

Structures and reaction dynamics of N₂ and H₂ binding at FeMo-co, the active site of nitrogenase.

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S1. Calculation of transition states

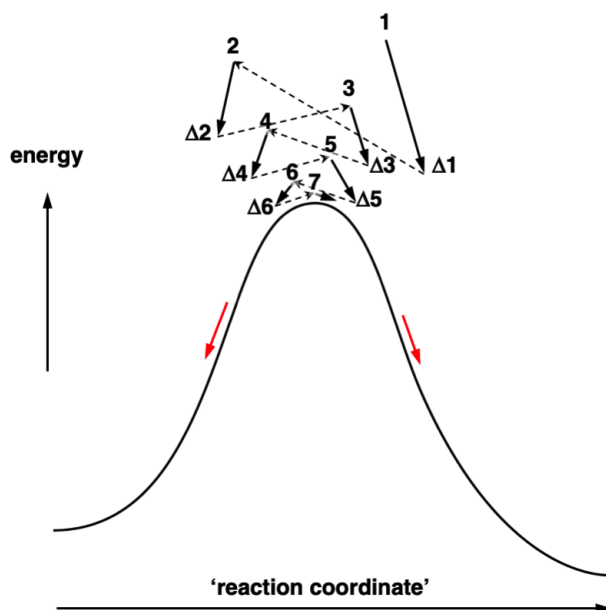


Fig. S1 Generalised diagram of the procedure for locating a reaction transition state. The solid arrows represent the course of limited small-step energy reductions from the numbered positions, which are generated (broken arrows) from D positions partway along the previous energy reduction, chosen according 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).

S2. Density functional procedures and validation

Density functional (DF) calculations use the DMol methodology of Delley,¹⁻⁵ with accurate DNP (double numerical plus polarisation) basis sets.⁴ 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 PBE⁶ was used because validation tests demonstrate that it is more accurate than other commonly used functionals when used with DMol.⁷ The calculations were all-electron, spin-unrestricted, with no imposed symmetry. The conductor-like screening model (COSMO)⁸⁻¹⁰ was used with a dielectric constant of 5. Constraints on interatomic distances used the Lagrange Multiplier Algorithm. Spin populations are calculated by the Mulliken method.¹¹

The DMol method uses numerical solutions of DFT-free atoms as part of its basis set, and thus gives highly accurate DFT solutions for the separated atoms limit.⁴ These numerical basis sets avoid the need for basis set superposition corrections, and provide reliable energies at long intermolecular distances. This advantage of the DMol methodology obviates the need for empirical treatment¹² of the long-range dispersion energies that are involved when the computational model is comprised of separate molecular units. This ability of the DMol methodology to incorporate long-range dispersion has been well demonstrated. Zhang *et al* reported the excellent agreement between the experimental interatomic potential energy curves and the DMol/PBE calculated potential energy

curves for the inert-gas pairs He₂, Ne₂, Ar₂, HeNe, HeAr and NeAr.¹³ Todorova and Delley used DMol to optimize the crystal structures of a comprehensive set over 40 molecular crystals in which dispersion and intermolecular interactions determine the crystal packing and crystal lattice parameters.¹⁴ This set of molecular crystals ranged over amino acids, aliphatic and aromatic hydrocarbons, ice, H₂S, S₈, C₆₀, and the inert gases Ne, Ar, Kr and Xe. The PBE functional overestimates lattice parameters by about 4%, while the PBE_{sol} functional yields lattice parameters with an average systematic error of less than 1%. Todorova and Delley emphasise that the DMol numerical basis sets have low BSSE because of the accurate tails of the molecular orbitals.

The PBE/DMol method reproduces experimental enthalpy data on the binding of N₂. Relevant $\Delta H_{\text{exp}} / \Delta H_{\text{calc}}$ comparisons from ref ⁷ are (kcal mol⁻¹) (a) exp 17.6, calc 20.0, 18.8 (b) exp ~10, calc 10.2 (c) exp 22.8, calc 25.9. Other assessments of DMol accuracy vs experiment have examined the electron affinities of atoms and molecules,¹⁵ the enthalpies of formation for small (<100 electrons) molecular and atomic species,¹⁶ the structures of metal-sulfide clusters,¹⁷ photo-induced conversion of [Os(NH₃)₅(η^1 -N₂)²⁺ to [Os(NH₃)₅(η^2 -N₂)²⁺ (i.e. end-on to side-on bonding of N₂),¹⁸ the geometry and vibrational frequencies of [(NH₃)₅Ru(pyrazine)Ru(NH₃)₅]^{4+,5+,6+},¹⁹ and protonation reactions involving hydrogen bonding.²⁰

S3. Additional descriptions and analyses of the binding of H₂

Refer to Table 1.

S3.1. H₂ at endo positions

Endo H₂ is bound in transverse configuration when the exo ligand on Fe is H, but is closer to parallel conformation when the exo ligand is endo-on N₂, or absent; variations in the configuration of Fe-H₂ involve very small energy changes, as expected. The endo angle is large, 159-174°, in all structures except **1** and **2** where the exo Fe2 position contiguous to Fe2-H₂ is void and the endo angle is slightly smaller (149, 144°). For reference, the endo angles in unligated FeMo-co are 118 (Fe2), 116 (Fe6)°. In **1** and **2** the Fe2-C^c bond is contracted slightly to 1.95Å, compared with 2.12-2.24 in the others, but at Fe6 with endo H₂ (structure **8**) Fe6-C^c is elongated to 2.36Å. In **5** the HisN ϵ -H bond is directed between S2B and the *exo*-H atom on Fe2, such that there is a weak (1.72Å) HisN ϵ -H••H-Fe2 dihydrogen bond and a bent (142°) HisN ϵ -H→S2B hydrogen bond.

The adaptation energies, which range between 7 and 24 kcal mol⁻¹, correlate generally with the endo angles in the dissociated limit, and therefore with the difference in endo angle between associated and dissociated structures. The larger adaptation energies, 18-24 kcal mol⁻¹, occur in **1**, **2**, **3**, **5**, **6**, **8**, and **10-H₂** which have smaller (112 - 128) endo angles at the dissociated limit and in the optimized-sans-H₂ structure. This correlation of the dissociated endo angle with the adaptation energy continues for **4**, 135° and 16 kcal mol⁻¹; for **7**, 138° and 12 kcal mol⁻¹; for **9-H₂**, 152° and 9 kcal mol⁻¹; and for **11-H₂**, 162° and 7 kcal mol⁻¹. Interactions involving His195 influence the adaptation energies. The short strong HisN ϵ -H••H-Fe2 dihydrogen bond in **4** is associated with a smaller adaptation energy, 16 kcal mol⁻¹, than that of **3**, 22 kcal mol⁻¹, with a HisN ϵ -H→S2B hydrogen bond and the same ligated FeMo-co structure. The smaller adaptation energies and larger endo angles in dissociated **7** and **11-H₂** are related to the absence of any hydrogen bonding between His195 and S2B. Structure **9-H₂** does have a hydrogen bond from His195 to S2B, but the endo angle in both the dissociated state (152) and opt-sans-H₂ (155°) is unusually large: this appears to

be a consequence of the course of the dissociation trajectory on the PES of the transition state, because there is another deeper potential energy well for the opt-sans-H₂ form of **9-H₂**.

The association and dissociation trajectories of **11-H₂** are anomalous. H₂ introduced ca 2.9 Å from Fe2, and with no van der Waals interference, resides on a very flat energy surface. There is a small ridge, < 1 kcal mol⁻¹ with Fe2-H distances of 2.4, 2.6 Å, beyond which H₂ binds to Fe2, with enlargement of the endo angle to 173°. The barrier for the reverse dissociation is 6 kcal mol⁻¹. Structure **7**, also without hydrogen bonding between His195 and FeMo-co, similarly has a flat energy surface with small barriers for association (4 kcal mol⁻¹) and dissociation (10 kcal mol⁻¹).

S3.2. H₂ at exo positions

H₂ is not strongly bound in an exo-Fe position, as the barriers to dissociation are small, 3 - 8 kcal mol⁻¹. The adaptation energies in **13 -16** range from 11 to 26 kcal mol⁻¹, and correlate with the difference in Fe-C^c distance between the bound and dissociated structures, regarded as the main source of the adaptation energy. Similarly, the barriers to H₂ binding, ranging 7 - 20 kcal mol⁻¹, follow the adaptation energies. H₂ dissociated from Fe2 is located in the hydrophobic channel adjacent to Arg277, Ser278) while H₂ dissociated from Fe6 encounters the sidechain of Gln191 and its hydrogen bond with O1 of homocitrate.

S4. Additional descriptions and analyses of the binding of N₂

Refer to Table 2.

S4.1. Exo end-on-N₂, structures 9-11, 17, 25-27

In all structures the Fe-N distances are 1.81-1.83 Å, and the trans Fe-C^c bond ranges 2.16 - 2.23 Å, except in **17** and **26** where a Fe2-H-Fe6 bridge enforces shorter Fe-C^c distances (2.10, 2.07 Å). The stability of this end-on bonding of N₂ is shown by the barriers to dissociation which are 13 - 16 kcal mol⁻¹ in all structures except **25** (7 kcal mol⁻¹) and **26** (10 kcal mol⁻¹). Adaptation energies are ca 18 kcal mol⁻¹, except in **26** where movement of the symmetrical Fe2-H-Fe6 bridge in the bound structure to asymmetric endo-Fe6-H in the dissociated structure increases the adaptation energy to 26 kcal mol⁻¹.

The one structure with N₂ bound at exo-Fe6, **27**, is unusual, because the H atom bound to Fe2 is folded backwards towards the sidechain of Phe381. The C^c-Fe2-H angle is 135°. In the optimized-sans-N₂ form of **27** this angle is even more acute, 115°, and H on Fe2 is in van der Waals contact with Phe381. This unusual geometry arises because S2BH is folded far forward, such that the endo angles are 91° at Fe2 and 96° at Fe6, and H on Fe2 folds back to symmetrise the fivefold coordination of Fe2. N₂ on Fe6 is also tilted slightly backwards. See section S7.

Unbound N₂ approaching exo Fe2 is located within the N₂ pathway (Fig 2), adjacent to the sidechains of Arg277, Ser278 and Val70. Passage of N₂ towards binding at the exo-Fe2 site is easy. The calculated trajectory involves ca 3 kcal mol⁻¹ of diffusion as N₂ slides from 3.8 Å to about 3.3 Å from Fe2, the dissociated limit (see **10-N₂**, **11-N₂**, **17-N₂**, **25**, **26**). The barrier from this point to the transition state ranges from very small (2 kcal mol⁻¹) in structures **17** and **11** to 7 kcal mol⁻¹ in structure **26** (which also has the largest adaptation energy, contributing to the barrier for association). These potential energy barriers for the formation of end-on bound N₂ at exo-Fe2 are

remarkably small. At Fe6, when N₂ dissociates from the exo position it encounters the sidechains of Gln191 and Val70.

S4.2. Endo end-on-N₂, structures 22-24

Structures **22** and **23** have end-on N₂ bound at endo-Fe2, with endo angles 172, 168° and Fe2-C^c 2.19Å. The adaptation energies are 19, 20 kcal mol⁻¹. At endo-Fe6, structure **24**, N₂ bound end-on does not extend Fe6-C^c (2.17Å) as does endo side-on N₂ at Fe6 (Fe6-C^c = 2.74Å in **21**). However, the adaptation energy for **24** is larger, 31 kcal mol⁻¹, which is attributable to changes in the dihydrogen bond between the bound and dissociated states of **24**, causing a larger change in the endo angle.

S4.3. Endo side-on-N₂, structures 18-21

Three structures, **18**, **19**, **20**, have N₂ bound side-on at endo-Fe2, and one **21** at endo-Fe6. The geometry at Fe2 is normal, with endo angles 170-175 and Fe2-C^c = 2.20, but at endo Fe6 side-on N₂ causes large distortion of the coordination geometry, including extension of Fe6-C^c to 2.74Å. This distortion in **21** requires an unusually large adaptation energy of 36 kcal mol⁻¹. For the three structures binding N₂ at endo Fe2 the adaptation energies are significantly smaller, 25, 27 and 22 kcal mol⁻¹. Barriers to dissociation of endo side-on N₂, a measure of stability, range 3 to 8 kcal mol⁻¹.

The transition states for **18**, **19** and **20** and the trajectories from TS to the bound state are well defined. Beyond the TS the trajectories involve two stages, first the separation of N₂ and recovery of the adapted geometry of FeMo-co, and second the diffusion of the N₂ far from Fe2. The two stages are evident in the trajectory for **18**, described below. Structure **20** shows similar behaviour, with ca 11 kcal mol⁻¹ for the recovery of FeMo-co geometry (assessed as decrease in the Fe2 endo angle) and ca 6 kcal mol⁻¹ improvement as N₂ diffuses to ca 5Å from Fe2. For structure **19**, in both S=1 and S=0 spin states, the decrease in the Fe2 endo angle and diffusion of N₂ occur together as N₂ reaches 5Å from Fe2. The total downhill energy is ca 25 kcal mol⁻¹, similar to the total energy change for **18** and **20**, and the diffusion pathways are the same. Variations in the endo-Fe angle decreases during the dissociation trajectories of **18**, **19** and **20** are attributable to the different interactions involving His195 (short strong dihydrogen bond in **18**, weaker dihydrogen bond in **19**, nothing in **20**), because these interactions are involved in the flapping of S2B inherent in endo angle variations.

S5. Dissociation trajectory beyond the transition state for endo side-on N₂ of structure **18**.

Fig. S2 plots the endo-Fe2 angle with the energy improvement as N₂ separates from the transition state with Fe- N₂ = 2.5Å, to almost 5Å from Fe2. The decrease of the endo angle from 175 to 140° is complete when the Fe- N₂ separation is about 3.5Å. Then there is further energy reduction of at least 10 kcal mol⁻¹ as N₂ diffuses to 5Å away. The path of this diffusion of N₂ passes by residues Val70, Val71, His195 and Ser278, without any adverse van der Waals contacts. Fig S2 also illustrates a general property of dissociation trajectories from endo positions, which is that the endo angle undergoes small variations as the remainder of FeMo-co and connected protein adjust.

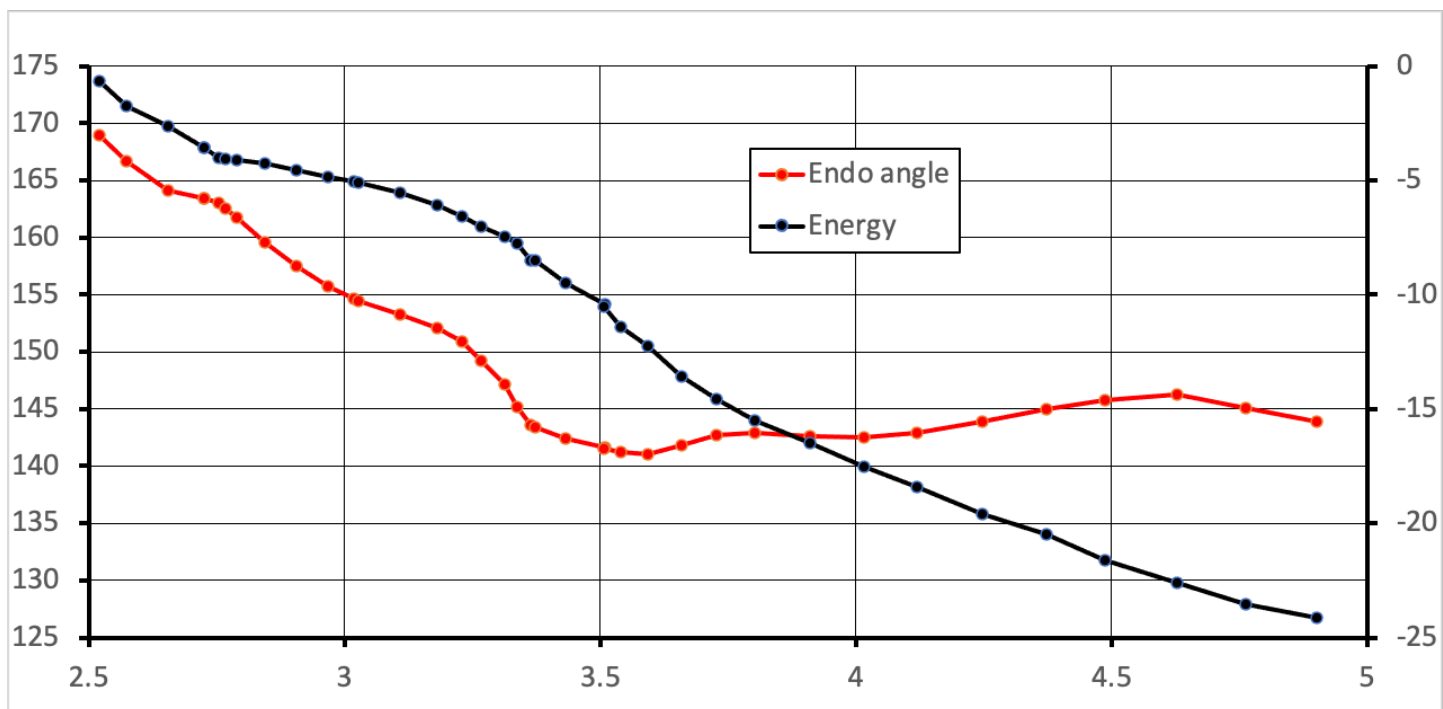


Fig. S2. The trajectory for dissociation of side-on N_2 from Fe_2 in structure **18**. The TS with mean Fe-N distance 2.5\AA is on the left. Energy minimisation causes N_2 to move to about 5\AA from Fe. Reduction in the endo angle at Fe_2 is complete when the Fe-N separation is about 3.5\AA : The further wobble in endo angle between 141 and 146° is due to adjustments in other parts of $FeMo-co$ and linked protein. The dihydrogen bond is short, $1.25 - 1.37\text{\AA}$, throughout this trajectory.

S6. Entropy data

There is no experimental or computational information on the entropy changes associated with the the binding of H_2 or N_2 to $FeMo-co$ within the $MoFe$ protein. There is experimental entropy data for the binding of H_2 and N_2 to metal sites that have chemical similarities with the Fe sites of $FeMo-co$. These data are for the ligand, H_2 or N_2 , in the gas phase, and the complex in non-aqueous solution. For the binding of H_2 or N_2 to $FeMo-co$, the relevant dissociated state for the small molecule ligand is not gas phase but condensed phase, considered to be a diffusible position within the protein. Here the ligand will have lost translational and rotational entropy relative to the gas phase.

The cobalt binding site shown in Figure S3 has analogous four-coordinate geometry, similar soft ligands in the trigonal positions, and the axial B ligand approximates C^c of $FeMo-co$.

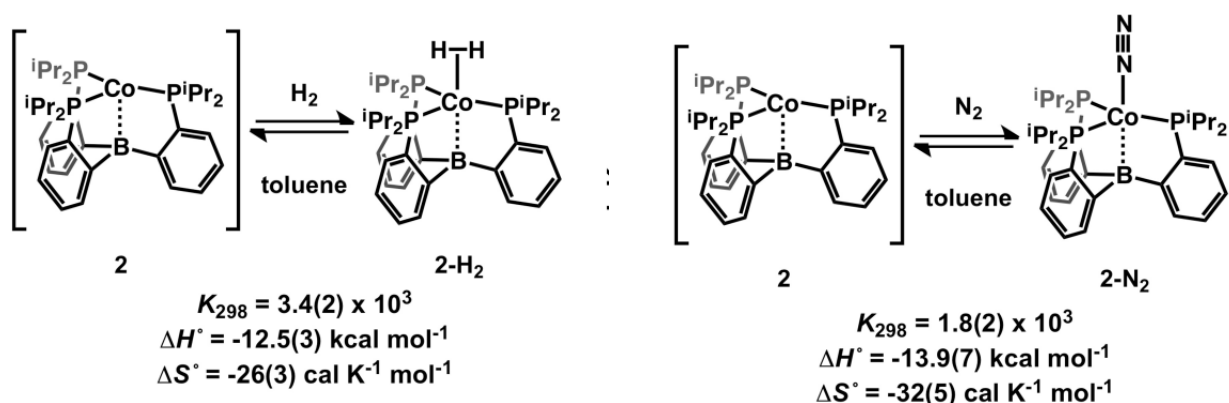


Fig. S3. Enthalpy and entropy data from ref ²¹

Gonzalez and Hoff²² measured enthalpy and entropy changes for the binding of H₂ and N₂ to [P(C₆H₁₁)₃]₂M(CO)₃ (M = Cr, Mo, W in THF. Relevant results are tabulated.

[P(C₆H₁₁)₃]₂M(CO)₃ + L(g) → [P(C₆H₁₁)₃]₂M(CO)₃L (in THF solution)

M	L	ΔS cal mol ⁻¹ K ⁻¹
Cr	N ₂	-35.4 ± 2.3
Cr	H ₂	-25.6 ± 1.7
Mo	N ₂	-32.1 ± 3.2
Mo	H ₂	-23.8 ± 2.1

Additional reports are cited in ref ²¹.

S7. Plasticity of FeMo-co and His195 involvement

When a dihydrogen bonded structure (right) changes to a linear HisNε-H ••• S2B structure (**27**) with Fe2-H folded backwards from the exo position, there are concomitant changes in the some dimentions of FeMo-co, as shown in Fig S4.

