

What triggers the coupling of proton transfer and electron transfer at the active site of nitrogenase?

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Supplementary Informations

1. Computational models

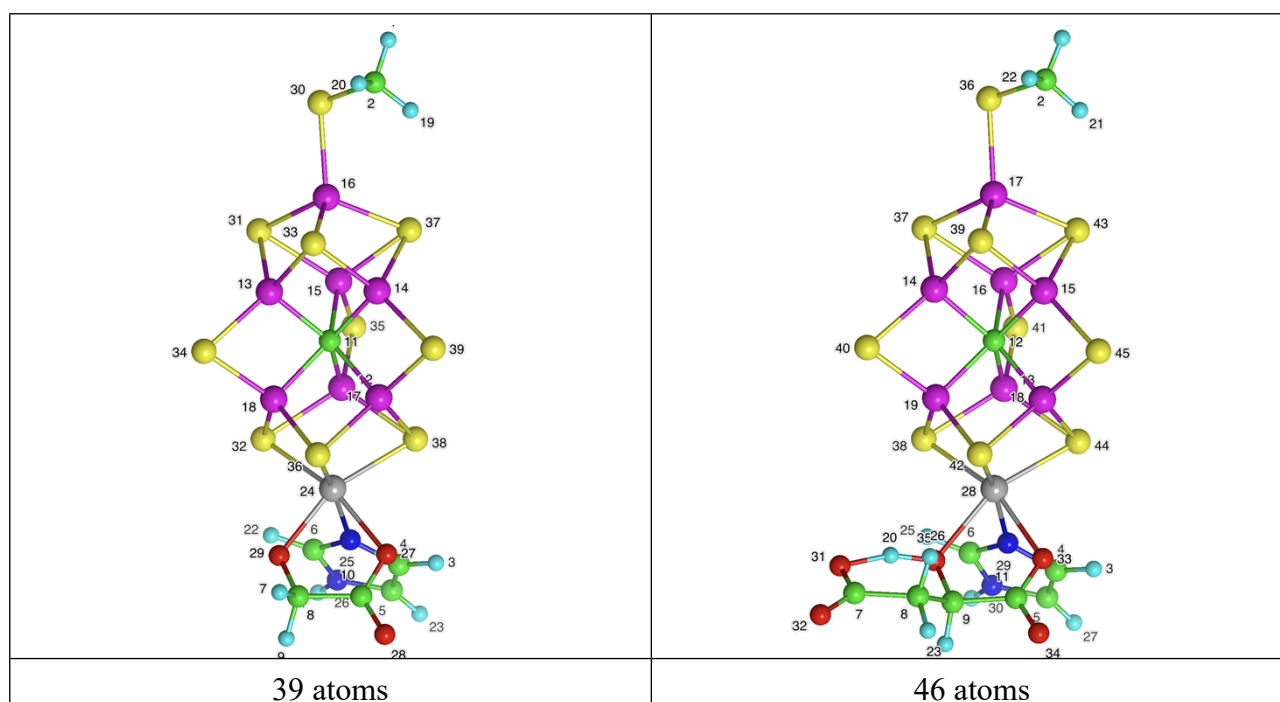


Fig S1. Minimal models.

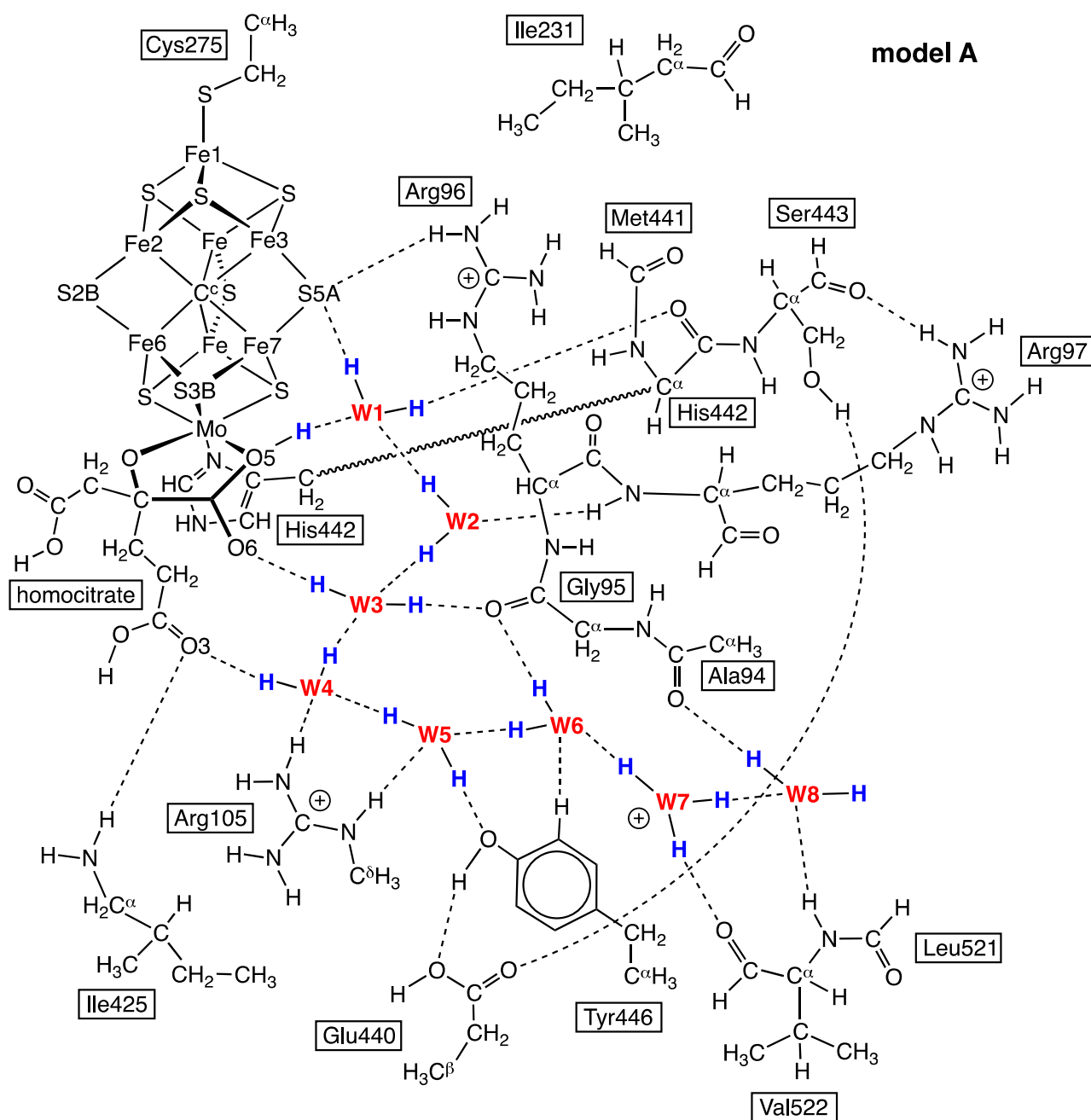


Fig S2. Water path model used for the calculation of proton transfer steps. Surrounding residues are truncated (with hydrogenation) according to their proximity to the water chain and its hydrogen bonds. Proximal parts of residues 231Ile and 425Ile are included because they provide van der Waals enclosures for the motions of W1, W2, W4 and W5. Atoms C α Arg96A, C α Ile231A, C α Ala94A, C α His442A, C α Ser443A, C α Tyr446A, C α Val522D, C δ Arg105B, C α Ile425A and C β Glu440A are fixed during the calculations.

2. Validation of computational procedure

Details of validation calculations have been published.¹ The following table provides additional results on the reproduction of the dimensions of the FeMo-co cluster.

Table S1. Dimensions (Å) for FeMo-co cluster, as calculated for full 483 atom model of the FeMo protein² in comparison with crystallographic dimensions.

Distance	Crystal (PDB 3U7Q)	Calc with HisO	Calc - crystal	Calc with HisH ⁺	Calc - crystal
Cc-Fe2	1.997	1.945	-0.052	1.962	-0.036
Cc-Fe3	1.984	1.982	-0.001	1.982	-0.002
Cc-Fe4	1.990	2.005	0.015	1.995	0.004
Cc-Fe5	2.008	2.045	0.036	2.023	0.015
Cc-Fe6	2.018	1.969	-0.049	2.009	-0.009
Cc-Fe7	1.997	2.011	0.014	1.998	0.000
Fe1-Fe2	2.668	2.673	0.005	2.671	0.003
Fe1-Fe3	2.668	2.653	-0.015	2.652	-0.015
Fe1-Fe4	2.655	2.681	0.027	2.687	0.032
Fe2-Fe6	2.576	2.630	0.054	2.643	0.067
Fe3-Fe7	2.583	2.603	0.021	2.606	0.024
Fe4-Fe5	2.612	2.573	-0.039	2.555	-0.057
Mo-Fe5	2.727	2.733	0.006	2.731	0.004
Mo-Fe6	2.674	2.717	0.044	2.730	0.056
Mo-Fe7	2.681	2.679	-0.002	2.687	0.006
Fe2-S1A	2.261	2.257	-0.004	2.252	-0.009
Fe2-S2A	2.254	2.291	0.037	2.296	0.042
Fe3-S2A	2.275	2.285	0.010	2.288	0.013
Fe3-S4A	2.254	2.233	-0.021	2.228	-0.026
Fe2-S2B	2.206	2.178	-0.028	2.219	0.013
Fe3-S5A	2.221	2.236	0.015	2.226	0.005
Fe6-S2B	2.173	2.160	-0.013	2.219	0.047
Fe7-S5A	2.210	2.209	0.000	2.199	-0.011
Fe6-S1B	2.235	2.226	-0.008	2.234	0.000
Fe6-S3B	2.218	2.238	0.020	2.250	0.032
Fe7-S3B	2.245	2.254	0.009	2.252	0.007
Fe7-S4B	2.220	2.228	0.009	2.222	0.002
average deviation			0.020		0.020

