

Calculating the chemical mechanism of nitrogenase: new working hypotheses.

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Supplementary Information

Figure S1

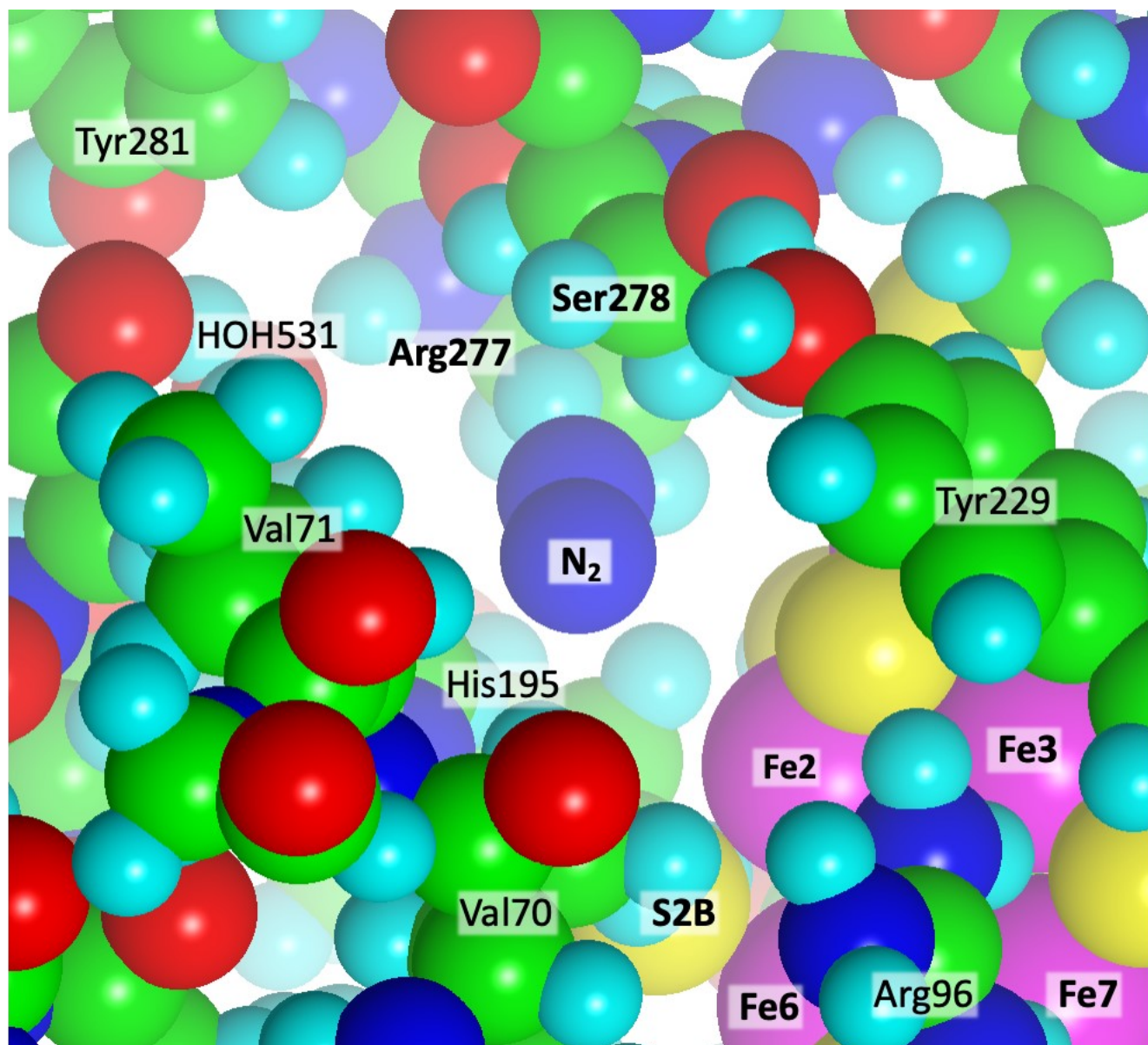


Figure S1. N_2 located in the N_2 ingress channel, engaging van der Waals contacts only with H atoms of Ser278 and Arg277. At this point N_2 is 3.5Å from Fe2 and not oriented for end-on bonding to Fe2. This is the ‘dissociated’ position for the calculated trajectory of end-on bonding to Fe2.

Atomic coordinates and Fe spin populations for the associated and dissociated forms, and the transition state between them, for structures A, B, C, D in different electronic and spin states.

Translation of Fe numbering

- Fe1 = Fe143
- Fe2 = Fe140
- Fe3 = Fe141
- Fe4 = Fe142
- Fe5 = Fe139
- Fe6 = Fe145
- Fe7 = Fe144

Structure A, 47(3/2)

structure, spin densities	filename, coordinates		
A, 47(3/2)	bm22n2xd47tg.car 2		
associated	C1	-1.849563959	-7.327444774 -5.712627250
	C2	-0.964308062	-7.592316043 -6.934285509
Fe(139) 0.541 2.342	C3	-4.152604957	-7.153505418 -4.870842651
Fe(140) 0.435 -1.635	C4	-4.065044420	-8.073349296 -3.654725683
Fe(141) 0.582 2.882	C5	-3.507062376	-10.286099705 -2.782801511
Fe(142) 0.555 -2.602	C6	-2.332545618	-9.949578043 -1.856512864
Fe(143) 0.563 2.927	C7	-0.156945358	-8.845875573 -1.637496793
Fe(144) 0.503 -2.193	C8	-0.514429081	-7.627808072 -0.781623677
Fe(145) 0.466 -0.209	C9	-1.743137061	-5.531026164 -0.603234763
	C10	-2.687550289	-5.925228730 0.541672634
	C11	-4.532087733	-7.309907380 1.297857242
	C12	-3.884522812	-8.121135579 2.427384411
	C13	-2.455470748	-10.015761661 3.017284636
	C14	-1.185998413	-9.567875543 3.753747678
	C15	0.964856052	-8.389241345 3.594984221
	C16	1.153017092	-6.925106814 4.004265606
	C17	0.193388578	-4.639160479 3.944738681
	C18	-0.894916600	-4.267241250 4.969160068
	C19	0.153970100	-3.773712196 2.656573306
	C20	-0.003070474	-2.282996389 2.975743184
	C21	1.403234687	-4.026839309 1.804982954
	C22	-3.304255412	-4.167131634 5.479664482
	C23	-3.480572542	-5.242428728 6.567717962
	C24	-4.599248826	-3.918595092 4.670879737
	C25	-5.804905246	-3.719574379 5.596960485
	C26	-4.434004738	-2.709769285 3.739989536
	C27	-3.755022567	-7.589301883 7.114626313
	C28	-2.731002515	-7.593649452 8.232811926
	C29	10.724075572	-7.538983352 3.234598733
	C30	10.418241045	-6.050343452 3.406351616
	C31	8.855204216	-4.470542388 4.556940827
	C32	9.196114993	-4.220565871 6.039486947
	C33	7.339381614	-4.395707446 4.299432449
	C34	6.719944852	-3.028802593 4.606858443
	C35	5.286527150	-2.954662508 4.078803489
	C36	3.475032652	-1.396111251 4.828382324
	C37	10.248639102	-2.693152230 7.639012399
	C38	9.411896739	-1.608299867 8.285138663
	C39	-1.262526617	-2.924296418 -5.239123510
	C40	-2.629428834	-2.415131417 -4.753523200
	C41	-0.193194686	-2.413592712 -4.248417292
	C42	1.195641867	-3.074494149 -4.358408020
	C43	2.158347258	-2.420310681 -5.348517133
	C44	-4.293187606	-0.644941769 -5.072724523
	C45	-5.628028120	-1.393149604 -5.103586279
	C46	-4.421729793	0.689143729 -5.836418685
	C47	-6.818804825	-3.466377371 -5.593745855
	C48	-7.001348846	-4.089795558 -4.203113274
	C49	-6.000534624	-4.537275568 -2.001843581
	C50	-5.924142787	-3.533416247 -0.853662034
	C51	-5.881036669	-1.176650526 -0.152867589
	C52	-7.257636160	-0.894110432 0.495244594
	C53	-5.390564405	0.171925496 -0.700054194

C54	-3.970656118	0.240494094	-1.165148362
C55	-2.832727187	-0.474173894	-0.878838070
C56	-2.250995505	1.197556739	-2.218597840
C57	-9.673081448	-0.710273365	0.058305992
C58	-10.127225700	-1.402148388	1.338592301
C59	-10.619764978	-1.082056471	-1.113617326
C60	-11.913718105	-0.327507025	-1.173856486
C61	-12.952816982	-0.254762978	-0.265170079
C62	-13.407842485	0.967194830	-2.056360949
C63	4.195208764	2.074680329	8.712038902
C64	5.680106891	1.764412870	8.750454933
C65	3.639020890	1.418030666	7.420476471
C66	2.150346062	1.608178653	7.250068009
C67	1.227004292	0.713216118	7.819884245
C68	1.643325724	2.688709035	6.504157370
C69	-0.152701819	0.882272361	7.652622035
C70	0.270812249	2.875087532	6.335292589
C71	-0.626501086	1.969478055	6.906925812
C72	-0.721927566	7.698060615	4.882751011
C73	-2.051767622	8.185958852	4.293430549
C74	-0.375941025	6.309532331	4.323830073
C75	-3.155321001	9.759006287	2.765353110
C76	-3.769759118	8.876070766	1.679275461
C77	-3.466452861	6.938256249	0.183402452
C78	-4.192773180	5.733808803	0.820166966
C79	-2.289624718	6.521967713	-0.718917893
C80	-2.595067548	5.578017393	-1.886282281
C81	-3.388423904	6.162786913	-3.071625914
C82	-5.808391153	6.787898578	-2.902401916
C83	-4.366415456	4.143935667	2.667015074
C84	-5.552520914	4.577313770	3.554032716
C85	-3.413194642	3.294690819	3.514429057
C86	-6.354064990	6.209846441	5.193291892
C87	-7.671272758	6.934741679	4.925399419
C88	-9.208796560	7.877438946	3.242954047
C89	-10.521481708	7.082831374	3.064395785
C90	-8.914678628	8.722634397	1.979876635
C91	-8.591477219	7.839584967	0.781493735
C92	-11.547559153	4.857993508	2.828275098
C93	-12.499218911	4.825030457	4.022159913
C94	-11.060947308	3.420098703	2.499831118
C95	-10.231254977	3.361418893	1.237863966
C96	-10.843944025	3.218173580	-0.015717856
C97	-8.833082742	3.486082398	1.282197111
C98	-10.092413712	3.226178788	-1.193256208
C99	-8.065406973	3.519430336	0.115360212
C100	-8.709930374	3.397474220	-1.113816242
C101	7.961226231	4.802229026	-5.204688650
C102	6.704217260	4.064625048	-5.640032592
C103	4.321371919	3.634504649	-5.084926197
C104	3.220329813	4.658860909	-5.383974775
C105	1.831769707	6.437325236	-4.420338160
C106	1.992150730	7.656594772	-3.516232540
C107	2.914704783	8.702750985	-1.527655313
C108	3.560621128	9.939890108	-2.116881678
C109	3.105240529	2.375234107	-9.371852899
C110	1.575923399	2.478898283	-9.437339783
C111	3.510588242	1.303137543	-8.332925614
C112	4.979717241	0.874737522	-8.516196960
C113	5.446389911	0.057008248	-7.332490684
C114	-0.465494233	3.443659520	-8.482749232
C115	-0.836282636	4.903033016	-8.289140025
C116	-1.174429186	2.460038852	-7.519929106
C117	-0.500474073	2.367266212	-6.173304551
C118	-0.729188657	3.329544787	-5.174880286
C119	0.450546205	1.362024436	-5.928556910
C120	-0.000895094	3.299091133	-3.979604275
C121	1.177916866	1.333629625	-4.733736925
C122	0.961905489	2.309237721	-3.757192106
C123	10.822821960	2.212205684	-0.500163277
C124	11.432068785	2.046976699	0.901299248
C125	10.040666129	0.960482755	-0.933977494
C126	9.259494011	1.077321751	-2.207834137

C127	9.764438418	1.293351680	-3.474825664
C128	7.592816839	0.883205292	-3.608133353
C129	12.728040475	0.716405746	2.471106007
C130	13.607364695	1.882203513	2.868485721
C131	5.268838699	-4.379836107	-1.817928236
C132	5.955110000	-3.658353317	-0.692030428
C133	7.008987239	-2.592770019	-1.196561623
C134	8.054464955	-3.295423057	-2.110633771
C135	9.254098209	-2.396956540	-2.460958155
C136	10.410799794	-3.127570782	-3.087174364
C137	7.771379095	-2.108550353	0.074664234
C138	3.514755862	2.467089627	0.419156262
Fe139	4.899110938	2.690885432	-0.925949792
Fe140	1.260204953	2.257165423	0.458168028
Fe141	3.340691280	3.175970152	2.294790007
Fe142	3.234673591	4.412971556	0.010431329
Fe143	1.241040133	4.762429810	1.694860590
Fe144	5.014295197	1.477013974	1.355052793
Fe145	3.405554856	0.747426524	-0.484555828
H146	0.823468639	-7.502763020	-5.954702060
H147	0.462104777	-6.135439635	-6.771708481
H148	-3.532257516	-7.562717624	-6.874090120
H149	-1.425947549	-7.134124062	-7.823457400
H150	-0.985415823	-8.683225308	-7.107172544
H151	-4.021251731	-6.130085931	-4.491039507
H152	-3.473881134	-9.643609616	-4.835988673
H153	-5.162490091	-7.238280283	-5.296146144
H154	-3.351339268	-11.289980937	-3.199130621
H155	-1.363319623	-8.987636977	-3.389992131
H156	-4.407649392	-10.308593298	-2.155814359
H157	-0.899737359	-4.996856499	-0.148513921
H158	-1.502128490	-6.743225825	-2.369529217
H159	0.669288069	-8.589740586	-2.314605439
H160	-5.006092650	-6.432389419	1.757047941
H161	-3.699465356	-7.252686359	-0.685723267
H162	0.184898404	-9.629871301	-0.952180319
H163	-2.258074242	-4.841641385	-1.286926626
H164	-2.856277633	-9.277547070	1.052811468
H165	-5.311242493	-7.924280041	0.824778196
H166	1.511786276	-5.090437651	1.546896426
H167	1.351578835	-3.447045520	0.871699918
H168	2.312958018	-3.707022911	2.336845527
H169	-0.729503034	-4.094101692	2.080297739
H170	-2.221312390	-10.957017222	2.499383733
H171	-3.604809836	-2.844818336	3.030936143
H172	-3.551657072	-6.779154702	5.159093746
H173	-5.996813919	-4.598978012	6.227889313
H174	-0.012970218	-1.694841289	2.046319168
H175	0.838169657	-1.911087002	3.577980841
H176	3.724101475	1.576807614	9.581648809
H177	-5.353720483	-2.556461627	3.156949492
H178	-6.706760320	-3.528527683	4.997127632
H179	-4.245309416	-1.796753120	4.328259580
H180	-5.648338207	-2.855964096	6.262137056
H181	-4.785518005	-4.814062815	4.050734462
H182	-3.044095864	-3.252665588	6.032858469
H183	-2.389149390	-4.820970319	3.645197242
H184	-0.935198794	-2.073331699	3.521747073
H185	-2.531604213	3.034789453	2.905068749
H186	-3.950362276	2.367393091	3.772482193
H187	-2.644347886	3.372323982	5.316852055
H188	-2.492957534	1.476282100	7.107060257
H189	-0.103001621	3.703335964	5.731956657
H190	2.334547467	3.380490094	6.016885229
H191	1.588119678	-0.137342563	8.405890649
H192	-0.616411176	-6.440684523	3.105970787
H193	1.748966185	-8.615984923	2.856727440
H194	1.155926795	-9.000247293	4.486805956
H195	-0.510173339	-8.556645071	2.072646426
H196	-3.202404332	-10.226893206	3.793066595
H197	-0.852578296	0.164967899	8.089335248
H198	1.144874263	-4.465968021	4.464833502
H199	-4.761849335	-7.541352231	7.561479254

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H201	-1.745212590	-7.139769322	7.973582810
H202	11.305324028	-2.384981782	7.642831949
H203	4.136884764	-1.969780060	-5.617030286
H204	6.523666873	-5.820654923	-1.558946051
H205	5.063603598	0.253635345	-9.419385038
H206	5.621787990	1.759064585	-8.641370816
H207	2.865885332	0.415397297	-8.427135052
H208	-0.105846010	5.620915708	-8.732949828
H209	3.382050303	1.993502729	-10.365783354
H210	-0.103973921	-1.320833515	-4.357086732
H211	1.086604433	-4.131040186	-4.661412089
H212	1.549193139	3.784543135	-7.825274753
H213	-0.813090588	3.210989605	-9.508655569
H214	3.655629852	4.041446943	-8.262117441
H215	3.770890796	-2.736194148	-4.071197628
H216	3.342192752	1.707715424	-7.322925489
H217	4.727157658	3.632414603	-9.443773268
H218	-1.269643366	-3.209185309	-7.282576652
H219	-0.574702955	-2.602165577	-3.234266870
H220	6.248906168	1.696483712	-6.586233680
H221	1.661531755	-3.092749591	-3.363137653
H222	-5.231746497	-1.526504043	0.662235998
H223	-2.678165675	-1.348044244	-0.257319387
H224	-6.952097241	-5.077122853	-1.898609768
H225	-5.056821333	-3.575223024	-3.653639813
H226	-8.184840656	-1.638366168	-1.174099232
H227	-13.105018134	-0.693363959	0.715430729
H228	-9.745193628	-2.446896928	1.444971201
H229	-10.791530117	-2.172041461	-1.102224653
H230	-9.680928053	0.377670155	0.224133670
H231	-13.962077852	1.622174707	-2.723048774
H232	-5.526433923	0.907884915	0.109580441
H233	-6.056114939	0.488142894	-1.520615658
H234	-14.779629860	0.846112292	-0.431693020
H235	-10.087136054	-0.855878069	-2.049664561
H236	-5.943342425	-1.938904814	-2.168502396
H237	-5.196670992	-5.272547141	-1.853589721
H238	-7.741463125	-2.915358865	-5.817496631
H239	-1.649392235	1.877155602	-2.815390939
H240	-6.725548057	-4.277464279	-6.328179494
H241	4.174025336	3.920600966	9.606242273
H242	3.036869522	3.741716451	8.445832521
H243	-2.757171649	5.547061229	2.303075073
H244	-4.799054318	3.490297003	1.896401421
H245	-4.656793975	6.381384995	3.945454764
H246	-4.224219308	2.010777329	-2.368925624
H247	-5.479261012	2.627182762	-3.965879375
H248	-6.364129971	3.034668132	-2.706711998
H249	-3.490115803	1.260479460	-5.727264644
H250	-4.590477247	0.491908455	-6.907989443
H251	-8.085670918	9.409154164	2.208240403
H252	-9.811956656	9.311954473	1.753069273
H253	-6.514169402	8.103228644	1.019955601
H254	-7.015439423	6.863124621	-0.089787680
H255	-6.346794969	8.762453161	-2.941541703
H256	-3.024191766	5.725655204	-4.013201179
H257	-10.581535840	3.087964852	-2.160748291
H258	-8.312698779	3.549846057	2.241760755
H259	-7.273770591	5.393809317	-2.469344972
H260	-1.521034318	6.040797670	-0.094340781
H261	-2.072086584	7.705360417	1.611332732
H262	-3.089004545	4.660543282	-1.529140529
H263	-4.818180211	-2.920024324	-6.172782502
H264	-2.900267475	10.724846737	2.309634280
H265	-2.557379513	-1.177527064	-6.324789523
H266	-1.837650974	7.448553495	-1.110542751
H267	-6.986206824	3.677523312	0.167067713
H268	-6.204758496	0.850245930	-5.046981008
H269	-3.946923340	9.933977773	3.506879243
H270	-4.756581160	8.442297510	-3.522277855
H271	-7.846114058	7.004387395	-2.778011231
H272	-0.001781206	-2.276052082	-6.727207597

H273	-1.311371463	-4.025339469	-5.138156493
H274	-11.926686139	3.090438071	-0.080334609
H275	-4.150415547	-0.408481793	-4.005955103
H276	-4.236972375	7.451418811	-0.408350098
H277	-3.214291806	7.243703001	-3.141357618
H278	-1.619023340	5.258113847	-2.276875378
H279	-5.094797261	4.890285682	-3.018915322
H280	-6.609172012	5.302070181	5.760281181
H281	-7.385844477	6.794320560	2.898634712
H282	-9.403706264	8.566860115	4.077931945
H283	-5.767007364	6.862726384	5.852919929
H284	-9.493295938	5.330602209	3.248720627
H285	7.685837584	5.750745061	-4.719500272
H286	8.428884564	4.165810939	-4.423738949
H287	10.123941026	3.056440210	-0.411508861
H288	9.752763983	5.334124053	-6.019221488
H289	8.945355721	4.195961992	-6.878978419
H290	0.601083403	6.012305370	4.723623278
H291	-1.599840329	7.074377753	6.611884028
H292	-1.060573540	9.593994139	3.166726891
H293	-1.141239474	5.593107810	4.652671116
H294	-0.919945161	8.556032891	6.737769647
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C120	-0.016242137	3.317712574	-3.979554095
C121	1.185267697	1.361271234	-4.720402328
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C123	10.847601429	2.221394966	-0.514639144
C124	11.447335620	2.055056880	0.890658776
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C126	9.323939421	1.080789484	-2.250072537
C127	9.831095151	1.307361777	-3.514699757
C128	7.657091292	0.904145750	-3.649581956
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C130	13.617535882	1.873514505	2.869489245
C131	5.328375802	-4.395782889	-1.830556202
C132	5.996775730	-3.654130299	-0.706104581
C133	7.066790115	-2.602746702	-1.204284861
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C137	7.815591483	-2.114792353	0.074008310
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Fe139	4.948791486	2.685584796	-0.951030680
Fe140	1.425318755	2.325893274	0.496647524
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Fe142	3.264854636	4.391181277	0.003239490
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O427	-0.962904956	-9.992768594	4.897268748
O428	2.198419451	-6.608411900	4.600537927
O429	-0.590080829	-3.843759989	6.100657110
O430	-3.586740574	-4.949886059	7.784443351
O431	-2.951140243	-8.113161484	9.336008861
O432	11.145677120	-5.211586793	2.836911669
O433	8.922858654	-5.078423884	6.893345001
O434	9.814029582	-0.903828929	9.180342954
O435	-3.210969270	-2.882480987	-3.753340650
O436	1.765940825	-1.954740817	-6.440619709
O437	-6.625608443	-0.876657007	-4.548462282
O438	-5.477746246	1.492031469	-5.281458882
O439	-8.075303314	-4.653629026	-3.923705065
O440	-5.889501616	-3.932124802	0.315054121
O441	-7.348702999	-0.374334578	1.610182943