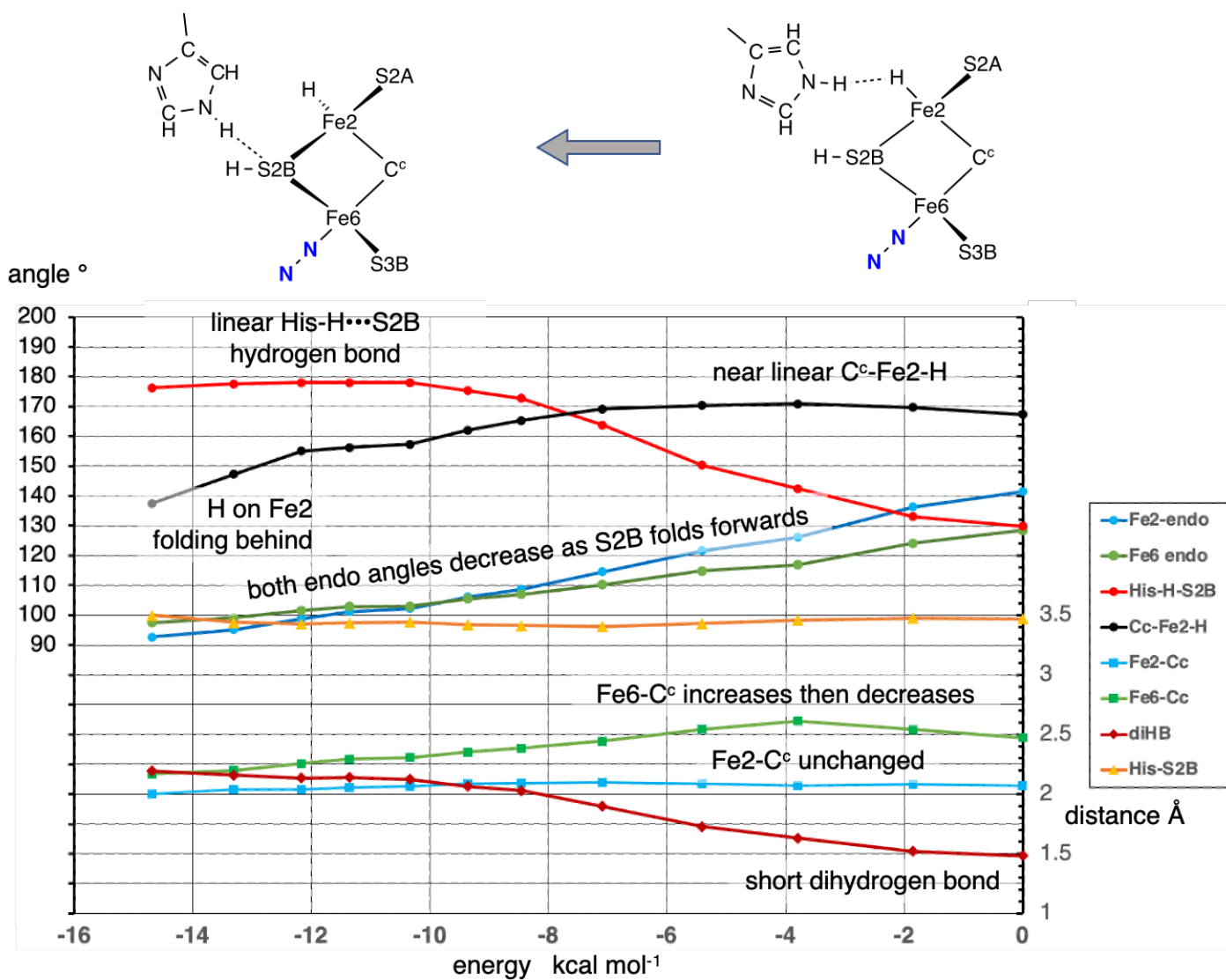


Fig. S4. Energyscape for concerted changes involving hydrogen bonding from His195 and the geometry of ligated FeMo-co.

S8. Additional mechanisms for H₂ / N₂ exchange.

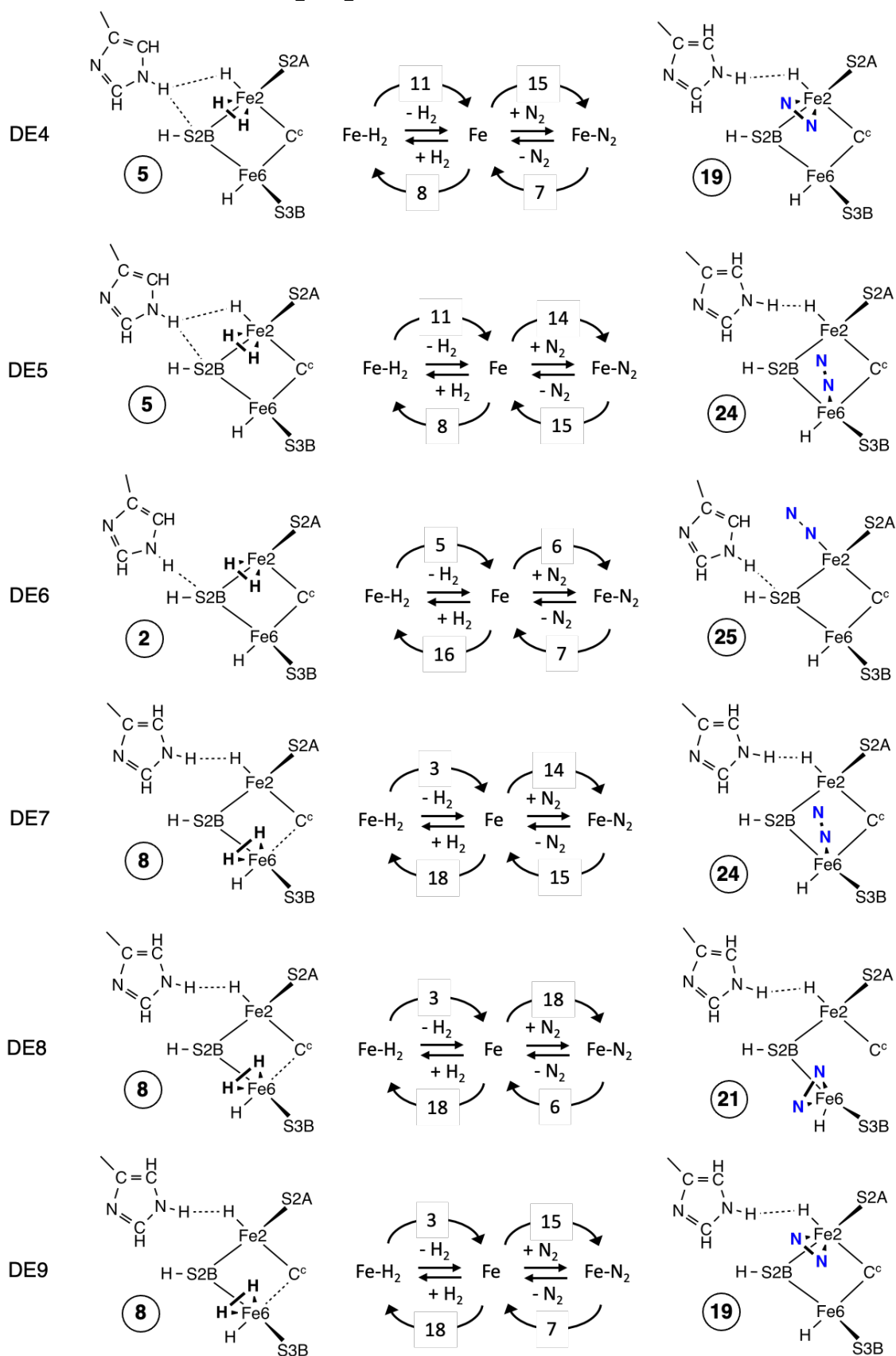


Fig S5. Additional mechanisms for dissociative exchange of H₂ and N₂, with potential energy barriers (kcal mol⁻¹, marked on the arrows) for the steps involved. These have some large reaction barriers and are less feasible than those described in Scheme 6.

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S9. Coordinates and spin densities for bound structures

Translation of Fe numbering

Fe1 = Fe143

Fe2 = Fe140

Fe3 = Fe141

Fe4 = Fe142

Fe5 = Fe139

Fe6 = Fe145

Fe7 = Fe144

structure, spin densities	filename, coordinates		
1 (S=1/2)	bm22b6x2h2nconexbdtmi.car_2		
Fe(139) 1.915	C1	-1.945094869	1.101572138 -9.457452011
Fe(140) -0.493	C2	-2.452749408	2.113158990 -8.425366185
Fe(141) 2.706	C3	-2.671431539	4.489244947 -7.831234344
Fe(142) -2.709	C4	-4.143615237	4.525428964 -7.423187057
Fe(143) 3.178	C5	-6.472878366	4.169100391 -8.068497659
Fe(144) -2.502	C6	-6.880433356	3.059142021 -7.092754476
Fe(145) -1.583	C7	-6.376916141	0.817613726 -6.245124771
	C8	-5.831805773	1.150253324 -4.854264769
	C9	-4.089522731	2.223086698 -3.538753819
	C10	-4.972005121	3.237838494 -2.796195299
	C11	-6.347962920	5.231604370 -2.902923428
	C12	-7.712056818	4.689838384 -2.453196057
	C13	-9.737092394	3.479496593 -3.101310946
	C14	-9.924841003	2.218857379 -2.246805044
	C15	-9.115061769	-0.045269077 -1.738966566
	C16	-8.119306049	-0.361804812 -0.622495822
	C17	-5.996095579	0.246314710 0.468441728
	C18	-6.034025079	1.229289933 1.651043006
	C19	-4.601856147	0.186635354 -0.219867196
	C20	-3.442170345	0.159374451 0.782231699
	C21	-4.524967403	-1.009105414 -1.174362533
	C22	-6.185468170	3.616554544 2.321666696
	C23	-7.664647159	3.950694170 2.605524239
	C24	-5.354476911	4.856793669 1.916705783
	C25	-5.585289018	6.017545214 2.892478662
	C26	-3.863447596	4.509523011 1.832738699
	C27	-9.840633761	4.626354902 1.766445830
	C28	-10.585438511	3.533281247 2.508308105
	C29	-9.067774689	-9.597353728 -1.968802027
	C30	-7.977026689	-9.438354369 -0.909993218
	C31	-7.261860372	-7.986887155 0.996709798
	C32	-7.993751661	-8.189792231 2.336917804
	C33	-6.828281106	-6.523018741 0.797364773
	C34	-5.883888081	-5.996953734 1.881828641
	C35	-5.242897432	-4.680955113 1.440489081
	C36	-4.311039513	-2.932214553 2.974908295
	C37	-7.841541074	-9.153825035 4.584982210
	C38	-7.141705402	-8.416487095 5.704831241
	C39	0.742204561	1.498241715 -5.659804110
	C40	1.136030879	2.753692096 -4.869382890
	C41	0.624169567	0.343315335 -4.636203351
	C42	-0.072887186	-0.941848096 -5.126187662
	C43	0.841037916	-1.967518464 -5.792642078
	C44	2.998466762	4.222340381 -4.270260536
	C45	2.540361713	5.633660029 -4.668335856
	C46	4.536182172	4.143553030 -4.229955034
	C47	1.022744592	6.955124931 -6.078704484
	C48	-0.330694524	7.090145780 -5.362255488
	C49	-1.986151837	5.995724510 -3.902593221
	C50	-1.794429731	6.107938621 -2.385552140
	C51	-0.356400684	5.850291523 -0.426424920
	C52	-0.385448912	7.341537979 -0.016778274
	C53	1.035475753	5.355502619 0.003617825
	C54	1.307457324	3.888242423 -0.073893030
	C55	0.514870037	2.773764586 0.072043738
	C56	2.606758382	2.078172137 -0.181411292

C57	0.510066440	9.561617019	-0.611098686
C58	-0.778975630	10.304435587	-0.261596197
C59	1.172430164	10.184988254	-1.860251605
C60	1.981591392	11.427142835	-1.626484455
C61	1.846943438	12.427679271	-0.684371554
C62	3.581445554	12.832616154	-2.003155042
C63	-3.681894187	-3.244236321	8.309725261
C64	-4.210255485	-4.665693801	8.367296267
C65	-3.746057117	-2.800744101	6.826469031
C66	-3.308890660	-1.368980060	6.624679822
C67	-4.222779342	-0.303059802	6.719167255
C68	-1.967584083	-1.062376527	6.335513092
C69	-3.817116919	1.020922706	6.519652947
C70	-1.545630219	0.254016148	6.142984519
C71	-2.475067207	1.293618434	6.229172655
C72	3.407637785	0.758721881	8.217835627
C73	4.287946432	1.987744546	7.950011432
C74	2.705094093	0.317505115	6.924489715
C75	6.589470021	2.820550208	7.677981747
C76	6.695369758	3.289517360	6.225773269
C77	6.051231654	2.885281542	3.876953855
C78	4.738788520	3.622451787	3.527997690
C79	6.278983633	1.637353631	3.000297097
C80	6.304186538	1.849588102	1.482836846
C81	7.487858506	2.645292971	0.909524490
C82	8.054144807	5.050520494	1.255984452
C83	2.331024494	3.811514427	3.797254805
C84	2.073595716	5.086801148	4.619640441
C85	1.114890932	2.885033512	3.973962827
C86	2.102413719	6.019365124	6.881980806
C87	2.974016482	7.181454019	7.342294259
C88	5.066644749	8.439767221	7.080741056
C89	4.696250040	9.866930812	6.624825145
C90	6.510578591	8.081599252	6.677232356
C91	6.708216418	8.058642625	5.164670510
C92	3.479520276	11.223685727	4.986334437
C93	2.875756447	12.210601870	5.975945131
C94	2.493842751	10.997823355	3.807594593
C95	3.085173207	10.081089208	2.761600276
C96	3.959313410	10.586118887	1.786176597
C97	2.848320918	8.696564519	2.788382433
C98	4.594045184	9.738870843	0.875007377
C99	3.499788248	7.830175779	1.904437014
C100	4.374401393	8.362876067	0.961023923
C101	6.482102565	-8.555275399	-1.188133074
C102	6.243342086	-7.302589573	-2.014686378
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C104	6.654443179	-3.800534649	-1.582811174
C105	7.478674177	-2.334087263	0.195413155
C106	7.908157222	-2.399153718	1.657648171
C107	7.721317364	-3.457023869	3.859362991
C108	8.664282643	-4.595011222	4.190701053
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C110	7.434667813	-2.457733472	-6.209298968
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C113	4.096444807	-6.204275279	-5.809447867
C114	7.639589321	-0.329247980	-5.019341379
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C117	5.401308091	-0.137477049	-3.855919199
C118	5.587120213	0.217251495	-2.508806896
C119	4.457448310	-1.131912243	-4.167725936
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C134	-2.235088400	-7.938343919	-3.537234183
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Fe140	1.068481558	-1.854675586	1.599493005
Fe141	1.054192209	-3.322837041	3.686484326
Fe142	3.357525356	-3.497398526	2.452288979
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H191	-5.274828373	-0.507596307	6.932445753
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	O459	8.709530562	-1.542758394	2.066838938
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	S479	3.883740590	0.076124491	5.517141770
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Fe(139) 1.919	C1	-2.043339037	-3.061182463	-8.992707147
Fe(140) -0.544	C2	-2.414220312	-1.664438634	-8.485142126
Fe(141) 2.690	C3	-2.510180974	0.738204889	-9.003564140
Fe(142) -2.696	C4	-3.960567020	1.026495339	-8.618367634
Fe(143) 3.187	C5	-6.320607873	0.478481748	-8.918496487
Fe(144) -2.502	C6	-6.681230525	-0.011426798	-7.511288228
Fe(145) -1.578	C7	-6.106013735	-1.524431287	-5.672354911
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	C9	-3.771239977	0.991269099	-4.002622408
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	C24	-5.020592361	5.781064929	0.077659274
	C25	-5.136080814	7.251036486	0.500030114
	C26	-3.545856973	5.360554067	0.010464015
	C27	-9.522172356	5.596212049	0.471066777
	C28	-10.150075902	5.094059517	1.756697546
	C29	-9.481732576	-9.134565742	2.825949698
	C30	-8.278618249	-8.646432606	3.636249493
	C31	-7.320266012	-6.595239042	4.705382610
	C32	-7.940742820	-6.206430081	6.062495249
	C33	-6.861586250	-5.365700364	3.902667268
	C34	-5.834613998	-4.486143404	4.623007982
	C35	-5.156326636	-3.546387523	3.625003100
	C36	-4.076170343	-1.375146451	4.237542076

C37	-7.649219550	-6.258906804	8.495320226
C38	-6.907692592	-5.134515778	9.184728880
C39	0.176615556	-0.959448160	-5.763749781
C40	0.648658586	0.496292338	-5.636872760
C41	0.129043908	-1.549617327	-4.332511571
C42	-0.614864852	-2.892254995	-4.166239721
C43	0.239806662	-4.142228259	-4.374609779
C44	2.593497469	1.968869058	-5.825108948
C45	2.145382106	3.089100163	-6.773623746
C46	4.127205377	1.834385106	-5.859452077
C47	0.647422700	3.724786533	-8.614291369
C48	-0.660274473	4.253495429	-8.005887888
C49	-2.273213090	4.045623756	-6.154413013
C50	-1.969218649	4.712591995	-4.808511351
C51	-0.446027955	5.081325680	-2.936296690
C52	-0.352325418	6.614798013	-3.137451344
C53	0.944385209	4.696867207	-2.401453908
C54	1.190322542	3.294531936	-1.952013452
C55	0.407311209	2.322703884	-1.376580307
C56	2.490345555	1.563613023	-1.418536593
C57	0.689441924	8.340872483	-4.565580991
C58	-0.536926061	9.252054280	-4.611350970
C59	1.423819588	8.333585124	-5.923071103
C60	2.266476211	9.534095951	-6.241470795
C61	2.185529004	10.841130078	-5.803187826
C62	3.891034662	10.596289255	-7.196791924
C63	-3.187479832	0.782440129	8.995780691
C64	-3.798873211	-0.453751401	9.630437588
C65	-3.337922904	0.614582457	7.463106946
C66	-2.809049024	1.797113738	6.685678966
C67	-3.633793763	2.882838695	6.338280115
C68	-1.458528453	1.848982163	6.298528941
C69	-3.132863183	3.976677978	5.623414579
C70	-0.940695775	2.939332891	5.598960919
C71	-1.782046208	4.000844617	5.256075089
C72	4.373045836	3.757675510	6.908383945
C73	5.220025006	4.711347836	6.057712057
C74	3.501004552	2.875769681	6.005454603
C75	7.488098879	5.278495469	5.286548600
C76	7.441658392	5.136016401	3.765742546
C77	6.587186417	3.851202964	1.838093493
C78	5.236443745	4.409770998	1.340499506
C79	6.773613745	2.356078032	1.518993182
C80	6.613201432	1.924108443	0.056704546
C81	7.673641663	2.409764245	-0.943530102
C82	8.193991633	4.707898579	-1.741356750
C83	2.850767001	4.697579542	1.686830566
C84	2.646176550	6.202661609	1.926095463
C85	1.678689755	3.943736538	2.344937753
C86	2.877552412	7.994327886	3.579189592
C87	3.815967934	9.191799794	3.501606430
C88	5.873871127	10.167436803	2.583010477
C89	5.474984242	11.327746275	1.645193182
C90	7.273437089	9.626978136	2.237294497
C91	7.346923373	9.014978706	0.840432655
C92	4.082235098	12.021453064	-0.248449114
C93	3.581604458	13.337691570	0.330033505
C94	2.976540073	11.401521496	-1.146852334
C95	3.438972547	10.109952454	-1.779494990
C96	4.220847995	10.128028616	-2.944381488
C97	3.167241520	8.868465345	-1.179521152
C98	4.732528969	8.948577187	-3.487189570
C99	3.692801184	7.680628818	-1.695127802
C100	4.475123461	7.736741861	-2.845351678
C101	6.207875470	-8.569053488	1.910031477
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C103	5.232445712	-5.481512665	-0.120067519
C104	6.252109603	-4.351367503	-0.308777781
C105	7.148957722	-2.291378921	0.671910687
C106	7.779531920	-1.806944257	1.972886643
C107	7.824989024	-1.810756273	4.419070645
C108	8.726282292	-2.777699034	5.156549073
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H184	-3.317651256	2.079441653	1.370433639
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	O460	8.400709377	-1.693018339	2.643133638
	O461	8.238508324	-2.562024477	7.294164590
	O462	6.407139532	-6.953208785	-4.887555223
	O463	1.422396522	-8.760389713	-1.982442062
	O464	2.338902044	-8.838119781	0.051738345
	O465	8.453898260	-2.573616067	-3.352373861
	O466	-1.620847642	-7.486179371	9.080632333
	O467	-4.193569125	-8.167018813	11.422267391
	O468	-2.991567531	-5.326980091	-1.162606825
	O469	-4.800115281	-6.621607456	-1.207592515
	O470	-4.459759368	-11.173393208	3.144433387
	O471	-3.715488306	-11.023360441	1.017095333
	O472	-2.941652265	-6.072248452	4.145880912
	O473	-5.082406222	-6.553229985	3.628155624
	O474	-2.044287203	-6.517852867	1.724844933
	O475	-5.889783679	-5.638147829	7.665184423
	O476	-3.789211473	-4.381422957	6.237585643
	O477	5.541831989	2.788448344	-3.176394196
	O478	-5.330010573	-10.534296016	6.046625670
	O479	-6.068599123	-7.760620322	5.846408231
	S480	4.254230203	2.345409747	4.595628059
	S481	3.150640313	-0.576716637	2.256990531
	S482	0.835608711	-5.151573331	1.663442435
	S483	0.568935066	1.015381173	3.963268026
	S484	0.582594793	-1.812038729	0.364846697
	S485	3.653875412	-4.145289489	4.054412119
	S486	-2.179091811	-3.404650226	2.857734517
	S487	2.747400997	-0.960433805	5.845032267
	S488	0.108533646	-5.045767475	5.283852259
	S489	-1.195872065	-1.519084441	5.965231708
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Fe(139) 2.222	C1	-3.094260160	0.889311539	-9.218326863
Fe(140) -0.049	C2	-3.395525309	1.917393620	-8.122624940
Fe(141) 2.226	C3	-3.505120965	4.303423173	-7.537291397
Fe(142) -2.702	C4	-4.896739197	4.339676787	-6.906247213
Fe(143) 3.166	C5	-7.286973835	3.905043157	-7.150501172
Fe(144) -2.433	C6	-7.488348070	2.840891954	-6.067879988
Fe(145) -0.835	C7	-6.756282504	0.687425781	-5.162881568
	C8	-6.085781915	1.137468246	-3.860838065
	C9	-4.250555970	2.349909236	-2.808599884
	C10	-5.047222591	3.436800402	-2.071790824
	C11	-6.523388004	5.360875530	-2.222071976
	C12	-7.820577241	4.858405923	-1.571384634
	C13	-9.878256754	3.560890767	-1.849373655
	C14	-9.935307780	2.322316832	-0.948312329