3. Calculated atom charges

Table S2. Calculated charges for the minimal model with various electron populations for Chart 1.

		minus 1 electron		resting E0		plus 1 electron		plus 2 electrons	
		S=1		S=3/2		S=1		S=3/2	
FeMo-co	atom	Mulliken	Hirshfeld	Mulliken	Hirshfeld	Mulliken	Hirshfeld	Mulliken	Hirshfeld
	H 1	0.110	0.025	0.097	0.017	0.080	0.007	0.051	-0.009
	C 2	-0.235	-0.138	-0.233	-0.146	-0.234	-0.156	-0.233	-0.173
	H 3	0.133	0.054	0.124	0.051	0.120	0.047	0.113	0.043

	C 4	0.016	-0.034	0.011	-0.038	0.015	-0.040	0.018	-0.042
	C 5	-0.035	-0.035	-0.044	-0.045	-0.053	-0.052	-0.061	-0.061
	C 6	0.193	0.048	0.188	0.043	0.185	0.039	0.184	0.035
	H 7	0.096	0.021	0.074	0.007	0.059	-0.004	0.043	-0.015
	C 8	-0.035	-0.050	-0.028	-0.060	-0.021	-0.069	-0.016	-0.077
	H 9	0.096	0.021	0.074	0.007	0.055	-0.004	0.034	-0.017
	C 10	0.415	0.111	0.408	0.102	0.399	0.094	0.392	0.086
	C 11	-0.762	-0.176	-0.769	-0.183	-0.759	-0.186	-0.785	-0.191
Fe5	Fe12	0.543	-0.032	0.552	-0.045	0.558	-0.060	0.535	-0.111
Fe2	Fe13	0.530	-0.008	0.535	-0.026	0.548	-0.040	0.563	-0.055
Fe3	Fe14	0.525	-0.007	0.535	-0.028	0.552	-0.037	0.568	-0.049
Fe4	Fe15	0.564	0.011	0.565	-0.010	0.538	-0.063	0.565	-0.052
Fe1	Fe16	0.570	-0.004	0.578	-0.024	0.587	-0.042	0.559	-0.121
Fe7	Fe17	0.499	-0.055	0.536	-0.058	0.538	-0.079	0.552	-0.083
Fe6	Fe18	0.521	-0.044	0.529	-0.061	0.531	-0.081	0.548	-0.084
	H 19	0.133	0.027	0.127	0.023	0.120	0.015	0.111	0.007
	H 20	0.116	0.026	0.106	0.019	0.100	0.012	0.084	0.001
	H 21	0.243	0.174	0.236	0.168	0.229	0.163	0.223	0.158
	H 22	0.143	0.067	0.135	0.062	0.129	0.057	0.124	0.051
	H 23	0.123	0.069	0.113	0.063	0.105	0.057	0.096	0.052
	Mo24	0.793	0.428	0.771	0.402	0.754	0.380	0.725	0.355
	N 25	-0.374	-0.115	-0.356	-0.114	-0.346	-0.111	-0.341	-0.107
	N 26	-0.250	-0.040	-0.255	-0.047	-0.260	-0.053	-0.266	-0.060
	O 27	-0.537	-0.276	-0.537	-0.283	-0.537	-0.287	-0.536	-0.296
	O 28	-0.559	-0.414	-0.587	-0.438	-0.611	-0.459	-0.635	-0.480
	O 29	-0.618	-0.321	-0.637	-0.344	-0.646	-0.362	-0.656	-0.378
Scys	S 30	-0.628	-0.288	-0.683	-0.335	-0.741	-0.388	-0.789	-0.433
S1A	S 31	-0.602	-0.197	-0.694	-0.265	-0.794	-0.344	-0.890	-0.414
S1B	S 32	-0.539	-0.169	-0.606	-0.215	-0.670	-0.255	-0.722	-0.297
S2A	S 33	-0.607	-0.195	-0.671	-0.245	-0.774	-0.323	-0.881	-0.407
S2B	S 34	-0.665	-0.327	-0.767	-0.406	-0.873	-0.489	-0.969	-0.566
S3A	S 35	-0.708	-0.359	-0.797	-0.429	-0.907	-0.517	-1.016	-0.608
S3B	S 36	-0.460	-0.142	-0.573	-0.224	-0.634	-0.265	-0.716	-0.322
S4A	S 37	-0.618	-0.205	-0.695	-0.261	-0.802	-0.341	-0.876	-0.393
S4B	S 38	-0.502	-0.159	-0.592	-0.223	-0.661	-0.268	-0.721	-0.316
S5A	S 39	-0.627	-0.290	-0.771	-0.410	-0.881	-0.496	-0.977	-0.572
Fe total		3.752	-0.140	3.830	-0.251	3.852	-0.403	3.890	-0.555
core S total		-5.328	-2.042	-6.166	-2.678	-6.996	-3.296	-7.768	-3.894
total S double bridge		-2.000	-0.976	-2.335	-1.245	-2.661	-1.502	-2.962	-1.746
total S triple bridge		-3.328	-1.066	-3.831	-1.433	-4.335	-1.794	-4.806	-2.148
mean S double		-0.667	-0.325	-0.778	-0.415	-0.887	-0.501	-0.987	-0.582
mean S triple		-0.555	-0.178	-0.639	-0.239	-0.723	-0.299	-0.801	-0.358
mean Mo bound S		-0.500	-0.157	-0.590	-0.221	-0.655	-0.262	-0.720	-0.311

Hirshfeld charges

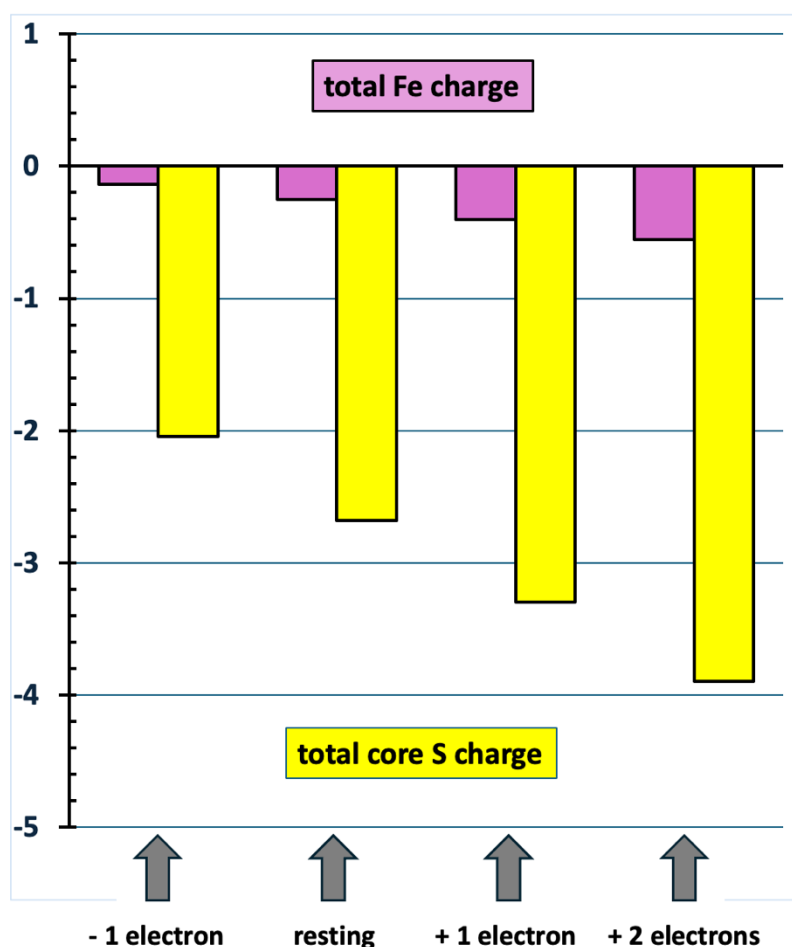


Chart S1. Hirshfeld calculated total charges for the seven Fe atoms and nine S atoms of FeMo-co as dependent on the total number of electrons. The resting $S=3/2$ state of the enzyme is labelled as 'resting', with results for the removal of one electron or addition of one or two electrons. This the Hirshfeld equivalent of Chart 1(a).