	O442	-10.895839859	-0.945369318	2.156211288
	O443	6.166021587	0.817129165	9.344913762
	O444	-1.979763084	2.176907138	6.683799928
	O445	-3.151334948	7.676673888	4.609871119
	O446	-4.940964043	9.120782136	1.286014477
	O447	-5.190307924	5.259635490	0.258871980
	O448	-6.461709500	3.771887946	3.784565812
	O449	-3.074332613	4.025820129	4.720917474
	O450	-8.360315373	7.301166410	5.884188785
	O451	-11.598031538	7.678585886	2.934714019
	O452	-9.493051345	7.342362552	0.081558788
	O453	-13.672153293	4.454377407	3.923947136
	O454	-7.946269591	3.495852682	-2.275179245
	O455	6.731594066	3.286969137	-6.622476784
	O456	2.735304106	4.791057385	-6.538870003
	O457	1.271603599	8.650750174	-3.743125880
	O458	3.521716670	11.006797960	-1.552702193
	O459	0.916197638	1.796574745	-10.259375474
	O460	5.215373813	-1.141804865	-7.193531909
	O461	6.129097956	0.718934339	-6.376279142
	O462	-1.862918023	5.277760279	-7.745021714
	O463	11.379244116	2.963096411	1.740204229
	O464	13.905844096	2.134275025	4.028534126
	O465	4.395817640	-3.982680758	-2.504668384
	O466	5.830323517	-5.639224161	-2.122553586
	O467	11.608403092	-3.180555999	-2.669825352
	O468	10.114810558	-3.806770154	-4.243965671
	O469	7.701440363	-0.853555320	0.332902425
	O470	8.500635285	-2.918865041	0.747037418
	O471	6.443308134	-1.557354912	-1.860813267
	O472	10.314167850	-1.154151916	4.220811114
	O473	7.938673510	-0.137314957	3.056658675
	O474	-5.469220717	3.110516369	-3.070569001
	O475	13.001522425	-2.194668861	-0.066650894
	O476	10.943411876	-2.600625543	1.905069456
	S477	-0.316827370	6.296337358	2.480904356
	S478	1.070268159	4.467543118	-0.504317551
	S479	4.546087099	1.037790112	-2.441149720
	S480	1.180016216	2.749041352	2.771145939
	S481	1.279556496	0.286135214	-0.660773128
	S482	4.703468863	4.808854057	-1.639090131
	S483	4.610914205	-0.662215419	0.798466931
	S484	3.453557749	5.405838907	1.974941326
	S485	6.806010266	2.263274085	0.252126753
	S486	4.900607216	2.059648283	3.448478006
A 47(3/2) dissociated	bm22n2xd47tf.car_6			
	C1	-1.841467894	-7.320004239	-5.706047916
	C2	-0.951890643	-7.584559252	-6.924667580
	C3	-4.144580817	-7.137065488	-4.870866474
	C4	-4.062514052	-8.062131791	-3.658171576
	C5	-3.511104309	-10.280815661	-2.793353086
	C6	-2.336161962	-9.950791399	-1.865860071
	C7	-0.154970772	-8.858222450	-1.644161880
	C8	-0.505668700	-7.640308753	-0.785420518
	C9	-1.720438643	-5.537802238	-0.600095696
	C10	-2.668351356	-5.932312429	0.542891898
	C11	-4.522134692	-7.309850564	1.290010277
	C12	-3.879351000	-8.123875635	2.419899870
	C13	-2.452096771	-10.018413698	3.013872626
	C14	-1.192460200	-9.557452998	3.758199268
	C15	0.956397940	-8.375351809	3.600508004
	C16	1.145246894	-6.910647165	4.007548654
	C17	0.196922348	-4.621828122	3.935458445
	C18	-0.893136645	-4.236408209	4.953138427
	C19	0.173443120	-3.762723791	2.643806339
	C20	0.044356389	-2.267679401	2.954827594
	C21	1.420240385	-4.039156514	1.794905696
	C22	-3.304933420	-4.156261496	5.461878159
	C23	-3.479179412	-5.235217284	6.548735579
	C24	-4.598891538	-3.911232011	4.650308385
	C25	-5.809404467	-3.728145554	5.573748203
	C26	-4.438709742	-2.695349065	3.728793851

C27	-3.732271840	-7.586782648	7.094140729
C28	-2.713795326	-7.564188015	8.215670477
C29	10.726664393	-7.546384420	3.249473528
C30	10.421864180	-6.058210953	3.419419193
C31	8.858794317	-4.476536925	4.569470117
C32	9.195216600	-4.218428204	6.051942284
C33	7.344324439	-4.407484644	4.306350008
C34	6.722171426	-3.040658074	4.607340463
C35	5.292988627	-2.969095782	4.068494579
C36	3.478992735	-1.419030466	4.828826362
C37	10.259010311	-2.691772353	7.645227818
C38	9.435001978	-1.591344585	8.281883852
C39	-1.256380891	-2.913997373	-5.232885237
C40	-2.622364584	-2.402249975	-4.747774783
C41	-0.183194951	-2.408865041	-4.243864814
C42	1.203765697	-3.073735514	-4.355690649
C43	2.165058102	-2.428311095	-5.351495242
C44	-4.291420526	-0.639261089	-5.085124782
C45	-5.622343052	-1.394321514	-5.110656023
C46	-4.423762928	0.685119839	-5.865000653
C47	-6.803101730	-3.474923455	-5.597086011
C48	-6.987820509	-4.100878832	-4.207887001
C49	-5.991632143	-4.550911779	-2.003919510
C50	-5.915263274	-3.545700229	-0.856640855
C51	-5.862374617	-1.184911562	-0.166730218
C52	-7.232721271	-0.889673480	0.487183426
C53	-5.368535401	0.152922382	-0.732224725
C54	-3.950533670	0.210542900	-1.201426157
C55	-2.803891594	-0.472211089	-0.868061648
C56	-2.228765914	1.154059961	-2.265357950
C57	-9.648656374	-0.685100077	0.064144733
C58	-10.086632896	-1.342658107	1.368166120
C59	-10.613139422	-1.087040138	-1.084349120
C60	-11.908661223	-0.335305673	-1.143225820
C61	-12.948923143	-0.271003130	-0.235057956
C62	-13.404514454	0.962616102	-2.017984207
C63	4.207209461	2.075041121	8.704362545
C64	5.692241326	1.764541021	8.748627890
C65	3.654016157	1.422665272	7.409829260
C66	2.164428648	1.612967151	7.239320148
C67	1.241896754	0.721480722	7.816247050
C68	1.656861000	2.690167161	6.488660347
C69	-0.137399549	0.892374178	7.651922336
C70	0.284156417	2.879276608	6.325498874
C71	-0.612335483	1.977795406	6.904723864
C72	-0.721211103	7.684249386	4.867200775
C73	-2.051466229	8.187899322	4.291395094
C74	-0.399843250	6.288710651	4.310236875
C75	-3.143374898	9.765319111	2.756997280
C76	-3.772890355	8.881407816	1.677606265
C77	-3.484340635	6.923214922	0.200814391
C78	-4.207223264	5.725150310	0.856866056
C79	-2.311253936	6.501223794	-0.706711261
C80	-2.614228718	5.558497602	-1.876259899
C81	-3.392580580	6.145432769	-3.069880691
C82	-5.811335274	6.767086640	-2.882936114
C83	-4.399498526	4.186973542	2.753697243
C84	-5.593447998	4.639087217	3.616856775
C85	-3.457785596	3.361756317	3.643821470
C86	-6.385116701	6.284737829	5.238615704
C87	-7.706890004	6.990400995	4.945521657
C88	-9.223741436	7.896624012	3.226747376
C89	-10.523900662	7.084543527	3.037365793
C90	-8.918807020	8.731482574	1.960024714
C91	-8.584653941	7.843308511	0.768186678
C92	-11.521398272	4.846722232	2.814344299
C93	-12.464628082	4.807253043	4.013424398
C94	-11.027068290	3.411422579	2.490504338
C95	-10.200492262	3.350277432	1.226333768
C96	-10.813194156	3.206869010	-0.027934877
C97	-8.801613025	3.467818727	1.270897753
C98	-10.060405754	3.208617277	-1.205648250
C99	-8.033525990	3.491890453	0.103753489

C100	-8.676388638	3.367490297	-1.125915306
C101	7.971729098	4.807090212	-5.228775218
C102	6.709082731	4.068628318	-5.645164199
C103	4.332444923	3.635877920	-5.062155401
C104	3.229726087	4.656051502	-5.363937883
C105	1.836783947	6.432983874	-4.405024591
C106	2.009819815	7.657324654	-3.510136318
C107	2.943525710	8.709121875	-1.532850828
C108	3.511707551	9.967434627	-2.154729387
C109	3.111942439	2.394959601	-9.379858942
C110	1.583367777	2.507610524	-9.446898276
C111	3.513394405	1.324413819	-8.337131870
C112	4.978746040	0.883843517	-8.522005650
C113	5.441545070	0.061056562	-7.339404902
C114	-0.453608867	3.468351749	-8.481526347
C115	-0.818232775	4.925835546	-8.268089664
C116	-1.171238529	2.476009790	-7.531651700
C117	-0.498593283	2.363326976	-6.186180939
C118	-0.717329490	3.318573730	-5.178678315
C119	0.445601973	1.348782578	-5.953759915
C120	0.014608135	3.272710818	-3.986819589
C121	1.175376265	1.304163842	-4.761297332
C122	0.970236234	2.273063924	-3.776078588
C123	10.823182378	2.191843657	-0.488855536
C124	11.428014653	2.024227646	0.914437998
C125	10.038409784	0.942507459	-0.920719602
C126	9.273401086	1.056906054	-2.203322488
C127	9.787005073	1.274274163	-3.466871048
C128	7.616688833	0.857328030	-3.614021698
C129	12.752895596	0.707589470	2.471384462
C130	13.612627256	1.890675270	2.863557655
C131	5.227143619	-4.363938822	-1.812179162
C132	5.933980546	-3.665335133	-0.684920743
C133	7.000219487	-2.615361915	-1.187917958
C134	8.033246393	-3.315750182	-2.117260695
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C136	10.387503142	-3.128613418	-3.099144855
C137	7.773499055	-2.145584180	0.082113339
C138	3.544346880	2.472390784	0.410290775
Fe139	4.995570876	2.719476299	-0.921613961
Fe140	1.574867915	2.341934397	0.414077668
Fe141	3.239553364	3.098901884	2.289363735
Fe142	3.211051152	4.392205766	0.010308957
Fe143	1.115979613	4.697704623	1.634526545
Fe144	5.015285213	1.496208886	1.378957445
Fe145	3.439817086	0.706478032	-0.516923571
H146	0.830784888	-7.509556538	-5.937901076
H147	0.478746805	-6.134642448	-6.744345114
H148	-3.519545602	-7.541862232	-6.875078628
H149	-1.409464729	-7.123962620	-7.814410345
H150	-0.977925224	-8.674728916	-7.099073134
H151	-4.008630463	-6.116014077	-4.486325796
H152	-3.472949803	-9.629222803	-4.843991227
H153	-5.153250953	-7.215490335	-5.298544562
H154	-3.357986098	-11.283253166	-3.215235230
H155	-1.362571583	-8.988527183	-3.396417401
H156	-4.412543496	-10.304259816	-2.167171007
H157	-0.873186764	-5.012059745	-0.142000412
H158	-1.487210826	-6.744547614	-2.371927956
H159	0.672857899	-8.606416088	-2.321355390
H160	-4.995245505	-6.432429835	1.749614863
H161	-3.686675560	-7.248028198	-0.692170782
H162	0.182763884	-9.645377341	-0.960357012
H163	-2.231304230	-4.840815844	-1.279295945
H164	-2.851927712	-9.284955634	1.047248707
H165	-5.301246488	-7.921299449	0.813454648
H166	1.506440026	-5.103023494	1.529604574
H167	1.386324293	-3.452467950	0.864615023
H168	2.334646482	-3.743093611	2.332786776
H169	-0.714279519	-4.071278315	2.068129267
H170	-2.202672052	-10.955870084	2.495946341
H171	-3.607349860	-2.821251731	3.020499752
H172	-3.555497468	-6.771360409	5.136018121

H173	-5.997416630	-4.613900929	6.197628844
H174	0.043749957	-1.684518603	2.021630734
H175	0.893372171	-1.907158653	3.553386052
H176	3.733564047	1.573549718	9.570336758
H177	-5.357663598	-2.541781130	3.144781867
H178	-6.710267509	-3.538717188	4.971545451
H179	-4.254910709	-1.785832431	4.323880204
H180	-5.661245623	-2.867885321	6.245793997
H181	-4.776742185	-4.803368634	4.023053074
H182	-3.049971687	-3.243456507	6.019519944
H183	-2.382924478	-4.817634291	3.635082672
H184	-0.881565688	-2.034877125	3.502056456
H185	-2.542295925	3.121166128	3.081473368
H186	-3.982145500	2.419261769	3.874491018
H187	-2.713638770	3.449700839	5.447649670
H188	-2.479222580	1.493747407	7.128788267
H189	-0.090941343	3.708984637	5.725795300
H190	2.348536354	3.378655927	5.997836225
H191	1.602987523	-0.127813806	8.404205573
H192	-0.620435120	-6.420955250	3.099327793
H193	1.741194333	-8.601815834	2.863133482
H194	1.147167043	-8.984288957	4.493593901
H195	-0.512444980	-8.553807562	2.074103594
H196	-3.202454183	-10.238941582	3.783380012
H197	-0.838034231	0.180823815	8.095620207
H198	1.146301276	-4.453432687	4.459285467
H199	-4.742597175	-7.564150443	7.534003815
H200	-3.613136046	-8.546694411	6.567330249
H201	-1.732504298	-7.104412063	7.954014319
H202	11.319666335	-2.398449527	7.650988642
H203	4.142165164	-1.977717975	-5.624759051
H204	6.469336416	-5.822866367	-1.591532885
H205	5.056560137	0.261514158	-9.425315592
H206	5.628036363	1.763280052	-8.648047249
H207	2.861924614	0.440358246	-8.423418151
H208	-0.084021149	5.645451640	-8.700976973
H209	3.387594594	2.010644163	-10.373624154
H210	-0.089830638	-1.316342174	-4.349738756
H211	1.091237013	-4.131597845	-4.652070749
H212	1.560956661	3.788294015	-7.814556927
H213	-0.802957895	3.250149083	-9.510298559
H214	3.670590881	4.055357753	-8.267525676
H215	3.773044279	-2.726905529	-4.069596520
H216	3.350869110	1.736189823	-7.328715435
H217	4.739012309	3.643609876	-9.449709202
H218	-1.268093604	-3.201791856	-7.275149096
H219	-0.564870909	-2.598168970	-3.229999485
H220	6.247026224	1.696648996	-6.585821598
H221	1.672776727	-3.088500354	-3.362078844
H222	-5.210364676	-1.530823453	0.647313015
H223	-2.641714224	-1.313905276	-0.204315498
H224	-6.944997331	-5.088804538	-1.903750404
H225	-5.043849710	-3.586301168	-3.654250176
H226	-8.176398581	-1.626163393	-1.178758478
H227	-13.100270789	-0.717000930	0.742299607
H228	-9.696240580	-2.381228349	1.502372505
H229	-10.782215422	-2.176395948	-1.040315386
H230	-9.653004545	0.407046979	0.204364238
H231	-13.959320482	1.622094653	-2.679392055
H232	-5.497635691	0.902247663	0.065780968
H233	-6.033255302	0.459794905	-1.556029740
H234	-14.776703994	0.828551032	-0.394907217
H235	-10.093836177	-0.886122098	-2.033917992
H236	-5.934118769	-1.957112314	-2.176835168
H237	-5.188501488	-5.286832817	-1.854280067
H238	-7.726717656	-2.927314504	-5.824802562
H239	-1.627926073	1.822011958	-2.877301633
H240	-6.704764995	-4.285591434	-6.330538628
H241	4.181329080	3.915770493	9.607046047
H242	3.048860762	3.742044135	8.440740777
H243	-2.787725872	5.583443606	2.357497976
H244	-4.823931526	3.511270844	1.998402633
H245	-4.671819035	6.430409346	4.008112422

H246	-4.209643977	1.939943467	-2.461515693
H247	-5.466712787	2.621326514	-4.001606690
H248	-6.324059941	3.010531324	-2.720556254
H249	-3.495485802	1.262359403	-5.758407439
H250	-4.588074353	0.474389743	-6.934829285
H251	-8.093715321	9.421440504	2.190753758
H252	-9.813983967	9.317722620	1.719875479
H253	-6.508926663	8.100967438	1.023064023
H254	-7.006782851	6.852909027	-0.080340205
H255	-6.352817976	8.739729819	-2.882551393
H256	-3.019121806	5.706862096	-4.006980859
H257	-10.551993283	3.072605023	-2.172302857
H258	-8.280815907	3.536641302	2.230471120
H259	-7.267312133	5.357724802	-2.479698111
H260	-1.541954641	6.018537313	-0.083912978
H261	-2.082711911	7.699002695	1.612409677
H262	-3.121378649	4.647020348	-1.524650351
H263	-4.803278350	-2.922514063	-6.171670698
H264	-2.877254131	10.725286120	2.294207786
H265	-2.548415782	-1.174439974	-6.327045686
H266	-1.856744525	7.427002921	-1.098120350
H267	-6.954006006	3.645435928	0.155512226
H268	-6.211682348	0.849445873	-5.085881603
H269	-3.930147643	9.953713840	3.500562599
H270	-4.768580257	8.432658263	-3.478822035
H271	-7.848262668	6.974946033	-2.733413632
H272	0.004651367	-2.273374849	-6.725773279
H273	-1.308696829	-4.015147675	-5.133960556
H274	-11.897399499	3.084932793	-0.092657478
H275	-4.152520907	-0.389272987	-4.021221371
H276	-4.258688368	7.428493398	-0.392786084
H277	-3.216664986	7.225589561	-3.139133557
H278	-1.636016448	5.230384410	-2.255295612
H279	-5.097306557	4.872556317	-3.031974335
H280	-6.635628707	5.386380405	5.822997465
H281	-7.387193154	6.824998925	2.924360131
H282	-9.438871742	8.593357031	4.050871111
H283	-5.806773433	6.956839188	5.886004741
H284	-9.473886896	5.345140097	3.241728642
H285	7.704869685	5.757553776	-4.743552582
H286	8.445917768	4.172613609	-4.451500162
H287	10.125741593	3.038217535	-0.404147299
H288	9.756204487	5.328192815	-6.064062821
H289	8.935296306	4.191602299	-6.911023360
H290	0.584320034	5.983697422	4.687325797
H291	-1.580383687	7.080095659	6.612807864
H292	-1.048545601	9.571345481	3.144596143
H293	-1.163859953	5.581445388	4.662632029
H294	-0.881417435	8.555372347	6.716641772
H295	3.613826662	8.410704435	-0.711020472
H296	0.083975406	8.376531012	4.574185633
H297	6.846838008	-5.192263171	4.900277794
H298	9.371367899	-3.742095864	3.935639515
H299	3.386814654	6.740321578	-2.226635078
H300	2.146857197	0.071439618	5.222362961
H301	1.825508275	6.780678562	-5.445765774
H302	1.915835629	0.517562363	-4.600074127
H303	0.826912535	6.039253906	-4.197035669
H304	4.660511222	-3.738414531	4.530239773
H305	3.207692825	5.098940053	-3.372975466
H306	5.294278075	-3.168422334	2.983968314
H307	7.194909467	-4.656549830	3.243196471
H308	7.311190319	-2.240347545	4.133796249
H309	6.714729624	-2.845795900	5.692209685
H310	-1.183333038	1.494244471	-8.026731365
H311	8.946738123	-6.628454578	4.640362545
H312	10.446275354	-7.796659602	2.214886578
H313	1.528614867	2.235926240	-2.839274198
H314	10.527320249	-8.576707480	5.022197079
H315	9.811150335	-9.320562751	3.750479786
H316	5.061314041	-0.884702961	3.715517976
H317	-0.139717336	4.020321035	-3.205633061
H318	0.620103694	0.586682578	-6.717113905

H319	12.328386015	-2.404510963	0.612565201
H320	10.748724096	0.101832875	-1.023988988
H321	10.044542787	-2.636320056	1.451967905
H322	12.596710126	-2.471311224	-0.903695670
H323	4.141371526	9.798222361	-3.061322200
H324	7.890460945	-0.409148229	2.109377959
H325	6.429327708	-4.387005939	-0.018795138
H326	5.725534861	4.835454458	-4.018744654
H327	8.400205016	-4.218583172	-1.604975128
H328	8.765411593	1.222259804	-5.350415104
H329	6.642868661	0.686544691	-4.056638963
H330	11.823333351	-7.649380781	3.312292289
H331	3.336501801	0.466630958	4.021627616
H332	9.515544530	-0.715578728	3.889205013
H333	7.511953713	0.718992324	3.108945129
H334	10.017316900	-2.377893240	5.526066233
H335	3.424428268	-3.084329539	6.043610529
H336	10.859466842	-4.226717009	-4.565375665
H337	8.895042937	-1.619481312	-3.144609243
H338	9.625538899	-1.933228509	-1.558941637
H339	7.528655726	-3.626183255	-3.044110871
H340	4.092871974	3.054381193	-4.158709156
H341	-1.445264748	4.116863873	-5.347483848
H342	-2.211727787	2.821664232	-7.431899046
H343	5.188051063	-3.096283664	-0.113850161
H344	10.639159253	-1.657892194	3.383405782
H345	11.028880677	-3.550903634	2.238997183
H346	1.958849429	-2.173490628	5.996156588
H347	10.793128209	1.501414761	-3.797842641
H348	9.340685882	0.663811866	-0.121306307
H349	4.408763020	2.957793681	-5.914842463
H350	1.958478553	8.933292958	-1.094526619
H351	3.895285412	0.349565507	7.455046006
H352	4.184839723	1.849080189	6.543789042
H353	12.303261259	3.433774464	-1.183568390
H354	12.592785498	1.854015405	-1.492159490
H355	13.412916583	-0.173519749	2.413438352
H356	12.198014856	0.120577393	0.499311929
H357	14.013174083	2.486150081	2.008075256
H358	12.009230204	0.513542182	3.260751214
H359	6.325124030	2.478475849	8.167339412
H360	-12.021716619	5.154463004	4.976798867
H361	10.147136794	-3.587321872	8.280484225
H362	8.395247135	-1.484517588	7.887794461
H363	-12.100198644	5.229759909	1.958823110
H364	-10.443352574	3.031289292	3.344337526
H365	-11.918867445	2.774670660	2.399221725
H366	-8.475979877	3.306028311	-3.063945063
H367	-0.725180163	0.004018739	-1.353497888
Mo368	6.105850692	0.241864473	-0.799071944
N369	0.431667444	-7.154299699	-6.810878422
N370	-3.181951548	-7.432409003	-5.921933876
N371	-3.676113097	-9.340432796	-3.890129265
N372	-1.271573803	-9.339468341	-2.443611506
N373	-1.258473656	-6.678256626	-1.378843071
N374	-3.582192256	-6.891471236	0.261108131
N375	-3.008293522	-9.093528446	2.040194406
N376	-0.341331126	-8.749057123	3.064757069
N377	0.156704281	-6.052393651	3.645253762
N378	-2.182347998	-4.461414607	4.572594084
N379	-3.515761290	-6.526055465	6.128352158
N380	9.981947848	-8.407863198	4.174580664
N381	9.362919943	-5.796288654	4.208056630
N382	4.676678391	-1.653380344	4.273431469
N383	2.882977482	-2.344270850	5.610727356
N384	2.836876987	-0.271969395	4.556790239
N385	9.821801965	-3.042262587	6.306097832
N386	-1.006227806	-2.471345227	-6.609630602
N387	3.458643205	-2.384857132	-4.978954958
N388	-3.149694698	-1.415494585	-5.521790776
N389	-5.654402363	-2.594759665	-5.719662851
N390	-5.934283385	-3.997784587	-3.346130481
N391	-5.914412839	-2.217472093	-1.192049821