C15	-8.958120732	0.128766137	-0.409772103
C16	-7.884249527	-0.072951662	0.662552888
C17	-5.839396483	0.867821652	1.698895692
C18	-5.881389165	2.021739221	2.714173097
C19	-4.495476795	0.751186183	0.930325518
C20	-3.292068165	0.773008624	1.880363867
C21	-4.473133269	-0.507374291	0.055535322
C22	-5.760657004	4.444460009	3.104263888
C23	-7.215141341	4.771168041	3.496701709
C24	-5.004409439	5.647345496	2.493965333
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C28	-10.090419637	4.115437072	3.794918484
C29	-9.695852305	-9.261615562	-0.563180640
C30	-8.466751414	-9.122700370	0.338130055
C31	-7.442001705	-7.622295854	2.063891749
C32	-8.022437546	-7.749684604	3.484899109
C33	-6.992516131	-6.184679361	1.746928293
C34	-5.845676626	-5.673056738	2.620971269
C35	-5.296974767	-4.354202476	2.069391945
C36	-3.927078129	-2.805353115	3.493879204
C37	-7.710125207	-8.700134299	5.717902276
C38	-7.042355268	-7.833322519	6.765973397
C39	0.090542377	1.216398048	-5.837189879
C40	0.588351334	2.502691077	-5.159424380
C41	0.052100416	0.121143953	-4.742042445
C42	-0.701511136	-1.178726319	-5.100946203
C43	0.173805384	-2.261379166	-5.726389430
C44	2.566477515	3.919064651	-4.799512271
C45	2.139908397	5.317759759	-5.265405204
C46	4.094029934	3.757422266	-4.917618538
C47	0.519257508	6.603393681	-6.590666889
C48	-0.734495435	6.864855044	-5.740265837
C49	-2.222059498	6.012537077	-3.972623491
C50	-1.885014434	6.185114927	-2.486866064
C51	-0.292303696	5.931308840	-0.640409603
C52	-0.189047931	7.433413208	-0.311031348
C53	1.100198467	5.353912819	-0.329411286
C54	1.295656047	3.876535977	-0.469394254
C55	0.537151962	2.823707418	0.002994578
C56	2.402924250	2.053647224	-0.891617525
C57	0.847339314	9.530391879	-1.111564669
C58	-0.378453306	10.432757660	-0.987823333
C59	1.683942387	9.920009566	-2.346862345
C60	2.499543039	11.174973301	-2.246983137
C61	2.476406490	12.202161376	-1.324740816
C62	4.053466528	12.556572506	-2.840848533
C63	-2.962055124	-2.699652433	8.762611743
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C68	-1.108142680	-0.659436799	6.811998180
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C71	-1.679914829	1.635769767	6.324713507
C72	4.564835688	0.979808960	7.596072127
C73	5.440486796	2.149685440	7.128814612
C74	3.626869178	0.535689710	6.467420263
C75	7.699776198	2.852411445	6.450884190
C76	7.607806090	3.248568891	4.975564211
C77	6.585505406	2.788898631	2.777816337
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C79	6.631511397	1.515350551	1.914435603
C80	6.437379968	1.701236910	0.403512522
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C82	8.340105433	4.793010777	-0.217131768
C83	2.903260920	3.808577018	3.148957320
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C85	1.700292399	2.931786205	3.537821895
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C92	4.608816582	11.241663040	3.883082127
C93	4.095095417	12.251972877	4.894823566
C94	3.527355252	11.014655110	2.789214371

C95	3.977259647	10.008396964	1.754668662
C96	4.909726082	10.372503352	0.767424910
C97	3.541007498	8.673805478	1.787485629
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C99	4.035913183	7.723033738	0.886665749
C100	4.966360166	8.108308635	-0.085900505
C101	5.987115213	-8.836829905	-1.390884787
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C104	6.355953989	-4.146782360	-2.197421483
C105	7.371924771	-2.641233030	-0.550317704
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C107	7.847972425	-3.584279223	3.136277828
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C116	5.626231392	-0.094535378	-5.627593796
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C118	5.187461984	-0.211641394	-3.130179796
C119	3.863732439	-1.577946837	-4.619996335
C120	4.584106247	-0.838655495	-2.036272952
C121	3.265507894	-2.208338846	-3.525771857
C122	3.646177887	-1.855675842	-2.228764279
C123	0.471799976	-10.859919261	1.469222632
C124	-0.537487215	-11.279133972	2.550149785
C125	-0.185584317	-10.298488724	0.197458841
C126	0.755357092	-9.718527593	-0.815780873
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C132	-3.509649787	-5.663040233	-2.040376352
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Fe139	2.162999490	-5.290396062	0.801294586
Fe140	0.984663130	-1.600111520	1.664412537
Fe141	1.276701975	-3.314103192	3.626496597
Fe142	3.366487791	-3.499460908	2.139397519
Fe143	3.221195256	-1.386470003	3.707232738
Fe144	0.049716708	-5.090179853	2.245083778
Fe145	0.269954765	-3.719114416	-0.029731257
H146	-3.524143993	-0.753429126	-8.084368392
H147	-1.920778301	-0.505653580	-8.289687417
H148	-2.910569150	3.449943928	-9.403864407
H149	-2.254882781	1.246506231	-9.835449715
H150	-3.977736001	0.881204438	-9.881839604
H151	-2.791129263	4.234474286	-6.704461666
H152	-5.756515102	3.666975993	-8.647582647
H153	-3.333207733	5.255786868	-8.056504444
H154	-7.982252606	3.701519559	-7.975899984
H155	-5.997667139	1.688036572	-6.884094366
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H158	-4.509007279	1.959051452	-4.912282589
H159	-6.239176629	-0.200485840	-5.551381950
H160	-5.941097913	5.857405841	-1.435224408
H161	-5.624979872	4.296820714	-3.862745058
H162	-7.786963487	0.407433607	-4.913116544
H163	-3.277914600	2.757024230	-3.118342574
H164	-8.274091127	3.735082218	-3.252176556
H165	-6.777622209	6.104240363	-2.990067523
H166	-5.307694966	-0.520780915	-0.658845830
H167	-3.535113447	-0.552281523	-0.519409757
H168	-4.527122616	-1.418547610	0.671424227
H169	-4.423058974	1.630106972	0.269025324
H170	-10.495988682	3.350863769	-2.734366893
H171	-3.342498271	4.419090176	1.736808923
H172	-7.855337573	4.768337768	1.507381996
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H176	-3.701931676	-1.996617266	9.191312088
H177	-2.992112517	6.158630599	1.847237878
H178	-4.623222798	7.741740061	2.900001706
H179	-3.050280204	5.171001345	3.327410581
H180	-4.800867132	6.746242576	4.365335438
H181	-5.429732750	5.842572261	1.492676595
H182	-5.280459854	4.165252511	4.054134856
H183	-5.486254057	3.418500860	1.229189567
H184	-3.286337407	1.656869838	2.535705548
H185	1.833609381	1.919842052	3.117485156
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H187	0.605365590	2.935479331	5.174055842
H188	-1.978467817	3.502456878	5.869899428
H189	0.342750223	0.891053977	6.411720847
H190	-0.342662872	-1.432697328	6.904914575
H191	-4.487467626	-0.220205594	6.820972713
H192	-7.056855792	1.715871442	0.147356286
H193	-8.836967931	-0.692155839	-1.133347762
H194	-9.936845002	0.010828949	0.074651220
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H196	-10.353023061	4.374836669	-1.286879534
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H205	4.687216380	-6.817927197	-7.234271398
H206	5.092780960	-6.830751703	-5.513116932
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H209	6.471584309	-5.035761767	-7.697121710
H210	1.087367107	-0.115211999	-4.447352798
H211	-1.521033679	-0.962876411	-5.807807609
H212	6.759269303	-2.806919701	-4.868397693
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H224	-2.787379550	6.905224126	-4.264179855
H225	-0.575776066	4.991502452	-4.857778848
H226	0.589533259	7.701280713	-2.185527387
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H229	1.020332406	9.973322895	-3.230119798
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H248	4.885896410	4.683679539	-2.435014658
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H252	7.913997237	7.006850991	5.720657270
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H259	2.805185020	8.350539082	2.529532116
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H261	5.857677796	0.815653590	2.267679238
H262	6.331627608	1.676483443	4.589462796
H263	5.468730088	2.177465455	0.186123993
H264	0.965227057	4.510697108	-6.716105857
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H266	2.305287532	2.195904607	-6.142885273
H267	7.603703876	1.028420528	2.095634424
H268	3.729107721	6.679731241	0.972441756
H269	4.245949140	5.601979636	-4.295917474
H270	7.565778421	3.780944888	7.023241762
H271	9.937700174	3.494887327	-0.323485581
H272	8.792015986	6.763931155	-0.352767986
H273	1.039723656	-0.183913966	-7.008912580
H274	-0.954393585	1.426406695	-6.133223142
H275	5.260139653	11.405959225	0.711303522
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		C3	-2.707642136
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Fe(141)	2.362	C5	-6.495779967	4.892859026	-7.495421076
Fe(142)	-2.695	C6	-6.845008391	3.713556392	-6.578924984
Fe(143)	3.169	C7	-6.240947602	1.449145707	-5.862566593
Fe(144)	-2.460	C8	-5.667924174	1.692125654	-4.463775679
Fe(145)	0.320	C9	-3.914513583	2.684935658	-3.098628745
		C10	-4.798781987	3.631280036	-2.273307419
		C11	-6.270697139	5.565338640	-2.246494889
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		C13	-9.644806244	3.793408100	-2.546423440
		C14	-9.801823673	2.447078447	-1.829638456
		C15	-8.902020125	0.183971265	-1.499123189
		C16	-7.936106668	-0.176610999	-0.368072116
		C17	-5.906948571	0.474096250	0.882382196
		C18	-6.037386479	1.428791418	2.081306803
		C19	-4.485784059	0.456756846	0.255255920
		C20	-3.395251251	0.318791363	1.323347084
		C21	-4.367310949	-0.658568799	-0.789403591
		C22	-6.049019106	3.761465627	2.871832437
		C23	-7.533322122	4.030626534	3.182726442
		C24	-5.258154920	5.048446408	2.539937180
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		C31	-7.273046270	-8.071333941	0.197705201
		C32	-7.993513020	-8.437450219	1.509960632
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		C34	-5.864991112	-6.222467825	1.314511222
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C92	3.733401974	10.490113126	6.251630165
C93	3.183954999	11.321582834	7.400353613
C94	2.701338175	10.463374339	5.091787711
C95	3.211297509	9.669455976	3.912266608
C96	4.110188101	10.242541947	3.000735540
C97	2.859366453	8.319758489	3.740893676
C98	4.650062714	9.497042414	1.951027046
C99	3.409682851	7.550996439	2.710720538
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C101	6.457320149	-8.322005212	-2.187645558
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C104	6.516979496	-3.570528240	-2.087170118
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C106	7.803845165	-2.575752368	1.267171957
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C108	8.550191401	-5.051365690	3.558984698
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C110	7.292950277	-1.804054392	-6.551160743
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C112	5.202392039	-5.056709333	-6.804936068
C113	3.719848969	-5.356087225	-6.828080688
C114	7.438458352	0.193088998	-5.139372919
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C116	6.081080088	0.927223214	-5.011961672
C117	5.177637719	0.254626201	-4.013890947
C118	5.337371279	0.463954532	-2.633905207
C119	4.244612808	-0.700753054	-4.448315004
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C121	3.533043117	-1.477670463	-3.529211749
C122	3.742570206	-1.302937070	-2.158644854
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C126	1.115607533	-9.473519468	-2.126234396
C127	2.013228345	-10.019797746	-3.020241051
C128	2.135245521	-7.810948292	-3.108350951
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Fe141	1.063802915	-3.845074476	3.276591742
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Fe(141) 2.397	C3	-3.416396433	7.557040314	-4.318139805
Fe(142) -2.752	C4	-4.855889227	7.284807336	-3.883570422
Fe(143) 3.180	C5	-7.206839272	7.099782923	-4.514563143
Fe(144) -2.463	C6	-7.459164997	5.632535122	-4.142436034
Fe(145) -0.705	C7	-6.736045593	3.309769767	-4.452440770
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	C38	8.171834179	-7.478215807	5.667340227
	C39	-4.808136952	-1.045877706	-3.414156222
	C40	-5.137073523	0.289710063	-2.735287953
	C41	-3.347487352	-1.401230245	-3.047096452
	C42	-2.960471425	-2.892434813	-3.126207758
	C43	-2.535541694	-3.399686099	-4.498328713
	C44	-5.152599380	2.742090104	-3.046085463
	C45	-6.407161819	3.070471329	-2.233231067
	C46	-4.967345270	3.707516707	-4.246466133
	C47	-8.784226035	2.597628193	-1.854192547
	C48	-8.755467998	2.040492787	-0.424562859
	C49	-7.518689008	0.723205046	1.238679787
	C50	-6.409215796	1.418139616	2.037739555
	C51	-4.711070498	3.181798011	2.114235203
	C52	-5.518610302	4.233773407	2.893525385
	C53	-3.791615783	3.997072717	1.185614939
	C54	-2.690128296	3.278767388	0.476810187
	C55	-1.744558304	2.394469182	0.954939492
	C56	-1.319032879	2.877807509	-1.157254161
	C57	-7.127527471	6.051825678	2.609048113
	C58	-7.684135036	5.847363560	4.016676166
	C59	-8.268284434	6.386714613	1.620774778
	C60	-8.791227164	7.792966103	1.648509400
	C61	-8.885338142	8.708752831	2.677917576
	C62	-9.690970404	9.571111548	0.801579941
	C63	7.071412969	-0.997638819	6.496095186
	C64	8.001670973	-2.189823022	6.374083364
	C65	5.824513726	-1.300034572	5.629697928

C66	4.773407806	-0.218759295	5.735430108
C67	3.848367508	-0.206241421	6.797593651
C68	4.684867921	0.802676710	4.771699222
C69	2.868338522	0.785691912	6.897045654
C70	3.713935049	1.801141598	4.859146894
C71	2.804700044	1.789973872	5.922269973
C72	5.793610926	6.252996323	2.732017674
C73	4.938496621	7.486614439	2.415113380
C74	5.035359880	4.971464357	2.351321244
C75	4.626746876	9.428043037	0.937050999
C76	3.315812782	9.178433142	0.188389767
C77	1.855699655	7.513662949	-0.906636768
C78	0.824112503	7.022542565	0.132305815
C79	2.163812098	6.466271350	-1.992227167
C80	0.975324270	5.857259234	-2.743640391
C81	0.231517159	6.769640683	-3.733003129
C82	-1.059929284	8.809106644	-3.100287502
C83	0.339724383	5.687999249	2.107089463
C84	0.009740379	6.698177753	3.221706203
C85	0.817429812	4.385803592	2.765204486
C86	0.953119978	8.332901163	4.777752126
C87	0.599100000	9.815614350	4.772885930
C88	-0.172671604	11.764932716	3.492039004
C89	-1.586500444	12.162733943	3.965531835
C90	0.086029009	12.284135020	2.062056794
C91	-0.850964071	11.644432825	1.041928261
C92	-3.878369924	11.418968008	4.387985877
C93	-4.062022281	12.061125389	5.756554599
C94	-4.699344379	10.103579845	4.318848248
C95	-4.635695763	9.463736351	2.949914728
C96	-5.502353244	9.876297161	1.926083546
C97	-3.670835233	8.488293554	2.648748091
C98	-5.405686661	9.343687931	0.638264982
C99	-3.540642165	7.964121038	1.359707771
C100	-4.415935849	8.397000763	0.364720151
C101	6.779471024	-1.596041765	-8.227294132
C102	5.290276973	-1.292643351	-8.179766402
C103	3.479922320	-0.237660956	-6.853147934
C104	3.179481927	1.262772624	-6.976884597
C105	3.513546146	3.461455204	-5.943288536
C106	4.702308652	4.325123757	-5.531236188
C107	6.861381558	4.511731423	-4.391395810
C108	8.131087775	4.408842530	-5.206407663
C109	0.547878599	-0.292732389	-10.402816744
C110	-0.594825286	0.677947175	-10.084036940
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C112	1.328452007	-2.669396999	-9.963716749
C113	1.598846042	-3.712808843	-8.900862214
C114	-1.382107647	2.588698206	-8.774494831
C115	-0.810348510	3.991560455	-8.705943117
C116	-2.225123472	2.171330336	-7.544385115
C117	-1.338758498	1.789102390	-6.390352255
C118	-0.774239026	2.774844509	-5.564851683
C119	-0.940036264	0.451751846	-6.219137714
C120	0.231494402	2.437683579	-4.655266707
C121	0.060393913	0.115389478	-5.302025864
C122	0.676890567	1.118589940	-4.549807497
C123	8.479765961	-5.605232912	-3.775562548
C124	9.309441637	-6.226333479	-2.638768680
C125	7.088323105	-6.241536824	-3.922131438
C126	6.142509317	-5.563162244	-4.866564347
C127	6.101609857	-5.698486488	-6.239808387
C128	4.396265651	-4.457164639	-5.576410278
C129	9.921803276	-8.161335190	-1.296936666
C130	11.408477305	-7.971909473	-1.502811433
C131	0.194825890	-6.810626097	-1.779916166
C132	1.566548051	-6.717814383	-1.171272528
C133	2.738649540	-6.698728008	-2.236715721
C134	2.612963521	-7.933321416	-3.178382293
C135	3.809775786	-8.058533025	-4.137013180
C136	3.863188207	-9.375447509	-4.856910026
C137	4.063219267	-6.895234722	-1.438305186
C138	4.082057481	-0.541860417	-1.265666014
Fe139	4.735069647	-1.370682159	-2.890885818
Fe140	2.575881986	0.902192058	-0.913705986
Fe141	4.869376646	0.205778773	0.389176844
Fe142	4.907895169	1.036477877	-2.069485764
Fe143	4.310411090	2.801049544	-0.182783569
Fe144	4.956394730	-2.194265881	-0.489558104
Fe145	2.366946208	-2.167691673	-1.245246419

H146	-5.861875798	-5.496370815	-3.897255006
H147	-5.720690663	-4.168400147	-4.843546717
H148	-9.518466415	-3.020724500	-3.371557720
H149	-8.080655973	-3.898225063	-4.993447871
H150	-8.300315421	-5.442947512	-4.177490870
H151	-8.232150122	-1.648046677	-1.277476262
H152	-9.922044752	-4.799377624	-1.064150944
H153	-9.990349124	-1.870571488	-1.445044927
H154	-10.105635094	-6.259927841	0.726869744
H155	-7.452279121	-5.588145223	-0.534700265
H156	-9.985680099	-4.880472147	1.844964507
H157	-3.616786358	-2.710163470	1.403970468
H158	-5.886089226	-3.720316537	-0.049689548
H159	-5.320069048	-6.494446290	-0.268108058
H160	-6.606691586	-1.406207048	4.843983307
H161	-7.128597858	-2.810661368	2.357306201
H162	-5.734452066	-7.062255767	1.367269345
H163	-4.981751185	-1.758788264	0.774422559
H164	-7.057403122	-4.943382110	4.128349471
H165	-8.061981138	-2.351275499	4.427264818
H166	-1.513621777	-4.656709970	2.389103298
H167	-0.954951029	-3.293558817	1.394337304
H168	0.188733707	-4.126176491	2.475248921
H169	-2.232719532	-2.431066283	3.343241630
H170	-7.109295774	-6.674953892	5.653474277
H171	-2.797370153	0.404199522	4.692286200
H172	-4.465382762	-2.496499344	7.615917997
H173	-4.054365518	0.967329467	8.836624661
H174	-0.425051446	-1.048030789	2.449611904
H175	0.783604902	-1.840685841	3.463627125
H176	6.742300296	-0.946509809	7.552178608
H177	-3.524748302	1.918365595	5.269990167
H178	-4.296076281	2.213239261	7.590595489
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H180	-2.659325763	1.867812573	8.202738981
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H182	-1.506462134	-0.368108148	7.451789731
H183	-3.106449927	-1.867610014	5.496448977
H184	-0.469452608	-0.818943333	4.208780412
H185	1.185557890	3.696808295	1.984304364
H186	-0.059148327	3.929881709	3.251456584
H187	1.755841222	4.013726512	4.451888392
H188	1.259818546	2.664696054	6.713139112
H189	3.636813657	2.563426201	4.083458899
H190	5.359137426	0.796069501	3.911598741
H191	3.880161802	-0.995870410	7.553232361
H192	-3.123499773	-4.336343374	4.823560628
H193	-2.766821798	-7.450467545	4.031474615
H194	-2.790096163	-7.555060770	5.802457572
H195	-4.627145858	-5.949590489	4.106726186
H196	-6.761363339	-5.541885451	6.979332696
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H198	-0.188127456	-3.971805195	4.994013155
H199	-4.891198748	-2.251998910	10.405983366
H200	-5.242473887	-3.678537795	9.392912798
H201	-2.533872537	-4.090461932	9.732881595
H202	8.865299562	-9.288960178	4.747710387
H203	-1.177243958	-4.631209258	-5.397161197
H204	0.295815135	-8.722736865	-1.543121912
H205	0.742858695	-3.146374669	-10.762787612
H206	2.278003992	-2.319513433	-10.394003304
H207	-0.503699128	-1.794120011	-9.211559655
H208	0.112572263	4.144365394	-9.315474555
H209	0.266643228	-0.700018174	-11.386231844
H210	-2.670558339	-0.794397794	-3.670202127
H211	-3.811686239	-3.516029377	-2.800657459
H212	0.551691127	1.657631362	-8.658788086
H213	-2.067948223	2.621822896	-9.644862741
H214	2.210381610	0.702686197	-9.664648152
H215	-0.6797182700	-4.541500480	-3.661677910
H216	0.947523219	-1.139135888	-8.441235205
H217	2.513456457	-0.226538811	-10.986002990
H218	-5.963079547	-1.152077999	-5.121102802
H219	-3.185276926	-1.086632715	-2.006034502
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H221	-2.151001005	-3.081419701	-2.406391728
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H223	-1.5992260694	1.940454217	1.930108048
H224	-8.446567111	0.881432001	1.803791613
H225	-7.006262079	0.983158945	-0.809086390