4. Protonated homocitrate

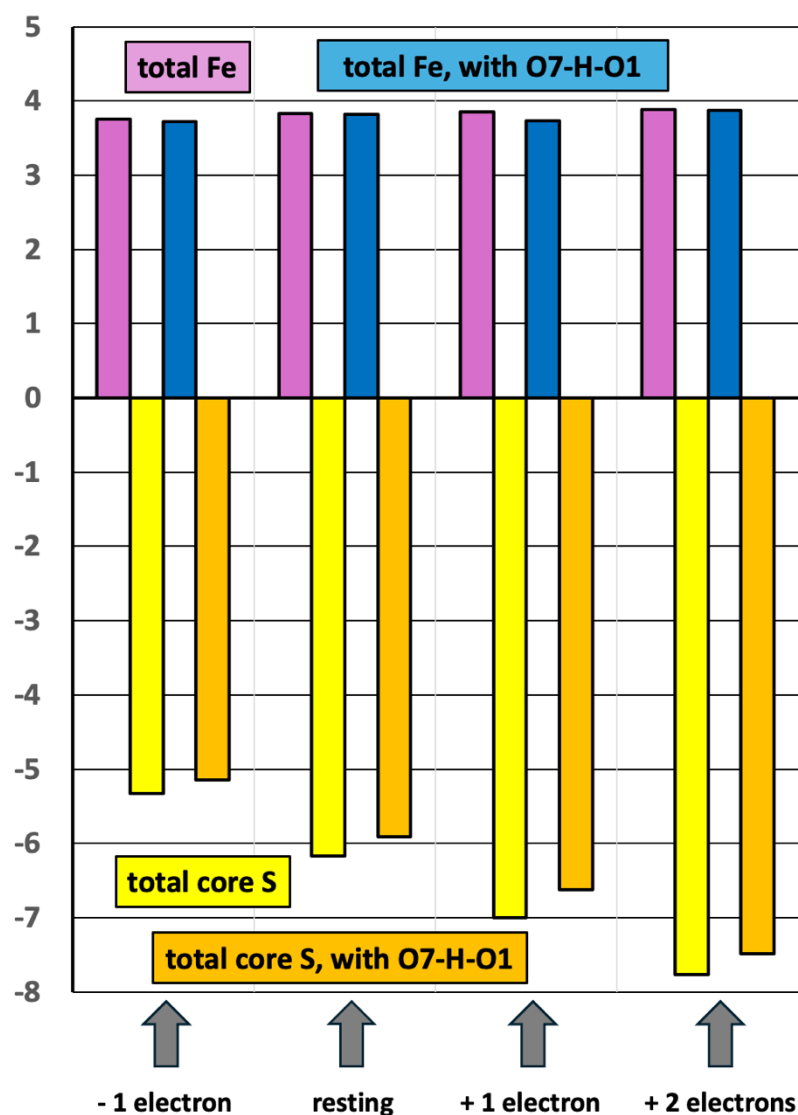


Chart S2. Comparison of Fe and S total charges for structures with and without a proton hydrogen bonded between O7 and O1 of homocitrate..

5. References

1. I. Dance, *Molecular Simulation*, 2018, **44**, 568-581.
2. I. Dance, *Chembiochem*, 2020, **21**, 1671-1709.

6. Atomic coordinates

39 atom model, resting file femocob.car_2	1	1.306017198	8.992112663	0.656461218	H
	2	1.030910469	8.002788031	1.051708397	C
	3	2.033375301	-3.951519009	-1.604106721	H
	4	1.056091805	-4.064870132	-2.064465995	C
	5	0.695363995	-4.809607721	-3.164724121	C
	6	-1.073000572	-3.754059566	-2.333494930	C
	7	-1.032294625	-4.190328405	2.981517898	H
	8	-0.753834788	-4.401420801	1.919389697	C
	9	-1.077599764	-5.450323271	1.732651252	H
	10	0.780071217	-4.382801200	1.869770693	C
	11	-0.212041349	1.631822674	0.327235555	C

	12	-0.176680229	0.326995780	-1.196027047	Fe
	13	-1.559496801	2.885064416	1.075139716	Fe
	14	1.073461886	2.944900126	1.074655511	Fe
	15	-0.241512350	2.902936454	-1.201313539	Fe
	16	-0.274675866	5.116259046	0.366788743	Fe
	17	1.103228919	0.350259497	1.081337290	Fe
	18	-1.466497610	0.280349298	1.074997391	Fe
	19	1.882702972	7.321433437	0.918343811	H
	20	0.818771457	8.090473811	2.127035093	H
	21	-1.252453300	-4.994193930	-4.046050290	H
	22	-2.094494936	-3.405683062	-2.222653917	H
	23	1.259348584	-5.448512965	-3.836312934	H
	24	-0.157276027	-1.950840940	0.350922156	Mo
	25	-0.050141968	-3.412505421	-1.561694069	N
	26	-0.662560387	-4.598487147	-3.320508529	N
	27	1.284003550	-3.439066032	1.140025499	O
	28	1.453205956	-5.232077460	2.505902810	O
	29	-1.361272013	-3.520998666	1.025986683	O
	30	-0.453274711	7.387145815	0.129358162	S
	31	-2.098473697	4.158704734	-0.690931477	S
	32	-2.028961926	-0.898936884	-0.739256706	S
	33	-0.259925833	4.226224756	2.421827469	S
	34	-3.006002967	1.529323152	2.038118394	S
	35	-0.175778142	1.593523914	-2.993084552	S
	36	-0.164638996	-0.892772627	2.494893827	S
	37	1.575750032	4.230751460	-0.691707647	S
	38	1.691881507	-0.849615243	-0.730356874	S
	39	2.588699915	1.677558075	2.032602884	S
FeMoco 46 atom model, resting file femocaaa4.car_1	1	1.664003544	9.511929518	0.205110671	H
	2	1.348159939	8.540361544	0.616402268	C
	3	2.365894532	-3.390666861	-2.035391280	H
	4	1.386156677	-3.507287090	-2.486963588	C
	5	1.013511775	-4.258635842	-3.577113917	C
	6	-0.743967061	-3.183369024	-2.750041721	C
	7	-2.617503069	-3.707204990	2.877945882	C
	8	-1.078271446	-3.720810281	2.912879703	C
	9	-0.458594850	-3.959245763	1.522874604	C
	10	-0.662265160	-5.003662224	1.217332682	H
	11	1.067016226	-3.808760763	1.516290868	C
	12	0.137287968	2.177784222	-0.117776317	C
	13	0.162328117	0.893638691	-1.652848256	Fe
	14	-1.211811721	3.428305940	0.642581546	Fe
	15	1.434861481	3.486409873	0.634670262	Fe
	16	0.104091163	3.470672120	-1.632930332	Fe
	17	0.059876251	5.673280434	-0.054613242	Fe
	18	1.449038390	0.879947422	0.623772872	Fe
	19	-1.116580342	0.821255799	0.623831905	Fe
	20	-2.065648921	-2.951062973	1.000489329	H
	21	2.176789678	7.826821966	0.501873372	H
	22	1.127575778	8.658982938	1.687595998	H
	23	-0.711311966	-4.469205448	3.628876038	H
	24	-0.943424490	-4.438140119	-4.442776668	H
	25	-1.762421380	-2.827304897	-2.635316034	H
	26	-0.754214002	-2.727019639	3.268306656	H
	27	1.569849228	-4.905854522	-4.245374965	H
	28	0.220222049	-1.375280898	-0.142223704	Mo
	29	0.286464386	-2.842632194	-1.985714165	N
	30	-0.343230172	-4.039890156	-3.727137816	N
	31	-3.147429903	-3.170674670	1.819965713	O
	32	-3.273970089	-4.166049162	3.839828582	O
	33	1.561171767	-2.920786548	0.717011213	O
	34	1.747145150	-4.561831596	2.247672491	O
	35	-1.063876708	-3.081639497	0.567220723	O

	36	-0.144717422	7.945579857	-0.300925203	S
	37	-1.762192553	4.709853174	-1.113074925	S
	38	-1.671933337	-0.348500076	-1.203888651	S
	39	0.091525639	4.752689516	1.992069198	S
	40	-2.652869182	2.056829940	1.588622343	S
	41	0.127851444	2.181213631	-3.437233755	S
	42	0.190416838	-0.352513518	2.020664679	S
	43	1.920872159	4.792163505	-1.125789607	S
	44	2.044800935	-0.269124648	-1.204454400	S
	45	2.929337000	2.179411546	1.597700229	S
FeMoco 46 atom model + 1 electron file femocaaa5.car_1	1	1.664277629	9.498928417	0.194155100	H
	2	1.341198576	8.528486290	0.606310391	C
	3	2.362161889	-3.372459202	-2.041568485	H
	4	1.381116635	-3.494343594	-2.490011855	C
	5	1.003757939	-4.253404789	-3.574335741	C
	6	-0.747405165	-3.163071219	-2.748810318	C
	7	-2.633908899	-3.713180225	2.883958706	C
	8	-1.093397853	-3.704358085	2.905041145	C
	9	-0.458621150	-3.943361090	1.525711894	C
	10	-0.644213273	-4.993530175	1.226341043	H
	11	1.072391174	-3.778957541	1.531557912	C
	12	0.129046044	2.145439797	-0.107071725	C
	13	0.168541111	0.893493820	-1.649198685	Fe
	14	-1.176328334	3.386148377	0.662502721	Fe
	15	1.439258852	3.455960932	0.650601557	Fe
	16	0.103494909	3.465422601	-1.646239923	Fe
	17	0.052822831	5.623648342	-0.046978329	Fe
	18	1.473953186	0.879620365	0.633735035	Fe
	19	-1.103558855	0.847592262	0.618400547	Fe
	20	-2.016580960	-2.926014527	0.928271339	H
	21	2.170662381	7.812866113	0.505192934	H
	22	1.116063840	8.655924067	1.676417472	H
	23	-0.724619838	-4.455678893	3.615664482	H
	24	-0.956495789	-4.426933113	-4.437850368	H
	25	-1.761293821	-2.792334292	-2.631194798	H
	26	-0.776059920	-2.711475830	3.267488226	H
	27	1.557618831	-4.901411992	-4.244922486	H
	28	0.223518618	-1.342514185	-0.164340819	Mo
	29	0.286823837	-2.819782209	-1.992364406	N
	30	-0.354362130	-4.031311501	-3.722271347	N
	31	-3.191124657	-3.200599370	1.840481292	O
	32	-3.253312555	-4.181746579	3.875086866	O
	33	1.571732549	-2.910667606	0.725305313	O
	34	1.745921464	-4.522346948	2.287564978	O
	35	-1.061988634	-3.086683751	0.542841263	O
	36	-0.144535641	7.918008980	-0.313916452	S
	37	-1.781316501	4.663982391	-1.088988917	S
	38	-1.685457610	-0.334426659	-1.200358896	S
	39	0.090204536	4.705270713	2.007584234	S
	40	-2.689412957	2.038843427	1.549064110	S
	41	0.120068992	2.163212520	-3.462009187	S
	42	0.197130748	-0.318832226	2.012717890	S
	43	1.940956113	4.777172381	-1.102206397	S
	44	2.063052346	-0.249793913	-1.213016047	S
	45	2.978233849	2.169175959	1.605660010	S
TS for H transfer without added electron file mhohv4w2w13b0tc_1_26596.61	C1	0.705007463	2.817227612	8.302544776	
	C2	-7.505477059	10.710533571	-9.317337507	
	C3	0.740569937	1.761017317	7.214910915	
	C4	-0.613880572	0.601779331	4.399875719	
	C5	-7.362152740	9.641755786	-8.227189081	
	C6	-0.555660430	0.134463231	5.864486226	
	C7	-0.974992537	2.607227612	2.907544776	