N392	-3.559657912	1.205835060	-2.086391705
N393	-1.760400871	0.132647900	-1.540763619
N394	-8.311749926	-1.142694417	-0.294394356
N395	-12.208526540	0.439256310	-2.253737784
N396	-13.886630625	0.560667648	-0.807143605
N397	4.022805838	3.528143952	8.673507108
N398	-0.750023056	7.613912377	6.335495647
N399	-1.966298336	9.220253783	3.405314981
N400	-2.999407722	7.892753151	1.178463624
N401	-4.833766967	5.873211429	-3.021807606
N402	-5.573624075	8.093708816	-2.962197494
N403	-7.059226429	6.352272671	-2.587302517
N404	-3.726676437	5.277969921	2.049852763
N405	-5.551080317	5.911381348	4.104652139
N406	-8.067855845	7.104710638	3.633346844
N407	-7.267360645	7.520199673	0.644701312
N408	-10.396881953	5.734480940	3.062920413
N409	8.823715867	5.066603229	-6.391246495
N410	5.622634354	4.289187405	-4.879385981
N411	2.830695226	5.380484115	-4.296889153
N412	2.878582680	7.600361440	-2.470907380
N413	3.742364801	3.712620876	-9.233422636
N414	0.991987365	3.324809630	-8.530303633
N415	11.852709454	2.563002678	-1.479895111
N416	7.907229665	0.802879908	-2.316563035
N417	8.727008419	1.145941097	-4.337655478
N418	12.140244709	0.889984525	1.166314355
N419	-2.756782260	2.206098944	0.841517797
N420	-1.923069739	2.702638912	0.299175755
O421	-1.379075372	-7.079911760	-4.575560234
O422	-4.350033410	-7.643785350	-2.524064606
O423	-2.373492385	-10.266714322	-0.665832957
O424	-0.131326593	-7.548958567	0.394361148
O425	-2.597381132	-5.393865105	1.659211293
O426	-4.186223508	-7.924250789	3.607540077
O427	-0.976610686	-9.961310030	4.908847723
O428	2.176334841	-6.577829751	4.610590737
O429	-0.593773527	-3.740309165	6.051194399
O430	-3.580855086	-4.936782507	7.750577227
O431	-2.915105823	-8.066820332	9.310634363
O432	11.126042715	-5.213478160	2.825487419
O433	8.908303111	-5.059907874	6.921506047
O434	9.854503932	-0.871460824	9.174227822
O435	-3.192314188	-2.848838801	-3.731234945
O436	1.780912220	-1.980242158	-6.455468834
O437	-6.616800352	-0.889953512	-4.541679261
O438	-5.499381505	1.484878802	-5.347662761
O439	-8.055879871	-4.662011819	-3.933906275
O440	-5.877030498	-3.940385835	0.311614596
O441	-7.304560284	-0.365243144	1.602529207
O442	-10.835970894	-0.828637482	2.180261453
O443	6.181160491	0.813894397	9.342027597
O444	-1.959557857	2.199328084	6.701545751
O445	-3.147359341	7.694522681	4.615217318
O446	-4.934311388	9.127962251	1.292310199
O447	-5.200436544	5.230134095	0.293548601
O448	-6.509950923	3.844914581	3.873669623
O449	-3.147415452	4.082789562	4.837416208
O450	-8.400981726	7.410450519	5.880534828
O451	-11.605984176	7.664652470	2.874785609
O452	-9.465270811	7.369359866	0.033701537
O453	-13.613492653	4.404022415	3.943147446
O454	-7.890465099	3.440754691	-2.293401254
O455	6.725192216	3.281776132	-6.625350364
O456	2.770614201	4.806404559	-6.517040640
O457	1.320778754	8.666900816	-3.737159417
O458	3.338369284	11.084621355	-1.695104870
O459	0.924617519	1.866504917	-10.282861902
O460	5.202389130	-1.136360472	-7.211375939
O461	6.116759550	0.718282038	-6.376536583
O462	-1.838599264	5.315182531	-7.718670334
O463	11.345358985	2.922142836	1.772796273
O464	13.923065961	2.142881217	4.018990152

O465	4.273298645	-3.923827567	-2.437631828
O466	5.721746460	-5.590392175	-2.175156540
O467	11.544639550	-3.118495757	-2.685134512
O468	10.041190844	-3.805045092	-4.225607514
O469	7.664248814	-0.887242900	0.356420110
O470	8.473744578	-2.956936316	0.730145114
O471	6.368635152	-1.562049390	-1.825632979
O472	10.332486374	-1.181554245	4.199479061
O473	7.939268396	-0.157937019	3.067157466
O474	-5.419400071	3.069183930	-3.113567763
O475	13.023204641	-2.203325616	-0.064400473
O476	10.947513098	-2.630034673	1.876743883
S477	-0.398259483	6.228421060	2.461048967
S478	1.009816726	4.354963937	-0.566002344
S479	4.570925750	1.075553736	-2.424066888
S480	1.017819600	2.585056467	2.563584442
S481	1.238544298	0.378313612	-0.607678836
S482	4.709890512	4.840284610	-1.594483877
S483	4.587639254	-0.642720093	0.844588356
S484	3.290056310	5.375094236	2.012300703
S485	6.824765884	2.239270672	0.301047798
S486	4.842620976	2.097043786	3.487719587

Structure A, 35(3/2)

A, 35(3/2) associated	bm22n2xd35td.car_2
C1	-1.849981071 -7.330177219 -5.712980393
C2	-0.962578610 -7.593336296 -6.935259201
C3	-4.152370796 -7.152067754 -4.871981690
C4	-4.065634333 -8.071558238 -3.656139104
C5	-3.507837852 -10.285449840 -2.783781364
C6	-2.333125283 -9.949944589 -1.858547831
C7	-0.156877333 -8.847495106 -1.638706948
C8	-0.513794426 -7.629777999 -0.782189552
C9	-1.739641205 -5.531446859 -0.603494670
C10	-2.685448838 -5.925384960 0.541734337
C11	-4.530442516 -7.309458171 1.296019029
C12	-3.883892625 -8.121316607 2.425923857
C13	-2.455493854 -10.016324664 3.017544005
C14	-1.187741566 -9.566232400 3.754640269
C15	0.964293348 -8.387955255 3.594542864
C16	1.151121405 -6.924291795 4.004439317
C17	0.193565130 -4.638443780 3.945253694
C18	-0.895564854 -4.263945651 4.967319178
C19	0.157709184 -3.773607021 2.657144179
C20	0.007224701 -2.281478244 2.974130416
C21	1.406321133 -4.029980232 1.804386335
C22	-3.304371899 -4.167650594 5.477532830
C23	-3.482535322 -5.243011781 6.565727775
C24	-4.599789355 -3.918674276 4.667428745
C25	-5.805908948 -3.721453963 5.593405440
C26	-4.434836082 -2.708464867 3.738254181
C27	-3.754093295 -7.590562356 7.113851755
C28	-2.730126893 -7.590333979 8.230935608
C29	10.721837095 -7.536074216 3.232430049
C30	10.415703627 -6.047255018 3.406422988
C31	8.852430588 -4.467968776 4.557149272
C32	9.192434678 -4.215837833 6.039240968
C33	7.337269563 -4.395121744 4.298451482
C34	6.716718590 -3.027695004 4.602004069
C35	5.284699334 -2.955838148 4.069081416
C36	3.470101357 -1.404031756 4.826770594
C37	10.245876564 -2.687193722 7.637936652
C38	9.410661517 -1.599999825 8.282373259
C39	-1.264801360 -2.927093156 -5.240203016
C40	-2.630010671 -2.415483169 -4.753743047
C41	-0.194360121 -2.417902964 -4.249780990
C42	1.195501957 -3.076877394 -4.358497086
C43	2.157954829 -2.422927590 -5.347801374
C44	-4.292423749 -0.644293455 -5.075126888
C45	-5.626538914 -1.394068998 -5.103226955

C46	-4.422478307	0.687667619	-5.842624207
C47	-6.817095881	-3.467320689	-5.593880640
C48	-7.000044636	-4.090990913	-4.203509038
C49	-5.999216853	-4.537800208	-2.001233922
C50	-5.923033014	-3.531005425	-0.853941246
C51	-5.882334781	-1.172893014	-0.156843438
C52	-7.258237329	-0.888489282	0.491453951
C53	-5.386635841	0.173872881	-0.701882046
C54	-3.964350435	0.241569720	-1.157288799
C55	-2.828295315	-0.470564219	-0.858844138
C56	-2.237521720	1.192561443	-2.207171136
C57	-9.677124000	-0.710999253	0.058155480
C58	-10.126811938	-1.400682643	1.342154704
C59	-10.625498472	-1.087110140	-1.112111317
C60	-11.918724181	-0.330880787	-1.172455339
C61	-12.956834556	-0.258486089	-0.262888152
C62	-13.412566606	0.966841754	-2.051471210
C63	4.197398316	2.074307316	8.708420259
C64	5.682492602	1.763632879	8.747953458
C65	3.641066144	1.419755293	7.416801149
C66	2.151327396	1.610982815	7.248449401
C67	1.229214808	0.715571476	7.819798663
C68	1.643648191	2.692172256	6.504380322
C69	-0.150284016	0.884411817	7.652562467
C70	0.271105141	2.880511350	6.339464325
C71	-0.625249648	1.973328044	6.909628611
C72	-0.732566118	7.702849139	4.877649468
C73	-2.061422436	8.196087212	4.292770704
C74	-0.386605705	6.318131055	4.305529718
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C76	-3.775245682	8.878866285	1.674405043
C77	-3.470515302	6.937108208	0.183460990
C78	-4.193464551	5.731860952	0.822092099
C79	-2.293855037	6.520041670	-0.718781450
C80	-2.597983706	5.573622384	-1.884470250
C81	-3.388205876	6.155344778	-3.073288244
C82	-5.806855668	6.782849072	-2.899935638
C83	-4.370325751	4.147199524	2.673162107
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C85	-3.418982566	3.299113389	3.524811869
C86	-6.357169934	6.216083847	5.193840821
C87	-7.675763359	6.938553471	4.925360341
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C89	-10.526127016	7.084750955	3.060192824
C90	-8.916442867	8.722193724	1.977244663
C91	-8.592563662	7.839035626	0.778334287
C92	-11.551427422	4.858755325	2.828983965
C93	-12.500333438	4.823096744	4.023715065
C94	-11.063456449	3.421590759	2.500588459
C95	-10.234802425	3.362858254	1.238082900
C96	-10.847438837	3.219373407	-0.015825963
C97	-8.836522046	3.485859194	1.282540914
C98	-10.095153820	3.224853061	-1.193306201
C99	-8.068776186	3.516529243	0.115371304
C100	-8.712396271	3.393736863	-1.114194329
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C102	6.703402917	4.068037534	-5.637037901
C103	4.319286863	3.641975595	-5.080542445
C104	3.217822806	4.665177613	-5.380493730
C105	1.821986482	6.439235713	-4.419346448
C106	1.987719959	7.660346572	-3.518361577
C107	2.921255524	8.704200705	-1.532917077
C108	3.549173088	9.949894447	-2.124217369
C109	3.105637450	2.378022670	-9.375072426
C110	1.576161827	2.482534358	-9.442986287
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C124	11.427927322	2.044748626	0.901340793
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C126	9.271948754	1.069912230	-2.216246062
C127	9.780989836	1.291377077	-3.481090625
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C131	5.258547253	-4.382543604	-1.818286931
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H150	-0.981851653	-8.690143707	-7.120845323
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H167	1.314648047	-3.443244802	0.873266022
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C28	-2.713851705	-7.573601487	8.217889454
C29	10.727439769	-7.543251488	3.247372998
C30	10.419155530	-6.055412595	3.416884692
C31	8.855069747	-4.472772177	4.563072625
C32	9.191649874	-4.217375536	6.045252699
C33	7.340355283	-4.401225495	4.300036734
C34	6.716313437	-3.033627877	4.598636439
C35	5.286589885	-2.963852296	4.058797087
C36	3.471450268	-1.418389546	4.822853286
C37	10.252430840	-2.693816454	7.643223398
C38	9.424020523	-1.597894615	8.282500875
C39	-1.259667663	-2.918193560	-5.232636595
C40	-2.623945669	-2.406075200	-4.745700009
C41	-0.186356276	-2.413338802	-4.242930868
C42	1.201278570	-3.076565191	-4.355101890
C43	2.163996299	-2.427961463	-5.347616642
C44	-4.291171160	-0.639525522	-5.076699003
C45	-5.623607717	-1.392758017	-5.103640616
C46	-4.424356078	0.688609284	-5.851496136
C47	-6.808350564	-3.468914703	-5.594474268
C48	-6.993450131	-4.092869720	-4.204481556
C49	-5.994138728	-4.544133481	-2.002901933
C50	-5.914939347	-3.540615480	-0.854090702
C51	-5.860934692	-1.180953811	-0.160552661
C52	-7.233814010	-0.889003859	0.491132733
C53	-5.365438689	0.160468641	-0.720575896
C54	-3.947431542	0.216003845	-1.191086407
C55	-2.805143215	-0.477525177	-0.868792246
C56	-2.220492915	1.166419718	-2.239602251
C57	-9.651051071	-0.687572627	0.059816552
C58	-10.091968774	-1.360695023	1.355568700
C59	-10.608547656	-1.079211375	-1.097931794
C60	-11.904262587	-0.328795471	-1.156554016
C61	-12.942962174	-0.263877526	-0.247636034
C62	-13.404529120	0.963947930	-2.032684574
C63	4.203222565	2.074713535	8.700486151
C64	5.688162317	1.764005717	8.741505437
C65	3.647354156	1.422124140	7.407322415
C66	2.158265172	1.613392799	7.239059510
C67	1.235786352	0.720651240	7.813605268
C68	1.650134561	2.693587187	6.493255527
C69	-0.143777232	0.891360989	7.650171969
C70	0.277141847	2.883253352	6.331621270
C71	-0.619165190	1.979410445	6.907228237
C72	-0.737958351	7.695592069	4.878993778
C73	-2.064407456	8.198180773	4.291549874
C74	-0.407782168	6.304560450	4.315833922
C75	-3.155252804	9.770487886	2.749531664
C76	-3.773639017	8.879313997	1.670260985
C77	-3.472456767	6.925404394	0.193396409
C78	-4.192591323	5.724508326	0.845824944
C79	-2.298375521	6.508066501	-0.712158485
C80	-2.602035681	5.562654922	-1.879524705
C81	-3.387158206	6.145645220	-3.071590569
C82	-5.806890731	6.771978180	-2.891075346
C83	-4.380225178	4.168534721	2.724717212
C84	-5.578254794	4.615510267	3.582840220
C85	-3.446479442	3.343578402	3.621257689
C86	-6.367860007	6.249070332	5.215743292
C87	-7.684515989	6.968619737	4.935989910
C88	-9.210612557	7.887724894	3.232824237
C89	-10.513608005	7.079514843	3.049224776
C90	-8.913918272	8.727435470	1.966700080
C91	-8.587572500	7.842857495	0.770416083

C92	-11.522474078	4.848279380	2.820673797
C93	-12.469623045	4.814036199	4.017609130
C94	-11.035626075	3.410503590	2.492805518
C95	-10.208929524	3.350157910	1.228452033
C96	-10.823009759	3.210120878	-0.025115362
C97	-8.810305817	3.471689065	1.272108238
C98	-10.071806242	3.215629121	-1.202858915
C99	-8.043550952	3.501575320	0.104387225
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C104	3.230409692	4.668343011	-5.371469574
C105	1.829787730	6.438683979	-4.410930700
C106	1.995478495	7.661330929	-3.512762056
C107	2.941683854	8.709115343	-1.536907012
C108	3.529545422	9.967246167	-2.143904757
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C110	1.578389262	2.496181262	-9.448347042
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C113	5.438099796	0.064037057	-7.335187379
C114	-0.459364258	3.460627295	-8.485074918
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C121	1.172876836	1.303056330	-4.744986399
C122	0.963741643	2.270486731	-3.758867438
C123	10.827616360	2.196080268	-0.494488992
C124	11.434600318	2.031204760	0.907511985
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C126	9.276526010	1.058793439	-2.208807783
C127	9.787002581	1.284206832	-3.472057195
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H336	10.876578883	-4.222632225	-4.560382302
H337	8.900172916	-1.625308958	-3.137647531
H338	9.631441358	-1.938319862	-1.553643180
H339	7.540720421	-3.639196281	-3.037358592
H340	4.090782504	3.062386324	-4.169417318
H341	-1.435382971	4.125411885	-5.342927595
H342	-2.208343773	2.816420892	-7.420178419
H343	5.195078171	-3.102800794	-0.117124596
H344	10.635045107	-1.647463717	3.390954035
H345	11.033565829	-3.542751803	2.248903392
H346	1.967517471	-2.170343754	6.009371873
H347	10.791128893	1.516271030	-3.804223758
H348	9.346771940	0.665195312	-0.127562637
H349	4.410116891	2.973240359	-5.924850157
H350	1.951324713	8.942026326	-1.114979834
H351	3.887753874	0.349159107	7.450226552
H352	4.176081000	1.848511102	6.540637574
H353	12.305122337	3.441472892	-1.184074390
H354	12.596675098	1.861996718	-1.499176587
H355	13.408558285	-0.171040170	2.412937108
H356	12.199420400	0.124798811	0.495811378
H357	14.017488842	2.485558563	2.008649965
H358	12.004408382	0.518238002	3.257916331
H359	6.319156493	2.477479407	8.157842900
H360	-12.028481560	5.165779034	4.980563270
H361	10.144556996	-3.591797414	8.275849776
H362	8.385009805	-1.492618850	7.886553618
H363	-12.097828309	5.235686835	1.964777396
H364	-10.453689022	3.026130739	3.346156338
H365	-11.930565907	2.777979745	2.398865669
H366	-8.490234088	3.319776227	-3.061509840
H367	-0.724527080	-0.003873317	-1.337845559
Mo368	6.099160977	0.234005870	-0.798073215
N369	0.427331547	-7.156417768	-6.817714061
N370	-3.185646330	-7.438951472	-5.922133045
N371	-3.675272818	-9.342941406	-3.887066039
N372	-1.271914157	-9.337462876	-2.440523130
N373	-1.264534022	-6.674619897	-1.379024914
N374	-3.588473085	-6.890406538	0.263024693
N375	-3.007511668	-9.091015004	2.042386259
N376	-0.340366049	-8.746954737	3.064678110
N377	0.158063684	-6.051550496	3.642018013
N378	-2.180294630	-4.459807913	4.574116562
N379	-3.507994510	-6.522130329	6.133601181
N380	9.980013055	-8.406103743	4.168634229
N381	9.355947163	-5.793815839	4.199963120
N382	4.666974868	-1.648998622	4.260486130
N383	2.888811488	-2.340979077	5.618081995

N384	2.819788580	-0.279291200	4.545099106
N385	9.816660670	-3.041686774	6.303200630
N386	-1.006799680	-2.472063759	-6.607250792
N387	3.457133730	-2.383733257	-4.972194939
N388	-3.151405815	-1.417452253	-5.517081730
N389	-5.658643604	-2.590867598	-5.717035934
N390	-5.939120334	-3.991276926	-3.344187982
N391	-5.910733970	-2.211829469	-1.188308520
N392	-3.550029129	1.225847945	-2.057839206
N393	-1.757393349	0.130354584	-1.532861789
N394	-8.310741185	-1.137319670	-0.295485234
N395	-12.206868596	0.443489051	-2.267518249
N396	-13.883802869	0.563614941	-0.820122781
N397	4.020094237	3.527393002	8.667662679
N398	-0.782921975	7.610854024	6.345446496
N399	-1.979356340	9.233627807	3.408732506
N400	-2.993599772	7.894887755	1.173697090
N401	-4.829931092	5.875227028	-3.018329383
N402	-5.565971895	8.096795228	-2.982041109
N403	-7.056725976	6.364285442	-2.592713797
N404	-3.702893918	5.262427728	2.029570735
N405	-5.541558235	5.886857306	4.073064659
N406	-8.054009028	7.090848378	3.627181188
N407	-7.271065830	7.521513356	0.639401933
N408	-10.393114799	5.728776116	3.072572207
N409	8.826031915	5.067913619	-6.392090817
N410	5.622817710	4.299528797	-4.885033700
N411	2.828431006	5.390391965	-4.303467214
N412	2.875781138	7.607309871	-2.482857582
N413	3.736159433	3.706933974	-9.239720710
N414	0.986715252	3.322657440	-8.539894980
N415	11.856469416	2.571127214	-1.485340796
N416	7.912179581	0.796059865	-2.320894003
N417	8.727176136	1.151486907	-4.342476460
N418	12.140993272	0.894273017	1.162788068
N419	-2.761200146	2.266346560	0.702666437
N420	-1.682945390	2.455278359	0.517852665
O421	-1.381377858	-7.075625761	-4.579434098
O422	-4.353836233	-7.647986017	-2.522959167
O423	-2.373059635	-10.263652643	-0.661422273
O424	-0.137958483	-7.541758834	0.396100555
O425	-2.604481619	-5.388386945	1.657437239
O426	-4.187113016	-7.922838178	3.609687635
O427	-0.970536227	-9.964845867	4.906555319
O428	2.177667059	-6.576289381	4.607654537
O429	-0.589163694	-3.745004711	6.052756222
O430	-3.576373755	-4.932075764	7.753723973
O431	-2.916068859	-8.082517638	9.309688665
O432	11.125106701	-5.210113235	2.825800365
O433	8.907089502	-5.061605862	6.912729074
O434	9.840004170	-0.878039389	9.176565413
O435	-3.193800939	-2.852239181	-3.729101702
O436	1.780738514	-1.978014182	-6.451147585
O437	-6.616383862	-0.888777038	-4.531258656
O438	-5.497222949	1.486250206	-5.326543332
O439	-8.060233775	-4.655678485	-3.929590327
O440	-5.875543592	-3.936498905	0.313813849
O441	-7.308061885	-0.367352201	1.607366665
O442	-10.836067368	-0.854475303	2.177054302
O443	6.179369126	0.813404402	9.333173604
O444	-1.966455297	2.200777016	6.703047191
O445	-3.160146504	7.695906080	4.602296597
O446	-4.934644190	9.119634860	1.280124334
O447	-5.194145797	5.239333579	0.289428134
O448	-6.490928458	3.816797755	3.838620836
O449	-3.142734549	4.068626966	4.813440253
O450	-8.370771482	7.386956915	5.877535505
O451	-11.594857305	7.662678658	2.892066376
O452	-9.473004180	7.372478029	0.038965221
O453	-13.618605084	4.411132061	3.944957465
O454	-7.905582953	3.459961015	-2.291467093
O455	6.726065062	3.284434053	-6.625545891
O456	2.773909367	4.819600526	-6.525243157

