	-1.539517352	3.897999044
H170	-6.726326340	-4.595164083	7.869663731
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H172	-3.909346970	-0.390224162	8.289723524
H173	-3.695041000	3.084165846	8.483172535
H174	-0.149513702	-0.561864172	2.499801616
H175	1.089720096	-1.021817382	3.674325937
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H178	-4.110503208	3.985205886	7.005352444
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H184	-0.127785293	0.209261648	4.097326521
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H186	0.272565086	5.060917375	2.334500638
H187	2.333532159	5.261275150	3.136939412
H188	2.159565581	4.605438941	5.662764663
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	O456	1.725154673	-0.586039199	-8.320529608
	O457	3.821489407	3.870433019	-7.387496325
	O458	8.454636927	3.643672123	-6.786951228
	O459	-2.863500158	-2.177116860	-9.849685811
	O460	-0.270526474	-6.301755479	-6.250053932
	O461	1.798865914	-5.574974759	-6.656774396
	O462	-1.725863740	2.697534333	-8.912248420
	O463	10.173218621	-5.980998232	-1.261110416
	O464	12.344550270	-7.838709192	0.754083255
	O465	-0.467322868	-6.031085880	-0.694270006
	O466	-0.394962330	-8.116984955	0.076984112
	O467	4.669864097	-11.041363951	-2.184971258
	O468	2.621642689	-10.681032746	-3.065547025
	O469	4.879452344	-6.021807439	-0.256650697
	O470	4.284116682	-7.742547213	1.071772897
	O471	2.624285730	-6.015890058	-1.605384676
	O472	8.039155173	-7.184231554	2.919362561
	O473	6.610615124	-5.027658447	1.743037607
	O474	-3.184371326	5.141352904	-3.318111107
	O475	7.346703338	-10.916348594	-0.599157272
	O476	6.590384832	-9.139741450	1.533955330
	S477	4.309049070	4.903716643	-0.961879539
	S478	2.717004140	1.849666581	-2.676374210
	S479	2.690223312	-3.176367424	-3.141819896
	S480	3.295116289	1.479221908	0.800879357
	S481	0.598177796	-1.112972118	-1.153729446
	S482	5.254933125	-0.618597775	-4.468745910
	S483	3.317782597	-3.505792366	0.466370402
	S484	6.126693929	1.703012781	-1.518476634
	S485	6.175703393	-3.398219770	-1.868721763
	S486	6.170229434	-1.180879282	1.224103347
	15(b)			
	Fe(139)	0.578	-2.646	
	Fe(140)	0.369	1.055	
	Fe(141)	0.544	-2.650	
	Fe(142)	0.579	2.807	
	Fe(143)	0.596	3.172	
	Fe(144)	0.490	1.629	
	Fe(145)	0.345	-0.777	
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	C1	-5.813186058	-7.371631562	0.549776816
	C2	-5.534571916	-8.573154541	-0.359707288
	C3	-7.518584057	-5.852643516	1.454107509
	C4	-7.154952998	-5.914184528	2.937194601
	C5	-6.852465198	-7.298350442	4.928248565
	C6	-5.374605023	-7.031080781	5.231561141
	C7	-3.084074560	-7.041129352	4.359815102
	C8	-2.790868964	-5.542464689	4.247022295
	C9	-3.282915008	-3.434402302	3.124351678
	C10	-3.767492788	-2.630396296	4.340467007
	C11	-5.405239758	-2.386809933	6.121481832
	C12	-4.608259702	-2.663668980	7.403883611
	C13	-3.712746855	-4.362496053	8.923807311
	C14	-2.184481804	-4.282474402	9.029231983
	C15	-0.034160904	-4.579525602	7.871762514
	C16	0.713787757	-3.413089772	7.221754445
	C17	0.476873170	-1.335425509	5.885865014
	C18	0.055284508	-0.017658767	6.562587621
	C19	0.141874813	-1.398605989	4.371344987
	C20	0.556267351	-0.120821728	3.633342216
	C21	0.786181949	-2.633560199	3.731220861
	C22	-1.792111499	1.460785678	7.253496095
	C23	-1.804820927	1.330290404	8.789495025
	C24	-3.173871420	1.856398158	6.677982076
	C25	-3.770697095	3.043717411	7.444914224
	C26	-3.067332913	2.182139769	5.183237345