	C8	0.077395595	3.744041731	3.007275706
	C9	-2.418994438	3.154314225	2.735415170
	C10	-2.655296813	4.029726121	1.492165962
	C11	-4.143391044	4.420629358	1.373688105
	C12	-2.093193855	-1.419285066	-3.686378134
	C13	2.069716150	4.789135125	1.956791353
	C14	-4.396936846	6.601075590	0.134109421
	C15	1.626195645	6.201078746	1.541681434
	C16	3.235514879	4.253286486	1.098453930
	C17	3.901833276	3.000754474	1.695735405
	C18	-6.686992537	3.602227612	-5.196455224
	C19	4.919442604	2.335453861	0.755531928
	C20	6.776684347	3.374691675	-0.623702093
	C21	2.170007463	6.568227612	-2.814455224
	C22	-7.894074066	-0.409206198	0.819151999
	C23	3.602684219	6.780891410	-3.241411527
	C24	1.332199940	5.568821692	-3.631518588
	C25	-6.566260550	0.243125288	0.507980710
	C26	-5.682282837	-0.564056663	-0.530549808
	C27	-0.186647612	5.824640077	-3.433571645
	C28	1.739298479	4.111836545	-3.320364260
	C29	-5.496282563	-2.034886658	-0.026989740
	C30	-4.575763541	-2.845329161	-0.970149176
	C31	-0.683251449	5.828305056	-1.975419056
	C32	-4.314796112	-4.232014259	-0.455496862
	C33	-4.246042446	0.055592031	-0.558157652
	C34	7.089616969	-2.837155823	0.245542398
	C35	-0.947992537	-8.024772388	-0.673455224
	C36	5.948144510	-2.374585184	0.928914432
	C37	7.136703742	-4.201579930	-0.092082158
	C38	4.892324675	-3.227511345	1.256945477
	C39	-0.727118125	-7.751600402	0.834829592
	C40	6.086517779	-5.076419257	0.237131338
	C41	0.131662500	-8.859666657	1.501558617
	C42	4.960144971	-4.583254849	0.907502368
	C43	-2.070740293	-7.604862597	1.586746355
	C44	0.428007463	-5.599772388	5.405544776
	C45	1.631105819	-8.826713598	1.150464175
	C46	-1.569475561	-4.366455295	4.604827016
	C47	8.220758952	-1.882213220	-0.104403745
	C48	2.636007463	-4.850772388	-4.312455224
	C49	3.032703075	-6.146470650	-3.590625750
	C50	2.993729860	-6.032319248	-2.081255683
	C51	0.212720497	-1.249581824	-6.683358928
	C52	-1.043992537	-0.700772388	-4.599455224
	C53	-0.028944197	-0.036186955	-3.650940636
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	C58	3.273748363	0.334901097	-2.977378277
	C59	2.476175119	-1.520037785	-1.444061195
	C60	7.793007463	-0.731772388	-1.045455224
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	C66	3.626729436	-3.276428020	6.914320347
	Fe67	-7.783729635	6.556645339	-7.053387526
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	Fe69	-6.846393552	3.870375166	-7.141624129
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	Fe72	-7.424358517	2.587665753	-3.688350046
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	H75	-1.675168307	-8.858026586	-0.764244356
	H76	3.364011300	-4.054879515	-4.137799373
	H77	2.587767015	-5.040182382	-5.393472120
	H78	1.650950457	-4.502728997	-3.980623577
	H79	0.461598176	-2.099131639	-7.345410539
	H80	7.003287531	-0.121317536	-0.591758849
	H81	8.646196954	-0.072648307	-1.262660610
	H82	6.234966483	-0.271339371	8.741269851
	H83	-6.338269307	9.249746362	-8.205107592
	H84	-7.586432129	10.062715301	-7.240624930
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	H87	-7.250910451	10.308302005	-10.307496627
	H88	-6.772036569	1.219639218	0.058837247
	H89	-5.996221507	0.375355427	1.433123586
	H90	-5.072501132	-2.008189912	0.985354532
	H91	-6.476331024	-2.521627760	0.027732886
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	H93	-3.604363605	-2.355887124	-1.076688182
	H94	-0.304865707	1.172793015	0.027025214
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	H96	3.901797732	-7.754244085	-1.959720020
	H97	0.029471906	-8.761780531	2.594231428
	H98	-0.291136850	-9.844977205	1.244270853
	H99	1.809806927	-8.934808835	0.073221322
	H100	-1.725405286	-3.574026475	0.499810017
	H101	-0.009165359	-8.376331162	-1.119907213
	H102	-2.700629695	-6.819679289	1.153958695
	H103	-0.179146686	-6.799572209	0.915458575
	H104	-1.611627088	-7.083109371	-2.379700438
	H105	4.038402510	-6.477937946	-3.889540091
	H106	2.353105708	-6.969876487	-3.861370798
	H107	-2.630764987	-8.552636305	1.560696776
	H108	-2.204471009	-6.414506598	-1.012521023
	H109	-1.897129415	-7.345337814	2.640510833
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	H113	-0.269852395	6.671032722	-1.403490370
	H114	-1.776203090	5.911481627	-1.958519216
	H115	-0.423675581	4.899159597	-1.451789853
	H116	0.530449248	6.380058716	1.564134851
	H117	-4.643373393	6.701450580	-1.918878336
	H118	-4.561743425	8.226743075	-1.084679455
	H119	-4.166479076	8.339169339	1.180836570
	H120	-4.771150117	4.769319759	-0.639911021
	H121	-2.356659478	3.483873262	0.591435393
	H122	-2.039296782	4.936942349	1.532053249
	H123	-4.488042930	4.926586993	2.283868530
	H124	-4.762141856	3.521673849	1.270241832
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	H126	-3.090099417	2.286118767	2.709932695
	H127	-0.718441918	1.906650560	2.117177800
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	H130	0.301759122	-0.540243705	5.954759409
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	H132	3.153777614	-1.129254425	-0.671522445
	H133	2.884237362	-3.394456906	-1.940318128
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	H135	-1.466548590	-0.441400895	6.060036196