O457	1.290667943	8.662829774	-3.726970822
O458	3.391400919	11.077855684	-1.658268210
O459	0.919650649	1.840739220	-10.273003483
O460	5.197336196	-1.132359485	-7.202704112
O461	6.104797464	0.725761037	-6.369382577
O462	-1.846947841	5.309294976	-7.733488621
O463	11.356607931	2.933208207	1.762272852
O464	13.920702849	2.143005075	4.018829801
O465	4.287420859	-3.937966976	-2.442840649
O466	5.734411179	-5.604830196	-2.170967503
O467	11.554387632	-3.117446239	-2.677549966
O468	10.056699730	-3.803349541	-4.221035149
O469	7.660719672	-0.883878852	0.350808381
O470	8.475356355	-2.948325855	0.736507798
O471	6.375683619	-1.570674835	-1.825751603
O472	10.329079402	-1.170511295	4.206997432
O473	7.942945498	-0.147080138	3.063003070
O474	-5.431080699	3.074015938	-3.094452996
O475	13.019925941	-2.204753061	-0.061048212
O476	10.947277434	-2.622176293	1.886496913
S477	-0.360394132	6.274241692	2.463865231
S478	0.963776507	4.336826863	-0.503746621
S479	4.549100527	1.085543551	-2.420154227
S480	1.066946328	2.576125275	2.625228749
S481	1.228528845	0.340902354	-0.495967771
S482	4.722819930	4.877583483	-1.604821903
S483	4.594143686	-0.664356380	0.828022122
S484	3.348256555	5.332917824	2.082236953
S485	6.818878191	2.262674260	0.251014193
S486	4.807011338	2.026514063	3.452122739

Structure B 47(1)

B 47(1) associated	bm22b2n2xd47tf_car_3			
	C1	-1.678066606	-5.818882930	-7.291472803
	C2	-0.748216083	-5.799487303	-8.509182119
	C3	-4.010565294	-5.796645638	-6.514351340
	C4	-3.975386577	-6.969350569	-5.535646418
	C5	-3.481492472	-9.335304612	-5.171517926
	C6	-2.351062907	-9.231348522	-4.142592696
	C7	-0.171618419	-8.255926759	-3.595680201
	C8	-0.552653293	-7.253559950	-2.502397159
	C9	-1.768033450	-5.225296750	-1.911966903
	C10	-2.760558852	-5.842781114	-0.915815205
	C11	-4.651587383	-7.321652214	-0.550942818
	C12	-4.059485951	-8.378989485	0.389532810
	C13	-2.676859879	-10.386331626	0.593302433
	C14	-1.428162948	-10.144898980	1.452094171
	C15	0.735325742	-8.995175739	1.643738686
	C16	0.920291109	-7.662313458	2.373955726
	C17	-0.026167629	-5.413069137	2.808569287
	C18	-1.153455566	-5.261357643	3.846211885
	C19	-0.004812449	-4.280682148	1.746649000
	C20	-0.161187255	-2.896511867	2.385328009
	C21	1.273559589	-4.356876383	0.905305763
	C22	-3.582316186	-5.231050214	4.265062725
	C23	-3.818718309	-6.520014922	5.076736526
	C24	-4.836360461	-4.784313955	3.476454410
	C25	-6.081396681	-4.773233761	4.370030194
	C26	-4.618305425	-3.403199475	2.845694330
	C27	-4.131638611	-8.927308115	5.071753507
	C28	-3.166042692	-9.185939395	6.210842247
	C29	10.502613011	-8.271899190	1.883760860
	C30	10.214619943	-6.852698729	2.376199719
	C31	8.613109123	-5.534999244	3.775674356
	C32	8.890242596	-5.638122924	5.288298188
	C33	7.112953945	-5.367894380	3.477109566
	C34	6.491683611	-4.101853627	4.074058538
	C35	5.092618310	-3.873244267	3.501079258
	C36	3.258271105	-2.499526430	4.506082414
C37	9.882001734	-4.534435814	7.234167689	

C38	9.013054909	-3.630674831	8.083745952
C39	-1.061420815	-1.655269285	-5.814404543
C40	-2.444849216	-1.248061571	-5.280948360
C41	-0.029930509	-1.392657638	-4.695183483
C42	1.360149451	-2.026910054	-4.890248051
C43	2.365068334	-1.177481210	-5.667267235
C44	-4.078860406	0.578811401	-5.260877800
C45	-5.423778759	-0.103013771	-5.518721332
C46	-4.144524681	2.059173486	-5.691423228
C47	-6.619187602	-1.994781670	-6.490369854
C48	-6.873557640	-2.895562327	-5.272489545
C49	-5.954786157	-3.854411448	-3.200965140
C50	-5.896917727	-3.136058869	-1.854402291
C51	-5.881722120	-0.994439091	-0.645088452
C52	-7.278899828	-0.830414176	0.001216973
C53	-5.355265774	0.433078205	-0.857753711
C54	-3.922604675	0.581047106	-1.255674327
C55	-2.805382411	-0.210051162	-1.134501750
C56	-2.163322094	1.721549701	-2.023893753
C57	-9.680843704	-0.536033508	-0.476003355
C58	-10.210971528	-1.486648076	0.592266919
C59	-10.569186181	-0.604290903	-1.744685887
C60	-11.849829912	0.172578431	-1.685888272
C61	-12.923243561	0.070745961	-0.821542799
C62	-13.289099687	1.659640634	-2.321785321
C63	3.841601366	-0.006755726	9.117909691
C64	5.321518320	-0.342396993	9.136707069
C65	3.332705406	-0.345378787	7.691044536
C66	1.853411337	-0.099784724	7.510538473
C67	0.902707843	-1.088008243	7.829001113
C68	1.382406769	1.125368874	7.006779481
C69	-0.467059427	-0.867133989	7.645914350
C70	0.019189871	1.364537256	6.829298936
C71	-0.906224036	0.364893227	7.146660738
C72	-0.857771284	6.421036249	6.453059845
C73	-2.167160578	7.041783263	5.947517407
C74	-0.509833611	5.178144807	5.620564094
C75	-3.205515144	8.938440477	4.775503699
C76	-3.768847633	8.352098070	3.480135869
C77	-3.416407522	6.791043337	1.603038401
C78	-4.167276687	5.480096884	1.918042309
C79	-2.207045606	6.578852662	0.672302721
C80	-2.460660782	5.917688474	-0.687161872
C81	-3.194389004	6.757271544	-1.750966183
C82	-5.609875837	7.378116038	-1.521242549
C83	-4.438194262	3.526208024	3.357855610
C84	-5.662758254	3.768142702	4.265774485
C85	-3.522069754	2.496478224	4.031315772
C86	-6.518307050	4.994209090	6.204879631
C87	-7.814904157	5.790056224	6.058754125
C88	-9.266996566	7.119680136	4.572341365
C89	-10.580485761	6.408105980	4.175560943
C90	-8.913928965	8.213232341	3.535583123
C91	-8.550143442	7.604820871	2.185878171
C92	-11.620183869	4.322222727	3.382164200
C93	-12.643267584	4.053808665	4.480035699
C94	-11.125405670	2.983728515	2.769176934
C95	-10.237339970	3.190818046	1.562258568
C96	-10.802910995	3.362244650	0.290025526
C97	-8.839304723	3.263227181	1.679761031
C98	-10.009270624	3.628840464	-0.828526569
C99	-8.029655994	3.551322988	0.576303734
C100	-8.627623763	3.736641533	-0.667663345
C101	8.218634025	5.695038270	-3.663250301
C102	6.972965587	5.104982672	-4.302397005
C103	4.566301552	4.608144760	-3.962120110
C104	3.482354997	5.686350496	-4.066163744
C105	2.081178041	7.234388484	-2.779139630
C106	2.231322955	8.222713679	-1.625522599
C107	3.064759321	8.764185715	0.588058096
C108	3.718742512	10.099080930	0.301355348
C109	3.526914030	4.360441571	-8.464294665
C110	2.002665492	4.498931406	-8.564551055

C111	3.881816680	3.075440472	-7.680617297
C112	5.356734739	2.683894462	-7.893814253
C113	5.772911807	1.608044938	-6.916834984
C114	-0.069023771	5.263514771	-7.504707596
C115	-0.448385598	6.645402574	-7.006376010
C116	-0.813460482	4.097708250	-6.806608386
C117	-0.196168863	3.701579228	-5.488226568
C118	-0.466183623	4.420292740	-4.309973561
C119	0.732910198	2.647778519	-5.431366134
C120	0.200284056	4.106378786	-3.119896004
C121	1.401998561	2.336320538	-4.241642810
C122	1.143865668	3.072280901	-3.081157786
C123	10.848709830	2.056039996	0.430554197
C124	11.393460764	1.573244675	1.784461070
C125	10.072858894	0.948742855	-0.301922936
C126	9.354631924	1.367480962	-1.549081875
C127	9.907972870	1.858066992	-2.716365298
C128	7.736821197	1.535665667	-3.007410216
C129	12.609992096	-0.096549992	3.067443424
C130	13.481844273	0.924504819	3.763881531
C131	5.289689490	-3.951954958	-2.540977988
C132	5.916220412	-3.510711980	-1.248896034
C133	7.015175460	-2.389494377	-1.453704890
C134	8.086333746	-2.891098290	-2.463545478
C135	9.301138069	-1.952496258	-2.560284589
C136	10.475078071	-2.545938854	-3.288116593
C137	7.723688776	-2.233717422	-0.073387731
C138	3.508042134	2.239501968	1.103424993
Fe139	5.024451075	2.783249352	-0.110232117
Fe140	1.355938679	2.140343761	1.011989834
Fe141	3.270665305	2.514007797	3.099872331
Fe142	3.293900798	4.243813253	1.139124205
Fe143	1.215844200	4.246980752	2.765400153
Fe144	4.966939076	1.069130680	1.857006283
Fe145	3.483123060	0.828553267	-0.163950976
H146	0.998370190	-5.990440446	-7.474951034
H147	0.686211676	-4.457807454	-7.942744462
H148	-3.316010566	-5.751541384	-8.535290715
H149	-1.171446573	-5.130686586	-9.274752863
H150	-0.774493782	-6.813314102	-8.945433456
H151	-3.887114208	-4.887320730	-5.909833162
H152	-3.365251949	-8.244137707	-7.023676587
H153	-5.002979972	-5.768969111	-6.983764267
H154	-3.306789341	-10.217409012	-5.801519959
H155	-1.291286265	-7.990655706	-5.391169512
H156	-4.412329953	-9.489499290	-4.609845075
H157	-0.935621817	-4.821777446	-1.320520470
H158	-1.468749194	-6.026088232	-3.890667902
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O468	11.610137921	-2.673331407	-2.835102926
O469	10.167445920	-2.942997780	-4.551715061
O470	7.591173279	-1.076587665	0.484433763
O471	8.398217695	-3.179126970	0.398674121
O472	6.425063461	-1.210333056	-1.865095777
O473	10.111157753	-2.271611703	4.239795189
O474	7.780699820	-0.964800774	3.287398548
O475	-5.294671256	3.813430810	-2.523899894

	O476	12.969273946	-2.356267655	-0.036923304
	O477	10.813364958	-3.172705682	1.679937937
	S478	-0.411267644	5.522854084	3.804903447
	S479	1.137445268	4.440473478	0.542617521
	S480	4.610456402	1.516577077	-1.933798268
	S481	1.074687539	1.990078119	3.299731737
	S482	1.373942640	0.287897164	-0.562486190
	S483	4.823052396	5.000867350	-0.324444383
	S484	4.474400453	-0.860015013	0.844506876
	S485	3.385032275	4.799575934	3.298437324
	S486	6.809299456	2.028392419	1.049190577
	S487	4.754191258	1.130883247	4.046593914
B 47(1) TS	bm22b2n2xd47tf_orig			
	C2	-0.748	-5.824	-8.514
	C3	-4.012	-5.806	-6.521
	C4	-3.977	-6.973	-5.537
	C5	-3.478	-9.335	-5.158
	C6	-2.341	-9.230	-4.137
	C7	-0.169	-8.236	-3.594
	C8	-0.557	-7.241	-2.498
	C9	-1.781	-5.216	-1.908
	C10	-2.780	-5.829	-0.916
	C11	-4.659	-7.322	-0.552
	C12	-4.067	-8.380	0.389
	C13	-2.681	-10.387	0.589
	C14	-1.434	-10.148	1.451
	C15	0.740	-9.014	1.640
	C16	0.929	-7.682	2.372
	C17	-0.025	-5.433	2.810
	C18	-1.150	-5.294	3.852
	C19	-0.026	-4.300	1.749
	C20	-0.222	-2.921	2.387
	C21	1.256	-4.346	0.912
	C22	-3.576	-5.242	4.276
	C23	-3.816	-6.527	5.089
	C24	-4.831	-4.790	3.493
	C25	-6.070	-4.771	4.397
	C26	-4.608	-3.412	2.859
	C27	-4.152	-8.928	5.083
	C28	-3.175	-9.205	6.207
	C29	10.510	-8.286	1.878
	C30	10.211	-6.865	2.365
	C31	8.613	-5.545	3.768
	C32	8.893	-5.648	5.282
	C33	7.112	-5.373	3.478
	C34	6.502	-4.101	4.073
	C35	5.084	-3.884	3.541
	C36	3.266	-2.487	4.550
	C37	9.888	-4.542	7.230
	C38	9.021	-3.633	8.076
	C39	-1.075	-1.663	-5.825
	C40	-2.455	-1.247	-5.293
	C41	-0.047	-1.399	-4.700
	C42	1.344	-2.037	-4.883
	C43	2.352	-1.187	-5.654
	C44	-4.080	0.586	-5.262
	C45	-5.424	-0.099	-5.516
	C46	-4.153	2.068	-5.689
	C47	-6.621	-1.987	-6.495
	C48	-6.864	-2.905	-5.289
	C49	-5.954	-3.855	-3.211
	C50	-5.912	-3.138	-1.863
	C51	-5.895	-1.001	-0.647
	C52	-7.294	-0.850	-0.006
	C53	-5.384	0.432	-0.855
	C54	-3.952	0.600	-1.246
	C55	-2.821	-0.172	-1.118
	C56	-2.206	1.769	-2.004
	C57	-9.686	-0.538	-0.491
	C58	-10.221	-1.508	0.557
	C59	-10.577	-0.597	-1.760
	C60	-11.858	0.182	-1.704

C61	-12.937	0.081	-0.846
C62	-13.294	1.669	-2.350
C63	3.828	-0.014	9.111
C64	5.307	-0.353	9.137
C65	3.321	-0.354	7.686
C66	1.843	-0.103	7.506
C67	0.889	-1.088	7.826
C68	1.376	1.125	7.004
C69	-0.479	-0.863	7.640
C70	0.014	1.367	6.826
C71	-0.914	0.370	7.140
C72	-0.868	6.438	6.474
C73	-2.172	7.059	5.955
C74	-0.495	5.210	5.629
C75	-3.201	8.951	4.772
C76	-3.763	8.354	3.481
C77	-3.405	6.796	1.604
C78	-4.157	5.486	1.921
C79	-2.197	6.582	0.673
C80	-2.461	5.924	-0.686
C81	-3.197	6.772	-1.743
C82	-5.616	7.393	-1.540
C83	-4.426	3.528	3.355
C84	-5.658	3.773	4.250
C85	-3.526	2.497	4.048
C86	-6.511	4.986	6.195
C87	-7.814	5.772	6.053
C88	-9.262	7.118	4.580
C89	-10.576	6.409	4.186
C90	-8.911	8.216	3.546
C91	-8.554	7.611	2.194
C92	-11.615	4.323	3.401
C93	-12.639	4.052	4.500
C94	-11.134	2.984	2.781
C95	-10.252	3.191	1.571
C96	-10.816	3.348	0.296
C97	-8.855	3.280	1.692
C98	-10.021	3.614	-0.822
C99	-8.045	3.568	0.590
C100	-8.641	3.739	-0.657
C101	8.214	5.700	-3.658
C102	6.972	5.108	-4.306
C103	4.564	4.603	-3.970
C104	3.478	5.679	-4.076
C105	2.071	7.228	-2.797
C106	2.191	8.200	-1.626
C107	3.035	8.742	0.587
C108	3.771	10.045	0.355
C109	3.524	4.347	-8.473
C110	2.000	4.490	-8.575
C111	3.875	3.063	-7.685
C112	5.348	2.666	-7.897
C113	5.764	1.599	-6.910
C114	-0.069	5.257	-7.511
C115	-0.441	6.640	-7.013
C116	-0.820	4.095	-6.814
C117	-0.208	3.705	-5.491
C118	-0.489	4.425	-4.316
C119	0.733	2.661	-5.427
C120	0.181	4.126	-3.125
C121	1.404	2.364	-4.235
C122	1.137	3.104	-3.080
C123	10.877	2.076	0.430
C124	11.416	1.588	1.785
C125	10.143	0.962	-0.335
C126	9.424	1.384	-1.580
C127	9.985	1.873	-2.744
C128	7.811	1.567	-3.040
C129	12.611	-0.092	3.075
C130	13.501	0.923	3.756
C131	5.366	-3.966	-2.559
C132	5.984	-3.512	-1.268
C133	7.084	-2.391	-1.471

C134	8.168	-2.913	-2.460
C135	9.376	-1.970	-2.585
C136	10.546	-2.571	-3.316
C137	7.778	-2.224	-0.083
C138	3.506	2.219	1.093
Fe139	5.013	2.762	-0.130
Fe140	1.508	2.151	1.028
Fe141	3.263	2.475	3.101
Fe142	3.258	4.203	1.108
Fe143	1.197	4.237	2.771
Fe144	4.971	1.049	1.836
Fe145	3.485	0.795	-0.178
H146	0.996	-5.979	-7.469
H147	0.664	-4.456	-7.953
H148	-3.321	-5.767	-8.544
H149	-1.176	-5.172	-9.291
H150	-0.758	-6.844	-8.935
H151	-3.881	-4.894	-5.921
H152	-3.360	-8.255	-7.016
H153	-5.006	-5.775	-6.988
H154	-3.311	-10.223	-5.782
H155	-1.299	-7.970	-5.383
H156	-4.406	-9.483	-4.590
H157	-0.952	-4.812	-1.313
H158	-1.478	-6.016	-3.885
H159	0.683	-7.842	-4.166
H160	-5.142	-6.562	0.076
H161	-3.740	-6.852	-2.439
H162	0.147	-9.160	-3.095
H163	-2.261	-4.385	-2.446
H164	-2.988	-9.213	-1.170
H165	-5.427	-7.801	-1.175
H166	1.393	-5.327	0.433
H167	1.228	-3.582	0.120
H168	2.141	-4.143	1.535
H169	-0.883	-4.488	1.081
H170	-2.443	-11.193	-0.121
H171	-3.755	-3.408	2.168
H172	-3.857	-7.705	3.366
H173	-6.304	-5.765	4.804
H174	-0.248	-2.147	1.605
H175	0.602	-2.668	3.070
H176	3.318	-0.688	9.826
H177	-5.499	-3.111	2.291
H178	-6.942	-4.423	3.825
H179	-4.427	-2.655	3.639
H180	-5.923	-4.084	5.245
H181	-5.006	-5.522	2.684
H182	-3.328	-4.478	5.028
H183	-2.594	-5.472	2.376
H184	-1.166	-2.853	2.948
H185	-2.599	2.382	3.463
H186	-4.071	1.538	4.038
H187	-2.879	2.138	5.860
H188	-2.790	-0.130	7.140
H189	-0.326	2.315	6.407
H190	2.092	1.894	6.709
H191	1.218	-2.053	8.221
H192	-0.819	-6.995	1.571
H193	1.550	-9.093	0.900
H194	0.883	-9.812	2.380
H195	-0.677	-8.797	0.068
H196	-3.462	-10.749	1.269
H197	-1.203	-1.648	7.876
H198	0.908	-5.389	3.387
H199	-5.175	-8.953	5.492
H200	-4.054	-9.751	4.357
H201	-2.169	-8.737	6.087
H202	10.943	-4.250	7.349
H203	4.343	-0.721	-5.737
H204	6.547	-5.491	-2.502
H205	5.472	2.262	-8.912
H206	5.998	3.548	-7.793

H207	3.233	2.229	-8.007
H208	0.304	7.432	-7.263
H209	3.839	4.192	-9.517
H210	0.051	-0.309	-4.572
H211	1.255	-3.002	-5.414
H212	1.918	5.406	-6.715
H213	-0.380	5.257	-8.576
H214	4.034	5.714	-6.997
H215	3.910	-1.815	-4.424
H216	3.661	3.232	-6.619
H217	5.161	5.551	-8.186
H218	-0.983	-1.485	-7.880
H219	-0.481	-1.794	-3.770
H220	6.553	3.016	-5.788
H221	1.759	-2.277	-3.893
H222	-5.277	-1.532	0.091
H223	-2.683	-1.172	-0.722
H224	-6.916	-4.384	-3.265
H225	-4.936	-2.567	-4.570
H226	-8.156	-1.207	-1.833
H227	-13.136	-0.552	0.012
H228	-9.897	-2.566	0.400
H229	-10.762	-1.655	-2.017
H230	-9.687	0.476	-0.066
H231	-13.806	2.466	-2.881
H232	-5.551	0.966	0.095
H233	-6.020	0.931	-1.606
H234	-14.742	1.229	-0.852
H235	-9.993	-0.171	-2.591
H236	-5.888	-1.289	-2.785
H237	-5.165	-4.621	-3.207
H238	-7.526	-1.379	-6.620
H239	-1.591	2.571	-2.404
H240	-6.511	-2.613	-7.391
H241	3.785	1.578	10.400
H242	2.695	1.688	9.187
H243	-2.796	4.957	3.393
H244	-4.811	3.068	2.433
H245	-4.759	5.413	5.095
H246	-4.172	2.611	-2.014
H247	-5.291	3.576	-3.467
H248	-6.236	3.708	-2.190
H249	-3.216	2.570	-5.412
H250	-4.282	2.137	-6.782
H251	-8.083	8.817	3.948
H252	-9.792	8.858	3.424
H253	-6.484	7.802	2.545
H254	-6.954	6.849	1.169
H255	-6.135	9.337	-1.168
H256	-2.794	6.554	-2.743
H257	-10.477	3.717	-1.810
H258	-8.370	3.119	2.658
H259	-7.118	5.969	-1.493
H260	-1.449	5.967	1.199
H261	-2.073	7.195	3.228
H262	-2.981	4.962	-0.557
H263	-4.589	-1.379	-6.855
H264	-2.926	9.996	4.571
H265	-2.304	0.309	-6.543
H266	-1.732	7.568	0.512
H267	-6.968	3.692	0.715
H268	-5.962	2.082	-4.945
H269	-4.027	8.954	5.496
H270	-4.522	9.122	-1.733
H271	-7.653	7.619	-1.468
H272	0.257	-0.713	-7.070
H273	-1.134	-2.758	-5.973
H274	-11.898	3.263	0.166
H275	-3.977	0.557	-4.165
H276	-4.152	7.438	1.117
H277	-3.008	7.838	-1.561
H278	-1.471	5.683	-1.098
H279	-4.919	5.552	-2.034