	C27	-2.486086347	0.070782358	10.747869556

C28	-1.141291160	0.193245324	11.438295760
C29	8.355325352	-8.726359932	5.861735180
C30	8.605736008	-7.416393222	5.115862949
C31	8.176901963	-4.958654418	5.226442624
C32	9.081431599	-4.163921558	6.186749474
C33	6.777284917	-4.327444385	5.115504095
C34	6.798328681	-2.881826580	4.609067101
C35	5.390982771	-2.409890199	4.250230434
C36	4.557420472	-0.065019894	4.002843996
C37	11.012024345	-2.668174472	6.356349677
C38	10.833546910	-1.170509460	6.230676421
C39	-3.968335738	-4.088684652	-1.834173047
C40	-4.808604946	-2.812057635	-1.661309675
C41	-2.483431204	-3.703414358	-1.641906077
C42	-1.492679135	-4.874726203	-1.474500565
C43	-0.895135769	-5.407865233	-2.776005501
C44	-5.989913734	-1.049325762	-2.894742064
C45	-7.440459551	-1.034998157	-2.390750909
C46	-5.894806584	-0.429944170	-4.302906972
C47	-9.144150901	-2.251156376	-1.109674854
C48	-8.926857718	-1.968622742	0.385444740
C49	-7.295565855	-1.644595776	2.200082913
C50	-6.632535410	-0.290385841	2.460770351
C51	-5.463158202	1.680510130	1.594546644
C52	-6.460692650	2.749519299	2.095155486
C53	-4.900736673	2.259485083	0.287137810
C54	-3.777909946	1.528467595	-0.374736909
C55	-2.806909049	0.668472271	0.077455907
C56	-2.406592727	1.064226216	-2.069220696
C57	-8.680959629	3.725731604	1.668357320
C58	-8.989625926	3.967132568	3.144315395
C59	-9.953791911	3.281060599	0.909110312
C60	-10.912437044	4.367219832	0.519607936
C61	-11.373085591	5.461138700	1.227596393
C62	-12.285384588	5.406895004	-0.791143541
C63	7.380574875	4.230266184	4.828506652
C64	8.630347003	3.373357926	4.914470089
C65	6.229727988	3.291543157	4.382931412
C66	4.895962174	3.994412517	4.292596869
C67	4.051279483	4.094128345	5.413882014
C68	4.462166847	4.575166461	3.086948410
C69	2.817234909	4.748683038	5.339407401
C70	3.238333860	5.240291032	2.999381144
C71	2.415834213	5.323278351	4.126615145
C72	3.265761985	8.412945348	-1.198709956
C73	1.990037123	9.063520060	-1.747491936
C74	2.971133359	6.975841376	-0.744956726
C75	0.843862775	9.930597034	-3.742946104
C76	-0.343579994	8.994756630	-3.979617420
C77	-1.146299876	6.654162510	-3.940331496
C78	-1.845858959	6.370453160	-2.591269764
C79	-0.533001698	5.395615754	-4.582857218
C80	-1.460821377	4.206394065	-4.844447409
C81	-2.521189006	4.375676259	-5.944557529
C82	-4.499838017	5.898539331	-5.871035820
C83	-1.675258909	6.146274422	-0.169655000
C84	-2.256839898	7.425326372	0.465054959
C85	-0.707242837	5.508109010	0.838000324
C86	-1.879328734	9.807450829	0.878229392
C87	-2.887853085	10.845854333	0.396144082
C88	-4.521603431	11.518398735	-1.312215983

C89	-5.950148684	11.514130933	-0.727504861
C90	-4.557854729	11.391913823	-2.850943334
C91	-5.139519181	10.058421746	-3.306079390
C92	-7.625547708	10.263540060	0.559307935
C93	-7.982233088	11.336375526	1.583080873
C94	-7.759390126	8.858441971	1.203433452
C95	-7.555431538	7.750622158	0.194760537
C96	-8.620596803	7.327865746	-0.615603675
C97	-6.297038252	7.159101496	0.002174513
C98	-8.436751044	6.361795284	-1.605896116
C99	-6.087369432	6.205915936	-0.999427890
C100	-7.163917812	5.823521947	-1.796419211
C101	6.281740877	-2.729912834	-8.236414137
C102	4.822999912	-2.946277024	-7.867992386
C103	2.841329348	-1.928419750	-6.764461812
C104	1.976517314	-0.880961677	-7.473124149
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C106	2.156520877	2.851626241	-7.679636204
C107	4.089388038	4.231012014	-7.077434749