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H137	1.236217287	-1.647375938	-3.834716098
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H139	-1.290130623	1.431982281	7.402017456
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H146	2.860721064	4.027493133	0.087815467
H147	1.574344628	0.402373883	-1.713764247
H148	5.246281848	1.383877153	1.194086003
H149	1.551842738	5.751694996	-4.693678487
H150	3.967919684	5.062444755	0.991294185
H151	5.593407453	2.195273097	-1.879125005
H152	4.390104188	3.250832021	2.649638487
H153	4.444851374	2.119274093	-0.204474699
H154	1.571169708	3.869375558	-2.261859808
H155	6.897910232	3.044271988	-2.634726195
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H157	-0.436908711	6.793162257	-3.893880014
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H166	-2.029071312	2.485918755	-1.204607970
H167	0.239662397	1.979389540	-1.197533860
H168	-0.819799427	-0.237889412	1.717228800
H169	1.837845841	-2.518911075	2.914126098
H170	1.147553960	-1.211653558	3.442793638
H171	-1.015127873	-2.168942258	0.783865511
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H177	-1.832728042	-5.271600853	6.431587896
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H187	8.628704354	-1.446389202	0.823141538
H188	-3.775276816	2.815998478	-1.880663661
H189	-5.143963904	-5.926384987	-0.168773450
H190	-8.751541308	-1.524525732	2.117305893
H191	4.395014413	0.741991219	5.015084768
H192	3.809349502	-4.782563116	4.574427076
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	H204	-1.946153505	-0.100495388	0.605792302
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	H206	1.006917506	3.779142377	7.868048647
	H207	2.192844968	6.319463892	-1.742249570
	H208	1.723671778	7.580199743	-2.841438203
	H209	3.353273516	0.297021050	-4.082906129
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	N214	6.105649416	3.193247207	0.526732337
	N215	-4.442955598	5.258099235	0.195543014
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	N218	7.929156972	4.091660592	-0.597904610
	N219	-4.698923477	7.220650342	-1.023811927
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	N224	-2.195235551	-3.662357655	3.644621918
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	N228	1.084093655	-0.758381775	-3.361295356
	N229	5.870113505	-1.337311664	7.031082946
	O230	-8.912211045	-0.339095573	0.139202698
	O231	-7.861476125	-1.124500682	1.996296725
	O232	-3.246929391	-4.616542483	0.029712046
	O233	-5.389144803	-5.058885198	-0.560172913
	O234	-3.779937581	0.325872473	-1.733901125
	O235	-3.591480271	0.192148269	0.510290877
	O236	-6.249687577	-0.526531537	-1.809927994
	O237	0.124830112	4.472723307	4.017026386
	O238	-2.535793920	2.847642496	-1.983118318
	O239	-0.133599934	2.102585661	-0.300336868
	O240	-0.972793992	-0.327468418	0.740360634
	O241	3.889884342	-5.408741877	1.272193063
	O242	1.795772732	1.425804266	6.638949654
	O243	-0.423822479	-0.234772340	3.477795076
	O244	2.405069043	7.090458105	1.224081131
	O245	4.136635026	6.311740191	-4.244714234
	O246	2.518489717	-5.095899139	-1.447271240
	O247	3.525743680	-7.071349111	-1.365231189
	O248	0.518099844	-0.077191593	-6.942886931
	O249	-0.292971938	1.063868393	-3.119348772
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	O255	2.016139716	-1.677902009	3.403308416
	O256	4.560150517	1.061183707	5.944398394
	O257	-1.002307574	-3.137857187	1.013781611
	O258	4.290614687	-0.053626363	3.384402067
	S259	-8.531892398	8.184659055	-8.508185893
	S260	-9.062453790	4.576094997	-7.272823913
	S261	-7.424313767	0.478030891	-4.498278412
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	S264	-6.259084026	1.883729098	-8.024788256
	S265	-5.511746128	2.819936868	-1.952527377
	S266	-5.604258385	5.775220833	-7.570290282
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	C4	-0.615737274	0.603170046	4.398882148
	C5	-7.364568904	9.639801027	-8.230722984
	C6	-0.557108693	0.134236369	5.863467520
	C7	-0.974906716	2.607018657	2.907145522
	C8	0.077805358	3.743816942	3.011104517
	C9	-2.419629111	3.153848702	2.731494040
	C10	-2.657708101	4.025654874	1.486510148
	C11	-4.145502654	4.419012955	1.368315449
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	C13	2.071574763	4.790504410	1.956503085
	C14	-4.398083600	6.598932402	0.128750607
	C15	1.627708352	6.199633160	1.541859667
	C16	3.234328405	4.250584232	1.099850976
	C17	3.902915670	2.998481184	1.695282050
	C18	-6.686906716	3.602018657	-5.196854478
	C19	4.915079043	2.332088898	0.755407314
	C20	6.774886266	3.373696771	-0.626327768
	C21	2.170093284	6.568018657	-2.814854478
	C22	-7.895192178	-0.412230807	0.819934570
	C23	3.601828549	6.779395384	-3.241109676
	C24	1.332821491	5.568627502	-3.632341474
	C25	-6.572498360	0.242648805	0.512139985
	C26	-5.685825928	-0.565693507	-0.535593629
	C27	-0.186260961	5.822800691	-3.434529359
	C28	1.739646429	4.111841307	-3.321458770
	C29	-5.491746338	-2.033602440	-0.018826915
	C30	-4.571502584	-2.841119741	-0.966134110
	C31	-0.684010647	5.826579546	-1.976702690
	C32	-4.310037738	-4.227495563	-0.457717012
	C33	-4.247248251	0.060138895	-0.559341132
	C34	7.089922265	-2.838386118	0.247330963
	C35	-0.947906716	-8.024981343	-0.673854478
	C36	5.945879675	-2.374795897	0.927759286
	C37	7.135154848	-4.201188037	-0.094637678
	C38	4.891965453	-3.227888447	1.257758250
	C39	-0.727617083	-7.751389775	0.832348216
	C40	6.086399443	-5.076192891	0.237314339
	C41	0.130896118	-8.857019095	1.500906699
	C42	4.959048530	-4.582363979	0.905738850
	C43	-2.071269082	-7.605456237	1.584937779
	C44	0.428093284	-5.599981343	5.405145522
	C45	1.631413109	-8.824642708	1.149058848
	C46	-1.570642841	-4.367370621	4.603708069
	C47	8.221254873	-1.881285552	-0.104810410
	C48	2.636093284	-4.850981343	-4.312854478
	C49	3.033232040	-6.147927918	-3.589914484
	C50	2.995609655	-6.034030108	-2.083035679
	C51	0.213763420	-1.252761539	-6.682396240
	C52	-1.043906716	-0.700981343	-4.599854478
	C53	-0.029918132	-0.036564364	-3.653404312
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	C57	2.050093284	-0.350981343	-2.351854478
	C58	3.273256558	0.335502720	-2.978014539

C59	2.475124701	-1.518368155	-1.444984010
C60	7.793093284	-0.731981343	-1.045854478
C61	6.422255085	-1.254677066	8.271084320
C62	5.948093284	-2.544981343	6.171145522
C63	6.934872644	-2.123797252	5.075117977
C64	4.573931289	-3.079958607	5.709830472
C65	4.769475281	-4.407256304	4.944367265
C66	3.626984854	-3.276295029	6.912347092
Fe67	-7.770826169	6.563794181	-7.041889841
Fe68	-8.424795502	4.651200000	-5.103149997
Fe69	-6.814545777	3.854450789	-7.134603906
Fe70	-5.906502656	5.639553707	-5.323824704
Fe71	-6.050005452	1.811654419	-5.770356134
Fe72	-7.422066443	2.587614130	-3.677059805
Fe73	-5.021835146	3.577450580	-4.086893376
H74	1.444018978	2.554959106	9.071596492
H75	-1.672368589	-8.856003138	-0.764487648
H76	3.365470472	-4.053223835	-4.138280497
H77	2.586964284	-5.039882141	-5.391485880
H78	1.652192782	-4.503988308	-3.981055062
H79	0.456230989	-2.100444608	-7.347996752
H80	7.002319826	-0.120322009	-0.591991593
H81	8.643930983	-0.074511732	-1.263507375
H82	6.235454113	-0.271272810	8.740227184
H83	-6.339366826	9.249775163	-8.206707718
H84	-7.587154562	10.063493280	-7.242576562
H85	-6.824894299	11.559207424	-9.111227992
H86	-8.529113047	11.106551682	-9.363748237
H87	-7.248647861	10.309953546	-10.308903926
H88	-6.775420693	1.217678162	0.056539178
H89	-6.001625390	0.375359436	1.436429173
H90	-5.064773527	-2.005172794	0.991373086
H91	-6.469649428	-2.522755876	0.035225384
H92	-5.045534560	-2.885062739	-1.951572400
H93	-3.601831960	-2.350273475	-1.072469123
H94	-0.291262433	1.174014753	0.037566928
H95	2.173119841	-9.631194234	1.662023603
H96	3.903244549	-7.753852045	-1.960932182
H97	0.030486294	-8.759087235	2.593588685
H98	-0.290479791	-9.843849499	1.245021845
H99	1.808473084	-8.933719450	0.070570910
H100	-1.726184617	-3.573360778	0.500002273
H101	-0.006628682	-8.377340768	-1.121307547
H102	-2.702385843	-6.819696515	1.152008596
H103	-0.180904391	-6.797309659	0.913952262
H104	-1.610683063	-7.084429771	-2.380813048
H105	4.037061070	-6.479018060	-3.891803783
H106	2.351823537	-6.970578694	-3.862078300
H107	-2.631645151	-8.553460880	1.559651667
H108	-2.205518149	-6.415789183	-1.016361163
H109	-1.898636914	-7.344424412	2.639875430
H110	2.079641127	-7.870905123	1.461176039
H111	-4.093667005	6.912871274	2.137388964
H112	4.186973315	7.448421764	-2.567916185
H113	-0.271270756	6.669482987	-1.404257870
H114	-1.777329889	5.907030716	-1.962389567
H115	-0.423230350	4.898709357	-1.453999449
H116	0.530895245	6.380670484	1.564242424
H117	-4.642685417	6.697911322	-1.926072510
H118	-4.562900515	8.224203144	-1.082993808
H119	-4.168824408	8.333706730	1.181039024
H120	-4.766554849	4.762905889	-0.647424905
H121	-2.361346570	3.475895372	0.588031391
H122	-2.037718017	4.933110594	1.524307699

	H123	-4.488078618	4.924460044	2.279424355
	H124	-4.762402652	3.519188028	1.264397711
	H125	-2.670715370	3.731084698	3.633252635
	H126	-3.090096153	2.284360741	2.706925540
	H127	-0.717304664	1.905964885	2.117204380
	H128	0.656892662	-3.876846929	1.416616478
	H129	-1.007656941	2.482279056	5.025928537
	H130	0.300755385	-0.541725330	5.955018811
	H131	1.581919795	-1.932468971	-0.959830634
	H132	3.154526737	-1.131033417	-0.671874019
	H133	2.881106592	-3.395751905	-1.942227691
	H134	-6.491936514	-2.050349081	-5.074954289
	H135	-1.470545454	-0.441530361	6.059596184
	H136	-2.726441548	-3.974235953	-5.187756519
	H137	1.234557911	-1.648610005	-3.832367148
	H138	-5.193051004	-4.101335533	-5.845290233
	H139	-1.290726865	1.431721580	7.402663556
	H140	-1.533038618	0.107717929	-5.154876742
	H141	-0.732417846	-2.623670073	-5.513882213
	H142	0.785475362	3.239729346	1.148223978
	H143	3.150332742	2.233316110	1.926816397
	H144	-0.746339105	5.064631538	-3.998458270
	H145	8.105838375	4.698771889	0.198124063
	H146	2.858378460	4.029194035	0.088588914
	H147	1.573753163	0.400326247	-1.716701187
	H148	5.243647520	1.381559578	1.190736501
	H149	1.551885070	5.751691512	-4.695489691
	H150	3.967020693	5.060005891	0.990754897
	H151	5.592580952	2.191910941	-1.881909101
	H152	4.389804654	3.247945878	2.648234111
	H153	4.444247988	2.119357659	-0.207199235
	H154	1.570151070	3.869598207	-2.262955678
	H155	6.897760230	3.043585181	-2.636251022
	H156	8.324019161	4.404251807	-1.483525396
	H157	-0.437834584	6.791454436	-3.894328362
	H158	2.408663752	4.897693987	3.002267105
	H159	1.151144529	3.404454486	-3.921784301
	H160	2.802494588	3.943441650	-3.536772228
	H161	6.563137184	3.540404010	1.364337208
	H162	-1.575691918	-2.233735719	-3.164701094
	H163	2.076515640	-4.591334678	1.648137861
	H164	-2.404208396	-0.697235406	-2.925862256
	H165	-2.321897892	2.192956836	-2.707902974
	H166	-2.038525661	2.497372144	-1.200524545
	H167	0.292221047	1.990030037	-1.165339151
	H168	-0.825997452	-0.235470676	1.716301032
	H169	1.837050956	-2.519415279	2.910077714
	H170	1.148110680	-1.211566895	3.440428073
	H171	-1.017431053	-2.167979278	0.783511185
	H172	-1.735277757	-3.420984501	2.756574584
	H173	0.160168842	-4.616334790	3.526977954
	H174	3.476887678	-0.623565796	3.340555725
	H175	-3.101623348	-3.247734420	3.841679343
	H176	-3.183857638	-4.383382365	5.863582653
	H177	-1.833521730	-5.273856881	6.430031016
	H178	0.620430635	-4.988460512	6.298026788
	H179	-0.095169727	-6.519444687	5.698346544
	H180	1.384059226	-5.882915190	4.954166099
	H181	3.823469381	-6.136556367	0.619310189
	H182	4.015802650	-2.847002895	1.774264636
	H183	5.878884264	-1.326467095	1.213897826
	H184	8.007514320	-4.597660429	-0.615234602
	H185	6.146920935	-6.131292955	-0.027054638
	H186	9.040821399	-2.447496267	-0.568645071