H280	-6.791	3.974	6.525
H281	-7.434	6.112	4.065
H282	-9.478	7.608	5.541
H283	-5.949	5.463	7.009
H284	-9.573	4.642	3.994
H285	7.924	6.522	-2.987
H286	8.630	4.895	-3.016
H287	10.159	2.872	0.673
H288	10.052	6.358	-4.240
H289	9.283	5.458	-5.372
H290	0.471	4.827	5.982
H291	-1.822	5.451	7.981
H292	-1.127	8.663	5.207
H293	-1.267	4.440	5.765
H294	-1.136	6.853	8.467
H295	3.559	8.197	1.388
H296	-0.057	7.179	6.400
H297	6.576	-6.264	3.848
H298	9.167	-4.700	3.342
H299	3.508	6.992	-0.536
H300	1.945	-1.084	5.207
H301	2.117	7.821	-3.719
H302	2.150	1.567	-4.211
H303	1.051	6.809	-2.748
H304	4.433	-4.722	3.822
H305	3.407	5.686	-2.038
H306	5.100	-3.848	2.439
H307	7.002	-5.356	2.381
H308	7.111	-3.224	3.804
H309	6.473	-4.156	5.173
H310	-0.806	3.235	-7.499
H311	8.658	-7.657	3.337
H312	10.312	-8.282	0.795
H313	1.672	2.903	-2.149
H314	10.171	-9.716	3.324
H315	9.508	-10.084	1.871
H316	4.914	-1.766	3.660
H317	-0.014	4.697	-2.215
H318	0.954	2.076	-6.322
H319	12.249	-2.698	0.548
H320	10.878	0.185	-0.613
H321	9.944	-3.061	1.249
H322	12.588	-2.458	-0.939
H323	4.432	10.063	-0.545
H324	7.795	-1.002	2.271
H325	6.431	-4.354	-0.720
H326	5.901	5.494	-2.598
H327	8.515	-3.891	-2.091
H328	9.029	2.287	-4.616
H329	6.849	1.531	-3.536
H330	11.596	-8.435	1.996
H331	3.216	-0.463	4.196
H332	9.315	-1.729	4.025
H333	7.303	-0.151	3.475
H334	9.732	-3.741	5.236
H335	3.118	-4.374	5.361
H336	11.063	-3.316	-4.976
H337	9.065	-1.055	-3.112
H338	9.747	-1.679	-1.597
H339	7.712	-3.060	-3.450
H340	4.275	3.826	-3.243
H341	-1.216	5.241	-4.349
H342	-1.866	4.415	-6.689
H343	5.200	-3.052	-0.650
H344	10.455	-2.552	3.370
H345	10.894	-4.146	1.842
H346	1.692	-3.417	5.486
H347	11.007	2.139	-2.989
H348	9.417	0.483	0.335
H349	4.687	4.146	-4.954
H350	2.020	8.964	0.950
H351	3.552	-1.415	7.503
H352	3.891	0.245	6.957

H353	12.357	3.468	0.139
H354	12.711	2.009	-0.511
H355	13.231	-0.975	2.857
H356	12.152	-0.207	0.997
H357	14.001	1.649	3.072
H358	11.813	-0.410	3.765
H359	5.966	0.455	8.735
H360	-12.256	4.156	5.543
H361	9.768	-5.563	7.631
H362	7.997	-3.439	7.674
H363	-12.124	4.916	2.625
H364	-10.605	2.398	3.550
H365	-12.034	2.416	2.504
H366	-8.365	4.101	-2.551
H367	0.994	-0.627	0.346
H368	-0.744	0.348	-1.485
Mo369	6.135	0.323	-0.499
N370	0.627	-5.433	-8.253
N371	-3.015	-5.879	-7.580
N372	-3.596	-8.177	-6.030
N373	-1.252	-8.519	-4.525
N374	-1.288	-6.166	-2.894
N375	-3.682	-6.700	-1.430
N376	-3.184	-9.250	-0.166
N377	-0.543	-9.225	0.989
N378	-0.050	-6.757	2.195
N379	-2.426	-5.380	3.381
N380	-3.861	-7.690	4.389
N381	9.683	-9.315	2.520
N382	9.106	-6.759	3.126
N383	4.488	-2.628	4.016
N384	2.606	-3.549	5.064
N385	2.664	-1.288	4.516
N386	9.506	-4.569	5.830
N387	-0.757	-0.928	-7.053
N388	3.629	-1.252	-5.229
N389	-2.939	-0.097	-5.838
N390	-5.454	-1.131	-6.379
N391	-5.844	-3.012	-4.388
N392	-5.897	-1.768	-1.886
N393	-3.532	1.799	-1.806
N394	-1.762	0.572	-1.601
N395	-8.335	-0.923	-0.873
N396	-12.096	1.177	-2.640
N397	-13.835	1.037	-1.270
N398	3.657	1.412	9.399
N399	-0.980	6.027	7.882
N400	-2.054	8.266	5.334
N401	-2.964	7.500	2.805
N402	-4.642	6.522	-1.802
N403	-5.361	8.704	-1.347
N404	-6.885	6.959	-1.393
N405	-3.720	4.751	2.979
N406	-5.639	4.891	5.032
N407	-8.132	6.221	4.804
N408	-7.232	7.333	2.022
N409	-10.485	5.085	3.911
N410	9.142	6.197	-4.677
N411	5.844	5.173	-3.570
N412	3.059	6.168	-2.890
N413	3.003	7.887	-0.587
N414	4.155	5.589	-8.010
N415	1.377	5.114	-7.535
N416	11.951	2.685	-0.381
N417	8.055	1.205	-1.785
N418	8.952	1.980	-3.650
N419	12.086	0.402	1.813
N420	-1.876	2.303	1.070
N421	-0.792	2.039	1.030
O422	-1.262	-5.865	-6.129
O423	-4.298	-6.807	-4.349
O424	-2.425	-9.795	-3.035
O425	-0.234	-7.417	-1.313

	O426	-2.755	-5.533	0.289
	O427	-4.422	-8.449	1.578
	O428	-1.265	-10.814	2.481
	O429	1.946	-7.502	3.057
	O430	-0.890	-5.105	5.050
	O431	-3.968	-6.503	6.322
	O432	-3.434	-9.936	7.151
	O433	10.963	-5.926	2.027
	O434	8.575	-6.670	5.915
	O435	9.391	-3.150	9.135
	O436	-3.070	-1.900	-4.426
	O437	2.013	-0.478	-6.629
	O438	-6.433	0.297	-4.888
	O439	-5.229	2.745	-5.020
	O440	-7.945	-3.498	-5.184
	O441	-5.913	-3.785	-0.813
	O442	-7.418	-0.573	1.190
	O443	-10.973	-1.196	1.464
	O444	5.767	-1.413	9.533
	O445	-2.249	0.651	6.922
	O446	-3.274	6.499	6.098
	O447	-4.903	8.695	3.103
	O448	-5.130	5.156	1.220
	O449	-6.584	2.949	4.269
	O450	-3.245	2.914	5.386
	O451	-8.531	5.955	7.044
	O452	-11.641	7.041	4.137
	O453	-9.420	7.301	1.361
	O454	-13.790	3.722	4.267
	O455	-7.811	4.069	-1.747
	O456	7.037	4.570	-5.440
	O457	3.045	6.071	-5.183
	O458	1.511	9.241	-1.643
	O459	3.691	11.004	1.107
	O460	1.373	4.037	-9.547
	O461	5.504	0.407	-7.052
	O462	6.410	2.019	-5.806
	O463	-1.478	6.912	-6.425
	O464	11.319	2.286	2.811
	O465	13.732	0.918	4.958
	O466	4.484	-3.385	-3.175
	O467	5.863	-5.127	-3.097
	O468	11.676	-2.720	-2.859
	O469	10.241	-2.945	-4.587
	O470	7.638	-1.064	0.466
	O471	8.442	-3.169	0.404
	O472	6.498	-1.214	-1.895
	O473	10.110	-2.271	4.259
	O474	7.802	-0.964	3.263
	O475	-5.304	3.823	-2.502
	O476	12.972	-2.368	-0.043
	O477	10.829	-3.166	1.702
	S478	-0.377	5.573	3.817
	S479	1.078	4.381	0.538
	S480	4.607	1.495	-1.951
	S481	1.056	1.978	3.298
	S482	1.336	0.331	-0.568
	S483	4.788	4.979	-0.336
	S484	4.506	-0.885	0.810
	S485	3.385	4.769	3.257
	S486	6.808	2.024	1.025
	S487	4.794	1.128	4.033
B 47(1) dissociated	bm22b2n2xd47te.car_3			
	C1	-1.675256508	-5.811635529	-7.284981272
	C2	-0.745394043	-5.792864676	-8.503609565
	C3	-4.009647105	-5.793153206	-6.509294047
	C4	-3.974659300	-6.967796081	-5.533271754
	C5	-3.481554423	-9.332957540	-5.173939481
	C6	-2.350929167	-9.231252579	-4.144090672
	C7	-0.170942716	-8.258270063	-3.595855651
	C8	-0.551740400	-7.256484026	-2.503397869
	C9	-1.765454137	-5.226476813	-1.912899522

C10	-2.757526856	-5.842452022	-0.915436905
C11	-4.649668080	-7.320562878	-0.550796499
C12	-4.057087970	-8.378120245	0.390399524
C13	-2.674074175	-10.384028466	0.594605922
C14	-1.426933540	-10.139682856	1.454198388
C15	0.733418850	-8.982793036	1.648856873
C16	0.919506686	-7.648555481	2.375225593
C17	-0.019563435	-5.396488624	2.802674947
C18	-1.145461592	-5.241919506	3.841399566
C19	0.002178896	-4.264398289	1.739161911
C20	-0.151545824	-2.880385418	2.377271480
C21	1.279536880	-4.344921702	0.896684715
C22	-3.574599854	-5.216077386	4.260652657
C23	-3.805173509	-6.506795490	5.071910625
C24	-4.829580683	-4.776512972	3.470860836
C25	-6.075833611	-4.771430602	4.364088607
C26	-4.620853801	-3.394297100	2.840116184
C27	-4.111128742	-8.914597539	5.063394259
C28	-3.153205043	-9.173701471	6.208747796
C29	10.510692059	-8.284740987	1.895152860
C30	10.222048946	-6.863711594	2.384002131
C31	8.618764782	-5.541862748	3.776311373
C32	8.895118816	-5.645726478	5.290238077
C33	7.120110626	-5.373267646	3.475189285
C34	6.497351269	-4.109452176	4.075038820
C35	5.098865094	-3.876084478	3.497680190
C36	3.260954718	-2.508473493	4.505416363
C37	9.888021998	-4.546387180	7.237928270
C38	9.020088235	-3.641461598	8.085611610
C39	-1.056444465	-1.649697999	-5.805368790
C40	-2.441106128	-1.243349053	-5.273392395
C41	-0.023588680	-1.387500100	-4.687570291
C42	1.365047305	-2.024463349	-4.887068165
C43	2.370103748	-1.178056776	-5.667024170
C44	-4.079642915	0.580910879	-5.260149942
C45	-5.424319929	-0.100719459	-5.520259764
C46	-4.143681183	2.061510786	-5.689393135
C47	-6.617305406	-1.996002269	-6.489598571
C48	-6.871913104	-2.896853644	-5.271610624
C49	-5.953831434	-3.860734860	-3.201837897
C50	-5.890418899	-3.145118196	-1.854542503
C51	-5.859628097	-0.999948327	-0.648890955
C52	-7.250829566	-0.832307900	0.005315752
C53	-5.336631649	0.425564150	-0.875837504
C54	-3.909885251	0.568086273	-1.294473065
C55	-2.787179601	-0.214783416	-1.161905917
C56	-2.152791308	1.716527181	-2.059192908
C57	-9.651689088	-0.519427548	-0.465642260
C58	-10.182885747	-1.465242853	0.605139795
C59	-10.544420307	-0.591784361	-1.733064355
C60	-11.828860724	0.180590977	-1.675439113
C61	-12.903554560	0.072688927	-0.812711555
C62	-13.276967780	1.656837035	-2.315521660
C63	3.842651757	-0.003604286	9.110262906
C64	5.321690099	-0.340177327	9.128105257
C65	3.335527670	-0.341383124	7.682546395
C66	1.855548720	-0.097028298	7.503122257
C67	0.906540936	-1.086172154	7.825112046
C68	1.383015007	1.127307561	6.998827580
C69	-0.463294507	-0.866271867	7.643618115
C70	0.019643769	1.364431735	6.822979034
C71	-0.904087610	0.365188694	7.145283814
C72	-0.852576875	6.409066589	6.431394873
C73	-2.162688958	7.035259935	5.933698843
C74	-0.520287294	5.157508244	5.604606110
C75	-3.203668151	8.937658770	4.774588335
C76	-3.770351266	8.354913392	3.479077257
C77	-3.421479987	6.786545676	1.606034247
C78	-4.170401087	5.476662029	1.937283520
C79	-2.213827945	6.575430574	0.671646489
C80	-2.464865522	5.919253735	-0.689891007
C81	-3.193316224	6.760730049	-1.754083954
C82	-5.609974163	7.378486081	-1.518853077

C83	-4.443631877	3.538366456	3.395835323
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C85	-3.541657589	2.520186304	4.107963567
C86	-6.526624517	5.005437207	6.226618079
C87	-7.819395880	5.804152549	6.076100584
C88	-9.261933266	7.126644523	4.574812793
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C92	-11.587226361	4.313583186	3.374849194
C93	-12.615965673	4.052283841	4.470297778
C94	-11.097652284	2.973740764	2.762913482
C95	-10.211412111	3.180638626	1.554493822
C96	-10.779463065	3.354868136	0.283487802
C97	-8.813304709	3.253048750	1.670237267
C98	-9.987347055	3.624646897	-0.835853341
C99	-8.005683671	3.545561654	0.566752626
C100	-8.605365628	3.733168005	-0.676124561
C101	8.229590389	5.711171783	-3.685729529
C102	6.981204036	5.115318752	-4.313999050
C103	4.579454597	4.610596177	-3.956082259
C104	3.493284756	5.687382726	-4.063520054
C105	2.086090914	7.233213097	-2.778929337
C106	2.233487989	8.224362974	-1.626891878
C107	3.067154583	8.765612531	0.587233690
C108	3.713880579	10.104335430	0.297171944
C109	3.528331555	4.364286616	-8.473117925
C110	2.003023568	4.503118985	-8.568356436
C111	3.883058955	3.079845889	-7.688725611
C112	5.358487894	2.689296976	-7.898426257
C113	5.773403304	1.613436610	-6.919414721
C114	-0.066044877	5.263788260	-7.501587834
C115	-0.443669064	6.643934687	-7.001721970
C116	-0.812222839	4.097136253	-6.810385460
C117	-0.195795426	3.697152171	-5.492180867
C118	-0.463139688	4.416953886	-4.313558878
C119	0.734659905	2.643883493	-5.437215203
C120	0.206076987	4.102999157	-3.125382345
C121	1.406143111	2.333737264	-4.248545383
C122	1.149680128	3.069518082	-3.088609149
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C124	11.406113544	1.562959145	1.786115314
C125	10.079032916	0.942648851	-0.299706562
C126	9.361989898	1.365532077	-1.546251213
C127	9.915682003	1.856443419	-2.713148153
C128	7.743540367	1.537604019	-3.003053029
C129	12.641705673	-0.101935551	3.060432228
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C137	7.733602681	-2.241591855	-0.067305690
C138	3.542348889	2.242534852	1.094430001
Fe139	5.022060648	2.786219324	-0.111734055
Fe140	1.629654285	2.136564867	0.995664790
Fe141	3.146509481	2.438135851	3.083965085
Fe142	3.184865029	4.209596278	1.110957390
Fe143	1.056120277	4.135685650	2.695993794
Fe144	4.955248222	1.049351969	1.877059292
Fe145	3.501675588	0.791487347	-0.161260878
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H147	0.692907622	-4.454360602	-7.936937439
H148	-3.312908042	-5.747724222	-8.530583375
H149	-1.167802082	-5.123054804	-9.269192971
H150	-0.774685649	-6.806600547	-8.940705101
H151	-3.887356108	-4.883994767	-5.903575276
H152	-3.363277249	-8.238500225	-7.023566511
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H157	-0.932832896	-4.823382380	-1.321529400
H158	-1.466038481	-6.025834097	-3.891945349
H159	0.685528641	-7.873957459	-4.165455704
H160	-5.133861483	-6.561279999	0.077096743
H161	-3.738918920	-6.842545908	-2.439729632
H162	0.133253616	-9.184021524	-3.093388763
H163	-2.248003778	-4.395497931	-2.447828082
H164	-2.984265664	-9.217763571	-1.170119800
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H166	1.394239944	-5.331742182	0.424093048
H167	1.263091729	-3.585862952	0.100224143
H168	2.170811845	-4.155002059	1.514540706
H169	-0.862268162	-4.433491565	1.077202813
H170	-2.436812505	-11.194230885	-0.109958797
H171	-3.758194074	-3.375096854	2.158143139
H172	-3.819248011	-7.686343921	3.351463445
H173	-6.293147517	-5.765121781	4.783237613
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H176	3.335076825	-0.682765788	9.822494600
H177	-5.511533506	-3.104830741	2.265150332
H178	-6.951975185	-4.448156744	3.781676674
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H180	-5.948592258	-4.070019180	5.204677709
H181	-4.991406013	-5.509646661	2.659639331
H182	-3.340659275	-4.451723247	5.015598172
H183	-2.585092720	-5.447602394	2.367380575
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H197	-1.183585612	-1.654180972	7.879941359
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H206	6.005266419	3.572074570	-7.784088198
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H234	-14.719933499	1.201636807	-0.816879100
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H237	-5.175957392	-4.638379228	-3.208012275
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H239	-1.526053314	2.513548717	-2.453332844
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H241	3.798330774	1.589837127	10.398317593
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H248	-6.196679448	3.689879632	-2.194380958
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H250	-4.251847430	2.128767505	-6.784837601
H251	-8.084143667	8.823640364	3.933813364
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H257	-10.446480023	3.743969444	-1.820887220
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H262	-2.978377677	4.954726626	-0.565363188
H263	-4.580224234	-1.394826362	-6.839790069
H264	-2.932088759	9.985499015	4.586887271
H265	-2.301430006	0.302861412	-6.536400498
H266	-1.748999188	7.563483672	0.515144816
H267	-6.926398485	3.656117009	0.686559869
H268	-5.958529788	2.075251942	-4.962831079
H269	-4.025060103	8.929607212	5.503630619
H270	-4.509317066	9.109973288	-1.664452017
H271	-7.647302029	7.600569968	-1.418775387
H272	0.266055295	-0.681437973	-7.047255165
H273	-1.112301108	-2.744364569	-5.958036821
H274	-11.862577152	3.279152577	0.159030776
H275	-3.984115008	0.550341874	-4.162155313
H276	-4.171534601	7.424913401	1.118558082
H277	-3.000103302	7.827445194	-1.586180468
H278	-1.469084976	5.683330591	-1.091169873
H279	-4.914532584	5.545005600	-2.048381857
H280	-6.819896567	3.995802319	6.552346050
H281	-7.423202440	6.124484430	4.088905902
H282	-9.494777246	7.624066510	5.527745304
H283	-5.960997643	5.473834603	7.043210136
H284	-9.547442055	4.640043767	3.969015855
H285	7.948966761	6.541618084	-3.020482383
H286	8.651830554	4.913367458	-3.040173820
H287	10.160779873	2.863951053	0.679339546
H288	10.061456285	6.363037901	-4.300091271
H289	9.276307032	5.446866934	-5.410221265
H290	0.461449506	4.781792701	5.919406306
H291	-1.775838736	5.463132674	7.981389922
H292	-1.124378798	8.644779423	5.184434628
H293	-1.287400291	4.393962704	5.798596025
H294	-1.064655297	6.868463339	8.420033500
H295	3.677778868	8.265353411	1.356179588
H296	-0.032872846	7.135971300	6.315889031
H297	6.584911137	-6.268813212	3.831981935
H298	9.173923102	-4.696313827	3.352720386
H299	3.504661143	6.988815260	-0.509534097
H300	1.917294384	-1.132447013	5.165692200
H301	2.106539429	7.806054471	-3.714739003

H302	2.142721380	1.528548448	-4.231341310
H303	1.069823063	6.811217156	-2.689701572
H304	4.431477614	-4.717459379	3.727789609
H305	3.420980670	5.688953289	-2.023066858
H306	5.158666034	-3.814670558	2.397663130
H307	7.020590360	-5.345699955	2.377849016
H308	7.116736622	-3.229695569	3.842076277
H309	6.433766503	-4.183590278	5.173056101
H310	-0.802674454	3.239770329	-7.499131923
H311	8.658545435	-7.652133759	3.341904021
H312	10.298098786	-8.283786061	0.814461222
H313	1.679716708	2.852147651	-2.160539162
H314	10.183668127	-9.700825302	3.356098141
H315	9.512133148	-10.084382544	1.910631381
H316	4.903391785	-1.761918807	3.623970661
H317	0.017072175	4.666256773	-2.210007155
H318	0.945037875	2.057876282	-6.335278564
H319	12.265968525	-2.714055000	0.544364973
H320	10.782698676	0.131962813	-0.563796091
H321	9.945200842	-3.085993599	1.230127232
H322	12.601360886	-2.447374562	-0.935962617
H323	4.384140387	10.118658781	-0.595462290
H324	7.774003579	-1.024733964	2.298482286
H325	6.369032255	-4.363965768	-0.711992310
H326	5.929519515	5.517788144	-2.602136673
H327	8.430158313	-3.889568903	-2.133345345
H328	8.949321025	2.259117891	-4.583129774
H329	6.778342004	1.498213289	-3.492860685
H330	11.597827751	-8.437246393	1.998224660
H331	3.180182213	-0.482137159	4.165809568
H332	9.334176796	-1.743060993	4.009989283
H333	7.367227129	-0.130760790	3.501725715
H334	9.748068720	-3.747161663	5.238940305
H335	3.141858764	-4.395666840	5.315011457
H336	10.993037889	-3.308165469	-4.944436438
H337	9.002041559	-1.031260228	-3.071357577
H338	9.665462447	-1.686169350	-1.563490754
H339	7.620943492	-2.999958307	-3.451025692
H340	4.293830590	3.834945581	-3.227810648
H341	-1.179022488	5.242416718	-4.340139523
H342	-1.858538025	4.414446743	-6.678822301
H343	5.142717750	-3.059431939	-0.612937938
H344	10.469281819	-2.567028117	3.347225575
H345	10.895073786	-4.169806897	1.828577481
H346	1.698398892	-3.466678561	5.429364432
H347	10.935065408	2.128761081	-2.959997206
H348	9.344283587	0.503768845	0.387400527
H349	4.699072719	4.152600870	-4.939945727
H350	2.066043184	8.934157696	1.014344583
H351	3.571947889	-1.400268615	7.494168966
H352	3.900288061	0.263372317	6.954058592
H353	12.366796703	3.393759843	0.095869656
H354	12.664807248	1.920679833	-0.549243201
H355	13.290843461	-0.961904435	2.830762574
H356	12.180129949	-0.210192219	0.983947281
H357	13.976116468	1.686981991	3.092334977
H358	11.853339660	-0.453436677	3.745475459
H359	5.981584269	0.489797249	8.778776573
H360	-12.237519948	4.172982494	5.512507572
H361	9.763355893	-5.569283267	7.632849098
H362	8.004446064	-3.430636086	7.672579885
H363	-12.095113288	4.900507540	2.592206476
H364	-10.570532636	2.395412807	3.538522420
H365	-11.992161580	2.399407411	2.482316253
H366	-8.326114802	4.086198887	-2.572588377
H367	0.991913219	-0.602274838	0.398458549
H368	-0.702653121	0.302419697	-1.506594378
Mo369	6.115636075	0.320455993	-0.459887706
N370	0.637364283	-5.427975017	-8.245847464
N371	-3.008655975	-5.854196216	-7.565389878
N372	-3.595448872	-8.167477199	-6.035736404
N373	-1.253325459	-8.532123506	-4.528944884
N374	-1.277705666	-6.179491874	-2.900580514