C108	5.161617033	4.386542463	-8.136071858
C109	-0.181177188	-4.610394329	-9.061631661
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C111	0.292772915	-5.005285969	-7.643216826
C112	1.429883207	-6.041941679	-7.696184493
C113	2.072816486	-6.188136303	-6.335468145
C114	-2.748296112	-1.833793536	-8.485872945
C115	-2.650762431	-0.481664205	-9.164863606
C116	-3.274300021	-1.798685419	-7.030581405
C117	-2.207948436	-1.381152917	-6.053347417
C118	-1.901583217	-0.025246954	-5.846935795
C119	-1.419576950	-2.354525929	-5.413861955
C120	-0.797642117	0.335823303	-5.069795002
C121	-0.315666887	-1.991314893	-4.636930211
C122	0.010778949	-0.640976174	-4.480143104
C123	10.011900015	-3.531387170	-3.035847015
C124	11.022831263	-3.251674026	-1.913160011
C125	8.845247620	-4.420427551	-2.577965363
C126	7.730973520	-4.595700182	-3.565503261
C127	7.768103711	-5.296435297	-4.754702771
C128	5.693563606	-4.632791106	-4.355288186
C129	12.348992062	-4.060707970	-0.042247907
C130	13.630445232	-3.442880872	-0.557483417
C131	2.712405925	-6.331465684	0.645288777
C132	3.975958288	-5.598064175	1.001786205
C133	5.045596884	-5.609608882	-0.166224849
C134	5.402223798	-7.083311141	-0.521199265
C135	6.566123671	-7.182042342	-1.521583764
C136	7.122365920	-8.568965314	-1.683304403
C137	6.338216826	-4.963128633	0.418272750
C138	4.019689791	0.393630459	-1.757355326
Fe139	4.812353034	-0.730627340	-3.185771546
Fe140	2.272710615	0.959233126	-1.176301981
Fe141	4.645156569	2.005374728	-0.705008888
Fe142	3.757356449	1.702281043	-3.191711871
Fe143	2.842188820	3.713290298	-1.652678102
Fe144	5.471793724	-0.433008355	-0.677801260
Fe145	3.119163545	-1.278937702	-1.189247181
H146	-3.564300453	-8.801252468	0.115415818
H147	-3.803099565	-8.018341524	-1.296640592
H148	-7.817362260	-7.474879630	0.093622958
H149	-6.146075058	-8.486554168	-1.271556248

H150	-5.913017622	-9.462102321	0.173784183
H151	-7.047030371	-4.940920193	1.059534429
H152	-7.475541086	-7.942378926	2.971868784
H153	-8.608263520	-5.739693020	1.370091794
H154	-7.093002876	-8.326603601	5.227994998
H155	-4.864382099	-7.615049912	3.332615074
H156	-7.435962197	-6.610669718	5.554199751
H157	-2.223375562	-3.181465016	2.983427844
H158	-4.047484488	-5.381398285	2.611675370
H159	-2.545043452	-7.577298818	3.567286615
H160	-5.384530835	-1.302469017	5.953712468
H161	-5.421481841	-3.859463008	4.549000648
H162	-2.695702760	-7.373423438	5.329767340
H163	-3.832920390	-3.110901440	2.228587034
H164	-4.638621762	-4.702135417	7.031417082
H165	-6.448432868	-2.695769929	6.278704466
H166	0.461121559	-3.563609594	4.219789568
H167	0.512148394	-2.698754365	2.666633062
H168	1.885081042	-2.578917030	3.785376831
H169	-0.952634527	-1.495886832	4.287564073
H170	-3.999978440	-5.406091820	9.120742368
H171	-2.713760720	1.324461202	4.593543233
H172	-2.866959357	-0.461960432	8.716569059
H173	-3.950649721	2.805621918	8.503675966
H174	0.245638682	-0.177147885	2.579098894
H175	1.646470460	0.017558498	3.636541271
H176	7.152871052	4.592667923	5.849238912
H177	-4.049575773	2.482671939	4.790927749
H178	-4.729821150	3.336538672	6.992677097
H179	-2.370003370	3.020475602	5.023826485
H180	-3.097056440	3.914979815	7.404357339
H181	-3.852075223	0.992793725	6.804735652
H182	-1.077450204	2.272616730	7.051192948
H183	-1.941966007	-0.364014909	6.125051093
H184	0.094372585	0.779790385	4.065097701
H185	-0.189238345	4.664329188	0.347259237
H186	-1.314306988	5.118499699	1.670903133