	H187	8.627822664	-1.445804873	0.822705625
	H188	-3.780500701	2.808075331	-1.882005387
	H189	-5.139483506	-5.923213717	-0.169179828
	H190	-8.755947148	-1.529426800	2.115242956
	H191	4.392953100	0.741749633	5.015359515
	H192	3.807562504	-4.782342321	4.574374903
	H193	3.459150601	-2.338478710	7.458219577
	H194	8.004486980	-2.256229072	5.335961977
	H195	4.031998442	-4.017434015	7.618446851
	H196	4.114567960	-2.349547687	5.032834314
	H197	5.202737965	-5.174794749	5.601957924
	H198	2.650957228	-3.639338731	6.564667528
	H199	6.449375058	-3.310832836	6.780667479
	H200	5.428083978	-4.285287804	4.074656903
	H201	5.032495063	-0.685610976	3.510527966
	H202	5.379227811	-0.499054461	6.666873450
	H203	3.657566076	1.224522359	6.303246479
	H204	-1.953461388	-0.093388159	0.603165786
	H205	-0.283319425	2.925403793	8.766462040
	H206	1.005132236	3.778479369	7.867790063
	H207	2.192258146	6.318530684	-1.739282305
	H208	1.723361818	7.578984688	-2.842229581
	H209	3.352949565	0.295827540	-4.082302427
	H210	7.409506678	-1.125952724	-1.997525321
	Mo211	-5.385411870	0.725329318	-3.307776751
	N212	-0.460982032	1.201428711	6.863038058
	N213	-0.911485065	1.896266905	4.197496460
	N214	6.105302528	3.189721310	0.525011793
	N215	-4.445228989	5.256326588	0.190717155
	N216	6.362089529	2.855212759	-1.794128488
	N217	-4.039209118	7.327376360	1.212598448
	N218	7.930460251	4.089427994	-0.598698638
	N219	-4.704222414	7.218930722	-1.027020430
	N220	0.932599436	3.853881718	1.960440385
	N221	-0.335350373	-4.850884862	4.397840279
	N222	-2.186344639	-4.563802463	5.796145634
	N223	-1.356338313	-6.813512265	-1.425953989
	N224	-2.196867971	-3.662241639	3.645462687
	N225	-0.441016201	-1.649450020	-5.550016896
	N226	-4.601648068	-1.366680312	-4.304676926
	N227	-4.774544040	-3.315764965	-5.355671640
	N228	1.084303030	-0.758784860	-3.362822610
	N229	5.869760562	-1.337503226	7.030138952
	O230	-8.914948963	-0.348149281	0.140449557
	O231	-7.864740166	-1.129815524	2.001785273
	O232	-3.243314458	-4.617038148	0.027342519
	O233	-5.386487316	-5.055488594	-0.559198121
	O234	-3.775778282	0.324481194	-1.729483530
	O235	-3.594040784	0.196465866	0.515426957
	O236	-6.253972409	-0.550795362	-1.801601619
	O237	0.120902813	4.474407635	4.020272709
	O238	-2.531954645	2.838289830	-1.988561834
	O239	-0.105596791	2.103886529	-0.278388565
	O240	-0.977573304	-0.322584993	0.739091956
	O241	3.890532115	-5.408319335	1.270460471
	O242	1.791701150	1.427069284	6.636274099
	O243	-0.421096516	-0.234932628	3.479661319
	O244	2.406067666	7.088490389	1.224250328
	O245	4.137110746	6.312197038	-4.244640627
	O246	2.519251137	-5.098774696	-1.447886747
	O247	3.527510419	-7.070704446	-1.368339237
	O248	0.517505213	-0.079889579	-6.944674000
	O249	-0.286771856	1.063865087	-3.122021321
	O250	4.114151109	0.909302320	-2.297178113

	O251	3.129684816	-2.498847686	-2.263078268
	O252	7.061071902	-2.150404090	8.852970269
	O253	6.629334330	-1.590746378	4.010874378
	O254	1.340395143	-4.112648154	2.091706374
	O255	2.016621067	-1.678114460	3.398778263
	O256	4.558032750	1.060543920	5.944737013
	O257	-1.003276623	-3.135955887	1.013014612
	O258	4.289418431	-0.052748306	3.384598090
	S259	-8.534871148	8.190054925	-8.521933154
	S260	-9.065847106	4.576170877	-7.296157582
	S261	-7.436800561	0.485640003	-4.525571916
	S262	-7.788611271	6.924229199	-4.786280700
	S263	-9.452702830	3.513615363	-3.423603879
	S264	-6.248949024	1.877769101	-8.013353246
	S265	-5.521660420	2.821874173	-1.941820992
	S266	-5.581174840	5.786784202	-7.578016710
	S267	-3.878180908	1.767247648	-4.977290332
	S268	-4.121734664	5.641528377	-3.939461470
Full model for validation, His0 file bm51E0.car_3	C1	-7.528034222	-5.174529630	2.937012163
	C2	-8.144590512	-6.350866639	2.169719978
	C3	-7.995730363	-3.079025823	4.133144880
	C4	-7.143651065	-3.239321954	5.388815150
	C5	-6.451072175	-4.673290194	7.240264630
	C6	-4.955306947	-4.765895378	6.920292799
	C7	-3.238710650	-5.235072592	5.248342087
	C8	-2.673882606	-3.833003018	5.013057996
	C9	-3.106202011	-1.560259874	4.213913758
	C10	-2.790502652	-0.840455462	5.531987297
	C11	-3.438598578	-0.393122181	7.825508258
	C12	-2.262930168	-0.949175882	8.640262571
	C13	-1.233203982	-2.932152175	9.640837197
	C14	0.133795798	-3.289561483	9.038404630
	C15	1.318181440	-4.104067217	7.034723421
	C16	1.965329854	-3.127196004	6.046888190
	C17	1.651502958	-1.245880122	4.462482187
	C18	2.129524635	0.003508936	5.238168144
	C19	0.626612833	-0.929329025	3.357173145
	C20	1.130178834	0.197882355	2.449838318
	C21	0.310046828	-2.187318192	2.540506946
	C22	1.499175511	1.858635429	6.743724871
	C23	2.075737763	1.564654323	8.144906373
	C24	0.266110563	2.794820934	6.801454849
	C25	0.530584468	4.007431981	7.702920810
	C26	-0.135252054	3.249172618	5.392945155
	C27	1.797877115	0.539529210	10.330433985
	C28	3.258903928	0.152371077	10.422129206
	C29	6.412633805	-11.406264313	3.710634413
	C30	6.856321947	-10.182624269	2.911785019
	C31	7.147149400	-7.706587437	3.075756151
	C32	8.486737375	-7.301291437	3.718969290
	C33	6.040598793	-6.679954967	3.373866911
	C34	6.352191508	-5.275310227	2.851701110
	C35	5.117036374	-4.373799819	2.909870175
	C36	5.218662142	-1.860843922	2.881439616
	C37	10.765865604	-6.516906471	3.305103918
	C38	11.065150140	-5.045305066	3.132033812
	C39	-5.582353889	-2.724253780	-0.433307918
	C40	-5.884100755	-1.273656224	-0.013504434
	C41	-4.053568653	-2.877091219	-0.591630734
	C42	-3.535962583	-4.327557446	-0.693445536
	C43	-3.496299757	-4.934498905	-2.096431722
	C44	-6.363424264	0.954354349	-0.993242535
	C45	-7.347600472	1.499185064	0.048949744