H226	-6.663523732	4.517529169	1.202723683
H227	-8.585957206	8.668148553	3.719221076
H228	-8.098850205	4.826376665	4.193785024
H229	-9.092573047	5.664446593	1.763494460
H230	-6.395301846	6.875444588	2.638998731
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H232	-3.358627005	4.797126814	1.810095393
H233	-4.411520112	4.494027453	0.424738765
H234	-9.660823087	10.701856124	2.606014058
H235	-7.886017541	6.212694128	0.602000147
H236	-5.751367289	2.471919436	0.382681812
H237	-7.322337388	-0.358629959	1.238057100
H238	-9.054694351	3.658942213	-1.762377852
H239	-0.814972793	2.862509642	-2.119352175
H240	-9.592466876	2.097041517	-2.403383246
H241	0.045327329	1.697804748	-0.101308835
H242	8.419378972	0.530809795	6.723271417
H243	7.074559817	0.958280143	5.895004355
H244	2.230985409	5.786492549	1.047967852
H245	-0.613245845	5.480998522	1.599169132
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H247	-2.822520620	5.022846891	-1.677541695
H248	-4.276574188	5.300783109	-3.287558515
H249	-3.551217227	6.431276635	-1.518176840
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H251	-5.772183179	3.523025076	-4.976481427
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H253	-0.100814837	13.366695501	2.065595338
H254	0.698310452	10.437670867	0.280500961
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H256	-0.400962460	10.651740609	-3.701166493
H257	-0.171192140	6.167179410	-4.561437944
H258	-6.097875819	9.666780545	-0.142981435
H259	-3.002409999	8.109378465	3.426313001
H260	-2.684629037	8.737392263	-1.835676299
H261	2.718869160	5.635370274	-1.528797100
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H263	0.253578206	5.408510933	-2.043637494
H264	-7.513164217	1.782192066	-3.378082880
H265	5.276742287	10.030970243	0.288790179
H266	-4.905461554	1.149387950	-4.528451455
H267	2.848992255	6.934662064	-2.718223407
H268	-2.746884954	7.252527242	1.128343084
H269	-5.028197567	8.111385141	-1.463322585
H270	4.364349147	10.038564810	1.812337382
H271	0.304410225	9.327346060	-4.554895458
H272	-2.413979898	10.250285493	-2.612271545
H273	-4.398785966	-1.681836227	-5.314113737
H274	-5.463765266	-1.789243423	-2.922350675
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H276	-4.315033841	2.883457191	-2.343289165
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H278	0.936921918	7.482218865	-4.178630578
H279	1.387552137	5.021160168	-3.326271818
H280	-1.636393529	6.903741010	-2.691669608
H281	0.221664653	7.841374022	5.437523736
H282	0.137312425	9.746194381	2.774170600
H283	0.512142610	12.289390762	4.174362423
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H290	6.532189254	-2.520773456	-10.017647210
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H292	5.301201348	6.268996571	4.709711607
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H294	4.147192075	4.867997771	2.990937630
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H302	3.190947379	3.796724167	-6.936136099
H303	0.368096761	-0.925940886	-5.176796510
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H307	2.566950730	-5.966900371	2.163905247
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H313	2.932011309	-12.743404857	0.970384211
H314	1.485204924	0.886259837	-3.859067975
H315	3.392778702	-13.473145953	3.759013697
H316	2.007175765	-13.511585964	2.885989978
H317	4.102894660	-4.146591570	2.349784100
H318	0.692791173	3.201248711	-4.026565291
H319	-1.409082535	-0.326531186	-6.827169025
H320	7.002493331	-10.103429539	-2.110404288
H321	7.212188518	-7.282467554	-4.269591844
H322	5.740212523	-8.683065168	-0.624485379
H323	6.488611745	-10.394719470	-3.538948180
H324	8.000405496	3.985413141	-6.232084924
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H326	1.739699970	-7.546880918	-0.468718847
H327	5.539030681	-0.285705828	-6.399141765
H328	2.549534107	-8.838696902	-2.554091047
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H345	7.407834474	-8.346318332	0.782489082
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	O473	-2.964926937	-3.498396429	6.417206903	
	O474	-5.143377908	-4.028653263	6.180333970	
	O475	-2.180621728	-4.980328663	4.402631521	
	O476	-5.772205781	-1.453755303	9.439894276	
	O477	-3.685933835	-1.018845851	7.567242633	
	O478	5.386132951	0.881722502	-4.241473739	
	O479	-5.466459927	-6.577067201	10.044277182	
	O480	-6.087590350	-4.121395445	8.703651851	
	S481	4.510525917	4.038145845	3.176802889	
	S482	3.277839951	0.474277243	2.339979303	
	S483	0.743389961	-3.899002303	3.689983149	
	S484	0.779869946	2.767844251	3.417105224	
	S485	0.582576173	-1.371689215	1.098727734	
	S486	3.718094855	-2.139539707	5.340622627	
	S487	-2.156512926	-1.651289475	4.144315116	
	S488	3.086841346	1.527657478	5.810940929	
	S489	0.209297239	-2.273409824	6.932339464	
	S490	-1.022861431	1.210422223	6.257603381	
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Fe(139)	2.435	C1	-2.198880321	-5.183028445	-8.037343413
Fe(140)	-0.022	C2	-2.567225358	-3.701439951	-7.906438777
Fe(141)	1.901	C3	-2.542960923	-1.487149960	-8.974091214
Fe(142)	-2.607	C4	-3.976174727	-1.037378585	-8.702389831
Fe(143)	2.555	C5	-6.361319046	-1.499168338	-8.909935823
Fe(144)	-2.242	C6	-6.737334408	-1.567136302	-7.425104764
Fe(145)	-1.111	C7	-6.260857835	-2.604614809	-5.254138111
		C8	-5.593987674	-1.465115404	-4.478090402
		C9	-3.660799873	-0.008715597	-4.213333919
		C10	-4.365982295	1.343293543	-4.399454932
		C11	-5.619735422	2.812284114	-5.882910673
		C12	-7.016857404	2.892435833	-5.250227541
		C13	-9.209409945	1.828089148	-5.008110620
		C14	-9.518030764	1.431657033	-3.560572833
		C15	-8.903500436	0.001647193	-1.655826778
		C16	-7.958196632	0.440369848	-0.535237268
		C17	-5.885787269	1.685754460	0.011034322
		C18	-5.877004158	3.221455377	0.093016966
		C19	-4.495810829	1.070485239	-0.308412734
		C20	-3.397555409	1.651727085	0.590531810
		C21	-4.538859784	-0.456533088	-0.192170189
		C22	-5.482076742	5.355926002	-1.062626512
		C23	-6.900533840	5.949537256	-1.164027764
		C24	-4.530976614	5.875553263	-2.167325271
		C25	-4.598692183	7.403817721	-2.275931006
		C26	-3.090714794	5.420701989	-1.900231344
		C27	-9.047220744	5.983177922	-2.291259653
		C28	-9.854547275	5.888253805	-1.011169356
		C29	-10.355883518	-7.396649869	4.512289100
		C30	-9.169240436	-6.752134217	5.234057539
		C31	-8.132731806	-4.540549521	5.761152257
		C32	-8.807490454	-3.757459121	6.902264095
		C33	-7.520937293	-3.605909771	4.701946416
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		C35	-5.672753585	-1.995378175	4.119989859
		C36	-4.357204448	0.125789028	4.289466092
		C37	-8.665214338	-3.110569649	9.260372400
		C38	-7.967866877	-1.801520265	9.566478518
		C39	0.476511608	-2.636080273	-5.277129267
		C40	0.991660803	-1.212287125	-5.546964894
		C41	0.246494021	-2.790786591	-3.756857907
		C42	-0.672483738	-3.951266251	-3.312350887
		C43	-0.007072933	-5.315737466	-3.162130854

C44	3.054539214	0.135658114	-5.813069759
C45	2.625862086	1.038525044	-6.972568768
C46	4.572727277	-0.178408959	-5.827565885
C47	1.642515625	1.154948953	-9.214285984
C48	0.328209001	1.897937358	-8.941117135
C49	-1.562035640	2.222769329	-7.407217406
C50	-1.354850377	3.224159326	-6.263006123
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C52	0.299247312	5.436775583	-5.014009384
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C57	1.560787112	6.651967040	-6.754727386
C58	0.384792423	7.450770830	-7.314605131
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C68	-1.498869912	3.842195626	5.706953346
C69	-3.182269188	5.419056830	4.132086605
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C71	-1.791545654	5.518130736	3.995132563
C72	4.550504293	5.253761710	6.065052486
C73	5.479700884	5.877574183	5.016867893
C74	3.517286984	4.345486233	5.381486484
C75	7.753613170	5.918782576	4.080075029
C76	7.648009886	5.372496122	2.656176158
C77	6.543147038	3.764358738	1.144513537
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C86	3.725735531	8.892189282	1.746617513
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C92	5.219619621	11.201373750	-3.303627886
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H167	-3.565197143	-0.886826713	-0.473417320
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Fe(142)	-2.647	C4	-5.291884961	3.687246051	-7.078006924
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Fe(144)	-2.317	C6	-7.869993645	2.221853952	-6.209920010
Fe(145)	-1.025	C7	-7.124504979	0.123579566	-5.183878702
		C8	-6.341279979	0.620817439	-3.964820230
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		C10	-5.179950888	2.872295553	-2.306927829
		C11	-6.747594122	4.736275658	-2.323345827
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		C14	-10.169709334	1.710644459	-1.049283226
		C15	-9.202661940	-0.489570075	-0.532461868
		C16	-8.119243095	-0.642396762	0.538764237
		C17	-5.863042113	0.033856134	1.271721343
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		C22	-6.034442300	3.496793555	2.950161569
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C100	3.889603975	8.634812757	-0.006349828
C101	6.391223452	-8.510500424	-1.878312145
C102	5.935079603	-7.317269135	-2.701916385
C103	5.291926730	-4.927772345	-2.614509157
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C105	6.859578140	-1.831733389	-1.044062878
C106	7.821520716	-1.920569841	0.140591753
C107	8.494917793	-3.105117771	2.177300904
C108	9.406137940	-4.313323007	2.170346427
C109	6.596337969	-4.315487447	-6.988827774
C110	6.987068372	-2.837083706	-7.121679470
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C113	3.251293842	-6.091999500	-6.121312609
C114	7.539520444	-0.754259632	-5.971137579
C115	8.544116640	-0.505167882	-4.865808879
C116	6.424526656	0.310256904	-6.101248793
C117	5.524984918	0.381834559	-4.897825340
C118	5.668000808	1.414749750	-3.957549809
C119	4.571308673	-0.620823396	-4.658716206
C120	4.908145328	1.417058299	-2.785128541
C121	3.838688464	-0.638417015	-3.470050948
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C123	1.473966969	-10.808809699	1.468884427
C124	0.663656212	-11.218752309	2.705947670
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C126	1.334844046	-9.604467107	-0.791352974
C127	2.028022246	-10.285385212	-1.772337686
C128	1.992012604	-8.124095669	-2.255446093
C129	-1.300764881	-12.289057061	3.652653764
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C132	-3.219370580	-5.845660425	-1.818237429
C133	-2.186920322	-7.041614566	-1.697454067
C134	-2.543406774	-8.145396924	-2.734134318
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	O447	-0.885974452	2.558274656	6.892834553
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	O459	7.069462259	-3.455974557	-3.374832401
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	O467	-0.761374522	-13.347541203	5.754902432
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	O472	-1.390108863	-7.595245811	0.511924748
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	O474	-0.894569300	-6.595533652	-1.865268411
	O475	-3.519660899	-9.647155837	4.024976868
	O476	-1.901777557	-7.437523970	3.276536512
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	O479	-3.799914650	-10.542581913	1.379113197
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	S481	4.156889934	-1.232587910	1.484347818
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	S487	4.014881417	-3.505826077	4.293047762
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	Fe(143)	1.377	C5	-6.273141544
	Fe(144)	-2.364	C6	-6.579899088
	Fe(145)	0.198	C7	-5.873575600
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			C9	-3.633891697
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H220	4.434228910	-9.824034021	1.383990182
H221	-0.622042216	-3.933433570	-2.124036574
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H223	-0.950574672	1.467582769	-2.382010158
H224	-2.312976087	2.135262277	-8.307032670
H225	-0.095323272	0.463282372	-7.205269272
H226	0.801892987	4.297904063	-6.693428192
H227	1.441909868	9.147810626	-8.288019023
H228	-1.055781782	6.157597612	-8.230831134
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H230	1.157932255	7.168156727	-6.318879465
H231	5.050340061	8.471346656	-10.398878336
H232	0.864076006	4.430960615	-3.004387697
H233	1.695833959	3.765418323	-4.411246308
H234	3.350086291	10.207078511	-9.613722422
H235	2.667831261	5.477849274	-7.545085064
H236	-0.017352322	1.939104715	-5.530006109
H237	-2.527473269	0.884751113	-7.078207722
H238	2.040034520	1.720913586	-9.642975041
H239	2.986927206	0.015550654	-1.865984631
H240	1.348732476	0.147537390	-10.081731801
H241	0.560251660	-0.338270810	-1.303629076
H242	-3.014034175	4.594291390	9.250627580
H243	-2.362565337	4.429113785	7.761081410
H244	3.647119789	4.766350414	1.998051087
H245	2.137100578	5.013728427	-0.440872253
H246	3.358628300	7.457394404	1.804665878
H247	3.817497101	2.571167146	-3.476155800
H248	5.002737883	1.873479001	-5.234133235
H249	4.422202447	3.827405627	-4.264762962
H250	4.827004585	-0.465261894	-4.948455882
H251	4.845197004	-0.566278108	-6.729203686
H252	7.177673749	9.800600112	0.285372762
H253	7.597307819	11.042982134	-0.923458335
H254	7.085007484	7.612840824	-0.442843511
H255	6.999877546	7.190998126	-2.141813897
H256	9.786352669	4.907093450	-2.526497777
H257	7.363179740	1.325529343	-1.732245882
H258	5.424881085	7.375493880	-6.620742302
H259	2.196918836	8.375874359	-2.964876526
H260	6.540710702	5.205595957	-3.862868957
H261	5.260293970	2.688233542	1.681888866

H262	5.745741213	4.813952079	2.937011916
H263	5.055408789	2.338528129	-0.805271985
H264	2.109946618	-0.750429097	-8.064276639
H265	7.981632456	6.922432923	3.969443377
H266	2.983437647	-1.971860197	-5.675990461
H267	7.016493303	2.804571053	1.529019981
H268	3.216810738	6.127978756	-3.131808475
H269	5.255393498	5.200602401	-5.878495825
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H275	4.480608952	9.659618328	-6.405634542
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	O424	-4.283214520	-0.780383644	-7.952576709
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	O426	-6.009898100	-1.657389573	-3.321359162
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	O428	-7.887775461	2.827644148	-4.609590676
	O429	-10.687380960	0.487481183	-2.771689487
	O430	-8.091978263	-0.711310135	0.850221084
	O431	-6.579307397	3.092806671	1.120269239
	O432	-8.145837631	5.884958110	-0.471655911
	O433	-11.616673269	5.108936684	-0.684222173
	O434	-7.300024897	-8.220713176	5.990766187
	O435	-9.343565855	-4.092510186	6.973855824
	O436	-7.758560845	-1.794521328	10.792648781
	O437	0.238665075	-0.430204585	-5.483924932
	O438	1.663247199	-5.760326192	-3.651948865
	O439	2.417637482	2.240428016	-7.045532964
	O440	5.232364150	1.293881370	-6.011437654
	O441	-0.474780568	2.229248204	-9.849256642
	O442	-2.619505895	3.616868363	-6.276363019
	O443	-0.806909791	6.212511214	-4.725755280
	O444	-0.758612969	8.127505046	-7.799417893
	O445	-5.818178516	2.165850344	9.221644880
	O446	-1.961812331	6.217007157	2.666047314
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	O448	7.425503025	6.971301775	1.270103631
	O449	4.593241371	5.250503220	-1.022013944
	O450	1.356998156	7.435317666	-0.653618804
	O451	0.947788188	6.135404590	2.498167312
	O452	3.185241080	11.537926429	0.865135616
	O453	5.617333716	12.715647919	-2.118836498
	O454	6.941524290	9.563153398	-3.000443871
	O455	3.173801004	13.722699852	-4.748532345
	O456	4.903462674	5.334208005	-4.977315321
	O457	6.676617083	-7.475899974	2.823902173
	O458	7.331425092	-3.954059535	0.651374357
	O459	8.515161171	0.248281482	2.791839089
	O460	8.301248242	0.026386653	7.620060715
	O461	7.596033817	-6.489273676	-3.771613571
	O462	3.013767470	-8.053475681	-0.615257800
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	O469	-2.438835620	-11.187058845	4.391374554
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	O472	-3.923223284	-6.637772047	4.556428980
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	O474	-4.858239118	-5.455908154	8.498510554
	O475	-2.812981990	-4.091147897	7.108579786
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	O477	-3.603454282	-10.394435025	7.023939876
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	S480	3.401369364	0.279646403	2.566410032
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	Fe(139) 2.327	C1 -2.655651330	-3.050113620	-8.938677576
	Fe(140) -1.120	C2 -3.267982828	-3.615772196	-7.652598380
	Fe(141) 2.773	C3 -5.343284097	-4.179771587	-6.455551622
	Fe(142) -2.662	C4 -5.002186605	-5.579219765	-5.948588183
	Fe(143) 2.869	C5 -4.303358262	-7.857830655	-6.476869689
	Fe(144) -2.280	C6 -2.975630977	-7.909061164	-5.709569937
		C7 -0.773363579	-6.874500742	-5.408179510
		C8 -0.938665122	-6.196943330	-4.045792708
		C9 -2.103532613	-4.533121033	-2.701616962
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		C11 -4.277987079	-7.262002039	-1.156657362

Fe(145) 0.959
xt constrained model

C12	-3.313891940	-8.357764749	-0.684817641
C13	-1.755829728	-10.119802384	-1.343286908
C14	-0.382090872	-9.822263367	-0.725063740
C15	1.625571257	-8.408318568	-0.798356737
C16	1.839768010	-7.173282255	0.080720550
C17	0.875014156	-5.115040628	1.036075042
C18	0.225439060	-5.403020287	2.400442678
C19	0.333984389	-3.836265379	0.361974659
C20	0.218097244	-2.706622071	1.390049188
C21	1.219590243	-3.451277100	-0.828113144
C22	-1.826946115	-6.065172303	3.600111154
C23	-1.448534429	-7.500018435	4.024746437
C24	-3.347406015	-5.852010292	3.417599846
C25	-4.130537017	-6.416245972	4.609274473
C26	-3.663306939	-4.365391534	3.209328179
C27	-1.111730663	-9.801903454	3.305197978
C28	-2.061758900	-10.660622615	4.108661386
C29	10.638143690	-7.622418598	-3.081008414
C30	10.436242255	-6.432240873	-2.142733999
C31	9.159794727	-5.698793213	-0.116088409
C32	9.762271889	-6.204625899	1.209501203
C33	7.628477458	-5.573494270	-0.054708363
C34	7.114206823	-4.598227997	1.009240368
C35	5.641819897	-4.262674687	0.753994765
C36	4.099270237	-3.562180109	2.604663256
C37	11.253180472	-5.666161790	3.076955558
C38	10.660895655	-5.054999129	4.329590024
C39	-2.757117317	-0.353217839	-5.224375602
C40	-3.888599785	-0.166629378	-4.201035605
C41	-1.410212785	-0.206910530	-4.482639960
C42	-0.160443279	-0.750420664	-5.216562891
C43	0.503721435	0.238062912	-6.170736941
C44	-5.436236571	1.517775547	-3.240189165
C45	-6.686115979	0.644241119	-3.106144654
C46	-5.788663264	2.992443988	-3.560537055
C47	-8.254971528	-0.871231154	-4.223622964
C48	-8.011122035	-2.186099845	-3.470586635
C49	-6.378650544	-3.619269759	-2.326629135
C50	-6.078578824	-3.302594849	-0.856728456
C51	-5.805645429	-1.587796106	0.876301302
C52	-7.180016703	-1.707128284	1.567025067
C53	-5.359052707	-0.122812060	1.034792765
C54	-4.054056574	0.264268467	0.413943231
C55	-2.876619586	-0.440555399	0.276778735
C56	-2.635598580	1.591249267	-0.561798709
C57	-9.547263580	-1.078344895	1.386663625
C58	-10.064171141	-2.466822520	1.764994254
C59	-10.448156919	-0.431015189	0.314984254
C60	-11.754542809	0.126489578	0.799200642
C61	-12.495950084	-0.157216533	1.928668481
C62	-13.499543778	1.402799840	0.715799532
C63	5.510215979	-2.159235687	7.734810958
C64	7.000427081	-2.349665327	7.528452492
C65	4.840207212	-2.271977506	6.341500732
C66	3.337767393	-2.133919339	6.411661573
C67	2.513375059	-3.244030639	6.672332912
C68	2.721018086	-0.885959629	6.210952507
C69	1.120652280	-3.118894933	6.719851132
C70	1.334418916	-0.743757464	6.267446854
C71	0.536260969	-1.863698990	6.519592761
C72	0.223282938	4.259915853	7.849064255
C73	-1.151692953	4.931135750	7.733366051
C74	0.520821872	3.438346173	6.585476773
C75	-2.360358764	7.037219441	7.331307686
C76	-3.136168510	6.813936749	6.032229791
C77	-3.122971163	5.851868762	3.757700633
C78	-3.701537116	4.422008811	3.809297107
C79	-2.141681898	6.057182296	2.589026967
C80	-2.650770694	5.699084687	1.186659008
C81	-3.744654660	6.602797816	0.594558352
C82	-6.075471872	6.883422588	1.434922797
C83	-3.391442899	2.068508088	4.314364613
C84	-4.407387693	1.768955342	5.431643066
C85	-2.265919323	1.028908080	4.416294439
C86	-4.838738633	2.025352457	7.826506913
C87	-5.995342173	2.795344407	8.452547939
C88	-7.630499005	4.615019871	8.242416155
C89	-9.035402769	3.978838990	8.189946730
C90	-7.622067778	6.013458846	7.591256101
C91	-7.956934311	5.967104761	6.102912933