N375	-3.672639735	-6.698645736	-1.429316290
N376	-3.176119317	-9.250543850	-0.165165039
N377	-0.549486374	-9.199148258	1.000994457
N378	-0.056600856	-6.720871877	2.191784212
N379	-2.420437586	-5.338178756	3.370055918
N380	-3.825969647	-7.671000635	4.373626270
N381	9.689785976	-9.309675404	2.551253566
N382	9.111688098	-6.754562247	3.135990682
N383	4.486916993	-2.630032254	3.976262633
N384	2.614388124	-3.585510925	5.006859541
N385	2.642777979	-1.319180753	4.477451046
N386	9.512974221	-4.569210181	5.837158971
N387	-0.744923638	-0.910233242	-7.034156903
N388	3.656059870	-1.288866723	-5.282137178
N389	-2.935613801	-0.102894636	-5.828709647
N390	-5.448974934	-1.141716233	-6.373316591
N391	-5.844902896	-3.017255430	-4.379260307
N392	-5.880273936	-1.775637575	-1.880301854
N393	-3.479991537	1.758662184	-1.865410671
N394	-1.720642468	0.518434257	-1.649206240
N395	-8.301997706	-0.917512716	-0.848513740
N396	-12.075660340	1.174150230	-2.609982215
N397	-13.810068690	1.021484425	-1.233724077
N398	3.667262699	1.421281675	9.398292789
N399	-0.930935836	6.028813520	7.849574005
N400	-2.051088846	8.249122228	5.322608637
N401	-2.976312657	7.499313018	2.799972024
N402	-4.639527383	6.514487798	-1.814552867
N403	-5.353766984	8.684530187	-1.298127312
N404	-6.877043944	6.940317683	-1.368116275
N405	-3.745579723	4.763548015	3.013554449
N406	-5.655843552	4.903693625	5.063321180
N407	-8.125977958	6.244458778	4.820911470
N408	-7.224459722	7.318603208	2.024599015
N409	-10.460879777	5.079683131	3.886450754
N410	9.145522886	6.194571834	-4.722403978
N411	5.862118602	5.182371602	-3.567200463
N412	3.075487115	6.174281952	-2.876235703
N413	3.024204148	7.897066902	-0.576188508
N414	4.158278871	5.608156384	-8.010620253
N415	1.380362861	5.127979591	-7.528140187
N416	11.927214626	2.617418573	-0.406148764
N417	7.994037439	1.180074532	-1.748005033
N418	8.879347173	1.955621435	-3.616072799
N419	12.101002031	0.391071310	1.804266122
N420	-2.258015539	2.660862502	0.895513577
N421	-1.865119641	1.677012109	1.225841254
O422	-1.251705420	-5.840193677	-6.114319603
O423	-4.296349029	-6.809808504	-4.343743384
O424	-2.446478381	-9.792732621	-3.041098148
O425	-0.226956863	-7.429912778	-1.318281967
O426	-2.716104039	-5.562836629	0.293548181
O427	-4.409790618	-8.445646037	1.580106076
O428	-1.244842757	-10.817993646	2.473994348
O429	1.933109607	-7.467436216	3.065442656
O430	-0.886266848	-5.037767223	5.037613819
O431	-3.965470227	-6.482564656	6.303693345
O432	-3.423891888	-9.898482334	7.154165752
O433	10.983007831	-5.928991359	2.053031161
O434	8.569797894	-6.665511601	5.923152965
O435	9.379987526	-3.180433336	9.156810582
O436	-3.051688662	-1.898486888	-4.404981276
O437	2.024234614	-0.439451567	-6.616612239
O438	-6.437169951	0.305336804	-4.906522344
O439	-5.228683036	2.741212994	-5.040976448
O440	-7.960874147	-3.469812571	-5.154049952
O441	-5.879823915	-3.793517142	-0.805057021
O442	-7.360077972	-0.529939072	1.197160874
O443	-10.912154013	-1.128325845	1.521122523
O444	5.778892518	-1.422256481	9.467275217
O445	-2.240406528	0.642059079	6.937863374
O446	-3.263662271	6.477579351	6.093937191
O447	-4.907049903	8.708078354	3.102686292

O448	-5.136942516	5.134723691	1.230952407
O449	-6.610813895	2.965476384	4.299501219
O450	-3.326617656	2.914464141	5.464971012
O451	-8.540594420	6.002165823	7.062255613
O452	-11.636748189	7.020380337	4.126827052
O453	-9.407785923	7.301367799	1.345344506
O454	-13.764714311	3.714910280	4.236001577
O455	-7.775609729	4.062115277	-1.765762841
O456	7.032216196	4.574253930	-5.447429320
O457	3.061245003	6.080667273	-5.169633228
O458	1.590032901	9.288575692	-1.659395150
O459	3.562194177	11.093076181	0.997658482
O460	1.374742810	4.043521715	-9.536719704
O461	5.516674514	0.422628481	-7.073413064
O462	6.416839906	2.025143652	-5.809680084
O463	-1.479503037	6.909976806	-6.409596785
O464	11.294137857	2.250147669	2.818146060
O465	13.735099423	0.901776248	4.959648707
O466	4.392585086	-3.360467425	-3.127024529
O467	5.786853320	-5.092460273	-3.105337335
O468	11.614541322	-2.667187263	-2.841522709
O469	10.168299077	-2.947444779	-4.554189862
O470	7.600152693	-1.086860046	0.494649520
O471	8.407913935	-3.190671132	0.398759831
O472	6.433647412	-1.213514660	-1.856172584
O473	10.131780788	-2.283823330	4.237608157
O474	7.794200601	-0.981957740	3.289265942
O475	-5.268174923	3.808089717	-2.517523555
O476	12.991896116	-2.378473045	-0.040798259
O477	10.831772578	-3.190444437	1.676786296
S478	-0.491877980	5.472630965	3.780691786
S479	0.987643029	4.261517915	0.461199015
S480	4.610438152	1.505649248	-1.920230644
S481	0.934928239	1.864974592	3.101372730
S482	1.314972836	0.394770958	-0.481031834
S483	4.745991830	4.999978125	-0.295730529
S484	4.478988088	-0.884858558	0.848916834
S485	3.203316054	4.723616591	3.290217671
S486	6.799733118	2.026665892	1.070069107
S487	4.694364852	1.160161009	4.063454502

Structure B 35 (1)

B 35 (1)		bm22b2n2xd35tc.car_3	
associated		C1	-1.678937629 -5.823096998 -7.293422277
Fe(139)	0.539 -2.252	C2	-0.749448952 -5.803272067 -8.510909246
Fe(140)	0.441 -1.695	C3	-4.010769255 -5.797623770 -6.515558788
Fe(141)	0.547 -2.557	C4	-3.975173824 -6.969447318 -5.536141637
Fe(142)	0.588 2.946	C5	-3.481523566 -9.335190146 -5.170161938
Fe(143)	0.564 2.959	C6	-2.350085781 -9.231661329 -4.142085222
Fe(144)	0.506 2.307	C7	-0.171073193 -8.254505444 -3.595853885
Fe(145)	0.469 -0.264	C8	-0.552913991 -7.252532849 -2.502555742
		C9	-1.768581279 -5.224076023 -1.912078465
		C10	-2.761516016 -5.841416123 -0.915911206
		C11	-4.651551494 -7.321479778 -0.550926936
		C12	-4.058916640 -8.378447796 0.389788005
		C13	-2.676367358 -10.385983352 0.593614812
		C14	-1.427823308 -10.144449876 1.451938480
		C15	0.735294705 -8.993132848 1.644744468
		C16	0.922291012 -7.660273532 2.374465122
		C17	-0.023636283 -5.409621227 2.807951168
		C18	-1.150643579 -5.259612319 3.846487599
		C19	-0.005938392 -4.278319233 1.744983413
		C20	-0.166381620 -2.893985895 2.383118553
		C21	1.272470720 -4.352514632 0.903665174
		C22	-3.579372598 -5.228570452 4.265161123
		C23	-3.814953800 -6.517937652 5.076306856
		C24	-4.834760966 -4.783205693 3.477124770
		C25	-6.079160964 -4.773278508 4.371282102
		C26	-4.617727167 -3.402273525 2.846234942
		C27	-4.128540749 -8.924184344 5.071063882
		C28	-3.164299361 -9.184996292 6.211026570
		C29	10.500187020 -8.268114518 1.880239476

C30	10.211250708	-6.849409583	2.374383387
C31	8.609662318	-5.531481254	3.773300990
C32	8.887145644	-5.632959682	5.286683088
C33	7.110087151	-5.365953458	3.475852484
C34	6.486772043	-4.099888994	4.071899260
C35	5.086958743	-3.876984934	3.498243934
C36	3.246415345	-2.520136738	4.513769725
C37	9.876684801	-4.526681462	7.233269991
C38	9.007518575	-3.622710985	8.082737229
C39	-1.063615234	-1.657888434	-5.819563924
C40	-2.446295882	-1.249807563	-5.285683644
C41	-0.033562117	-1.395122538	-4.698563463
C42	1.357182520	-2.028676864	-4.891194665
C43	2.362179551	-1.178825618	-5.667062444
C44	-4.078535313	0.578645273	-5.261749303
C45	-5.423579440	-0.104011121	-5.517851789
C46	-4.145792174	2.059686591	-5.693091934
C47	-6.619666673	-1.995349436	-6.490982755
C48	-6.873243682	-2.896995964	-5.273591333
C49	-5.954730641	-3.854006637	-3.201981143
C50	-5.899264172	-3.134735998	-1.855620794
C51	-5.884993295	-0.993237268	-0.646364534
C52	-7.282128865	-0.830967555	-0.001172216
C53	-5.361154615	0.434516449	-0.859738821
C54	-3.926217366	0.583647079	-1.249555760
C55	-2.808683050	-0.206571328	-1.125034915
C56	-2.163016612	1.729436744	-2.002871887
C57	-9.682613670	-0.537649129	-0.477228131
C58	-10.212986625	-1.490319096	0.588775174
C59	-10.571416999	-0.604736750	-1.745552342
C60	-11.852786914	0.172347903	-1.687260818
C61	-12.926839659	0.070881124	-0.823702386
C62	-13.291511203	1.659673003	-2.324496880
C63	3.841579688	-0.003454808	9.108861260
C64	5.321422938	-0.340283372	9.127397999
C65	3.331173082	-0.342550100	7.682091227
C66	1.851405022	-0.096499287	7.505360505
C67	0.901620149	-1.085636091	7.824851307
C68	1.378260716	1.129505767	7.005473305
C69	-0.468580019	-0.865196192	7.644780418
C70	0.014447916	1.368903656	6.833553614
C71	-0.909633716	0.367831268	7.149701037
C72	-0.860870989	6.427983667	6.441763370
C73	-2.169886069	7.050031512	5.941114487
C74	-0.508402357	5.193607869	5.597688434
C75	-3.208339088	8.944837713	4.768233914
C76	-3.771814657	8.354448538	3.475207460
C77	-3.417172753	6.790781043	1.599433639
C78	-4.167340641	5.480089252	1.918594746
C79	-2.207543004	6.574993962	0.670543395
C80	-2.462946814	5.913189520	-0.688111344
C81	-3.194326230	6.754661872	-1.752790087
C82	-5.609744440	7.377636669	-1.524077526
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N415	1.375244865	5.133516590	-7.541499249
N416	11.923247816	2.630713032	-0.409511984
N417	7.987425544	1.187549026	-1.751212764
N418	8.871164321	1.957511181	-3.622714073
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O423	-4.294475684	-6.808525942	-4.346388165
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O429	1.937215660	-7.479437363	3.062809419
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O455	-7.804323392	4.063566644	-1.757956516
O456	7.031288146	4.570343788	-5.437537050
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	O470	7.620385547	-1.073396613	0.474860214
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	O472	6.433251803	-1.210011169	-1.863227256
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	O477	10.811348093	-3.167911497	1.681899837
	S478	-0.384248164	5.558623815	3.783348433
	S479	1.115781118	4.438406453	0.588250142
	S480	4.601486278	1.520449553	-1.892518362
	S481	1.138469611	1.967749331	3.341183398
	S482	1.387674011	0.289214858	-0.585201050
	S483	4.880453323	5.008986084	-0.289961713
	S484	4.506986748	-0.905749303	0.856243219
	S485	3.445292769	4.709883914	3.392469359
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	C4	-3.976710882	-6.972697244	-5.536647709
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	C6	-2.343428275	-9.228878142	-4.137440176
	C7	-0.169411277	-8.238868108	-3.593900105
	C8	-0.557173693	-7.241726697	-2.498720953
	C9	-1.779663789	-5.216847663	-1.909149405
	C10	-2.776040642	-5.832806690	-0.915871494
	C11	-4.658376549	-7.322265252	-0.551369593
	C12	-4.065329200	-8.379521403	0.389002107
	C13	-2.680504513	-10.386878005	0.589299940
	C14	-1.432947884	-10.146633511	1.450447416
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	C16	0.927355352	-7.677101627	2.371574980
	C17	-0.024565789	-5.426408757	2.809573488
	C18	-1.149720181	-5.286689920	3.851136308
	C19	-0.022081252	-4.294312175	1.748105551
	C20	-0.209828385	-2.914675382	2.386628042
	C21	1.259591310	-4.347178756	0.910176484
	C22	-3.576145363	-5.238515406	4.274142571
	C23	-3.815366713	-6.524759262	5.086397158
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	C27	-4.145392409	-8.926028183	5.079581577
	C28	-3.171436811	-9.200568968	6.208213524
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	C30	10.212063303	-6.863115110	2.368533007
	C31	8.613065565	-5.544282407	3.769442625
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C80	-2.461239563	5.923699154	-0.686412611
C81	-3.196790908	6.769982433	-1.743850929
C82	-5.614506922	7.390719858	-1.537050789
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C116	-0.818805557	4.095724360	-6.813992115
C117	-0.204697157	3.705179132	-5.491467907
C118	-0.484445972	4.424992104	-4.315825887
C119	0.733183504	2.659393270	-5.429005266
C120	0.182754975	4.120843292	-3.123519412
C121	1.402380112	2.357891187	-4.236576172
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H149	-1.176437054	-5.164806643	-9.287996803
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H151	-3.883052839	-4.892935725	-5.920359343
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H161	-3.740913227	-6.849034382	-2.439850621
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H202	10.940447514	-4.251757340	7.348900531
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H206	5.999450352	3.551342431	-7.792168757
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Fe(141) 0.532 -2.399	C4	-3.974321628	-6.966219564	-5.533486135
Fe(142) 0.583 2.934	C5	-3.482485571	-9.332655863	-5.176592685
Fe(143) 0.563 2.973	C6	-2.352357405	-9.232371784	-4.146617748
Fe(144) 0.511 2.259	C7	-0.169888302	-8.262262884	-3.598798356
Fe(145) 0.442 0.230	C8	-0.549229155	-7.259453031	-2.505290844
	C9	-1.760985202	-5.228624111	-1.913306525
	C10	-2.753625934	-5.844124396	-0.916922860
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	C13	-2.670785982	-10.385065037	0.594927991
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	C16	0.922079471	-7.643665250	2.377200567
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	C18	-1.145527710	-5.236189912	3.841055485
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	C23	-3.802290005	-6.501837867	5.069028391
	C24	-4.829301186	-4.777024062	3.465667303
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	C28	-3.151126109	-9.166279727	6.210980922
	C29	10.508670467	-8.283580480	1.896971581
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	C32	8.885744723	-5.638136110	5.290703775
	C33	7.114308362	-5.367539203	3.469893547
	C34	6.484041049	-4.107867521	4.071195226
	C35	5.096636273	-3.870453033	3.473225229
	C36	3.248133267	-2.541187420	4.507337449
	C37	9.884284899	-4.542998376	7.239822652
	C38	9.016354598	-3.637418110	8.089040380
	C39	-1.054429798	-1.649707040	-5.805662521
	C40	-2.437748874	-1.243526726	-5.275210265
	C41	-0.020533909	-1.386964705	-4.687594144
	C42	1.367526132	-2.023928461	-4.886907004
	C43	2.372234744	-1.179971086	-5.669786140
	C44	-4.076946714	0.580540012	-5.265720609
	C45	-5.421382098	-0.103770374	-5.526070314
	C46	-4.141005887	2.059564961	-5.697976596
	C47	-6.613331388	-2.003430249	-6.490340776
	C48	-6.869204442	-2.900373173	-5.270823694
	C49	-5.955028395	-3.863802769	-3.200247531
	C50	-5.892864781	-3.146336033	-1.853858229
	C51	-5.858274369	-0.999051858	-0.652124347
	C52	-7.246556540	-0.824952784	0.004068253
	C53	-5.330285290	0.424684517	-0.884139234
	C54	-3.898342563	0.565157311	-1.291609674
	C55	-2.775433852	-0.212893071	-1.135549892
	C56	-2.138405505	1.700326921	-2.068855766
	C57	-9.647620304	-0.517014233	-0.460932646
	C58	-10.178107719	-1.460969453	0.613596736
	C59	-10.544817093	-0.594066806	-1.725291205
	C60	-11.830460687	0.175533002	-1.665896004
	C61	-12.904728721	0.069289171	-0.802919325
	C62	-13.277572088	1.652853198	-2.306505889
	C63	3.847790263	0.000805598	9.105150257
	C64	5.327886199	-0.337499908	9.125077342
	C65	3.338524671	-0.335690095	7.678044528
	C66	1.858497573	-0.093071895	7.500730733
	C67	0.910158637	-1.081851302	7.825849091
	C68	1.383246389	1.130711487	6.997759939
	C69	-0.460679444	-0.862633344	7.648763873
	C70	0.019104637	1.367082399	6.826292738
	C71	-0.903769831	0.368804229	7.153003756
	C72	-0.856493286	6.406688233	6.415561580
	C73	-2.167415035	7.041477843	5.928357473

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C76	-3.774364927	8.356324519	3.472897414
C77	-3.429052517	6.779460262	1.604538596
C78	-4.185294761	5.474796041	1.948172857
C79	-2.220665011	6.563089533	0.672881747
C80	-2.471687608	5.904260687	-0.686554362
C81	-3.194278768	6.747417850	-1.754318515
C82	-5.612075767	7.369907729	-1.516733495
C83	-4.453222367	3.544369128	3.423065234
C84	-5.688693906	3.797997974	4.310481038
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C86	-6.540012678	5.025748404	6.246911766
C87	-7.835912740	5.817551567	6.083502875
C88	-9.271438120	7.133388547	4.571700268
C89	-10.571975766	6.406114344	4.167598588
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C93	-12.613516005	4.049077413	4.464304641
C94	-11.091363303	2.975026225	2.759781824
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C99	-8.002956989	3.535586360	0.563493313
C100	-8.602247958	3.722689984	-0.679548466
C101	8.238128277	5.715117229	-3.687634050
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C107	3.095758184	8.772519186	0.584208713
C108	3.709354966	10.126383026	0.289767350
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C115	-0.445932281	6.650213448	-7.005654169
C116	-0.810301857	4.102636387	-6.808809856
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C118	-0.451676504	4.416002331	-4.311289304
C119	0.736265531	2.643185210	-5.443871514
C120	0.216420966	4.094459266	-3.123994414
C121	1.407116737	2.324153796	-4.256775020
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C126	9.362189255	1.366266711	-1.546763981
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C132	5.908650182	-3.508922419	-1.245932480
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Fe140	1.632317183	2.155432180	0.981492246
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Fe144	4.973838317	1.051070037	1.857467463
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H334	9.742806768	-3.741378656	5.243729525
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H336	10.978964500	-3.310153183	-4.946127648
H337	8.988775504	-1.036655998	-3.064828082
H338	9.657732906	-1.694813584	-1.560695808
H339	7.613181477	-3.011316957	-3.449096346
H340	4.298224760	3.836472403	-3.217404625
H341	-1.164934907	5.243637347	-4.332502700
H342	-1.855526882	4.423128106	-6.675352212
H343	5.135481876	-3.054217335	-0.610867828
H344	10.467411685	-2.566513466	3.342768037
H345	10.892044993	-4.173273167	1.823080835
H346	1.706138437	-3.538191168	5.433697981
H347	10.938115075	2.116936029	-2.961229894
H348	9.340510275	0.506856128	0.387340414
H349	4.700642959	4.149282988	-4.932104938
H350	2.098300070	8.920304220	1.026135418
H351	3.574772610	-1.393905546	7.489139497
H352	3.900325973	0.270227963	6.949207568
H353	12.372845601	3.387989428	0.086168338
H354	12.665107065	1.910628669	-0.552069305
H355	13.290857996	-0.965239783	2.830963523
H356	12.181225756	-0.211844724	0.982390074
H357	13.969514313	1.685521214	3.091114877
H358	11.853842077	-0.457953680	3.743847784
H359	5.989859055	0.489791742	8.769913464
H360	-12.238806677	4.167343268	5.509034375
H361	9.765929019	-5.563533232	7.636706137
H362	8.001331131	-3.425014006	7.674015184
H363	-12.091808003	4.899136524	2.586093569
H364	-10.559768764	2.398432492	3.533686288
H365	-11.986869563	2.398525979	2.486234315

H366	-8.322831287	4.084068077	-2.577187460
H367	1.064271380	-0.652814899	0.399565984
H368	-0.694869978	0.296388988	-1.477307623
Mo369	6.128941982	0.329545468	-0.462234275
N370	0.638535059	-5.425574683	-8.241279360
N371	-3.009047508	-5.851806416	-7.564191550
N372	-3.595565697	-8.165580982	-6.038367210
N373	-1.253172176	-8.535744057	-4.530735546
N374	-1.274426810	-6.181571626	-2.901557546
N375	-3.669360146	-6.699337282	-1.430394584
N376	-3.174671428	-9.250735607	-0.165280575
N377	-0.549075732	-9.196667761	1.005352805
N378	-0.053350520	-6.715005889	2.192937321
N379	-2.419567288	-5.333270906	3.367134713
N380	-3.818651316	-7.666141092	4.371985731
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N382	9.109905772	-6.749275830	3.137886530
N383	4.467595939	-2.636481285	3.957981923
N384	2.630142072	-3.629741592	5.020029663
N385	2.603908420	-1.363435463	4.488572812
N386	9.505919821	-4.564115562	5.839761085
N387	-0.742861981	-0.910756594	-7.035307026
N388	3.659038875	-1.295006742	-5.289407787
N389	-2.932155878	-0.103819166	-5.831269663
N390	-5.443912038	-1.148198554	-6.376211983
N391	-5.842596671	-3.022194543	-4.378335329
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N393	-3.466306159	1.745195656	-1.884177547
N394	-1.708519493	0.513216352	-1.629143875
N395	-8.299703049	-0.915814098	-0.845454570
N396	-12.077224953	1.168383173	-2.600784993
N397	-13.809686976	1.018876786	-1.224090159
N398	3.672868426	1.425295234	9.397312129
N399	-0.926410409	6.023421189	7.835291065
N400	-2.053170908	8.251335259	5.309727252
N401	-2.983282034	7.496272675	2.796281486
N402	-4.642274993	6.506116756	-1.817584715
N403	-5.352078408	8.673311079	-1.281768751
N404	-6.879881264	6.933385480	-1.374563127
N405	-3.754486053	4.766392265	3.027294900
N406	-5.660988552	4.917467035	5.090111553
N407	-8.139053836	6.250591720	4.825188263
N408	-7.228340374	7.314927611	2.024490884
N409	-10.459994917	5.085624063	3.882107929
N410	9.149435930	6.198057689	-4.727380926
N411	5.866602727	5.185238323	-3.561827777
N412	3.071893289	6.168166562	-2.867647148
N413	3.050653783	7.907110579	-0.581174564
N414	4.154733339	5.613771303	-8.008682228
N415	1.380757769	5.133409009	-7.530961075
N416	11.929402465	2.610263992	-0.411123021
N417	7.994127117	1.185311125	-1.749887448
N418	8.883155291	1.950127449	-3.619563707
N419	12.102103584	0.388817426	1.803426551
N420	-2.589941117	2.643995359	0.977845799
N421	-1.783242110	1.877697220	1.092479602
O422	-1.253714888	-5.841584062	-6.111868762
O423	-4.295558969	-6.810516025	-4.343426696
O424	-2.449273966	-9.795133665	-3.044571981
O425	-0.222931755	-7.433428172	-1.320459863
O426	-2.710737773	-5.565551114	0.292248242
O427	-4.405401089	-8.444319971	1.580840768
O428	-1.244613737	-10.819289196	2.475926060
O429	1.936300113	-7.462945268	3.066973766
O430	-0.888731237	-5.033577547	5.038196499
O431	-3.966325746	-6.478033521	6.300262033
O432	-3.425499617	-9.889266713	7.157182332
O433	10.982058547	-5.927020657	2.051501048
O434	8.557127976	-6.657822526	5.921836311
O435	9.376304135	-3.173589773	9.158944433
O436	-3.049138098	-1.897883677	-4.406533741
O437	2.026073738	-0.441285969	-6.619332025
O438	-6.436892691	0.301730131	-4.916900514