C46	-6.687520310	1.457086553	-2.407728338
C47	-9.324062893	1.051440172	1.419455691
C48	-8.702301101	1.183444962	2.816114601
C49	-6.755778923	0.780255186	4.252103891
C50	-5.544794530	1.715185584	4.213869495
C51	-4.169803953	3.317939975	2.978582865
C52	-4.533744284	4.627441968	3.690483379
C53	-3.832891755	3.692258531	1.525023146
C54	-3.226828795	2.583887877	0.729716841
C55	-2.699279441	1.352869628	1.062589606
C56	-2.506846070	1.504762841	-1.071346910
C57	-6.297958068	6.305998985	3.929674090
C58	-5.984800323	6.542186674	5.405920300
C59	-7.826071354	6.359954341	3.680042781
C60	-8.442804324	7.725399248	3.584932262
C61	-8.211024644	8.875516174	4.314601160
C62	-9.784197189	9.229378098	2.793850672
C63	9.603203850	1.562007937	2.021930837
C64	10.573681338	0.425462481	1.767646876
C65	8.178205783	0.948825948	2.056429660
C66	7.111702467	1.977969319	2.348023607
C67	6.764368705	2.311212921	3.669388725
C68	6.432441375	2.627430728	1.303472986
C69	5.764802192	3.251259618	3.941999341
C70	5.442170880	3.576340175	1.559741902
C71	5.106797175	3.882996739	2.881059104
C72	5.098960661	6.618776255	-2.545780659
C73	4.068935416	7.752977364	-2.664246099
C74	4.434397456	5.371717935	-1.969101077
C75	2.826112297	9.222312825	-4.214594572
C76	1.342747275	8.850303246	-4.129968678
C77	-0.275727266	7.004276676	-3.717831198
C78	-0.571408573	6.777792646	-2.213180392
C79	-0.367940578	5.696182572	-4.538365985
C80	-1.637518049	4.843137530	-4.436626029
C81	-2.876086021	5.363405271	-5.184639662
C82	-4.318543565	7.324403273	-4.595879799
C83	0.174942009	5.947229772	-0.042997473
C84	0.246388928	7.235444550	0.790519086
C85	1.160972869	4.932640604	0.562650029
C86	1.516544675	9.293923977	1.165069554
C87	0.856752659	10.634271924	0.876324938
C88	-0.748588999	11.857287440	-0.491171192
C89	-1.888567754	12.492882891	0.344852458
C90	-1.145388986	11.785487229	-1.970566505
C91	-2.370402868	10.916981867	-2.235290562
C92	-3.611708765	12.142917227	2.056385465
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	N397	3.772510820	8.160248305	-3.933880675
	N398	1.063178539	7.547977779	-3.931559803
	N399	-3.763028860	6.149337029	-4.318236119
	N400	-4.261098352	7.882488189	-5.821912137
	N401	-4.939441141	8.021224832	-3.612426636
	N402	0.399501266	6.180029521	-1.470040875
	N403	1.099674526	8.191999494	0.319764401
	N404	-0.215291225	10.610156995	0.026592316
	N405	-2.266374838	10.079636048	-3.302155362
	N406	-2.396860197	11.745862611	1.355425149
	N407	2.345388239	-5.407153671	-10.362778596
	N408	1.188367633	-3.090499215	-7.819022000
	N409	0.233770948	-0.247655017	-7.337753579
	N410	2.260999412	1.732333225	-7.812543255
	N411	-3.277969664	-3.609985540	-9.391178777
	N412	-4.599377890	-1.671043456	-7.750277429
	N413	6.994397474	-7.533668187	-6.655683824
	N414	3.425077993	-6.004922374	-4.569294460
	N415	2.541461078	-7.076398479	-6.285947067
	N416	8.506638007	-7.816729897	-3.892621221
	O417	-6.303618314	-5.016197983	3.071676277
	O418	-6.361876062	-2.336373752	5.735872224
	O419	-4.109964070	-4.453372049	7.775502653
	O420	-1.523281041	-3.528163859	5.377039296
	O421	-1.803767530	-0.097068279	5.645222174
	O422	-1.455257251	-0.187181406	9.199918250
	O423	1.138196147	-3.307166190	9.764531643
	O424	3.194524668	-3.197691759	5.861604377
	O425	3.310623532	0.395445520	5.169568322
	O426	3.141140953	2.082341603	8.522949542
	O427	3.946562453	0.374009366	11.409357879
	O428	7.245449380	-10.321585796	1.733396735
	O429	8.649398362	-7.362072196	4.951220950

	O430	12.198034136	-4.597396857	3.039282843
	O431	-5.741780077	-0.858154134	1.153472830
	O432	-4.377433303	-4.683945267	-2.954785758
	O433	-7.155549192	2.595766706	0.601202300
	O434	-6.725158671	2.897418244	-2.424281803
	O435	-9.337295573	1.783241738	3.696531667
	O436	-4.880902429	1.889738292	5.244930609
	O437	-3.694002273	5.347284474	4.243756295
	O438	-5.757111830	7.633675921	5.901375712
	O439	11.222885258	-0.140645410	2.636599441
	O440	4.091885329	4.801349320	3.080673058
	O441	3.549296191	8.287120789	-1.667790785
	O442	0.486052529	9.750953219	-4.256039649
	O443	-1.659983695	7.141421974	-1.736737158
	O444	-0.400410409	7.356489771	1.839295903
	O445	2.437046988	5.544097799	0.775162597
	O446	1.279144913	11.671865658	1.403230861
	O447	-2.262020724	13.652213039	0.113034979
	O448	-3.397318456	11.011450926	-1.547231817
	O449	-4.219706593	14.039472137	3.423649965
	O450	-5.630253001	6.839218772	-0.863548898
	O451	0.284392807	-5.069654413	-8.556577845
	O452	-1.604911508	-1.299239705	-8.220961807
	O453	0.717361185	3.052367723	-8.840830269
	O454	4.351381004	3.683795366	-10.005833036
	O455	-6.357418679	-3.125496135	-7.733843662
	O456	-2.435078197	-6.998759870	-5.216845368
	O457	-0.683201538	-6.209564503	-6.351797062
	O458	-5.286196681	1.835138642	-7.782460285
	O459	9.162829369	-5.856103890	-4.816517479
	O460	12.052620282	-7.363526233	-3.588342003
	O461	-0.059090461	-6.322842245	-0.907532213
	O462	-0.311225078	-7.252391888	1.139280236
	O463	4.383363270	-11.225607447	-3.300163272
	O464	2.140919589	-11.199275825	-3.017507387
	O465	4.654815462	-5.990705028	-1.647251040
	O466	4.830381426	-7.645666030	-0.136347692
	O467	2.100823236	-6.324480654	-2.053320269
	O468	8.917922744	-6.712637081	0.062600956
	O469	6.948587589	-4.771015865	-0.570474447
	O470	-4.683635175	4.682854759	-2.034408040
	O471	7.066156380	-10.760421234	-2.886352486
	O472	7.245255296	-8.827100633	-0.613390097
	S473	3.019405436	4.792327933	-3.009348435
	S474	1.311811771	1.588579293	-3.695505397
	S475	1.410663167	-3.537395975	-3.715205420
	S476	3.103026526	1.611962435	-0.565715168
	S477	0.374902429	-1.105167088	-1.044714174
	S478	3.178965313	-0.991695450	-5.996556255
	S479	3.205260570	-3.508596967	-0.505195303
	S480	4.995475776	1.617460554	-3.636254032
	S481	5.106030292	-3.389722741	-3.705334033
	S482	6.029626190	-0.984102379	-0.974877202
Full model for validation, HisH+ file bm52E0.car_4	C1	-7.469526951	-5.674269046	2.062611282
	C2	-8.012752317	-6.792379854	1.165919880
	C3	-8.043785637	-3.716205301	3.428825028
	C4	-7.236094729	-3.974247177	4.697572195
	C5	-6.576430446	-5.558789471	6.436719064
	C6	-5.064972514	-5.561603067	6.187168552
	C7	-3.246173060	-5.806276272	4.578493180
	C8	-2.748921925	-4.363228159	4.503504597
	C9	-3.270761646	-2.051082665	3.900982330
	C10	-3.030031495	-1.438579086	5.287951070

	C11	-3.759909165	-1.250336913	7.596347515
	C12	-2.594067456	-1.843710812	8.398879202
	C13	-1.528915616	-3.871253405	9.258910661
	C14	-0.127691996	-4.116948742	8.682641072
	C15	1.174568596	-4.718427898	6.679232007
	C16	1.827725314	-3.643627765	5.804659308
	C17	1.500479890	-1.616286455	4.410248048
	C18	1.899655117	-0.428022542	5.316805753
	C19	0.493318459	-1.228258111	3.309299541
	C20	0.984557912	-0.000304285	2.535708451
	C21	0.236316244	-2.411262846	2.369228671
	C22	1.138636117	1.251160184	6.964283996
	C23	1.665857742	0.839274882	8.355025283
	C24	-0.127578107	2.139042212	7.055193005
	C25	0.054798711	3.264314431	8.081777713
	C26	-0.475527110	2.718745749	5.678029667
	C27	1.326390937	-0.397729730	10.419765292
	C28	2.796362618	-0.727245140	10.569054635
	C29	6.659650847	-11.512533613	2.913858757
	C30	7.094641273	-10.201634820	2.254911274
	C31	7.286946524	-7.743880652	2.665271705
	C32	8.576671257	-7.354185763	3.413190488
	C33	6.124349694	-6.792436617	3.000073450
	C34	6.405893533	-5.331707466	2.637241867
	C35	5.135102566	-4.483776213	2.733824605
	C36	5.148215811	-1.974842557	2.937847081
	C37	10.845798542	-6.462596271	3.186198663
	C38	11.095484856	-4.971310895	3.178438049
	C39	-5.458468472	-2.850975343	-0.953943651
	C40	-5.803576496	-1.445669920	-0.428078051
	C41	-3.916350735	-2.945565423	-1.059189640
	C42	-3.332729308	-4.357839999	-1.272418457
	C43	-3.211297340	-4.813818953	-2.726298710
	C44	-6.381501042	0.823107531	-1.212655175
	C45	-7.403999635	1.226360498	-0.140686791
	C46	-6.678748232	1.460214417	-2.577853850
	C47	-9.427778418	0.592534728	1.089794037
	C48	-8.872988567	0.602836388	2.518967560
	C49	-6.971943893	0.129227572	3.994065380
	C50	-5.796559974	1.103563093	4.084369354
	C51	-4.431316857	2.833570257	3.025251138
	C52	-4.852566828	4.094755673	3.813619315
	C53	-4.021734236	3.324345885	1.629423168
	C54	-3.323951537	2.357618876	0.725552150
	C55	-2.623663579	1.190229008	0.907991125
	C56	-2.463394189	1.721480292	-1.239030876
	C57	-6.700289214	5.677024938	4.207965099
	C58	-6.476556232	5.758948603	5.717622865
	C59	-8.208783914	5.710319680	3.872050815
	C60	-8.869687688	7.056940171	3.886762615
	C61	-8.730308335	8.127159366	4.749516533
	C62	-10.223512836	8.590582302	3.178832193
	C63	9.442185844	1.667957145	2.618049302
	C64	10.461974897	0.585993120	2.317218053
	C65	8.039775478	1.015118733	2.530494813
	C66	6.928149149	1.977905874	2.874605013
	C67	6.513248457	2.168233977	4.206071496
	C68	6.271115399	2.708086997	1.869152357
	C69	5.469290737	3.044431579	4.523887179
	C70	5.236835861	3.594872852	2.172183240
	C71	4.830263030	3.752858363	3.500399399
	C72	4.977889428	6.980434078	-1.662741689
	C73	3.909881264	8.085072591	-1.731490082
	C74	4.333804143	5.667168791	-1.227201270