C92	-10.501812140	2.362722177	7.083367687
C93	-11.114892898	1.787188145	8.351780698
C94	-10.385652371	1.242924609	6.014894915
C95	-9.806980414	1.761079058	4.719276673
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C98	-10.079867154	2.992814591	2.632733474
C99	-7.879226480	2.192143759	3.282159371
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C103	3.354407690	5.950686439	-3.413085336
C104	2.185428148	6.740709564	-2.818896562
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C106	1.421290073	8.177094970	0.526466583
C107	2.923037905	8.470745181	2.431420417
C108	3.811459561	9.696205214	2.389651210
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C112	3.364035102	5.418257717	-7.582488397
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C125	9.755187795	1.812941500	-2.303913175
C126	8.791639586	2.582769551	-3.153458012
C127	9.092305867	3.487795620	-4.152459937
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H164	-2.725551851	-8.716100320	-2.638939399
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H249	-6.618875028	3.246395929	0.453266409
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O473	10.764507310	-2.633285641	0.932625129
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S478	0.387355348	4.439600329	5.035141725
S479	1.358195208	4.438282739	1.403106028
S480	4.181716888	2.549122775	-2.437947738
S481	1.563833897	1.307457649	3.301281212
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S483	4.779347647	5.280468969	0.130453151
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Fe(140)	0.023	C3	-4.143284995	-0.352072509	-8.335382918
Fe(141)	1.481	C4	-4.543962747	-1.818319256	-8.186333969
Fe(142)	-2.609	C5	-4.630123219	-4.053045041	-9.166023805
Fe(143)	2.056	C6	-3.705902945	-4.807544274	-8.200278546
Fe(144)	-2.400	C7	-1.474820287	-4.903398112	-7.192901185
Fe(145)	1.401	C8	-1.761312479	-4.465184973	-5.753304168
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		C11	-5.994019722	-4.380011742	-4.057175692
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		C13	-4.776749985	-7.973072743	-4.489684612
		C14	-3.703755091	-8.406519231	-3.479454891
		C15	-1.397880339	-8.064635900	-2.698771211
		C16	-0.990638010	-7.209766770	-1.497972165
		C17	-1.316937330	-5.095450835	-0.262261857
		C18	-2.417618918	-5.217969266	0.805842830
		C19	-1.065733978	-3.643824047	-0.726585454
		C20	-0.980331184	-2.691312279	0.468208583
		C21	0.197154682	-3.579296077	-1.592787682
		C22	-4.835598017	-5.050380516	1.287253273
		C23	-5.331011475	-6.509952055	1.304276834
		C24	-5.945063907	-4.031552841	0.932983967
		C25	-7.215608085	-4.293308498	1.750785914
		C26	-5.450378469	-2.597045216	1.150910805
		C27	-6.079630882	-8.457052172	0.062712864
		C28	-5.195001333	-9.411458264	0.838565265
		C29	7.446292607	-11.022695865	-2.617146313
		C30	7.434035156	-10.028096793	-1.455222992
		C31	5.992146621	-9.172463780	0.399628579
		C32	5.925879092	-10.096667680	1.630401785
		C33	4.686795254	-8.386598281	0.182118978
		C34	4.296617906	-7.483086668	1.356601151
		C35	3.223150975	-6.481186138	0.926678111
		C36	1.621341915	-5.338241321	2.480711082
		C37	6.774123275	-10.494157095	3.894379192
		C38	6.093003338	-9.855188918	5.085790554
		C39	-0.748323715	1.722307924	-5.709701682
		C40	-2.017020370	2.198788834	-4.986330429
		C41	0.176374429	1.105935771	-4.631549083
		C42	1.331776198	0.212098487	-5.138463148
		C43	2.617112320	0.958523996	-5.478370290
		C44	-3.019712420	4.168294192	-3.861344074
		C45	-4.484423802	3.922858514	-4.230238950
		C46	-2.693206122	5.680938025	-3.786401040
		C47	-6.107909671	3.473371325	-6.007190553
		C48	-6.656138809	2.121743554	-5.530638570
		C49	-6.155613242	-0.034399002	-4.470117690
		C50	-6.184805672	-0.090430151	-2.938505946
		C51	-5.924250493	1.104457395	-0.817011108
		C52	-7.393785909	1.416925081	-0.462426299
		C53	-5.086205356	2.228468381	-0.181931374
		C54	-3.595946050	2.148297206	-0.312012449
		C55	-2.737394904	1.070280438	-0.384481638
		C56	-1.572077869	2.947483058	-0.386592376
		C57	-9.257149796	2.954036080	-0.941917639
		C58	-10.309919234	1.858138793	-0.797072250
		C59	-9.627559857	3.912159700	-2.096665843
		C60	-10.641665367	4.972889981	-1.784613193
		C61	-11.741086869	4.958389501	-0.948799132
		C62	-11.560335763	6.925259835	-1.954302113
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		C65	1.205657221	-5.257098027	6.326907880
		C66	-0.084971186	-4.496729491	6.133023327
		C67	-1.285438099	-5.156745499	5.810248922
		C68	-0.117795695	-3.096267947	6.255448034
		C69	-2.473316739	-4.446258117	5.604091917
		C70	-1.296225000	-2.374133211	6.061600258
		C71	-2.472835429	-3.051827172	5.730212963
		C72	-0.741789503	2.153120500	8.543366893
		C73	-1.655376116	3.371714674	8.364608674
		C74	-0.471789901	1.504838529	7.179493924
		C75	-1.788211833	5.830275955	8.369652315
		C76	-2.118435276	6.243806916	6.933861389
		C77	-1.758656261	5.823297276	4.527209160
		C78	-2.828440484	4.847441928	3.990617073
		C79	-0.445609937	5.788186449	3.723576200
		C80	-0.544434134	6.064723404	2.218582502
		C81	-0.951556772	7.489432708	1.806495073
		C82	-3.156006797	8.611763430	2.109531147

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C85	-3.146874851	1.139354081	3.797106151
C86	-5.982238315	2.571366609	6.867163006
C87	-6.915888553	3.655053574	7.391863257
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C90	-6.843114340	7.358912068	7.164838927
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C98	-8.644930381	6.720811556	1.133236015
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C102	8.640266325	4.492516158	-0.534932564
C103	6.190720000	4.399285720	-0.891100532
C104	5.320567856	5.563740257	-0.403342546
C105	3.934420462	6.389583168	1.444197734
C106	4.061431603	6.619590063	2.948991447
C107	4.746883898	5.784908162	5.146387881
C108	6.048516645	6.345967507	5.683198383
C109	6.107301928	6.555554024	-4.739170728
C110	4.703066432	7.153586007	-4.904779646
C111	6.011387712	5.011066564	-4.810892996
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C113	7.360410983	2.852944609	-4.982354500
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C115	2.338370956	8.720896634	-2.677373071
C116	1.513380274	6.638157431	-3.956051588
C117	1.749887738	5.490099377	-3.009573904
C118	1.334112192	5.549331141	-1.668691369
C119	2.492461034	4.375653008	-3.432937018
C120	1.696346031	4.539825499	-0.769942900
C121	2.859295499	3.369114805	-2.532801565
C122	2.476231258	3.459104950	-1.191322999
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C130	12.327078168	-5.573086587	3.807274252
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C137	6.866543053	-4.279142351	-1.126959546
C138	3.630674774	0.051536173	2.160399648
Fe139	5.426075507	0.629800014	1.408255609
Fe140	1.481782670	0.235536692	2.325566832
Fe141	3.474846453	-0.502806191	3.984893048
Fe142	3.808785698	1.825285193	2.986718440
Fe143	1.708476385	1.724109778	4.577931676
Fe144	4.627442917	-1.703206338	2.106748940
Fe145	3.656480591	-0.506502940	-0.085180729
H146	0.841837926	-1.143695330	-8.817853258
H147	0.849991424	0.477450565	-8.579576192
H148	-3.090008283	0.603048904	-9.930309995
H149	-0.812814726	0.853090407	-10.214489153
H150	-0.693149182	-0.829960859	-10.726401507
H151	-3.943174729	0.016448061	-7.319125490
H152	-3.947520934	-2.237880359	-10.107312989
H153	-5.002967498	0.204336798	-8.732198378
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H156	-5.658647808	-4.215221008	-8.818835465
H157	-1.741801700	-2.848785106	-3.549125781
H158	-2.176222560	-2.536393411	-6.369171375
H159	-0.463407200	-4.582355655	-7.477036975
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O472	9.891772369	-3.362152083	-5.214680824
O473	7.004433119	-3.567427405	-0.059631118
O474	7.092895183	-5.511713224	-1.194907799
O475	6.331826612	-2.142483498	-2.161265204
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O477	6.510354868	-4.943645082	2.380646020
O478	-3.630580621	5.895833968	-0.337770697
O479	-4.696206793	8.972232640	-3.519021267
O480	11.631882032	-6.083747713	-1.045122830
O481	9.082758189	-6.912191661	-0.024407238
S482	0.246884973	2.692685382	5.948119588

	S483	1.726938139	2.633861225	2.544420476
	S484	5.340202018	0.672968951	-0.848302448
	S485	1.338189456	-0.425400704	4.460615343
	S486	1.494403640	0.262797683	-0.000167271
	S487	5.754362917	2.663961538	2.310898881
	S488	4.047572462	-2.665335838	0.175712376
	S489	3.833282531	1.386700410	5.190802765
	S490	6.765262209	-1.062507819	2.079381582
	S491	4.134564350	-2.625158238	4.076219282
15 (S=1/2)	bm1s2b266h2xconex.car_4			
Fe(139) 2.439	C1	-7.914146286	-4.869973663	-3.414741763
Fe(140) -0.979	C2	-7.959445991	-3.665498755	-2.468934089
Fe(141) 2.770	C3	-8.899918844	-1.431677714	-2.042182454
Fe(142) -2.411	C4	-9.316505345	-1.604992563	-0.583555904
Fe(143) 3.089	C5	-10.586976071	-2.868223828	1.073895594
Fe(144) -2.354	C6	-9.449570125	-3.372985454	1.969830373
Fe(145) -0.029	C7	-7.301740884	-4.543659947	2.068223903
	C8	-6.336190549	-3.386571719	2.341521084
	C9	-5.332326016	-1.318433315	1.524418294
	C10	-5.863873659	-0.387523689	2.623992682
	C11	-7.781268628	0.693905275	3.643984000
	C12	-7.782500620	0.121154278	5.067510448
	C13	-8.362725006	-1.776588136	6.501295863
	C14	-7.135806471	-2.417011434	7.161422758
	C15	-5.054330326	-3.681726263	6.827125800
	C16	-3.680542443	-3.026960742	6.665011560
	C17	-2.387745726	-1.237144581	5.539807977
	C18	-2.340446080	0.168525348	6.167306444
	C19	-2.128094646	-1.241838044	4.005742505
	C20	-0.909680583	-0.399943185	3.614612186
	C21	-1.982465876	-2.678122755	3.489297194
	C22	-3.433749795	2.372968658	6.359411495
	C23	-4.106602302	2.372356087	7.748788755
	C24	-4.122807477	3.332792352	5.359854732
	C25	-4.348690855	4.715251540	5.981340647
	C26	-3.301851318	3.449214833	4.069751922
	C27	-6.018963359	1.783036990	9.123200408
	C28	-5.194347788	1.185367005	10.244650114
	C29	0.834888871	-11.423806218	7.071224245
	C30	1.902322161	-10.422377176	6.625175239
	C31	2.643246380	-8.056757882	6.925028812
	C32	3.460624175	-7.804305203	8.206977692
	C33	1.820655241	-6.814918264	6.539758279
	C34	2.685607174	-5.604693102	6.189489011
	C35	1.834543963	-4.413050788	5.761364263
	C36	2.343817707	-2.011836571	5.293341883
	C37	5.684008101	-7.373448708	9.130664165
	C38	6.181040524	-5.945094059	9.203148016
	C39	-4.569922448	-1.687730388	-3.526681367
	C40	-4.704654840	-0.161568370	-3.457340417
	C41	-3.348944793	-2.097092450	-2.671585880
	C42	-3.372382241	-3.519017675	-2.075241433
	C43	-2.972039274	-4.653232900	-3.009356108
	C44	-4.115877445	1.944693541	-4.625705607
	C45	-5.379750174	2.738125909	-4.295938983
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	C47	-7.828654128	2.814533522	-4.337479631
	C48	-8.136836719	2.942874762	-2.839851717
	C49	-7.482959533	2.317110982	-0.553920213
	C50	-6.346074906	3.069837095	0.143742435
	C51	-4.266764557	4.352997338	-0.049483085
	C52	-4.740010454	5.780636895	0.276629449
	C53	-3.082438791	4.529923018	-1.012481008
	C54	-2.309256858	3.304058619	-1.377484620
	C55	-2.186598882	2.080322871	-0.754117056
	C56	-0.924166698	2.125451982	-2.570121488
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	C58	-6.402421836	8.180229642	0.671724800
	C59	-6.946524978	7.946273304	-1.788034309
	C60	-7.139850138	9.350079548	-2.278438774
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	C62	-7.642455339	10.870380631	-3.734761371
	C63	6.485573969	0.452492363	7.444057047
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	C66	4.517115053	1.324544642	6.069571080
	C67	3.427354175	1.750063267	6.850293108
	C68	4.821276135	2.057728939	4.908669156
	C69	2.660443463	2.861730980	6.485826273

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C72	6.791235015	5.893395447	1.118564931
C73	6.254281994	7.013662007	0.220173132
C74	5.725706287	4.802431756	1.293384708
C75	6.419259574	8.119079785	-1.971281862
C76	5.117506218	7.804263226	-2.711788114
C77	3.359274765	6.125613592	-3.154735513
C78	2.182931516	6.376066586	-2.184140681
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C80	2.243028824	4.032929323	-4.278019980
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C82	1.163020185	6.858371145	-6.199499682
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C93	-2.032357623	13.849590792	0.110359611
C94	-2.851544406	11.571429554	-0.563630199
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C96	-3.469513974	10.555495168	-2.798064741
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H148	-9.278953264	-2.704939548	-3.715689892
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H159	-6.792723696	-5.311469704	1.468764292
H160	-7.228162397	1.641978830	3.670890427
H161	-7.793501571	-0.569855214	1.901953623
H162	-7.568186980	-4.979999604	3.038484570
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H165	-8.820705267	0.904844514	3.353523474
H166	-2.876198966	-3.283005914	3.697016804
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H181	-5.108647916	2.902398404	5.104924103
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H188	1.518954218	4.827232356	5.503395143
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H264	1.351138512	4.135548534	-3.639655318
H265	-6.552705130	1.271626906	-5.115714529
H266	7.211042743	8.249113691	-2.721106260
H267	-3.935914782	-0.125506565	-5.302166656
H268	4.333337128	4.589441219	-4.287929708
H269	-1.208048248	7.461021329	-2.156726314
H270	6.264888258	9.087122179	-1.474695846
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H280	0.042047106	5.439636602	-5.267617764
H281	1.789129527	9.573581099	2.239627143
H282	1.989080532	10.079714185	-1.066013192
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Fe(142) -2.472	C4	-8.999207687	0.766862842	-2.877367408
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C105	4.800043650	-5.635375926	-2.528364164
C106	6.249221956	-5.185795112	-2.350439678
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C108	9.092308480	-5.354578943	-0.652893774
C109	-0.002882474	-10.030545066	-2.485034367
C110	-0.331705383	-9.216341511	-3.743047927
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C112	-0.707290914	-10.410861445	-0.079439785
C113	-1.117308591	-9.772445351	1.230067437
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C116	-0.499617859	-6.223410993	-5.086272706
C117	-0.109538023	-5.488627882	-3.829145764
C118	1.002703088	-4.629882570	-3.800394148
C119	-0.805699240	-5.729937431	-2.633113924
C120	1.430575711	-4.062750949	-2.596159062
C121	-0.376142827	-5.165315694	-1.427630484
C122	0.752897250	-4.343070091	-1.405589943
C123	3.100335223	-6.683707304	8.151068271
C124	3.484468833	-5.861240406	9.390541561
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C126	1.269260048	-7.042798748	6.385727074
C127	1.087012798	-8.382381726	6.103982654
C128	0.538142826	-7.175517928	4.334191273
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C130	4.185719031	-5.427878139	12.207522328
C131	-3.794776786	-2.870848861	4.668286001
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N415	6.691239887	-4.892440401	-1.101224186
N416	1.425621547	-10.345918700	-2.384731155
N417	0.597478197	-8.312536598	-4.156178498
N418	3.354122834	-8.119522560	8.380739202
N419	0.922433942	-6.297887615	5.258748078
N420	0.628067328	-8.442154044	4.807059808
N421	2.559454005	-5.729754991	10.382390213
O422	-8.025270757	-1.589569274	-1.254669888
O423	-8.365226235	1.819458856	-2.695330712
O424	-10.102486323	2.775595218	0.477336585
O425	-6.842210173	2.025936840	2.151777599
O426	-4.730414986	3.909206406	0.109686570
O427	-6.800888437	6.872166987	0.450039871
O428	-8.077792506	6.598129692	4.266162946
O429	-4.525451936	3.998724079	5.933518554
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O433	-2.689404796	-2.539739005	12.066353018
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O435	3.237024842	2.458077092	12.748241477
O436	-4.257902181	-0.457974783	-3.812226209
O437	-4.724533820	-5.324868177	-0.819215536
O438	-2.783896678	0.657669035	-6.952529890
O439	-0.988007471	-1.806991756	-7.777362480
O440	-6.229378005	2.421613406	-7.534531275
O441	-4.352578698	4.462493997	-3.785735431
O442	-1.086273110	5.737496896	-5.239142322
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O444	4.912454817	4.254299922	9.277547237
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O447	8.187678764	1.570652420	-6.216196898
O448	4.237338144	1.832628916	-5.798894787
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O451	7.507746155	7.614972020	-6.186031571
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O455	1.462442687	1.557725670	-8.761644574
O456	2.384646339	-9.892490259	1.279243569
O457	2.980998092	-7.777002744	-2.315572074
O458	6.958930286	-5.067480474	-3.363923288
O459	10.261776891	-5.058406986	-0.462859779
O460	-1.404242521	-9.385056529	-4.348965673

	O461	-2.277354993	-9.558548288	1.554793153
	O462	-0.105504617	-9.413617195	2.058235980
	O463	1.931046206	-6.241501571	-6.708973585
	O464	4.635140943	-5.406905929	9.535514299
	O465	4.857369703	-4.722180310	12.947229313
	O466	-3.616702506	-2.784437563	3.458818411
	O467	-5.035623040	-3.251767553	5.108234184
	O468	-2.650599021	-7.516117523	9.150294780
	O469	-3.862119154	-7.740378170	7.255862895
	O470	0.334794767	-3.616146015	6.937538005
	O471	-1.378267099	-3.072694857	8.296331777
	O472	-1.230648101	-4.376129960	4.957960252
	O473	1.521088501	-1.772596319	10.918395335
	O474	1.919234070	-1.599635997	8.113358578
	O475	1.072033232	-0.238579568	-6.880749014
	O476	-0.717484701	-6.490238055	11.352523345
	O477	-0.503490296	-3.692969170	10.748091879
	S478	6.519064051	0.948621685	-0.996061664
	S479	3.950175913	-1.769321016	-0.694464103
	S480	0.721545234	-4.540331469	2.421285078
	S481	3.575254528	1.141086109	1.513513455
	S482	0.513091092	-1.396563919	0.473937566
	S483	4.535747799	-4.834506749	1.651885924
	S484	0.505859147	-1.562757480	4.684663432
	S485	6.118097964	-1.430044114	2.070136996
	S486	3.182508751	-4.038048185	5.108241489
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Fe(139)	1.775	C1	-9.570773097	1.682355187
Fe(140)	0.092	C2	-8.429622141	2.689095700
Fe(141)	2.741	C3	-7.614039137	4.962415153
Fe(142)	-2.684	C4	-7.156532486	5.392928385
Fe(143)	3.182	C5	-7.694133011	5.657412188
Fe(144)	-2.482	C6	-6.708937940	4.659967656
Fe(145)	-0.087	C7	-5.874494062	2.357916030
		C8	-4.501347265	2.532796241
		C9	-3.249332539	3.128809446
		C10	-2.484044672	4.321860456
		C11	-2.563200240	6.585674730
		C12	-2.071864519	6.421774804
		C13	-2.650703309	5.758920979
		C14	-1.822688247	4.569080515
		C15	-1.327587395	2.173122685
		C16	-0.203638953	1.615214704
		C17	0.938260768	1.766146985
		C18	2.049271077	2.808837358
		C19	0.221702189	1.311068702
		C20	1.215022156	0.941033533
		C21	-0.725096013	0.140785189
		C22	2.609814721	5.126919030
		C23	2.962980075	5.829870915
		C24	2.123194311	6.114134475
		C25	3.069391861	7.315659021
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		C27	2.226881462	7.021202642
		C28	3.119848305	6.221423931
		C29	-1.481613328	-7.231757765
		C30	-0.503454447	-7.371841933
		C31	1.357387700	-6.205184201
		C32	2.727796005	-6.412382158
		C33	1.291667616	-4.833560329
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		C35	2.199658083	-3.366185632
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		C37	4.898285325	-7.531053720
		C38	6.009191021	-6.818516226
		C39	-5.847850791	1.463066196
		C40	-5.118427926	2.635969702
		C41	-4.777642387	0.471128670
		C42	-5.173626338	-0.415551087
		C43	-6.005045862	-1.651359361
		C44	-4.286171034	3.477088878
		C45	-4.493719497	4.973355084
		C46	-4.500927801	3.094773809
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		C48	-5.300525159	7.306932818
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		C50	-2.422215346	6.600648922
		C51	-0.546257098	5.989648029