O439	-5.228868436	2.741576232	-5.053913252
O440	-7.959275029	-3.470854881	-5.153975437
O441	-5.882160465	-3.792570082	-0.802969240
O442	-7.353606190	-0.516454384	1.194677350
O443	-10.910228370	-1.123859994	1.526998982
O444	5.782916446	-1.418668977	9.468304739
O445	-2.241234821	0.646076741	6.951992347
O446	-3.269566099	6.487968442	6.095518792
O447	-4.912388547	8.706388641	3.097984734
O448	-5.161921273	5.135815974	1.256178722
O449	-6.625384253	2.985894406	4.323585238
O450	-3.330316008	2.931061727	5.496243066
O451	-8.562131880	6.017566798	7.065749607
O452	-11.647181458	7.019692140	4.115764912
O453	-9.410086637	7.300252412	1.341237221
O454	-13.761432686	3.710982692	4.225506649
O455	-7.770956004	4.048539202	-1.771204788
O456	7.036798413	4.571703552	-5.439942492
O457	3.063991912	6.078055866	-5.161326950
O458	1.587431953	9.279883402	-1.648044247
O459	3.528067948	11.114312655	0.983733119
O460	1.372161806	4.051877897	-9.538548792
O461	5.517442249	0.426240415	-7.085986527
O462	6.414522862	2.023299511	-5.811864886
O463	-1.480743540	6.915095453	-6.410909214
O464	11.292237991	2.244770689	2.819881564
O465	13.727723144	0.902162712	4.959590290
O466	4.377605350	-3.349963968	-3.126298220
O467	5.764453919	-5.088401149	-3.106139089
O468	11.606609077	-2.663101201	-2.847011176
O469	10.154216902	-2.951910638	-4.553716307
O470	7.612509072	-1.084622669	0.486367669
O471	8.393990657	-3.199760607	0.402993496
O472	6.440549189	-1.209048853	-1.856826150
O473	10.130917458	-2.285676030	4.234286069
O474	7.799546454	-0.976986237	3.282875246
O475	-5.264129594	3.799761508	-2.526739991
O476	12.992914663	-2.381621751	-0.042479571
O477	10.830817840	-3.192923123	1.671620492
S478	-0.476475715	5.478167122	3.756815849
S479	1.005749818	4.256001052	0.487297478
S480	4.625750978	1.526993113	-1.917680284
S481	0.988412266	1.807668082	3.141812794
S482	1.333921381	0.379561940	-0.458062999
S483	4.840226665	5.037590126	-0.264605255
S484	4.483804292	-0.876402383	0.832378423
S485	3.224150954	4.647032638	3.364665375
S486	6.816333049	2.036047005	1.062328371
S487	4.652059443	1.108875814	4.034593358

Structure C 47(3/2)

C 47(3/2)		bm22b6x2n2x47dtg.car_3	
associated		C1	-1.616251807 -8.942474568 -2.742886291
Fe(139)	0.534 2.273	C2	-0.657757345 -9.608548018 -3.733217689
Fe(140)	0.426 -1.176	C3	-3.955988808 -8.468153105 -2.172348783
Fe(141)	0.575 2.830	C4	-3.968887973 -8.882792083 -0.702110097
Fe(142)	0.551 -2.629	C5	-3.502235693 -10.617494142 0.956357426
Fe(143)	0.554 2.850	C6	-2.385479197 -9.947812987 1.763346422
Fe(144)	0.510 -2.292	C7	-0.206799092 -8.834248914 1.698309164
Fe(145)	0.334 0.942	C8	-0.597747249 -7.391889429 2.031509574
		C9	-1.799737081 -5.383206555 1.348358863
		C10	-2.827485781 -5.328442036 2.489495724
		C11	-4.737417247 -6.351636162 3.584280554
		C12	-4.181192235 -6.687866334 4.974103935
		C13	-2.823215712 -8.225695273 6.310418315
		C14	-1.591245023 -7.535323103 6.912083429
		C15	0.590291549 -6.487077357 6.462894603
		C16	0.776674538 -4.973225339 6.321388360
		C17	-0.157796620 -2.872952007 5.388781276
		C18	-1.304083974 -2.161240717 6.129294580
		C19	-0.105613908 -2.543798398 3.873874706
		C20	-0.266674370 -1.043057275 3.610084116

C21	1.189379316	-3.080832748	3.252257593
C22	-3.739180100	-1.904393735	6.404578335
C23	-4.003955890	-2.507522268	7.796305467
C24	-4.973264156	-1.971432543	5.473829646
C25	-6.229460538	-1.451549646	6.181685493
C26	-4.718288919	-1.180747368	4.183483402
C27	-4.355937569	-4.489043890	9.147832023
C28	-3.410169404	-4.060557182	10.250246026
C29	10.355774802	-5.734202475	6.465770250
C30	10.062690812	-4.287101237	6.062133244
C31	8.452840994	-2.413016899	6.442797015
C32	8.701110585	-1.637851209	7.752209923
C33	6.961123681	-2.445220733	6.066276142
C34	6.343596341	-1.063605952	5.824483364
C35	4.953179305	-1.205231434	5.202807785
C36	3.112608145	0.493316391	5.219917768
C37	9.664738176	0.379288576	8.748883935
C38	8.797855172	1.614396555	8.890657564
C39	-0.986125045	-4.670003535	-3.879466956
C40	-2.369528428	-4.025369108	-3.704055952
C41	0.025063483	-3.820707310	-3.074094023
C42	1.410929506	-4.459151998	-2.847055485
C43	2.443240950	-4.178857951	-3.937835834
C44	-3.973013710	-2.501296844	-4.760515915
C45	-5.320160997	-3.210135621	-4.610682506
C46	-4.015919344	-1.532084375	-5.961465388
C47	-6.518696196	-5.321952218	-4.373314565
C48	-6.800029086	-5.399826495	-2.864686840
C49	-5.950522630	-4.993870878	-0.591048150
C50	-5.916646502	-3.639209977	0.112284253
C51	-5.912235412	-1.186369430	-0.104618228
C52	-7.320175325	-0.693030197	0.307501309
C53	-5.374838503	-0.135290154	-1.087148410
C54	-3.926185023	-0.225125485	-1.442315902
C55	-2.831493437	-0.787177286	-0.833540172
C56	-2.113083425	0.280808598	-2.643554159
C57	-9.705332567	-0.717240434	-0.315557332
C58	-10.270463608	-0.899604828	1.088080849
C59	-10.569324185	-1.497251579	-1.341287116
C60	-11.842091213	-0.827395208	-1.763502688
C61	-12.942040298	-0.446034325	-1.019355140
C62	-13.250089161	0.041903903	-3.158970301
C63	3.651405330	5.155323805	7.601827605
C64	5.126505791	4.901682635	7.855424867
C65	3.172596524	4.066552225	6.606554817
C66	1.701344152	4.170208198	6.279144932
C67	0.728382026	3.548118457	7.083785352
C68	1.261019863	4.889909322	5.153770711
C69	-0.634487652	3.630314810	6.775562419
C70	-0.094503130	4.988749039	4.838388734
C71	-1.041704552	4.357084838	5.650749929
C72	-0.917439647	8.956879129	1.676529462
C73	-2.199845898	9.181241417	0.865459445
C74	-0.551645322	7.465829411	1.682066189
C75	-3.178791659	10.074860343	-1.201350467
C76	-3.733535468	8.853255601	-1.935917898
C77	-3.364027475	6.507482597	-2.602571161
C78	-4.147183540	5.610882464	-1.618521868
C79	-2.140312055	5.797337345	-3.215449905
C80	-2.385963905	4.480818656	-3.961614604
C81	-3.084580419	4.573417873	-5.332243609
C82	-5.496406058	5.209650867	-5.567682617
C83	-4.462608192	4.808196805	0.669332236
C84	-5.699213451	5.524556272	1.255299075
C85	-3.581751406	4.339802571	1.834152610
C86	-6.577337435	7.635836288	2.128285880
C87	-7.872588081	8.186385500	1.532193557
C88	-9.277564636	8.441582939	-0.478254214
C89	-10.595425651	7.635556251	-0.440940548
C90	-8.886205018	8.769175338	-1.940027146
C91	-8.506075243	7.508001568	-2.707394806
C92	-11.655611952	5.472584402	0.075336022
C93	-12.702603039	5.863846991	1.113347242

C94	-11.164059680	4.021203484	0.339462384
C95	-10.248825988	3.511352395	-0.750287436
C96	-10.784801077	2.935912150	-1.912570880
C97	-8.853612339	3.640559226	-0.660336052
C98	-9.965439856	2.520208546	-2.964148493
C99	-8.017058907	3.254507321	-1.712683393
C100	-8.586265791	2.705377330	-2.858627711
C101	8.355534705	2.618460237	-6.035490305
C102	7.114284332	1.774386406	-6.278418852
C103	4.694012401	1.552940252	-5.775736308
C104	3.620665451	2.381402257	-6.487550199
C105	2.211744587	4.381771526	-6.327252476
C106	2.339642531	5.849680318	-5.926689855
C107	3.150091576	7.559360465	-4.405761655
C108	3.851180930	8.501593605	-5.363017166
C109	3.732228716	-1.203063005	-9.364047561
C110	2.211065518	-1.151495966	-9.555695172
C111	4.056169232	-1.823441315	-7.984070616
C112	5.532401611	-2.255829085	-7.903296644
C113	5.907773786	-2.587347574	-6.475782220
C114	0.130532739	0.088028864	-9.176155672
C115	-0.226376312	1.513329323	-9.556747220
C116	-0.643564863	-0.464724079	-7.951771071
C117	-0.054299946	-0.046862585	-6.625692532
C118	-0.333778953	1.208393432	-6.054863917
C119	0.858807098	-0.891769798	-5.968315658
C120	0.304355962	1.610385766	-4.874396619
C121	1.498076674	-0.487373299	-4.790792702
C122	1.232496008	0.771848772	-4.243354140
C123	10.878007890	1.960409069	-0.564787533
C124	11.377577473	2.333506212	0.839982103
C125	10.121527898	0.621623456	-0.566558110
C126	9.448943554	0.258305887	-1.852866666
C127	10.044693324	0.011495574	-3.074524661
C128	7.878583258	-0.431342049	-3.204891879
C129	12.513021337	1.691763120	2.889537392
C130	13.398707811	2.918322294	2.883504532
C131	5.324785335	-4.713621803	0.257359084
C132	5.940040453	-3.618008103	1.079785523
C133	7.069046291	-2.815237687	0.316620757
C134	8.158361948	-3.804981746	-0.185600527
C135	9.373537885	-3.080610294	-0.787398214
C136	10.556574522	-3.969926621	-1.043391555
C137	7.742049024	-1.900410916	1.386281024
C138	3.485236337	2.469078112	-0.281406149
Fe139	5.021228901	2.204860492	-1.513742284
Fe140	1.238005518	2.479675371	-0.383351824
Fe141	3.252233030	3.782825505	1.180792684
Fe142	3.390158106	4.131356054	-1.372121668
Fe143	1.283955408	5.152341725	-0.119577246
Fe144	4.868382916	1.857434881	1.014601857
Fe145	3.525295410	0.300193083	-0.616474781
H146	1.059004453	-9.146230404	-2.735803950
H147	0.758997321	-8.161827855	-4.004346622
H148	-3.227792359	-9.580258381	-3.850037615
H149	-1.058162366	-9.502607511	-4.752973635
H150	-0.675179565	-10.689656008	-3.508343684
H151	-3.805484906	-7.378057569	-2.182166429
H152	-3.331019509	-10.770759521	-1.183939006
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	O464	-1.253459310	2.089300447	-9.228495635
	O465	11.271426334	3.492926388	1.282234245
	O466	13.613467202	3.601015438	3.875102446
	O467	4.431182101	-4.574854360	-0.566156449
	O468	5.826287335	-5.977115054	0.449128739
	O469	11.685923329	-3.804014027	-0.588673648
	O470	10.267489990	-5.013930592	-1.864681492
	O471	7.642973732	-0.632488223	1.167908575
	O472	8.361310976	-2.409712391	2.350066525
	O473	6.529825507	-2.074963765	-0.716908173
	O474	9.973966602	0.558920605	5.013476196
	O475	7.690193072	1.061374202	3.410424411
	O476	-5.223441248	1.706283736	-4.367919102
	O477	12.916066815	-1.943483552	1.596128452
	O478	10.727605433	-1.626528815	3.428876233
	S479	-0.360184446	6.768094310	-0.022108689
	S480	1.237055793	4.073978241	-2.073362284
	S481	4.786749170	0.154852938	-2.397192095
	S482	1.018678896	3.607613187	1.565871830
	S483	1.301714105	0.144322272	-0.292570684
	S484	4.926094075	3.919137344	-2.961068291
	S485	4.519066177	-0.338303865	1.251754439
	S486	3.469136740	5.811472413	0.109205899
	S487	6.769295550	2.258193302	-0.091488001
	S488	4.671547718	3.135712530	2.804375940
C 47(3/2) TS Fe(139) 0.535 2.264 Fe(140) 0.503 -1.471 Fe(141) 0.574 2.831 Fe(142) 0.545 -2.527 Fe(143) 0.559 2.922 Fe(144) 0.517 -2.298 Fe(145) 0.330 1.001	bm22b6x2n2x47dtg_1	53086.969		
	C1	-1.616695130	-8.934679225	-2.743864785
	C2	-0.657383561	-9.609369829	-3.730438010
	C3	-3.960687949	-8.474844222	-2.173462641
	C4	-3.966940601	-8.883979938	-0.701820059
	C5	-3.499199799	-10.615633783	0.957557996
	C6	-2.382924897	-9.945723900	1.765900202
	C7	-0.207547308	-8.824844614	1.701349896
	C8	-0.602014432	-7.381882206	2.030588688
	C9	-1.811276524	-5.379144702	1.344210444
	C10	-2.836939753	-5.324158526	2.486665347
	C11	-4.741996906	-6.348570403	3.587179457
	C12	-4.182747624	-6.687004173	4.975461770
	C13	-2.823556386	-8.225239675	6.308245453
	C14	-1.592231923	-7.537485098	6.911563348
	C15	0.589644364	-6.491660813	6.472484935
	C16	0.779152031	-4.978397895	6.326488570
	C17	-0.153569035	-2.878897879	5.389812996
	C18	-1.297310128	-2.171553034	6.138086594
	C19	-0.112965793	-2.545098197	3.874346928
	C20	-0.293209123	-1.045557362	3.614290215
	C21	1.184999072	-3.064010291	3.245305667
	C22	-3.731175941	-1.899851092	6.407796546
	C23	-3.999183626	-2.500120219	7.800796952
	C24	-4.965262428	-1.970555780	5.478269757
	C25	-6.221620249	-1.446446853	6.183454235
	C26	-4.712951447	-1.189316497	4.181859596
	C27	-4.362315128	-4.482449535	9.150420228
	C28	-3.410665802	-4.066204835	10.254327335
	C29	10.355838010	-5.742670445	6.470279455
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	C31	8.458839904	-2.419545279	6.445947567
	C32	8.708925608	-1.644833912	7.755254535
	C33	6.968559834	-2.447342484	6.070230795
	C34	6.359662235	-1.063647928	5.829316265
	C35	4.959155840	-1.192521590	5.228791855
	C36	3.136756159	0.525204665	5.225781934
	C37	9.679254091	0.368516657	8.751029292
	C38	8.806186795	1.596340695	8.912633077
	C39	-0.985203560	-4.660759785	-3.875929627
	C40	-2.369812047	-4.019408367	-3.703969974
	C41	0.025332767	-3.805968328	-3.075155302

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C43	2.444574341	-4.171197890	-3.931394630
C44	-3.974554342	-2.498754975	-4.759442547
C45	-5.322367695	-3.207476053	-4.610085741
C46	-4.020311852	-1.524035119	-5.954294507
C47	-6.522284969	-5.319259986	-4.374891532
C48	-6.801289689	-5.395759226	-2.866803803
C49	-5.942696746	-4.998650593	-0.595350080
C50	-5.918425294	-3.643369958	0.109805048
C51	-5.900513269	-1.192163520	-0.100516695
C52	-7.311545305	-0.704602935	0.313337049
C53	-5.365614094	-0.132429866	-1.075933864
C54	-3.922400471	-0.218105046	-1.458551452
C55	-2.809408053	-0.781084782	-0.882706733
C56	-2.142129542	0.303265976	-2.703066285
C57	-9.695900629	-0.725366132	-0.317270087
C58	-10.259464627	-0.920121276	1.085977948
C59	-10.557039342	-1.498116141	-1.350511541
C60	-11.827369948	-0.824097031	-1.776353537
C61	-12.924647628	-0.430016871	-1.034311895
C62	-13.233182144	0.038085310	-3.178128401
C63	3.646013431	5.158140285	7.612135397
C64	5.121370246	4.898537343	7.857959235
C65	3.163097521	4.071193976	6.617142289
C66	1.691618468	4.175036793	6.289217404
C67	0.718771876	3.546098546	7.088925273
C68	1.252541735	4.896017338	5.163607271
C69	-0.642855534	3.623752235	6.774911724
C70	-0.102339749	4.991821529	4.844569481
C71	-1.049515796	4.354184906	5.652269540
C72	-0.920210010	8.960670192	1.665894532
C73	-2.204899123	9.183506162	0.857153502
C74	-0.549621693	7.469840041	1.680898171
C75	-3.187007424	10.077819659	-1.207711574
C76	-3.735184372	8.855012028	-1.944705547
C77	-3.359262647	6.508856682	-2.602931538
C78	-4.136065088	5.607292192	-1.617779619
C79	-2.136357500	5.805878560	-3.222820147
C80	-2.381960673	4.492906102	-3.974258396
C81	-3.084126543	4.590162508	-5.342941810
C82	-5.498256015	5.216556189	-5.580430343
C83	-4.455830353	4.809574919	0.668676633
C84	-5.699549850	5.519169828	1.244198639
C85	-3.581606758	4.356282849	1.845177783
C86	-6.575382900	7.624142973	2.132302681
C87	-7.867499738	8.183588484	1.539386946
C88	-9.271158946	8.450622559	-0.470977561
C89	-10.588941226	7.645098499	-0.429957133
C90	-8.883322970	8.771556674	-1.933533907
C91	-8.506102138	7.508455860	-2.698582145
C92	-11.647282130	5.481941851	0.083357044
C93	-12.690504807	5.877464494	1.123262455
C94	-11.160317680	4.028926230	0.344053953
C95	-10.247207060	3.517664866	-0.747948915
C96	-10.784368227	2.926458796	-1.902978439
C97	-8.851712461	3.653839200	-0.663594270
C98	-9.965417208	2.511678319	-2.955761810
C99	-8.016142928	3.266430532	-1.716510953
C100	-8.586592476	2.705286975	-2.856551325
C101	8.344800735	2.630618047	-6.039807600
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C104	3.617316202	2.377912281	-6.491302146
C105	2.210867492	4.379250813	-6.345892826
C106	2.324631480	5.844970373	-5.935133483
C107	3.129216934	7.551771016	-4.404966234
C108	3.876299495	8.494159576	-5.326666295
C109	3.735557041	-1.203546318	-9.352801087
C110	2.215709758	-1.145772084	-9.551531755
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C112	5.528254186	-2.266599196	-7.891399753
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C114	0.134345663	0.084010678	-9.163032676