H187	0.490468719	6.239450292	2.217144569
H188	0.713072021	5.948686349	4.821459205
H189	2.906898053	5.670135356	2.053169345
H190	5.077507866	4.483847545	2.189081599
H191	4.357836714	3.646036073	6.363437333
H192	-1.065470005	-2.653555576	6.586534697
H193	0.281088944	-5.493208893	7.346655733
H194	0.312617650	-4.653406426	8.910112518
H195	-1.972609673	-4.760776093	7.017296349
H196	-4.110475534	-3.737671308	9.733957186
H197	2.165500384	4.800593650	6.216375874
H198	1.565504743	-1.386559318	6.018097625
H199	-3.181790899	0.799157772	11.194997822
H200	-2.868463139	-0.940265938	10.957497103
H201	-0.261671596	-0.083261874	10.810675814
H202	12.044310960	-2.937533441	6.085796866
H203	0.849532656	-6.145142761	-3.563210349
H204	3.445443713	-7.892977522	1.512845488
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H206	2.181067799	-5.738845744	-8.439456346
H207	-0.545370305	-5.421212355	-7.062808970
H208	-1.977059934	-0.465656233	-10.053566366
H209	-0.407000115	-5.538361815	-9.608697275
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H211	-1.984835926	-5.724655901	-0.969825579
H212	-0.617637768	-2.103313660	-8.497041979
H213	-3.501570050	-2.379209813	-9.091444720
H214	1.145072700	-3.041905924	-9.358362107
H215	0.956604072	-5.663105900	-1.870638410
H216	0.618638439	-4.095253254	-7.115960440
H217	1.563738513	-4.436124959	-10.125965811
H218	-4.895650276	-5.451680765	-3.082069843
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H220	3.507492298	-4.993666553	-6.958658191
H221	-0.679195302	-4.557512061	-0.807294265
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H223	-2.631167507	0.236979788	1.057270817
H224	-8.223584292	-1.653332943	2.785392879
H225	-6.866404788	-2.151816924	0.172672761
H226	-7.932138457	1.830624681	1.001649445
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H231	-12.902292625	5.708646085	-1.634373054
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H233	-5.727054527	2.368334725	-0.433785568
H234	-12.751172321	6.964457252	0.582975293
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H236	-5.928947740	-0.129289044	0.523269919
H237	-6.648796341	-2.430418252	2.617885891
H238	-9.862344759	-1.505580136	-1.473288214
H239	-1.933681848	1.033483248	-3.046125810
H240	-9.607348982	-3.241912927	-1.212910378
H241	8.195532240	6.018808666	4.242946398
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H244	-2.525294186	5.461180618	-0.303349079
H245	-0.844194062	8.572769927	-0.486114503
H246	-4.074955060	2.363538002	-2.366136813
H247	-5.543990052	2.368826983	-3.870663898
H248	-5.761130003	3.726665088	-3.072120248
H249	-4.840976632	-0.396592046	-4.610747072
H250	-6.451534248	-1.048848375	-5.026945752
H251	-3.538797283	11.544757492	-3.235958974
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H254	-4.580862353	8.178817295	-3.871837034
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H257	-9.278187166	6.030432201	-2.220068124
H258	-5.448593973	7.433388378	0.636406019
H259	-5.881995590	5.833811646	-4.343640032
H260	0.288426809	5.036341246	-3.943066331
H261	0.811183043	7.365908446	-3.476421920
H262	-1.940637759	3.877163884	-3.909029268
H263	-7.373472209	-3.033459267	-2.035305367
H264	1.162752172	10.328744465	-4.715945858
H265	-5.113219231	-2.934479676	-3.634644939
H266	-0.074229013	5.709567241	-5.535443126
H267	-5.087068041	5.807407847	-1.184313852
H268	-7.204943676	0.886018932	-3.720634018
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