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C60	-1.063939703	11.077875732	-4.491838886
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C62	-1.401876155	12.219886332	-6.298307636
C63	8.576896392	-3.001174524	3.850796806
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C65	7.120344699	-2.544413888	3.587461602
C66	7.042673574	-1.203874146	2.896952333
C67	7.058327064	-0.003381973	3.630224026
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C89	6.392319759	8.279165157	-7.768863433
C90	6.209325598	6.100782670	-9.065344794
C91	4.694944133	5.988951604	-8.918439225
C92	4.970035803	9.900569174	-6.602411832
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C105	-0.353562602	-4.032479872	-6.767996000
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C118	-2.965358704	-1.177436063	-5.201965470
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C120	-1.979852555	-1.753869096	-4.395928882
C121	-3.686201429	-2.734496007	-2.992419694
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C126	-1.573686276	-9.327078404	1.252996118
C127	-2.578502031	-10.003046028	0.590101257
C128	-2.723351668	-7.845490612	0.130714468
C129	2.197021042	-11.696229117	4.997648588
C130	3.045433837	-12.883392319	4.599414306
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C132	-2.219203576	-4.467709986	4.744171104
C133	-2.232111258	-5.869781584	3.996471161
C134	-3.448539190	-6.708654179	4.493522919
C135	-3.414480254	-8.154053949	3.969861633
C136	-4.415563036	-9.067809325	4.617425378
C137	-0.953545917	-6.628994750	4.462730366
C138	1.576080600	-3.902150100	-0.572518892
Fe139	0.492832777	-5.451371151	-0.976435440
Fe140	1.588142691	-1.805698794	-0.632112211
Fe141	3.576953146	-3.827530449	-0.465772993
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Fe144	2.074022245	-5.176440321	0.990808073
Fe145	-0.034976284	-3.335561838	0.793679750
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H147	-8.618470099	0.041384342	1.257721623
H148	-9.484121042	4.106374266	1.185279717
H149	-10.108665361	1.903654773	1.113969772
H150	-10.283896107	1.877279112	2.869030774
H151	-6.714856588	4.612945002	1.238290193
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H161	-4.218131724	5.448418774	4.156672932
H162	-5.719058389	2.397952990	7.229193173
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H164	-3.862352703	5.537562846	6.919012273
H165	-3.272686375	7.423856308	4.904230742
H166	-1.485026626	0.405534379	5.604778681
H167	-1.248184087	-0.164976415	3.936885656
H168	-0.163462955	-0.733707603	5.222740369
H169	-0.378594059	2.165994559	4.212616303
H170	-3.611373725	5.738226485	9.201059250
H171	1.262681601	4.578544538	2.604213789
H172	0.964645626	6.267869493	6.773533303
H173	3.118151533	7.897846429	4.739121993
H174	0.676402258	0.657626995	2.543126311
H175	1.829957738	0.080978175	3.757562188
H176	9.048482121	-2.262513987	4.526438927
H177	1.640161560	6.120860162	1.805483191
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H186	4.157871995	3.627709855	-1.343125170
H187	6.066824661	2.516515874	-0.935027436
H188	6.729601786	3.224064072	1.528086264
H189	6.762988762	0.158543822	-0.237549393
H190	6.886610572	-2.034725461	0.904125524
H191	7.126905698	-0.035917514	4.721465997
H192	-0.666325038	2.974126564	6.609297920
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H196	-2.108138396	6.663258869	8.967618568
H197	6.969544303	2.163126805	3.577587127
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H218	-7.663837738	1.336291632	-1.604005350
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H220	-4.687454775	-8.065100884	-2.984236963
H221	-4.255914817	-0.725750144	1.584334148
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H224	-4.112912048	7.834543275	0.828891061
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H231	-1.818512564	12.622697046	-7.218232324
H232	0.833239716	5.118953654	-2.386665707
H233	-0.729026415	5.508789708	-3.109251278
H234	0.378266952	13.380712984	-6.150507470
H235	-1.970064022	9.261588010	-3.954640687
H236	-2.637654980	5.853674905	-1.482473207
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H238	-5.753737399	7.422640265	-3.427127920
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H240	-7.109858479	6.862202030	-2.428716442
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Fe(141) 2.268	C3	-4.545	5.060	-6.453
Fe(142) -2.666	C4	-5.947	4.597	-6.055
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Fe(144) -2.385	C6	-8.125	2.360	-6.093
Fe(145) -0.948	C7	-6.941	0.237	-5.784
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	C9	-5.002	1.692	-2.839
	C10	-6.104	2.168	-1.882
	C11	-8.097	3.501	-1.532
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	C20	-3.500	-0.790	0.854
	C21	-4.227	-1.979	-1.256
	C22	-7.054	1.015	3.140
	C23	-8.509	0.683	3.537
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	C25	-7.300	3.295	4.222
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	C37	-5.049	-11.393	2.725
	C38	-4.550	-10.662	3.954
	C39	-0.117	2.806	-5.334
	C40	-0.031	3.930	-4.292

C41	0.137	1.486	-4.558
C42	-0.189	0.175	-5.302
C43	0.981	-0.431	-6.076
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C45	0.518	6.929	-3.323
C46	2.889	6.065	-3.387
C47	-1.445	8.064	-4.277
C48	-2.680	7.628	-3.476
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C68	-0.833	-2.837	6.092
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C73	4.624	1.234	8.118
C74	3.544	-0.560	6.725
C75	6.572	2.735	8.118
C76	6.459	3.542	6.824
C77	5.854	3.516	4.427
C78	4.370	3.919	4.278
C79	6.342	2.608	3.283
C80	6.065	3.071	1.848
C81	6.874	4.270	1.324
C82	6.822	6.605	2.186
C83	2.021	3.369	4.557
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C85	1.104	2.134	4.609
C86	1.425	4.913	7.979
C87	2.035	6.129	8.666
C88	3.739	7.899	8.647
C89	3.024	9.259	8.513
C90	5.198	7.993	8.153
C91	5.274	8.293	6.658
C92	1.427	10.594	7.226
C93	0.729	11.236	8.419
C94	0.403	10.386	6.079
C95	1.074	9.875	4.825
C96	1.654	10.774	3.918
C97	1.212	8.499	4.575
C98	2.367	10.324	2.804
C99	1.950	8.030	3.484
C100	2.522	8.951	2.609
C101	7.971	-6.302	-3.480
C102	7.331	-5.017	-3.976
C103	6.225	-2.908	-3.283
C104	6.972	-1.679	-2.761
C105	7.467	-0.332	-0.768
C106	8.205	-0.589	0.544
C107	8.750	-2.116	2.379
C108	9.991	-2.982	2.335
C109	7.326	-0.853	-7.290
C110	7.296	0.653	-7.019
C111	5.911	-1.439	-7.085
C112	5.781	-2.851	-7.686
C113	4.528	-3.530	-7.178
C114	7.302	2.441	-5.369
C115	8.316	2.682	-4.269
C116	5.944	3.164	-5.195
C117	5.201	2.607	-4.019
C118	5.375	3.167	-2.744
C119	4.460	1.420	-4.148
C120	4.883	2.510	-1.614

	C121	3.976	0.763	-3.017
	C122	4.210	1.293	-1.744
	C123	3.391	-10.482	-1.488
	C124	2.577	-11.326	-0.496
	C125	2.478	-9.568	-2.320
	C126	3.174	-8.561	-3.180
	C127	4.055	-8.799	-4.216
	C128	3.611	-6.632	-4.104
	C129	0.693	-12.806	-0.085
	C130	1.530	-13.765	0.732
	C131	-1.928	-4.390	-4.809
	C132	-1.909	-5.378	-3.678
	C133	-0.707	-6.404	-3.768
	C134	-0.780	-7.185	-5.111
	C135	0.287	-8.290	-5.185
	C136	0.131	-9.224	-6.351
	C137	-0.923	-7.442	-2.623
	C138	2.507	-3.425	0.847
	Fe139	3.548	-4.584	-0.420
	Fe140	1.865	-1.386	1.304
	Fe141	2.202	-3.568	2.749
	Fe142	4.373	-3.117	1.466
	Fe143	3.948	-1.569	3.559
	Fe144	1.367	-5.089	0.858
	Fe145	1.436	-3.214	-0.963
	H146	-2.977	0.592	-8.276
	H147	-1.539	1.376	-8.259
	H148	-3.660	4.982	-8.401
	H149	-2.429	3.271	-9.370
	H150	-3.931	2.395	-9.644
	H151	-3.904	4.885	-5.577
	H152	-6.453	4.303	-8.024
	H153	-4.575	6.141	-6.642
	H154	-8.662	3.656	-7.732
	H155	-6.397	1.852	-7.067
	H156	-8.656	4.425	-6.126
	H157	-4.539	0.809	-2.381
	H158	-5.078	1.868	-4.980
	H159	-6.232	-0.371	-6.363
	H160	-7.700	3.851	-0.570
	H161	-6.883	3.437	-3.318
	H162	-7.887	-0.311	-5.713
	H163	-4.230	2.468	-2.928
	H164	-9.227	1.882	-3.211
	H165	-8.597	4.339	-2.036
	H166	-5.054	-2.174	-1.954
	H167	-3.413	-1.503	-1.823
	H168	-3.845	-2.944	-0.888
	H169	-4.988	-0.107	-0.512
	H170	-11.151	0.628	-3.115
	H171	-4.984	2.373	1.778
	H172	-9.250	1.233	1.661
	H173	-8.373	3.154	4.414
	H174	-2.686	-0.310	0.293
	H175	-3.091	-1.708	1.301
	H176	-2.641	-5.369	8.282
	H177	-5.202	3.931	2.605
	H178	-7.117	4.372	4.097
	H179	-4.718	2.494	3.541
	H180	-6.750	2.959	5.116
	H181	-7.417	2.879	2.113
	H182	-6.441	0.641	3.973
	H183	-6.668	0.777	1.042
	H184	-3.785	-0.110	1.671
	H185	1.525	1.344	3.962
	H186	0.131	2.443	4.199
	H187	0.034	1.411	6.100
	H188	-2.526	1.100	6.863
	H189	0.232	-0.960	6.019
	H190	0.044	-3.413	5.788
	H191	-4.154	-3.187	6.775
	H192	-7.334	-0.773	-0.705
	H193	-8.550	-3.095	-2.554
	H194	-9.758	-3.069	-1.251
	H195	-8.598	-0.697	-2.621
	H196	-11.444	1.200	-1.454
	H197	-3.981	-0.719	6.938
	H198	-5.731	-2.717	0.854
	H199	-11.274	1.338	3.591
	H200	-11.430	0.609	1.971

H201	-10.317	-1.564	3.201
H202	-4.686	-12.432	2.751
H203	1.803	-2.244	-6.590
H204	-3.133	-5.581	-5.735
H205	5.713	-2.776	-8.781
H206	6.665	-3.455	-7.435
H207	5.157	-0.785	-7.550
H208	9.051	1.854	-4.128
H209	7.578	-0.931	-8.358
H210	1.190	1.478	-4.231
H211	-1.014	0.334	-6.018
H212	7.257	0.336	-4.960
H213	7.776	2.913	-6.256
H214	8.177	-1.558	-5.537
H215	0.380	-2.352	-5.565
H216	5.691	-1.453	-6.006
H217	8.553	-2.445	-6.869
H218	0.407	3.411	-7.242
H219	-0.480	1.523	-3.649
H220	5.656	-4.499	-5.894
H221	-0.566	-0.561	-4.579
H222	-2.375	4.902	1.622
H223	-1.100	2.504	1.290
H224	-4.680	6.416	-2.386
H225	-1.950	5.683	-3.319
H226	-1.592	7.951	-0.017
H227	-1.678	12.333	2.803
H228	-3.971	9.499	1.349
H229	-2.050	10.554	-0.330
H230	-1.065	9.461	2.376
H231	1.337	14.185	0.471
H232	-0.113	5.745	2.340
H233	0.215	6.300	0.696
H234	-0.108	14.337	2.570
H235	-0.431	9.876	-0.130
H236	-1.505	5.335	-1.039
H237	-4.012	4.780	-2.547
H238	-1.078	8.993	-3.819
H239	3.028	2.447	0.358
H240	-1.762	8.297	-5.302
H241	1.080	1.031	0.966
H242	-0.396	-5.712	8.993
H243	-0.293	-4.442	7.968
H244	3.707	2.063	4.953
H245	1.884	3.851	3.578
H246	2.751	3.588	7.006
H247	2.365	4.912	0.566
H248	3.661	6.312	-0.607
H249	3.392	6.980	0.791
H250	3.503	5.154	-3.365
H251	3.119	6.627	-4.308
H252	5.716	7.058	8.411
H253	5.680	8.821	8.692
H254	5.948	6.342	6.236
H255	5.607	7.382	4.858
H256	8.477	7.338	3.148
H257	7.030	4.169	0.240
H258	2.805	11.038	2.103
H259	0.737	7.760	5.227
H260	5.124	7.777	2.200
H261	5.873	1.619	3.408
H262	5.878	1.862	5.782
H263	4.990	3.262	1.707
H264	-0.364	6.392	-5.069
H265	7.638	2.637	8.364
H266	1.684	4.471	-5.183
H267	7.425	2.459	3.413
H268	2.104	6.959	3.347
H269	2.463	7.460	-2.096
H270	6.101	3.349	8.898
H271	8.770	5.908	2.211
H272	6.586	8.585	2.589
H273	1.276	2.099	-6.669
H274	-1.169	2.796	-5.673
H275	1.558	11.849	4.084
H276	1.209	5.185	-2.387
H277	6.407	4.464	4.426
H278	7.870	4.253	1.782
H279	6.322	2.218	1.204
H280	5.305	5.738	1.163

H281	0.405	5.199	7.678
H282	3.415	6.357	7.165
H283	3.760	7.699	9.729
H284	1.340	4.131	8.747
H285	1.909	8.528	6.978
H286	8.438	-6.135	-2.499
H287	7.131	-7.008	-3.317
H288	4.051	-9.857	-0.870
H289	9.250	-7.725	-4.180
H290	8.548	-6.829	-5.359
H291	3.261	-1.621	6.721
H292	2.389	0.223	9.040
H293	6.576	0.598	8.040
H294	2.643	0.049	6.563
H295	3.538	-0.339	10.059
H296	8.002	-2.586	3.037
H297	4.996	-0.891	8.289
H298	-6.042	-7.572	-0.418
H299	-4.063	-9.880	-0.786
H300	7.566	-2.556	0.665
H301	-2.665	-3.344	3.977
H302	8.187	0.114	-1.466
H303	3.423	-0.173	-3.109
H304	6.709	0.437	-0.549
H305	-4.697	-5.348	0.354
H306	6.218	-2.091	-0.905
H307	-3.219	-5.881	-0.443
H308	-4.578	-7.601	-1.429
H309	-3.252	-8.019	0.798
H310	-4.741	-7.552	1.641
H311	5.382	3.034	-6.131
H312	-6.870	-9.503	-1.767
H313	-6.284	-10.219	-4.670
H314	3.872	0.731	-0.872
H315	-8.506	-11.042	-2.964
H316	-8.490	-9.982	-4.212
H317	-1.982	-5.643	1.528
H318	5.063	2.938	-0.626
H319	4.282	0.997	-5.140
H320	-0.894	-11.910	-3.307
H321	1.849	-10.200	-2.973
H322	-1.792	-9.876	-2.239
H323	-0.165	-11.851	-4.665
H324	10.442	-3.125	1.323
H325	-0.495	-7.957	-0.054
H326	-2.855	-5.937	-3.621
H327	7.004	-4.422	-2.036
H328	-1.783	-7.632	-5.208
H329	4.906	-7.394	-5.591
H330	3.619	-5.579	-4.362
H331	-6.646	-11.865	-4.130
H332	-1.426	-4.022	2.960
H333	-1.488	-9.907	0.888
H334	-0.035	-7.844	1.426
H335	-3.697	-10.757	1.175
H336	-5.369	-4.814	2.232
H337	0.029	-9.272	-8.241
H338	1.276	-7.811	-5.239
H339	0.264	-8.914	-4.284
H340	-0.631	-6.481	-5.943
H341	5.226	-2.988	-2.825
H342	5.944	4.092	-2.639
H343	6.155	4.236	-5.066
H344	-1.757	-4.821	-2.744
H345	-1.877	-10.883	-0.262
H346	-2.815	-11.045	-2.324
H347	-4.992	-3.300	2.981
H348	4.497	-9.720	-4.577
H349	1.791	-9.036	-1.651
H350	6.119	-2.802	-4.364
H351	9.034	-1.152	2.833
H352	-3.154	-5.305	5.884
H353	-1.419	-5.368	5.468
H354	4.874	-11.876	-1.748
H355	3.671	-12.003	-2.850
H356	0.011	-13.415	-0.699
H357	1.193	-11.908	-1.954
H358	2.481	-14.092	0.248
H359	0.075	-12.184	0.582
H360	-1.159	-7.683	6.872

H361	0.391	10.529	9.212
H362	-6.150	-11.423	2.786
H363	-4.286	-9.588	3.797
H364	2.206	11.296	6.883
H365	-0.381	9.690	6.417
H366	-0.073	11.359	5.891
H367	1.968	0.114	1.553
H368	0.729	-0.466	-1.234
H369	0.388	-2.676	-1.918
H370	3.492	9.192	0.932
Mo371	1.489	-5.781	-1.777
N372	-2.397	1.253	-8.800
N373	-3.999	4.405	-7.635
N374	-6.778	4.231	-7.063
N375	-7.147	1.500	-6.477
N376	-5.490	1.389	-4.176
N377	-7.013	3.036	-2.385
N378	-9.570	1.676	-2.269
N379	-9.204	-1.194	-1.960
N380	-7.076	-1.643	-0.245
N381	-6.659	0.281	1.937
N382	-9.461	0.836	2.580
N383	-7.959	-10.297	-3.399
N384	-5.912	-9.865	-1.714
N385	-2.981	-5.424	1.562
N386	-4.666	-4.228	2.670
N387	-2.423	-3.768	3.083
N388	-4.695	-10.744	1.477
N389	0.849	3.007	-6.414
N390	1.054	-1.776	-6.073
N391	1.057	4.733	-4.407
N392	-0.371	7.087	-4.325
N393	-2.712	6.326	-3.074
N394	-2.180	5.661	-0.350
N395	1.684	4.120	0.659
N396	0.961	2.083	0.802
N397	-1.827	8.100	0.962
N398	0.304	12.324	0.125
N399	-0.153	13.574	1.901
N400	-0.490	-5.446	8.010
N401	3.127	-0.483	9.131
N402	5.975	1.415	8.102
N403	6.127	2.862	5.705
N404	6.249	5.581	1.559
N405	8.110	6.586	2.573
N406	6.089	7.699	2.527
N407	3.433	3.028	4.701
N408	2.114	4.368	6.815
N409	3.036	6.789	8.008
N410	5.611	7.241	5.868
N411	2.024	9.324	7.601
N412	8.981	-6.771	-4.432
N413	6.968	-4.136	-3.023
N414	6.848	-1.462	-1.434
N415	8.180	-1.841	1.072
N416	8.414	-1.490	-6.534
N417	7.225	1.035	-5.710
N418	4.249	-11.325	-2.343
N419	2.913	-7.194	-3.119
N420	4.317	-7.570	-4.783
N421	1.508	-12.010	-0.989
N422	-0.210	-0.781	1.231
N423	-0.231	-1.924	1.236
O424	-4.048	2.329	-6.696
O425	-6.287	4.570	-4.862
O426	-8.995	2.069	-5.256
O427	-6.834	-0.285	-3.420
O428	-6.149	1.775	-0.704
O429	-9.586	2.276	-0.065
O430	-11.226	-1.221	-0.871
O431	-7.468	-3.907	-0.204
O432	-6.013	-1.616	3.044
O433	-8.795	0.294	4.682
O434	-12.000	-1.072	4.242
O435	-4.480	-11.265	-2.876
O436	-6.834	-10.061	0.978
O437	-4.449	-11.193	5.048
O438	-0.887	4.082	-3.394
O439	1.807	0.286	-6.685
O440	0.637	7.729	-2.369

	O441	3.230	6.848	-2.232
	O442	-3.573	8.451	-3.239
	O443	-4.404	5.948	0.089
	O444	-2.501	7.109	2.908
	O445	-3.347	10.566	2.971
	O446	-3.059	-7.804	7.616
	O447	-1.685	0.676	6.611
	O448	3.837	2.198	8.149
	O449	6.699	4.766	6.858
	O450	4.068	5.021	3.787
	O451	0.578	5.148	5.292
	O452	0.968	1.662	5.949
	O453	1.593	6.499	9.761
	O454	3.346	10.216	9.231
	O455	4.982	9.412	6.205
	O456	0.504	12.434	8.486
	O457	3.290	8.458	1.543
	O458	7.136	-4.837	-5.205
	O459	7.638	-0.947	-3.526
	O460	8.786	0.369	1.080
	O461	10.485	-3.483	3.332
	O462	7.306	1.479	-7.948
	O463	3.401	-3.275	-7.594
	O464	4.693	-4.425	-6.184
	O465	8.385	3.711	-3.612
	O466	2.909	-11.441	0.698
	O467	1.171	-14.227	1.806
	O468	-1.312	-3.335	-4.845
	O469	-2.697	-4.722	-5.897
	O470	0.005	-10.444	-6.275
	O471	0.145	-8.584	-7.551
	O472	0.008	-7.478	-1.727
	O473	-1.918	-8.203	-2.638
	O474	0.498	-5.749	-3.631
	O475	-1.950	-10.767	0.723
	O476	-0.770	-8.174	0.874
	O477	3.701	6.139	0.373
	O478	-0.315	-12.448	-3.903
	O479	-1.871	-10.860	-2.075
	S480	4.711	-0.249	5.319
	S481	4.275	-0.888	1.447
	S482	2.843	-3.955	-2.456
	S483	1.655	-1.556	3.596
	S484	1.935	-1.049	-0.973
	S485	5.706	-4.205	0.063
	S486	-0.245	-4.595	-0.612
	S487	4.300	-3.814	3.592
	S488	2.755	-6.647	0.064
	S489	0.678	-5.175	2.963
19 (S=1)	bm12b2x6x2n22ndtitconextg.car_3			
Fe(139) 2.235	C1	-2.396877988	2.089920238	-9.198433395
Fe(140) -0.069	C2	-3.138594186	2.674701099	-7.994425456
Fe(141) 2.179	C3	-4.004224722	4.703433585	-6.910145952
Fe(142) -2.616	C4	-5.429990291	4.255831119	-6.589970706
Fe(143) 3.133	C5	-7.537051560	3.329480633	-7.412693555
Fe(144) -2.392	C6	-7.582406319	2.025930154	-6.607926978
Fe(145) -0.870	C7	-6.410265452	-0.042762161	-6.021614225
	C8	-6.012877766	0.249619989	-4.572284348
	C9	-4.672137058	1.613991080	-3.053696301
	C10	-5.844101426	2.140533184	-2.213493184
	C11	-7.818030670	3.547682390	-2.103054056
	C12	-8.938922336	2.538133898	-1.823766037
	C13	-10.491179819	0.906711924	-2.779122058
	C14	-10.314179773	-0.492251743	-2.175781634
	C15	-8.886044364	-2.487671279	-2.008096284
	C16	-7.838738271	-2.717506497	-0.917013005
	C17	-5.972626050	-1.691498909	0.350111018
	C18	-6.236660801	-0.958559942	1.678451314
	C19	-4.692033857	-1.215851060	-0.380949518
	C20	-3.512821598	-0.999505596	0.565924650
	C21	-4.316922546	-2.197509910	-1.496887591
	C22	-6.976642183	1.153647118	2.746844685
	C23	-8.486033189	1.079014306	3.064570316
	C24	-6.484441734	2.613019811	2.586813158
	C25	-6.939792379	3.479493296	3.767565835
	C26	-4.958681419	2.672850635	2.445323375
	C27	-10.784974175	1.429136724	2.355780296
	C28	-11.278871056	0.112812924	2.922422740
	C29	-6.331320415	-11.116272127	-3.732309984