C75	2.693019008	9.658519666	-3.195418451
C76	1.219646487	9.243228205	-3.193371071
C77	-0.346244025	7.316075912	-3.039235021
C78	-0.689829602	6.938762233	-1.576665505
C79	-0.367209530	6.085561686	-3.977102686
C80	-1.613025728	5.194204382	-3.996598448
C81	-2.838890733	5.740233860	-4.747100441
C82	-4.378314878	7.581987920	-4.048800123
C83	0.005354537	5.945100793	0.540701617
C84	-0.019821723	7.154666402	1.489984830
C85	1.008183313	4.918198823	1.097785733
C86	1.144940689	9.215368382	2.119242401
C87	0.443187677	10.547837098	1.905452050
C88	-1.165886631	11.812186009	0.585405546
C89	-2.363447323	12.320520091	1.426243655
C90	-1.504849196	11.859717208	-0.907903242
C91	-2.673020637	10.965904290	-1.301889365
C92	-4.133672745	11.761754826	3.028639118
C93	-3.951398797	12.835926148	4.089125869
C94	-4.687206369	10.462136007	3.682154527
C95	-5.022555945	9.401891337	2.656363523
C96	-6.293820272	9.364517692	2.060939108
C97	-4.064960372	8.468728972	2.225411126
C98	-6.592105185	8.449184248	1.048403979
C99	-4.335838268	7.561894364	1.197007442
C100	-5.600570205	7.569592689	0.612656447
C101	3.130672803	-3.565882579	-9.440441738
C102	1.764362793	-3.367055577	-8.807894732
C103	0.437387339	-1.949336635	-7.264239530
C104	-0.155055787	-0.605370814	-7.699837399
C105	0.165015516	1.825246497	-7.670112780
C106	1.275977035	2.840202148	-7.918738250
C107	3.576350428	3.556057471	-7.582154629
C108	4.086812606	3.747870888	-8.996953276
C109	-3.676383680	-3.352951601	-8.837945385
C110	-4.689292862	-2.306201398	-8.359597485
C111	-3.043018628	-4.061184017	-7.617001247
C112	-2.328653897	-5.361567379	-8.031237394
C113	-1.475437481	-5.883046544	-6.897128880
C114	-5.082372753	-0.019837124	-7.586004105
C115	-4.718738262	1.303267761	-8.231161151
C116	-5.258103042	0.044437298	-6.049275394
C117	-3.934373140	0.032629219	-5.334247990
C118	-3.171841231	1.206161823	-5.204724050
C119	-3.387095643	-1.182192622	-4.890903304
C120	-1.876531758	1.150197518	-4.679053759
C121	-2.094164941	-1.236084388	-4.360915290
C122	-1.329009659	-0.070340499	-4.266449011
C123	7.438379962	-5.886437628	-5.732847835
C124	8.729923115	-5.985681146	-4.908935502
C125	6.219607430	-6.348276943	-4.919616731
C126	4.882501252	-6.123803815	-5.552994292
C127	4.412590085	-6.683532128	-6.723420849
C128	2.769905456	-5.588083326	-5.724735754
C129	10.157655882	-7.235371997	-3.405410131
C130	11.404486631	-6.930078221	-4.205002186
C131	0.638183960	-6.840275239	-0.458103999
C132	2.169113600	-6.914249596	-0.313172281
C133	2.952287458	-7.009237088	-1.649562860
C134	2.862809010	-8.438783836	-2.238294385
C135	3.787675686	-8.723537564	-3.426168054
C136	3.802717198	-10.202706996	-3.871248669
C137	4.433170026	-6.676087372	-1.405110995
C138	3.281836453	-0.595761138	-2.511724096

	Fe139	3.464075305	-1.741393273	-4.169521102
	Fe140	1.874002320	0.537521474	-1.749124377
	Fe141	4.529726929	0.650939275	-1.607297694
	Fe142	3.312231306	0.798294725	-3.938130318
	Fe143	3.152217432	2.839214827	-2.198329153
	Fe144	4.598571671	-1.943296282	-1.848008638
	Fe145	2.035049670	-2.088067318	-2.007642864
	H146	-6.255128938	-7.773298647	0.820760818
	H147	-6.675613024	-6.751072075	-0.379358853
	H148	-9.391172560	-5.025562871	2.418105708
	H149	-8.850525009	-6.394640042	0.570494285
	H150	-8.454049396	-7.551845422	1.834089942
	H151	-7.436210935	-3.041387411	2.807479670
	H152	-7.984409446	-5.874309527	4.839784509
	H153	-8.961214497	-3.182450809	3.709494146
	H154	-6.882778305	-6.562637417	6.758554783
	H155	-5.341869137	-6.041687202	4.198255583
	H156	-6.758106125	-4.861301643	7.265747794
	H157	-2.361073585	-1.882641856	3.312852892
	H158	-4.498861878	-3.781205335	3.600074950
	H159	-3.089023893	-6.287084277	3.603099583
	H160	-3.592112477	-0.167193968	7.540238191
	H161	-4.719307809	-2.365497983	6.022025048
	H162	-2.627057439	-6.325521957	5.320327636
	H163	-4.100768220	-1.531044133	3.403348320
	H164	-3.177579136	-3.763103926	7.892721523
	H165	-4.695336996	-1.432724865	8.143375380
	H166	-0.135912694	-3.294215901	2.906927132
	H167	-0.498760279	-2.133318489	1.599893374
	H168	1.153546484	-2.688467319	1.827973546
	H169	-0.449759912	-0.956938015	3.814741665
	H170	-1.946348894	-4.847650221	9.544719833
	H171	-0.649165556	1.931209113	4.931584506
	H172	0.053019620	-0.436620636	8.717913180
	H173	0.225326602	2.881369480	9.098459563
	H174	0.246545519	0.292918233	1.777435138
	H175	1.914281057	-0.210729926	1.988482395
	H176	9.600846758	1.990009085	3.665346254
	H177	-1.386392819	3.332081481	5.740441572
	H178	-0.845227414	3.896097790	8.104535878
	H179	0.344198158	3.361297060	5.316514803
	H180	0.911365435	3.902676648	7.811326535
	H181	-0.965178901	1.500029460	7.388884545
	H182	1.958879580	1.837547705	6.526605514
	H183	-0.046368737	-0.240672557	5.972191461
	H184	1.156186034	0.865111618	3.192413295
	H185	1.171241189	4.120592472	0.351597661
	H186	0.546780654	4.471933215	1.992400589
	H187	2.615550106	5.129533819	2.228577151
	H188	3.577445814	4.630160512	4.695351961
	H189	4.720221743	4.133926105	1.378605293
	H190	6.546554646	2.555110175	0.822452797
	H191	6.996503054	1.604922313	5.008764607
	H192	-0.000492820	-2.848085688	5.327667788
	H193	1.004414391	-5.601182565	6.042858321
	H194	1.910911805	-4.987843132	7.445992021
	H195	-0.917447327	-4.348632966	6.783370728
	H196	-1.387761123	-3.280127566	10.171961137
	H197	5.139828197	3.157007629	5.560442460
	H198	2.431019369	-1.950091808	3.935152448
	H199	1.072927031	0.419436863	11.115082724
	H200	0.762409614	-1.293839334	10.721108454
	H201	3.275564605	-1.191072360	9.677116887
	H202	11.669831446	-6.972115787	2.663959563

H203	-2.060511028	-5.949035737	-3.965666809
H204	1.355573805	-5.967530291	-2.221032594
H205	-3.078814654	-6.126547332	-8.275438525
H206	-1.706707075	-5.187222464	-8.920844027
H207	-3.816003583	-4.299347919	-6.870634395
H208	-4.205162838	1.213363896	-9.217740722
H209	-4.298555534	-4.093654179	-9.361990419
H210	-3.582786486	-2.277049449	-1.869582373
H211	-3.953529634	-5.106771182	-0.750082201
H212	-3.190496001	-0.890738719	-8.107710805
H213	-6.075525186	-0.259059716	-8.016952323
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