C30	-5.288765513	-10.895344838	-2.635994326
C31	-4.896790817	-9.646368275	-0.506071755
C32	-5.516371610	-10.279915080	0.752944230
C33	-4.860263993	-8.110656961	-0.416167465
C34	-4.095575070	-7.569772778	0.794283713
C35	-3.790786210	-6.083626391	0.610288731
C36	-3.478306980	-4.479558137	2.499040619
C37	-5.061165693	-11.549786608	2.795915651
C38	-4.745165363	-10.758416855	4.049236166
C39	0.117424211	2.621565426	-5.253224993
C40	0.157186146	3.779979467	-4.246365406
C41	0.306684774	1.308773865	-4.456577280
C42	-0.133369414	0.008265050	-5.162253969
C43	0.912744754	-0.647240369	-6.057634945
C44	1.605854334	5.490609311	-3.217697752
C45	0.637320584	6.681018519	-3.243021891
C46	3.085745434	5.924227387	-3.379264771
C47	-0.918568421	8.012537813	-4.595941408
C48	-2.293339973	7.651803113	-4.010904012
C49	-3.677086937	5.892987176	-2.990445076
C50	-3.508177642	5.773800012	-1.467404085
C51	-1.975455482	5.671821048	0.445433813
C52	-2.351426943	7.057286768	1.000153589
C53	-0.478099574	5.510252210	0.758961436
C54	0.138370299	4.166943254	0.541001253
C55	-0.354804424	2.902439449	0.788894797
C56	1.746341376	2.770864150	0.118060641
C57	-1.880654250	9.439430177	0.819306629
C58	-3.313819800	9.808515808	1.203878083
C59	-1.322290670	10.412596560	-0.241661152
C60	-0.824077462	11.728632418	0.281662827
C61	-1.219364661	12.468293457	1.378717291
C62	0.431606221	13.491659654	0.313463912
C63	-2.479804414	-5.214250709	7.740357555
C64	-2.641889583	-6.711097503	7.552660700
C65	-2.645826876	-4.565152461	6.342150141
C66	-2.541567208	-3.058631883	6.390310735
C67	-3.661222878	-2.250162139	6.657951955
C68	-1.302568518	-2.423784654	6.188626225
C69	-3.550934296	-0.856463886	6.725092449
C70	-1.174862020	-1.037025262	6.263518007
C71	-2.300855543	-0.254375020	6.533139503
C72	3.903573448	0.401735539	8.250627380
C73	4.377370478	1.855800421	8.130222499
C74	3.301150295	-0.079159421	6.922043099
C75	6.316638704	3.350155277	7.906891008
C76	6.141259894	4.032428485	6.549343056
C77	5.465266720	3.801933706	4.189185732
C78	3.979048271	4.207448244	4.077210421
C79	5.902455176	2.804805839	3.100538824
C80	5.682823567	3.233068549	1.643882409
C81	6.524721551	4.417473732	1.142301929
C82	6.454736553	6.797868197	1.865525459
C83	1.636481036	3.605397513	4.370424110
C84	1.086864460	4.610119766	5.395066836
C85	0.769575285	2.333940793	4.429855743
C86	1.019403288	5.166709556	7.776232537
C87	1.537055488	6.455404530	8.405142988
C88	3.130323034	8.320059840	8.305867002
C89	2.354782245	9.643110780	8.128642443
C90	4.587368558	8.454477794	7.821378217
C91	4.690297419	8.741675413	6.325194346
C92	0.716644840	10.876142007	6.789430125
C93	-0.082653524	11.477144970	7.935518605
C94	-0.231009519	10.592236365	5.591940359
C95	0.521818951	10.019088781	4.414765390
C96	1.231468938	10.861312936	3.544896582
C97	0.599853569	8.631778201	4.207575691
C98	1.999056498	10.340774451	2.502260455
C99	1.382813397	8.091160046	3.181916740
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C102	7.763574601	-4.989246824	-3.085400685
C103	6.596945712	-2.871101073	-2.558864436
C104	7.294281103	-1.638354288	-1.973037974
C105	7.747776547	-0.351534957	0.052662067
C106	8.251378378	-0.527473594	1.480183997
C107	8.335203704	-1.845289029	3.542425060
C108	9.414462616	-2.880195184	3.768461189
C109	7.906329705	-0.884979365	-6.467464228

C110	7.665794627	0.624944295	-6.337390340
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C112	6.689207238	-3.051535820	-7.042252398
C113	5.445628577	-3.874708390	-6.770381684
C114	7.246535160	2.528944382	-4.857058992
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C116	5.727414917	2.818820414	-4.749157195
C117	5.064918492	1.843097959	-3.815699335
C118	5.147260016	2.007734031	-2.423148460
C119	4.501454831	0.661656435	-4.325102666
C120	4.755957217	0.974805147	-1.568274823
C121	4.111821054	-0.371726425	-3.468926217
C122	4.278982476	-0.228735939	-2.089586897
C123	3.520830967	-10.295109083	-0.674477921
C124	2.658782806	-11.200085787	0.217061655
C125	2.723980851	-9.651010544	-1.821741747
C126	3.461694531	-8.627315558	-2.626604919
C127	4.422481684	-8.856601525	-3.590540981
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C132	-1.691082500	-5.645547690	-3.458702583
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C134	-0.410662927	-7.436342567	-4.783490232
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H146	-2.252786647	0.193610405	-8.456404425
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H149	-1.719231329	2.845055179	-9.624998924
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H155	-5.752895192	1.476790848	-7.364197314
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H162	-7.357588553	-0.594474950	-5.991853251
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H168	-3.998678867	-3.164564661	-1.075670221
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H170	-10.893643619	0.776203106	-3.794227805
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H175	-3.189785559	-1.937641822	1.039673950
H176	-3.319219086	-4.866123983	8.372513919
H177	-4.641748656	3.716377366	2.296917656
H178	-6.583339130	4.510971189	3.629656196
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H180	-6.519331430	3.100577328	4.713372023
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H182	-6.485702815	0.697089270	3.617353465
H183	-6.581453346	0.800140678	0.669236095
H184	-3.735610388	-0.274355314	1.362328186
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H186	-0.208936482	2.578166358	3.991458485
H187	-0.328964069	1.781317064	5.970602719
H188	-2.977214386	1.556669698	6.716955167
H189	-0.211790793	-0.561909746	6.071708427

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H194	-9.835492331	-2.907655909	-1.652008831
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H198	-5.867261913	-2.749473266	0.620133578
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H200	-11.306681758	1.592263452	1.399860732
H201	-10.681036601	-0.779621438	2.623591641
H202	-4.613073504	-12.551365420	2.886423089
H203	1.664759819	-2.479638402	-6.562642544
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H208	9.075813127	2.603102758	-3.599737238
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H211	-1.022001236	0.201839559	-5.788290607
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H217	9.169960443	-2.329418512	-5.749023153
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H219	-0.291746050	1.397703788	-3.538513981
H220	6.387118888	-4.651982116	-5.236834170
H221	-0.456702476	-0.712824252	-4.398377194
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H223	-1.319397473	2.550849439	1.139864529
H224	-4.488732945	6.613140106	-3.150869393
H225	-1.742978284	5.662338945	-3.834503795
H226	-1.358560610	7.913115141	-0.595273424
H227	-1.975322029	12.295466059	2.137185126
H228	-4.087142653	9.364968724	0.531373349
H229	-2.075501598	10.565099303	-1.035077747
H230	-1.256118895	9.478689284	1.727668428
H231	1.179343498	14.247848174	0.088580208
H232	-0.351746933	5.796731084	1.817484833
H233	0.085263833	6.242126383	0.160640139
H234	-0.435489937	14.336232989	2.067055883
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H236	-1.476591081	5.404980781	-1.631047816
H237	-4.016086648	4.925845591	-3.388685619
H238	-0.609142357	8.941779760	-4.097269045
H239	2.691586660	2.319516479	-0.168586261
H240	-1.048075431	8.236350950	-5.663134927
H241	0.732153982	1.031026751	0.729465757
H242	-1.147562208	-5.141436101	9.294577379
H243	-0.941037696	-3.944211657	8.197542685
H244	3.355588564	2.360879724	4.805992430
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H246	2.422208863	3.933015619	6.798158191
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H248	3.415587518	6.600810648	-1.557038794
H249	2.896952093	6.852825850	0.595278781
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H252	5.135046925	7.543183822	8.101479359
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H256	8.172971659	7.677165066	2.547865585
H257	6.713607937	4.312740712	0.062514555
H258	2.536160265	11.006949543	1.823162214
H259	0.035488718	7.940892867	4.839422328
H260	4.709411518	7.883041671	1.954626677
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H262	5.541560868	2.261481440	5.677745011
H263	4.617230409	3.427450713	1.443580552
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H265	7.393838182	3.277688293	8.109837398
H266	2.002353120	4.156378497	-4.916909008
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H268	1.467014371	7.010707818	3.062378315
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H270	5.879833159	4.032408446	8.649304700
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H272	6.155802253	8.788942128	2.166406350
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H274	-0.914647761	2.621529376	-5.654480256
H275	1.185652381	11.943794068	3.682543921
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H282	2.863995517	6.722531353	6.869920834
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H291	3.026610849	-1.136259955	7.033903910
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H294	2.394154304	0.498205128	6.694530983
H295	3.326179183	0.485004164	10.214421193
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H299	-3.876748117	-10.021719827	-0.649609618
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H301	-2.866780960	-3.174066963	3.946370835
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H304	7.016413006	0.472865814	0.087941555
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H306	6.522165310	-2.139805358	-0.150474503
H307	-3.171506454	-5.939254971	-0.289027407
H308	-4.385563835	-7.755581553	-1.345167592
H309	-3.140264262	-8.100204611	0.922370903
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H315	-8.216936027	-11.330866560	-2.929505147
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H317	-2.045652692	-5.685249227	1.753412009
H318	4.823543849	1.087766645	-0.484323135
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H321	2.392602382	-10.445981950	-2.513344070
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H324	10.016693524	-3.145270224	2.865728294
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O470	0.764184753	-8.526083445	-7.434687709
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O472	-1.674912814	-8.329357741	-2.661511196
O473	0.722730672	-5.790130312	-3.470923878
O474	-1.842282206	-10.925854782	0.631653348
O475	-0.690962144	-8.339820824	0.920125339
O476	3.334636282	6.089751500	0.348479991
O477	0.053940242	-12.438988960	-3.976999932
O478	-1.607793153	-10.965591208	-2.150447612
S479	4.262103032	-0.084363060	5.365704797
S480	4.026359761	-0.859166731	1.758432028
S481	2.943202590	-3.915260448	-2.146215775
S482	1.470947515	-1.700804866	3.874181288
S483	1.554701058	-1.013471578	-0.673729262
S484	5.670715957	-4.175009868	0.517787672
S485	-0.240625401	-4.677593340	-0.492270687
S486	4.079946807	-3.764642273	3.956196944
S487	2.758226729	-6.662526909	0.346143055
S488	0.510462593	-5.232083271	3.159329867
20 (S=1)		bm202b2x6x2n22nconexadtd.car_3	
Fe(139) 2.172	C1	-2.920674081	0.625736582
Fe(140) -0.109	C2	-3.718736267	1.297706776
Fe(141) 2.365	C3	-4.747689091	3.372372581
Fe(142) -2.664	C4	-6.129551524	2.864646215
Fe(143) 3.146	C5	-8.173809160	1.691952691
	C6	-8.108741770	0.481338565
	C7	-6.767579909	-1.426591243
	C8	-6.285340365	-0.944988905
	C9	-4.957954744	0.665772057

Fe(144) -2.429

Fe(145) -0.899

C10	-6.116616581	1.212595292	-2.423777478
C11	-8.193636479	2.468987586	-2.346745127
C12	-9.211077434	1.409611607	-1.899355841
C13	-10.667076222	-0.434713390	-2.562388192
C14	-10.324456207	-1.692726079	-1.753027092
C15	-8.699493773	-3.495801716	-1.363567544
C16	-7.605818897	-3.427392028	-0.293555378
C17	-5.671515991	-2.184239117	0.602559246
C18	-6.023887698	-1.335874007	1.837271014
C19	-4.425409547	-1.666445528	-0.160235251
C20	-3.273315640	-1.276272101	0.766243773
C21	-3.962028300	-2.702705431	-1.191926325
C22	-7.127421550	0.732928389	2.647781919
C23	-8.580489831	0.386633891	3.027835050
C24	-6.951162949	2.220612722	2.258157492
C25	-7.593475837	3.145668722	3.298615761
C26	-5.466384286	2.553092411	2.077195311
C27	-10.890570480	0.102783364	2.343308639
C28	-11.075335474	-1.136875664	3.194409914
C29	-5.321471526	-12.107912721	-1.546908469
C30	-4.270234001	-11.639225131	-0.541480225
C31	-3.894976230	-10.013264629	1.318772707
C32	-4.381655755	-10.469523033	2.707153347
C33	-3.989172477	-8.487522553	1.139311744
C34	-3.212317273	-7.677064102	2.182089894
C35	-2.948229954	-6.264795239	1.656734507
C36	-2.811932764	-4.292421724	3.174271572
C37	-3.671576674	-11.293185852	4.906990232
C38	-3.186944527	-10.337242445	5.974235177
C39	-0.556843056	1.667533466	-5.668674732
C40	-0.762477851	3.027451923	-4.981448499
C41	-0.106802573	0.659628508	-4.583826504
C42	-0.219973032	-0.835690728	-4.950787138
C43	0.984345046	-1.438001716	-5.672371280
C44	0.487991649	5.023743704	-4.234530651
C45	-0.419912097	6.218388165	-4.533504647
C46	1.963477751	5.472802741	-4.244074619
C47	-2.300304806	7.092113424	-5.827073162
C48	-3.547741868	6.854408516	-4.961546421
C49	-4.736510534	5.349168469	-3.434155785
C50	-4.502219551	5.609514818	-1.940619126
C51	-2.938496350	5.573495042	-0.052437803
C52	-3.112809098	6.998785932	0.496062360
C53	-1.491624775	5.146579655	0.265474477
C54	-1.090053682	3.842581927	-0.342603059
C55	-1.788650325	2.713914879	-0.730410941
C56	0.272858498	2.293246365	-1.170830901
C57	-2.672846193	9.375196675	0.056235810
C58	-4.037307361	9.772529542	0.621972261
C59	-2.332486661	10.223300243	-1.187182038
C60	-1.878683913	11.631610578	-0.936165338
C61	-2.153646592	12.501698547	0.100422515
C62	-0.822665594	13.466156317	-1.385347536
C63	-1.429133035	-4.491512033	8.454408496
C64	-1.514634182	-6.005838919	8.470058961
C65	-1.757086572	-4.023809346	7.010934117
C66	-1.794812527	-2.518361415	6.898584763
C67	-2.961055648	-1.788465918	7.192371908
C68	-0.647928159	-1.800230176	6.518480294
C69	-2.986992724	-0.392008370	7.104358413
C70	-0.654577251	-0.407552608	6.439701335
C71	-1.825427163	0.296805903	6.731450761
C72	4.158316414	1.642658469	8.054889459
C73	4.512349838	3.114908244	7.801733912
C74	3.613864193	0.993866336	6.771677874
C75	6.329262654	4.726527892	7.400291656
C76	6.078632499	5.270476835	5.992591116
C77	5.393384651	4.760741457	3.675785335
C78	3.879478482	5.028547049	3.535498249
C79	5.906274681	3.695102346	2.689588204
C80	5.587613665	3.904986178	1.205658595
C81	6.308207920	5.060609866	0.493765052
C82	6.013777097	7.501845338	0.925526824
C83	1.593519146	4.321332971	3.979207334
C84	1.011030206	5.404173196	4.905441449
C85	0.808650561	3.019672169	4.214650222
C86	0.992969629	6.267477078	7.193361897
C87	1.495653345	7.632471644	7.648277219
C88	2.985685530	9.541520590	7.232113254
C89	2.116867098	10.780937351	6.931434440

C90	4.400983283	9.698049085	6.641173467
C91	4.389233720	9.777190701	5.116282503
C92	0.301656748	11.725528344	5.587048149
C93	-0.421881705	12.430467818	6.724424412
C94	-0.731525356	11.228243956	4.540582926
C95	-0.051199696	10.576955964	3.359091140
C96	0.516873271	11.364530592	2.344174779
C97	0.100171784	9.182161378	3.282966593
C98	1.233752656	10.782497425	1.298374268
C99	0.830452191	8.584011783	2.250765420
C100	1.398954053	9.395992114	1.270065970
C101	8.686721910	-5.881473955	-2.279706480
C102	7.894657195	-4.805408707	-3.002832379
C103	6.508953371	-2.769262307	-2.699921245
C104	7.066422507	-1.379759791	-2.389171919
C105	7.153838008	0.407360458	-0.701656935
C106	8.047422387	0.445690165	0.538109728
C107	8.940972905	-0.723655828	2.496601217
C108	10.282691235	-1.415386149	2.390004751
C109	7.636940844	-1.282091649	-6.911034919
C110	7.520614694	0.246248029	-6.875927730
C111	6.249986276	-1.914634782	-6.644201276
C112	6.222703135	-3.411690670	-7.005427991
C113	5.024150302	-4.098027565	-6.383080933
C114	7.342880021	2.259839476	-5.509921564
C115	8.255476417	2.723847874	-4.395728165
C116	5.938982428	2.910904514	-5.523187093
C117	5.120885471	2.581615662	-4.305678991
C118	4.983474273	3.516459404	-3.266544226
C119	4.535519279	1.314956185	-4.155681834
C120	4.319206010	3.174819113	-2.084311444
C121	3.897307834	0.962779582	-2.964326860
C122	3.804433292	1.885511515	-1.917080767
C123	4.534269654	-10.048345932	0.417669501
C124	3.834119432	-10.819975102	1.545182347
C125	3.534351496	-9.477609237	-0.599157295
C126	4.117600813	-8.550334155	-1.619467617
C127	5.039205464	-8.847147467	-2.604605303
C128	4.336388627	-6.761938829	-2.850432974
C129	2.196176509	-12.487272256	2.215612907
C130	3.166776004	-13.246764974	3.093186668
C131	-1.531608124	-5.454243221	-3.829316124
C132	-1.329183063	-6.166060547	-2.520539882
C133	0.001405942	-7.022128439	-2.466095689
C134	0.024609425	-8.027922304	-3.650959299
C135	1.211637801	-8.997674275	-3.556283986
C136	1.170972542	-10.123844869	-4.547276095
C137	-0.077301342	-7.864671880	-1.153338507
C138	2.850469574	-2.937986116	1.478703319
Fe139	4.010576849	-4.169605098	0.431227215
Fe140	2.021944166	-0.897817691	1.586252603
Fe141	2.555638687	-2.759372033	3.382869475
Fe142	4.671060804	-2.314546444	2.007476231
Fe143	4.094664722	-0.494359644	3.811244999
Fe144	1.885365407	-4.668721922	1.809749235
Fe145	1.789323774	-3.106868828	-0.322370576
H146	-2.666453411	-1.154093240	-8.341497112
H147	-1.329191634	-0.209730783	-8.324702560
H148	-3.708510777	3.083620783	-9.203945668
H149	-2.289033034	1.373486603	-9.809489297
H150	-3.663139144	0.297757792	-10.055192321
H151	-4.144365122	3.390241048	-6.439766644
H152	-6.489254884	2.169560904	-8.852535899
H153	-4.854040938	4.403372210	-7.723064357
H154	-8.655830803	1.387665659	-8.535246316
H155	-6.286080610	-0.029774299	-7.436360757
H156	-8.807355250	2.443603964	-7.106969827
H157	-4.435857625	-0.079446319	-2.656285699
H158	-4.998629184	0.414856512	-5.406086159
H159	-6.007947684	-2.082155283	-6.347332685
H160	-7.854714858	2.982567769	-1.437515613
H161	-6.936376321	2.163927764	-4.071922983
H162	-7.677127674	-2.015509913	-5.733861434
H163	-4.247409727	1.473644566	-3.500790113
H164	-9.208309529	0.545306574	-3.782000620
H165	-8.705181572	3.199142943	-2.989179918
H166	-4.766228270	-2.975541195	-1.890989364
H167	-3.117116973	-2.309807498	-1.778046756
H168	-3.612405990	-3.619097512	-0.689104746
H169	-4.747506539	-0.751394755	-0.682408643

H170	-11.080724498	-0.761939383	-3.526902214
H171	-4.997222261	1.925926775	1.306481329
H172	-9.272578215	0.643765816	1.070253184
H173	-8.678268179	2.986000400	3.381815981
H174	-2.474066002	-0.805433004	0.178894622
H175	-2.834197877	-2.150063045	1.265704021
H176	-2.229993120	-4.111864843	9.118087181
H177	-5.350184647	3.606672467	1.781671925
H178	-7.427759119	4.196595041	3.018055850
H179	-4.920377305	2.403599151	3.022717171
H180	-7.147888359	2.985513313	4.293286677
H181	-7.465846340	2.379216753	1.293147113
H182	-6.537842734	0.522508842	3.550541137
H183	-6.728801083	0.159659025	0.622578941
H184	-3.578147449	-0.557644329	1.540888392
H185	1.281643254	2.202592763	3.641704125
H186	-0.208149538	3.175471583	3.823223143
H187	-0.132174149	2.431568779	5.844354725
H188	-2.668378813	2.046989507	6.768020720
H189	0.238432610	0.124359484	6.109698836
H190	0.259085224	-2.337233083	6.229080849
H191	-3.873421029	-2.317648721	7.480675357
H192	-6.912045192	-1.648506988	-1.057778193
H193	-8.348925749	-4.195169468	-2.138968795
H194	-9.583708821	-3.937381911	-0.887893210
H195	-8.480509793	-1.832261245	-2.686824879
H196	-11.460485971	0.078376652	-2.004199884
H197	-3.909277798	0.156321449	7.313716031
H198	-5.470324690	-3.188455429	0.997769305
H199	-11.362526909	0.959484505	2.851120467
H200	-11.422868013	-0.069656888	1.394438509
H201	-10.320296125	-1.940272776	3.030792217
H202	-3.240956338	-12.290804302	5.084307316
H203	2.087795648	-3.162882044	-5.791852462
H204	-2.642818305	-6.935853964	-4.370878571
H205	6.150688681	-3.520896061	-8.097309151
H206	7.151204884	-3.898730547	-6.673755389
H207	5.476227269	-1.393145729	-7.229450300
H208	9.075518422	2.010826081	-4.142730948
H209	7.922470761	-1.506631407	-7.949233667
H210	0.932239411	0.898895481	-4.303211402
H211	-1.101414929	-1.003914724	-5.594099660
H212	7.413041103	0.237000743	-4.795492112
H213	7.846109967	2.630308040	-6.427868530
H214	8.473993209	-1.658557516	-5.055136535
H215	0.766746032	-3.225600485	-4.634101999
H216	5.993006523	-1.766783713	-5.583588997
H217	8.932353395	-2.720973083	-6.219738034
H218	0.020487031	2.047853473	-7.623697386
H219	-0.722138645	0.834414122	-3.689160550
H220	6.223432270	-4.795078678	-4.987851623
H221	-0.407150358	-1.408840844	-4.030803953
H222	-3.656195275	4.942224201	0.492150953
H223	-2.861423974	2.540557706	-0.670939026
H224	-5.599010521	5.959181311	-3.729620754
H225	-2.877801337	4.957132344	-4.424106960
H226	-2.471382337	7.729089108	-1.310451878
H227	-2.741076426	12.395667472	1.004772052
H228	-4.896130075	9.280201695	0.104074688
H229	-3.198390907	10.215168139	-1.873808911
H230	-1.911485956	9.519509383	0.839993676
H231	-0.208072347	14.231742928	-1.853388551
H232	-1.404868349	5.116464528	1.363864740
H233	-0.802523204	5.934410489	-0.081117320
H234	-1.456987304	14.509085512	0.358633190
H235	-1.515427139	9.714332560	-1.723095572
H236	-2.526100117	5.029038989	-2.074309201
H237	-5.018145420	4.292133923	-3.559107427
H238	-1.949583304	8.107663736	-5.604146276
H239	1.202304405	1.822628847	-1.477192549
H240	-2.603670279	7.067209487	-6.882206725
H241	0.024947975	-4.151772105	9.857166651
H242	0.066315412	-3.099473142	8.604491400
H243	3.403855967	3.247191280	4.497503166
H244	1.392067207	4.663645359	2.952869342
H245	2.420484395	4.973797137	6.333329929
H246	1.036996981	4.141466254	-0.427982981
H247	2.743321976	6.423187369	-1.642869883
H248	2.406470179	7.188697017	-0.312489450
H249	2.598892642	4.624809870	-3.951979876

H250	2.245827532	5.790089075	-5.263591495
H251	5.023895362	8.865056180	6.999377016
H252	4.820344585	10.639216584	7.024240378
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H254	4.789316901	8.645116330	3.455650374
H255	7.604301391	8.600550910	1.607078130
H256	6.479589786	4.795724685	-0.561301859
H257	1.674107366	11.406086720	0.515960840
H258	-0.358220882	8.531971684	4.034437206
H259	4.164505376	8.394213456	0.879226498
H260	5.485612829	2.720910539	2.984932763
H261	5.601244231	3.384633803	5.301064124
H262	4.500895706	3.989885463	1.049113091
H263	-1.150886900	5.314877150	-6.200239732
H264	7.413200255	4.747417687	7.580924236
H265	1.060994270	3.481707253	-5.674725501
H266	6.998141117	3.620115910	2.819493718
H267	0.970942823	7.502169906	2.228711848
H268	1.366670364	7.082268867	-3.312339764
H269	5.860229915	5.442249167	8.090088171
H270	8.033185203	7.084815571	0.885140409
H271	5.501018536	9.473937213	0.967374613
H272	0.934030458	0.872819404	-6.842994903
H273	-1.558801480	1.357800031	-6.020383713
H274	0.404214311	12.451446236	2.375757969
H275	0.229626999	4.733743251	-3.200773010
H276	5.871656196	5.729448081	3.482429293
H277	7.295760429	5.212989801	0.948259589
H278	5.893532511	2.981895557	0.693831592
H279	4.586789536	6.309829049	0.143026935
H280	-0.064734594	6.399909063	6.918824632
H281	2.748737159	7.754181024	6.032274652
H282	3.075615437	9.526000797	8.328428267
H283	1.033372136	5.607695305	8.071949981
H284	1.009136837	9.709079792	5.597822649
H285	9.090022227	-5.487203746	-1.335724209
H286	7.950194293	-6.667015553	-2.010041821
H287	5.048942095	-9.212651725	0.913016273
H288	10.185098472	-7.197024146	-2.701071356
H289	9.402013848	-6.639748701	-4.027604338
H290	3.448467274	-0.071895164	6.974792936
H291	2.354746161	2.081332555	8.891770346
H292	6.497022718	2.612069189	7.660914412
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C124	7.668956582	-0.137527517	8.735059855
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	S480	3.709522126	2.993302295	-0.700305091
	S481	5.010257757	-1.587366765	1.843875340
	S482	0.763688346	2.976482647	1.361563793
	S483	2.819114836	-0.549451342	0.014236566
	S484	6.667431201	2.017032451	1.516161688
	S485	2.397649815	-1.275962608	4.373703177
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Fe(140) 0.097	C2	-7.502964849	-4.560452440	-2.319726919
Fe(141) 1.385	C3	-8.887553446	-3.034782073	-0.972583525
Fe(142) -2.622	C4	-8.861161839	-3.768480332	0.365792319
Fe(143) 1.950	C5	-9.288282186	-5.831111812	1.603059896
Fe(144) -2.320	C6	-7.873571467	-6.191610194	2.073899738
Fe(145) -0.818	C7	-5.544545954	-6.570662839	1.420932265
	C8	-4.869229205	-5.320860575	1.997121694
	C9	-4.757495622	-2.882121772	2.025505248
	C10	-5.274883366	-2.636791545	3.450204418
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	C13	-5.830965995	-5.917399753	6.657918980
	C14	-4.310250072	-5.966050664	6.874872766
	C15	-2.096874304	-5.962694033	5.792846282
	C16	-1.216662942	-4.716995900	5.664661640
	C17	-1.175944198	-2.270648680	5.292543057
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	C19	-1.376662033	-1.666360716	3.882722380
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	C22	-3.196478816	0.117193581	7.513992571
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	C56	-1.347200076	2.667015329	-1.482902372
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	C54	-2.814847882	2.805032758	0.573623800
	C55	-2.553368623	1.475619599	0.844022899
	C56	-1.935151448	1.779333266	-1.191719175
	C57	-6.397152677	6.576561025	3.027472198
	C58	-6.504577346	6.670019789	4.547981286

C59	-7.790125266	6.741880181	2.375108661
C60	-8.323049299	8.139950496	2.263142674
C61	-8.241684601	9.211358164	3.130477338
C62	-9.392992694	9.769740739	1.320076342
C63	8.422425276	0.115271579	5.148359459
C64	9.461638782	-0.966662051	4.929481197
C65	7.064965778	-0.439264875	4.644834706
C66	5.935969483	0.546185382	4.831179079
C67	5.143647023	0.554394483	5.992676019
C68	5.656709716	1.500880922	3.838316563
C69	4.108433564	1.483018907	6.159667885
C70	4.646932539	2.446841344	4.001147177
C71	3.867392615	2.432592305	5.159036848
C72	6.087729061	6.505230962	1.071260001
C73	5.192900904	7.689157313	0.682417722
C74	5.319248393	5.184929167	0.903972173
C75	4.657196341	9.365902967	-1.032865605
C76	3.259225245	9.007820791	-1.543799840
C77	1.677982176	7.205542558	-2.140302389
C78	0.827840545	6.858543065	-0.899384182
C79	1.819834762	6.017807070	-3.112279801
C80	0.520324687	5.382897739	-3.623704827
C81	-0.329036819	6.226790979	-4.586530656
C82	-1.470354472	8.380167747	-4.031026142
C83	0.649735919	5.737957998	1.250272868
C84	0.475635546	6.864232849	2.287315919
C85	1.226834662	4.509960139	1.973070119
C86	1.649051170	8.634012092	3.506210167
C87	1.315140467	10.119446841	3.424308565
C88	0.407885962	11.974834238	2.094407747
C89	-0.893784101	12.476251577	2.757718365
C90	0.433101690	12.346098176	0.598124141
C91	-0.664925354	11.640806512	-0.192909504
C92	-3.121841162	11.878225353	3.573716401
C93	-3.085632394	12.678132702	4.866865020
C94	-3.965228639	10.591018352	3.774437250
C95	-4.096895354	9.815544642	2.485159029
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C97	-3.228259204	8.754635073	2.176257642
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Fe(141) 2.769	C3	-6.485022584	-0.864120625	6.785586701
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Fe(139) 2.433	C1	-9.669234126	1.293826827	0.623680427
Fe(140) -1.384	C2	-8.661332686	2.154436771	1.393540593
Fe(141) 2.730	C3	-8.000865350	4.445237409	2.019812698
Fe(142) -2.631	C4	-7.791615107	4.252866873	3.520403055
Fe(143) 2.830	C5	-8.727023796	3.575942740	5.666596551
Fe(144) -2.201	C6	-7.809602871	2.399644884	6.018233744
Fe(145) -1.131	C7	-6.858776756	0.266798295	5.284749830
	C8	-5.405040380	0.634902840	4.974678183
	C9	-3.854223859	1.911101639	3.591520991
	C10	-3.246085561	2.800537196	4.686181903
	C11	-3.586642191	4.550569136	6.335188163
	C12	-3.357629188	3.826797278	7.668733249
	C13	-4.298494554	2.358051451	9.383794778
	C14	-3.473848026	1.072117395	9.521170508
	C15	-2.820358288	-1.061595612	8.491188908
	C16	-1.562505251	-1.268523742	7.645557382
	C17	-0.037718778	-0.278427752	5.968577319
	C18	1.032927850	0.734080886	6.409962673
	C19	-0.429738785	-0.154444892	4.472662008
	C20	0.809172382	-0.091054492	3.571753488
	C21	-1.355835075	-1.303795613	4.056174910
	C22	1.633572642	3.091553548	6.767371877
	C23	1.670293176	3.202323194	8.302569247
	C24	1.344098365	4.441517354	6.070053156
	C25	2.250272164	5.548498185	6.622710188
	C26	1.527506892	4.312335825	4.552256970
	C27	0.445364637	3.457290252	10.379501234
	C28	1.144111395	2.320970711	11.098074631
	C29	-3.477717421	-10.486350293	7.509111668
	C30	-2.284049741	-10.270045582	6.575045755
	C31	-0.287338508	-8.804734668	6.219033950
	C32	0.923894023	-9.220675487	7.075950199
	C33	-0.325217723	-7.285863912	5.970282643
	C34	0.903505409	-6.739877371	5.238135472
	C35	0.640908413	-5.322152030	4.727531771
	C36	2.441170843	-3.684106034	4.136108144
	C37	3.087968882	-10.369480303	7.082964556
	C38	4.334234621	-9.556953671	6.801383455

C39	-5.382321586	1.952441837	-1.097567092
C40	-4.550892344	3.241019597	-1.202341162
C41	-4.434410798	0.743241902	-0.969963293
C42	-5.044059593	-0.535395447	-0.359862689
C43	-5.823401710	-1.441941231	-1.308047391
C44	-3.607108265	4.876882502	-2.800260981
C45	-3.956161890	6.199329538	-2.111302141
C46	-3.555508076	4.991901136	-4.344068353
C47	-5.692854409	7.515572573	-0.985916817
C48	-5.229087200	7.505529349	0.478126428
C49	-4.197349143	6.179634807	2.278464548
C50	-2.667107884	6.171887877	2.364850903
C51	-0.506067392	5.814439756	1.283368709
C52	0.058447948	7.230253677	1.494378506
C53	0.106762212	5.305278437	-0.035200019
C54	-0.322565237	3.953617635	-0.511768577
C55	-0.506419638	2.769288024	0.171525758
C56	-0.868265959	2.451045052	-1.984372729
C57	-0.079138029	9.557830981	0.719607970
C58	0.145494519	10.089320548	2.134244119
C59	-1.130428848	10.419603034	-0.014853775
C60	-0.659240948	11.744904073	-0.540330427
C61	0.329914090	12.598753701	-0.092309671
C62	-0.677911187	13.450341320	-1.872747903
C63	7.825069965	-4.401209976	4.023978584
C64	7.746217959	-5.899876985	4.246663758
C65	6.383050899	-3.907754900	3.737823646
C66	6.320895968	-2.409756414	3.557488638
C67	6.210489494	-1.542174541	4.660811721
C68	6.399254889	-1.838279364	2.274415047
C69	6.184412160	-0.153112249	4.493317602
C70	6.381759878	-0.455504696	2.092427208
C71	6.281226493	0.386319964	3.204396541
C72	8.768927477	0.459880041	-2.579748121
C73	8.634934396	1.802001866	-3.310251060
C74	7.420271646	0.060555622	-1.959801643
C75	8.448467846	2.925401981	-5.491664506
C76	7.049422931	3.544625257	-5.530172443
C77	4.656140231	3.276367518	-5.004079040
C78	4.410913123	3.989509429	-3.658178897
C79	3.663105992	2.127034844	-5.254134350
C80	2.169831204	2.472221179	-5.218716723
C81	1.630601164	3.326094403	-6.380483969
C82	2.210248282	5.726557583	-6.756643333
C83	4.688339663	4.005285032	-1.235644139
C84	5.669103345	5.143355683	-0.893717247
C85	4.721791833	2.984002524	-0.092021226
C86	8.006691224	5.864582651	-0.987612508
C87	8.421747984	7.147443670	-1.701337027
C88	7.978110518	8.751161726	-3.511515786
C89	7.468090505	10.107632930	-2.982193873
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C92	5.876314518	11.246397292	-1.494941521
C93	6.823588294	12.121331085	-0.682099382
C94	4.658412709	10.846148961	-0.621583760
C95	3.616470485	10.081543081	-1.404435114
C96	2.691983750	10.763879284	-2.211283983
C97	3.574202700	8.677427773	-1.384960024
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C101	-0.840835948	-7.514715533	-7.614148400
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C107	4.696981612	-2.609519461	-7.526216641
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C113	-5.756128563	-5.444096468	-5.749739165
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C115	-2.952174351	1.539311188	-8.782322672
C116	-4.225053270	1.386230494	-6.540117449
C117	-3.360338131	0.583541226	-5.598194059
C118	-1.978353116	0.817163900	-5.484555715

C119	-3.923747412	-0.469573460	-4.856673024
C120	-1.182760473	0.000877459	-4.673963159
C121	-3.128399947	-1.288721662	-4.049946988
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C127	-2.186075060	-9.769507256	-3.540826620
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H155	-8.232868207	1.503181180	4.221169922
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H163	-3.894929535	2.468145033	2.643590541
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H167	-1.694273795	-1.165404679	3.016993721
H168	-0.834446394	-2.273700237	4.104944219
H169	-0.981903848	0.792324178	4.358487782
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	O457	-1.524808724	-2.180748182	-7.836568274
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	O459	6.246941619	-4.189041802	-8.473783216
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C131	3.287535600	-6.045286762	0.744902701
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C133	5.455428114	-5.004880001	1.670377019
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Fe143	2.631181297	4.356128535	1.261220760
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	O439	-5.283839645	0.515000110	-5.609529558	
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	O441	-8.167709140	-2.279439974	-5.514388593	
	O442	-7.390751783	-1.486225319	-1.175801781	
	O443	-7.540225202	2.046403444	-0.678062643	
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	O445	3.187646228	1.737718020	10.804511805	
	O446	-2.806335293	4.270553296	5.111838128	
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	O449	-2.579733098	6.359276431	-2.433824591	
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	O451	-2.181852863	5.582319457	2.585915771	
	O452	-5.873057647	10.555807921	1.625232386	
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	O454	-5.703260626	9.795017786	-4.126269917	
	O455	-11.171113527	9.728204545	-1.456343199	
	O456	-5.091912311	5.063936534	-5.226021831	
	O457	8.860429726	-0.556387426	-4.656014766	
	O458	5.604628193	2.000256005	-5.855646569	
	O459	4.617319246	6.546473593	-4.155117092	
	O460	7.835299972	8.035288660	-0.927613466	
	O461	4.395240818	-1.190816078	-9.620903337	
	O462	6.653529349	-4.629204856	-5.205523484	
	O463	7.633893077	-2.877358221	-4.22291637	
	O464	1.693394239	2.956341364	-8.477157400	
	O465	10.645403951	-0.849896651	5.194695028	
	O466	11.987400165	-2.010173418	8.194616821	
	O467	2.686758114	-5.445450537	-0.133559013	
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	O469	9.575954478	-7.451442919	1.755572215	
	O470	8.388653852	-7.859146065	-0.121952340	
	O471	6.505866038	-3.337508205	3.071375040	
	O472	6.050893012	-5.336165907	4.010594038	
	O473	5.516186234	-4.006214082	0.724052576	
	O474	7.459657255	-3.550677122	7.537742476	
	O475	6.148795244	-2.008776230	5.556249690	
	O476	-2.898169622	3.633397404	-4.985292096	
	O477	10.477166350	-6.535647978	4.559437926	
	O478	8.030458707	-5.633655220	5.776038880	
	S479	1.466519330	6.247134321	1.146711571	
	S480	2.414963754	3.201277929	-0.658726124	
	S481	4.931640948	-1.294081636	-0.707493845	
	S482	1.787831137	2.955710219	2.778619361	
	S483	1.855597289	-0.263930065	-0.682714378	
	S484	6.369851111	2.370846892	-0.824313934	
	S485	3.934542959	-1.838697806	2.751883799	
	S486	4.764583648	4.350415318	1.856863906	
	S487	7.046693398	-0.056940006	2.004225703	
	S488	4.674325019	1.340052552	4.570917854	
	27 (S=1/2)		bm1s2b2x6n2xaconexdtl.car_3		
	Fe(139) 2.540	C1	-2.963870889	9.300326847	1.594052212
	Fe(140) -1.438	C2	-2.501576548	8.744918785	0.242763485
	Fe(141) 2.380	C3	-3.038723670	8.504683553	-2.148618873
	Fe(142) -2.575	C4	-1.707412179	8.939271028	-2.756952380
	Fe(143) 2.016	C5	0.046077266	10.626798692	-2.910910790
	Fe(144) -2.205	C6	1.234264979	9.802682934	-2.399474389
	Fe(145) 0.322	C7	2.128014388	8.427430592	-0.581522875
		C8	2.114751900	7.021239757	-1.188276033
		C9	0.798887181	5.162366054	-2.054810517
		C10	1.336438633	5.156934563	-3.494190059
		C11	1.547344316	6.325252681	-5.611529342
		C12	3.055598922	6.588334060	-5.712101767
		C13	4.936912734	7.983707930	-5.008543540
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		C15	6.542329979	5.872787915	-2.243028510
		C16	6.364919596	4.361752152	-2.076556744
		C17	4.959568958	2.393589732	-2.615848535
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		C19	3.614642480	2.123708203	-1.894542729

C20	3.235645513	0.640792824	-1.959669185
C21	3.667059669	2.619920307	-0.445066060
C22	4.137609704	1.646891876	-6.297387285
C23	5.293087576	2.240139658	-7.126255734
C24	2.757572233	1.835869484	-6.968777728
C25	2.792867067	1.405998405	-8.440013285
C26	1.671001177	1.060432128	-6.213832744
C27	6.473117685	4.217236661	-7.893873967
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C30	10.218529174	3.456056097	6.243429550
C31	9.650380834	1.698082778	4.555397139
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C33	8.599811487	1.841578364	3.441478971
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C35	6.778788609	0.729618087	2.102446565
C36	6.084566432	-0.930376050	0.366907171
C37	12.117287653	-1.208962267	4.337747952
C38	11.764071982	-2.401759406	3.475578882
C39	-3.461299783	4.786704592	0.474588112
C40	-3.933670307	3.967379544	-0.732625547
C41	-2.312085492	4.066689231	1.201036346
C42	-1.404689060	4.987979264	2.050629866
C43	-1.884376645	5.239923367	3.471640349
C44	-5.729330614	2.512765241	-1.607360350
C45	-5.925561272	3.211189221	-2.960161079
C46	-7.055585186	1.938538126	-1.053484874
C47	-6.375631365	5.329971323	-4.118812303
C48	-5.072923817	5.593720313	-4.886613356
C49	-2.629017890	5.327102314	-4.917639179
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C54	-2.591672081	0.152938281	-3.191382635
C55	-1.343629626	0.170173688	-2.600646824
C56	-2.849296346	-0.555578685	-1.153956605
C57	-4.644824014	1.469889073	-8.367915832
C58	-3.723203872	1.811894036	-9.536526112
C59	-5.959693678	2.277002879	-8.451529136
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C62	-8.977963601	1.403542113	-10.177681322
C63	7.736514677	-6.179010393	-0.455784316
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C116	-7.269518721	1.309415844	3.297221448
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H164	2.932055711	8.081722099	-4.280041260
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H167	2.700052134	2.446920683	0.050456574
H168	4.433210462	2.082190057	0.135848288
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H176	8.353854870	-6.108954776	-1.371861441
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H239	-3.259604327	-0.915671895	-0.216837201
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H241	-0.813760756	-0.456933424	-0.598608311
H242	7.401008321	-8.184739364	-0.698475197
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H244	-2.069190226	-5.470426342	-2.366830470
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