C115	-0.226165065	1.506605400	-9.544595871
C116	-0.645451887	-0.480568976	-7.947446391
C117	-0.063468258	-0.052742099	-6.621349169
C118	-0.351014591	1.206650068	-6.064396771
C119	0.858764007	-0.883740309	-5.959418650
C120	0.293426341	1.629188836	-4.896438999
C121	1.503817655	-0.459803665	-4.792202413
C122	1.232305364	0.805472066	-4.262080987
C123	10.880550958	1.963638428	-0.569167909
C124	11.386597762	2.331721887	0.833374351
C125	10.139686929	0.616653514	-0.578116361
C126	9.454782937	0.256894149	-1.860241806
C127	10.044069295	0.007789463	-3.084936471
C128	7.875154116	-0.421779465	-3.205959240
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C130	13.415083469	2.905454071	2.880419990
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C134	8.169869975	-3.796801458	-0.184380228
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C136	10.562652795	-3.974889223	-1.031804280
C137	7.756817510	-1.887565917	1.385316932
C138	3.492168993	2.471129874	-0.271087748
Fe139	4.991801342	2.161055501	-1.532764826
Fe140	1.502218857	2.385807748	-0.350047304
Fe141	3.240851969	3.791625302	1.205603763
Fe142	3.298994130	4.086259271	-1.383754438
Fe143	1.189028746	5.048191130	-0.095911832
Fe144	4.879177509	1.858186301	1.012582278
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H146	1.065672791	-9.152631401	-2.740289447
H147	0.765958693	-8.169087011	-4.008726911
H148	-3.227202155	-9.587843665	-3.845908141
H149	-1.058192988	-9.510618268	-4.751027685
H150	-0.677009326	-10.688688041	-3.498104536
H151	-3.820870051	-7.384400016	-2.186784466
H152	-3.329040623	-10.774916269	-1.181834570
H153	-4.945342442	-8.702634293	-2.604281785
H154	-3.325054141	-11.699594521	0.949789380
H155	-1.300085710	-9.617068604	0.050729276
H156	-4.440845906	-10.424130424	1.487959416
H157	-0.987722047	-4.709167743	1.626205181
H158	-1.475148206	-7.154342150	0.170320333
H159	0.662230548	-8.823030018	1.029471850
H160	-5.225301567	-5.365754644	3.660137587
H161	-3.780105045	-7.029396026	1.786493827
H162	0.085464105	-9.300457140	2.645418503
H163	-2.268604766	-4.997338771	0.420164313
H164	-3.085238024	-8.255717710	4.187907571
H165	-5.504835673	-7.094314326	3.325084129
H166	1.310801072	-4.142663496	3.415248909
H167	1.182378251	-2.887124940	2.158620565
H168	2.061405039	-2.543802781	3.660747269
H169	-0.959982013	-3.072640017	3.406841263
H170	-2.577211573	-9.289130900	6.181182637
H171	-3.845576139	-1.572139522	3.626856585
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H175	0.532070873	-0.454916770	4.038444928
H176	3.114940189	5.003866867	8.570808360
H177	-5.590031698	-1.262798395	3.522028656
H178	-7.079297502	-1.482730344	5.496028498
H179	-4.541263883	-0.124176354	4.405390880
H180	-6.083091356	-0.398840621	6.497004206
H181	-5.132392533	-3.032477685	5.218651193
H182	-3.486138408	-0.844385780	6.600978051
H183	-2.714379738	-3.166335323	4.997843453
H184	-1.239719536	-0.661487756	4.025488787
H185	-2.643502952	3.930905785	1.452633127
H186	-4.136951405	3.559271368	2.365635483
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H191	1.027168514	2.971952825	7.967353110
H192	-0.944146458	-4.867903279	5.234873594
H193	1.411317033	-6.972409856	5.920704520
H194	0.712337927	-6.730698889	7.536423172
H195	-0.793301939	-7.204821278	5.023854868
H196	-3.621758279	-8.142322806	7.056369948
H197	-1.383890050	3.115172464	7.398059887
H198	0.768391224	-2.516825872	5.863809869
H199	-5.394975857	-4.275890274	9.477270367
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H201	-2.400639787	-3.740405456	9.909940840
H202	10.735113420	0.676030621	8.712417861
H203	4.443809139	-3.846368191	-4.219524498
H204	6.518132890	-5.934179618	1.181712317
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H206	6.184578718	-1.479068601	-8.288620914
H207	3.408134079	-2.690661961	-7.782086199
H208	0.536904588	2.011880425	-10.181701697
H209	4.068505469	-1.919557911	-10.119742274
H210	0.138769565	-2.833373837	-3.580497721
H211	1.317661959	-5.535293261	-2.746171711
H212	2.105892613	0.665928788	-8.545379082
H213	-0.154285966	-0.522144656	-10.045165684
H214	4.237469053	0.759378428	-8.897557901
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H223	-5.303910875	-1.211906973	0.821948268
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H226	-4.885970759	-4.703768705	-2.423249843
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H231	-9.692396873	0.350489803	-0.549824044
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H233	-5.540303996	0.848544589	-0.602870307
H234	-5.981092306	-0.148198189	-1.990087753
H235	-14.715200573	0.515669132	-1.725725077
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H237	-5.851415852	-2.642853466	-1.697253447
H238	-5.163681577	-5.625828017	-0.137859151
H239	-7.416883275	-4.886145890	-4.840632235
H240	-1.504464774	0.733396615	-3.472533214
H241	-6.405148184	-6.341253156	-4.757999293
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H244	-2.806785178	6.005240327	-0.076047003
H245	-4.831008989	3.907437326	0.166632226
H246	-4.797621630	7.348043452	1.025176853
H247	-4.094749404	0.997528674	-3.238380564
H248	-5.188382051	0.973501410	-5.007517371
H249	-6.156375267	1.804792805	-4.052139954
H250	-3.085006505	-0.949073188	-5.988064608
H251	-4.123899897	-2.086046676	-6.896719601
H252	-8.056830481	9.496509858	-1.920943659
H253	-9.754450074	9.231534464	-2.416405020
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H257	-2.662710806	3.840518729	-6.029091414
H258	-10.399919615	2.036471047	-3.837781320
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H263	-2.919300952	3.771895141	-3.337718537
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H265	-2.895063414	10.823051904	-1.959740399
H266	-2.179122535	-3.456018005	-5.615958278
H267	-1.657281871	6.528703760	-3.903754633
H268	-6.939137906	3.436734910	-1.658812768
H269	-5.845360962	-1.094335043	-5.394223274
H270	-4.024654801	10.490041690	-0.628140143
H271	-4.374604898	6.539098928	-6.684650735
H272	-7.533072287	5.442820488	-5.692900370
H273	0.381101654	-4.581389147	-5.410794204
H274	-1.052118850	-5.646835420	-3.378022195
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C104	3.631180307	2.394740285	-6.486349302
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C106	2.349929871	5.855688794	-5.924817978
C107	3.173593143	7.575532640	-4.426370883
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C113	5.920919436	-2.588120396	-6.481127655
C114	0.135215130	0.110615314	-9.161869570
C115	-0.215307646	1.537994607	-9.536263685
C116	-0.650180126	-0.452265674	-7.949641920
C117	-0.057771947	-0.056615159	-6.618892012
C118	-0.327836020	1.194674002	-6.036713725
C119	0.853199833	-0.912466595	-5.974208275
C120	0.320770472	1.584568597	-4.859189249
C121	1.504083568	-0.520522206	-4.799042873
C122	1.246957826	0.735029499	-4.240756667
C123	10.876993294	1.947124380	-0.544640970
C124	11.382912253	2.323102163	0.855514010
C125	10.097589337	0.619268838	-0.537529670
C126	9.422491159	0.251731692	-1.823566864
C127	10.023604941	0.005167329	-3.042971745
C128	7.858830639	-0.440371143	-3.180757844
C129	12.551452786	1.689803225	2.893818767
C130	13.427106471	2.923037354	2.881088629
C131	5.298826524	-4.716618937	0.254588805
C132	5.922498351	-3.635048941	1.089649055
C133	7.045370684	-2.827309705	0.321867687
C134	8.136967801	-3.810369544	-0.187701426
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C137	7.716350510	-1.907113316	1.391835209
C138	3.529240413	2.500868889	-0.284523092
Fe139	5.015807064	2.186390338	-1.538738605
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Fe141	3.132751216	3.758251459	1.226254945
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N410	-10.501564066	6.375239681	0.071433869
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N412	5.988933593	2.255383499	-5.749037026
N413	3.188543202	3.455074656	-5.779033908
N414	3.147196640	6.195949276	-4.883049729
N415	4.366142162	0.098838073	-9.659770662
N416	1.579282193	-0.024075029	-9.068656136
N417	11.978619010	1.936166034	-1.527397149
N418	8.060752932	-0.025946669	-1.932883900
N419	9.020394659	-0.430984805	-3.880987007
N420	12.044594077	1.368585523	1.567858651
N421	-2.277010905	2.747019301	-0.910350876
N422	-1.999775401	2.225182499	0.032819860
O423	-1.207451115	-8.261728470	-1.742518273
O424	-4.315847792	-8.068818606	0.185644973
O425	-2.500489234	-9.790383672	2.984152487
O426	-0.289389591	-6.880308329	3.117549215
O427	-2.807097422	-4.408561789	3.324495095

O428	-4.559161395	-6.068145928	5.978904614
O429	-1.437148691	-7.480230069	8.137699895
O430	1.786063482	-4.406938152	6.783871111
O431	-1.044539670	-1.265039486	6.951816893
O432	-4.150778447	-1.784332150	8.778158412
O433	-3.689331851	-4.104510678	11.414054906
O434	10.828771454	-3.697300178	5.272206046
O435	8.324497522	-2.105281627	8.852234361
O436	9.160997029	2.612051411	9.505981995
O437	-2.990366277	-4.020053066	-2.610231996
O438	2.145653295	-4.114404217	-5.139891920
O439	-6.338329749	-2.532771598	-4.371120746
O440	-5.101470618	-0.606385327	-5.858545365
O441	-7.879239248	-5.853550567	-2.480527830
O442	-5.919341457	-3.588849499	1.351742858
O443	-7.415090449	0.226576676	1.131058900
O444	-10.990527911	-0.035034253	1.613343642
O445	5.565060643	4.255075974	8.807423400
O446	-2.355873338	4.467938543	5.284665519
O447	-3.294218525	8.796136635	1.263349307
O448	-4.869114921	8.927503714	-2.448164643
O449	-5.137844578	4.957018548	-1.989902788
O450	-6.675479565	4.920919227	1.730900492
O451	-3.404215956	5.541639759	2.788009561
O452	-8.639796962	8.954680092	2.202563210
O453	-11.645932419	8.101436648	-0.890800202
O454	-9.347968396	6.791861062	-3.271752030
O455	-13.827620618	5.446930723	1.051777089
O456	-7.686369164	2.345314154	-3.924049004
O457	7.196321070	0.687590230	-6.917028767
O458	3.225468925	2.105433192	-7.634025674
O459	1.693015330	6.702491182	-6.556174432
O460	3.683299721	9.725631018	-5.392432303
O461	1.591592473	-2.069455971	-10.077922436
O462	5.649687741	-3.657372331	-5.942218937
O463	6.550826954	-1.625095391	-5.780927210
O464	-1.243211895	2.113584831	-9.210282018
O465	11.270068034	3.481476811	1.298008035
O466	13.648895796	3.604805337	3.871593867
O467	4.392160939	-4.563288895	-0.552634328
O468	5.807837560	-5.981255607	0.412441946
O469	11.666008972	-3.796958740	-0.596669494
O470	10.243827327	-5.007824119	-1.867386277
O471	7.589217533	-0.640243704	1.181709152
O472	8.355982433	-2.410546327	2.345829392
O473	6.493923918	-2.090127232	-0.709025175
O474	9.995036900	0.538428485	5.019287260
O475	7.701137867	1.047198811	3.426947638
O476	-5.177909526	1.689445433	-4.364919309
O477	12.937474345	-1.957006560	1.599324306
O478	10.743465804	-1.644211978	3.425646448
S479	-0.463100732	6.622244811	-0.017878149
S480	1.103146631	3.774183035	-2.058928244
S481	4.716641348	0.138071470	-2.379827426
S482	0.887461969	3.315811872	1.466513669
S483	1.214966309	0.210733991	-0.432034079
S484	4.840370584	3.927165376	-2.960599028
S485	4.447462637	-0.348000861	1.250810362
S486	3.236517812	5.765452112	0.086654001
S487	6.756949889	2.241156763	-0.094555101
S488	4.591965457	3.161059591	2.813639953

Structure C 35(3/2)

C 35(3/2)		bm22b6x2n2xd35tc.car 4	
associated		C1	-1.850830777 -8.159785533 -4.499557399
Fe(139) 0.543 -2.417		C2	-0.922254805 -8.620563710 -5.626838484
Fe(140) 0.441 -1.282		C3	-4.171764466 -7.774362912 -3.796101537
Fe(141) 0.546 -2.581		C4	-4.155964551 -8.480584907 -2.442152764
Fe(142) 0.578 2.858		C5	-3.702284326 -10.531837839 -1.192979473
		C6	-2.560193665 -10.065955846 -0.283348019
		C7	-0.364432494 -8.987104933 -0.156261606
		C8	-0.721059189 -7.638061742 0.475277097

Fe(143)	0.557	2.894	C9	-1.892601594	-5.511873325	0.240401850
Fe(144)	0.500	2.176	C10	-2.902228514	-5.669087136	1.388026550
Fe(145)	0.358	1.071	C11	-4.803601720	-6.876295196	2.295772282
			C12	-4.227819576	-7.502562194	3.573062418
			C13	-2.883053391	-9.306240741	4.535440936
			C14	-1.622070325	-8.781645151	5.234088668
			C15	0.567990252	-7.697177401	4.965236332
			C16	0.778787186	-6.189906774	5.131305098
			C17	-0.132584780	-3.930562396	4.679719584
			C18	-1.248746839	-3.376622589	5.585283291
			C19	-0.100293453	-3.285426989	3.267576505
			C20	-0.225083419	-1.759534658	3.337108893
			C21	1.167242283	-3.700345040	2.512094460
			C22	-3.670858299	-3.118686935	5.952741384
			C23	-3.931593531	-3.993002466	7.196585048
			C24	-4.922362553	-2.976423171	5.052277482
			C25	-6.156519897	-2.593074417	5.876273503
			C26	-4.678772504	-1.947327958	3.941353474
			C27	-4.307519611	-6.206116572	8.116052552
			C28	-3.310859121	-6.047647787	9.247476816
			C29	10.349234880	-7.116307913	4.931215753
			C30	10.083278040	-5.611655317	4.839664228
			C31	8.507892066	-3.829193203	5.618919316
			C32	8.789228968	-3.351968317	7.057847618
			C33	7.008922739	-3.761324738	5.278230035
			C34	6.413494996	-2.352117284	5.354765065
			C35	5.007908808	-2.331661554	4.752138920
			C36	3.212632314	-0.634635952	5.155643063
			C37	9.812537981	-1.603065000	8.437518585
			C38	8.979450949	-0.406390032	8.848985791
			C39	-1.143769148	-3.753987781	-4.750921739
			C40	-2.513720514	-3.139575032	-4.418821204
			C41	-0.109053440	-3.102222852	-3.804287073
			C42	1.275380098	-3.778504193	-3.721166191
			C43	2.293326595	-3.306445694	-4.758817430
			C44	-4.099558831	-1.395534833	-5.090775721
			C45	-5.457485926	-2.100175390	-5.056044127
			C46	-4.154882499	-0.197779907	-6.061875061
			C47	-6.701826896	-4.190291516	-5.245966784
			C48	-6.959712627	-4.567053609	-3.779258819
			C49	-6.055798880	-4.663746870	-1.492764535
			C50	-5.996087444	-3.481196584	-0.528249786
			C51	-5.938362836	-1.042880595	-0.227606980
			C52	-7.331339660	-0.632070356	0.311589709
			C53	-5.402614001	0.190817547	-0.968370830
			C54	-3.965838368	0.168546025	-1.383782116
			C55	-2.855751435	-0.524587372	-0.965100338
			C56	-2.197735226	0.915508701	-2.524729112
			C57	-9.726648500	-0.484632333	-0.253600067
			C58	-10.262739663	-0.957736535	1.092148564
			C59	-10.627016765	-1.017730353	-1.400071333
			C60	-11.885001932	-0.243711134	-1.656004852
			C61	-12.966233378	0.007255865	-0.832189738
			C62	-13.281204938	0.930845785	-2.821397314
			C63	3.883248419	3.411716888	8.423864924
			C64	5.359159065	3.093823086	8.576091566
			C65	3.362107942	2.558120144	7.237130839
			C66	1.887858282	2.751798963	6.973085534
			C67	0.917080137	1.989413998	7.651282385
			C68	1.438685565	3.703072804	6.040180024
			C69	-0.449381642	2.160297005	7.402154148
			C70	0.079215805	3.894011549	5.790381988
			C71	-0.866021486	3.119013437	6.469470987
			C72	-0.702275860	8.434706064	3.495691073
			C73	-1.991710965	8.845574568	2.774103586
			C74	-0.365482560	6.969138205	3.182030687
			C75	-2.980066697	10.163457038	0.956743038
			C76	-3.583552017	9.121764451	0.013754563
			C77	-3.271894307	6.961622805	-1.136928513
			C78	-4.049345566	5.895665722	-0.334890068
			C79	-2.075536299	6.372504509	-1.908277044
			C80	-2.363070689	5.245627395	-2.905413600
			C81	-3.082891566	5.633117224	-4.211642586

C82	-5.484642724	6.348772615	-4.250575277
C83	-4.339954777	4.644648253	1.741816344
C84	-5.560682073	5.239752101	2.475046923
C85	-3.451883287	3.942560131	2.776916750
C86	-6.396440687	7.123368407	3.794015837
C87	-7.671681297	7.838157176	3.349440229
C88	-9.107582805	8.522480985	1.464208854
C89	-10.440741656	7.750477919	1.361075002
C90	-8.729377540	9.129711626	0.091219156
C91	-8.392367597	8.043453982	-0.922975593
C92	-11.537774269	5.547683536	1.446405264
C93	-12.563712221	5.732922017	2.559961895
C94	-11.080073777	4.064868556	1.391198064
C95	-10.197422488	3.770561053	0.199115497
C96	-10.767906356	3.453320924	-1.044074088
C97	-8.797629821	3.848996279	0.284881085
C98	-9.973207401	3.243602884	-2.174856888
C99	-7.986481411	3.666463147	-0.841023729
C100	-8.589164557	3.376963190	-2.063807869
C101	8.291374349	3.688649866	-5.537885314
C102	7.039723401	2.913488769	-5.916004319
C103	4.622661179	2.619994598	-5.428593873
C104	3.563241303	3.604888462	-5.934906342
C105	2.199082284	5.552303079	-5.334651524
C106	2.365403771	6.903948711	-4.645321261
C107	3.229174177	8.245563963	-2.815460168
C108	3.939677838	9.359162568	-3.556300259
C109	3.556002974	0.697511492	-9.487207354
C110	2.034767022	0.821619190	-9.643405239
C111	3.883008013	-0.198522360	-8.270256297
C112	5.347868658	-0.671793065	-8.306042031
C113	5.751111052	-1.291194384	-6.987111472
C114	-0.016268213	1.976648788	-8.965293894
C115	-0.369144849	3.451496837	-9.029306063
C116	-0.768568172	1.179912962	-7.868848832
C117	-0.154847665	1.323022996	-6.497429610
C118	-0.422026170	2.442056349	-5.689106242
C119	0.760175161	0.363369196	-6.030455665
C120	0.235480964	2.605141708	-4.463912049
C121	1.418698671	0.527434409	-4.806155369
C122	1.166796093	1.658430102	-4.024059429
C123	10.917254442	1.856437310	-0.381636947
C124	11.444137438	1.923300148	1.060803085
C125	10.140605419	0.557171580	-0.649013572
C126	9.430869557	0.478558540	-1.964589338
C127	9.995864748	0.479110125	-3.225418989
C128	7.818545750	0.109867811	-3.391298393
C129	12.588512971	0.849204376	2.916026256
C130	13.508224877	2.026815512	3.153962364
C131	5.269379329	-4.766630226	-0.835099412
C132	5.892973627	-3.857482211	0.186877268
C133	7.036696510	-2.938710944	-0.407143067
C134	8.096352788	-3.823491514	-1.125979066
C135	9.317231809	-3.012297383	-1.591021430
C136	10.477278271	-3.860134560	-2.031525919
C137	7.751368226	-2.276098678	0.812403863
C138	3.524970119	2.407857664	0.162339426
Fe139	5.007404374	2.368579205	-1.189041792
Fe140	1.286478457	2.455972782	0.190877840
Fe141	3.391390521	3.413897262	1.875243528
Fe142	3.394282793	4.232868154	-0.573466474
Fe143	1.386338406	4.971547437	1.133459693
Fe144	4.969544179	1.567516073	1.237414507
Fe145	3.561968549	0.285341784	-0.481543785
H146	0.819418304	-8.408904360	-4.587555962
H147	0.527840529	-7.178756686	-5.619762978
H148	-3.494075543	-8.513615542	-5.684715214
H149	-1.336764224	-8.295805004	-6.593697038
H150	-0.961730721	-9.723734773	-5.633008759
H151	-4.017140458	-6.706766754	-3.584545172
H152	-3.570269355	-10.241069758	-3.320009229
H153	-5.168817751	-7.900003000	-4.239844887
H154	-3.550689096	-11.592260262	-1.434892621

H155	-1.500607692	-9.397733605	-1.911100800
H156	-4.628769458	-10.439633698	-0.612509471
H157	-1.049522574	-4.927606806	0.632251925
H158	-1.630976523	-7.020175591	-1.273648409
H159	0.488791215	-8.852669339	-0.835253055
H160	-5.266809028	-5.923293269	2.582908880
H161	-3.876183526	-7.194378934	0.381457095
H162	-0.058586675	-9.652521434	0.659745226
H163	-2.356421692	-4.938865159	-0.575242393
H164	-3.186229084	-8.902350904	2.458704731
H165	-5.584073299	-7.539681869	1.898234927
H166	1.252650209	-4.793844988	2.432380324
H167	1.158819076	-3.281999831	1.493894264
H168	2.070844876	-3.319344373	3.013425709
H169	-0.972088268	-3.672140753	2.715710478
H170	-2.667170856	-10.328763527	4.193397531
H171	-3.816246810	-2.212690170	3.314454773
H172	-4.007214707	-5.741739095	6.059163901
H173	-6.406708441	-3.352273081	6.630788626
H174	-0.227597148	-1.335954225	2.321242544
H175	0.620147043	-1.305431597	3.872960145
H176	3.371203281	3.064930787	9.342079610
H177	-5.559544405	-1.886827444	3.285896143
H178	-7.025582150	-2.472527360	5.212355079
H179	-4.501320646	-0.949664711	4.374468339
H180	-5.994169063	-1.636449681	6.397677488
H181	-5.109517546	-3.959713865	4.583532423
H182	-3.404121243	-2.132342759	6.361172127
H183	-2.705064437	-4.068382064	4.283828273
H184	-1.156707195	-1.438847055	3.827373592
H185	-2.533032572	3.591381282	2.278254587
H186	-4.016195252	3.066968108	3.138172417
H187	-2.814278954	4.295988025	4.596363508
H188	-2.749714084	2.701459419	6.671001232
H189	-0.248431516	4.617533793	5.044259632
H190	2.165202787	4.285559775	5.469003092
H191	1.232672325	1.238942462	8.381360184
H192	-0.969051620	-5.831197687	4.136863060
H193	1.371239727	-8.058845441	4.306067302
H194	0.711939684	-8.154319645	5.953254567
H195	-0.862737642	-8.072712829	3.437342504
H196	-3.664205812	-9.359410806	5.304149223
H197	-1.187982756	1.541740422	7.920497259
H198	0.803071002	-3.693071719	5.202979586
H199	-5.325601131	-6.057145157	8.511764205
H200	-4.230112404	-7.245002816	7.759167318
H201	-2.310529769	-5.661908244	8.939815355
H202	10.876690247	-1.322130105	8.446685843
H203	4.292730806	-2.953927696	-5.015229756
H204	6.430890967	-6.164359556	-0.187152241
H205	5.464942520	-1.431373629	-9.092106650
H206	6.013246150	0.172322773	-8.540784945
H207	3.221999708	-1.078882187	-8.253995229
H208	0.389496528	4.080545049	-9.551699810
H209	3.863610533	0.152090858	-10.392747017
H210	0.012002844	-2.045562714	-4.095543050
H211	1.178767121	-4.872175726	-3.835754482
H212	1.978426860	2.392303006	-8.289819404
H213	-0.339871067	1.570087363	-9.944338267
H214	4.103695066	2.511339035	-8.638164243
H215	3.847369477	-3.441897768	-3.381230176
H216	3.677605663	0.367913951	-7.348657452
H217	5.218622304	1.883146425	-9.674164605
H218	-1.061157070	-4.370716692	-6.718662555
H219	-0.550538122	-3.109601290	-2.796939016
H220	6.574572111	0.432421273	-6.489905193
H221	1.687447563	-3.619540435	-2.714017001
H222	-5.325468361	-1.262814639	0.657663198
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H227	-13.182364475	-0.259650503	0.196406334

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H229	-10.844335665	-2.084458830	-1.219434548
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H231	-13.772958944	1.487846930	-3.614544605
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H233	-6.027440528	0.372620486	-1.858160368
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H237	-5.280783984	-5.381412420	-1.187267613
H238	-7.595101258	-3.656249079	-5.594594291
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H240	-6.612772608	-5.113849573	-5.831946829
H241	3.872912920	5.377320244	9.005229942
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H243	-2.676720148	5.933352226	1.219232379
H244	-4.747048503	3.874704929	1.071261497
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H260	-1.338251574	5.993140281	-1.182836552
H261	-1.905503424	7.935936194	0.188081543
H262	-2.909771422	4.424273972	-2.416476803
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H334	9.670544025	-1.629940404	6.287046699
H335	3.065572933	-2.055437647	6.640221577
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O435	8.443532898	-4.042852157	8.032216590
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O455	-13.717284054	5.346098678	2.471356693
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O459	1.709152879	7.871302205	-5.069333690
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O462	5.473451132	-2.441937798	-6.662682603
O463	6.415742251	-0.495269420	-6.127149085
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O465	11.367148885	2.967232341	1.734825455
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O473	6.501287236	-1.989468308	-1.253226266
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O475	7.774032295	0.213243627	3.390657908
O476	-5.267341761	2.671812552	-3.806045597
O477	12.899983760	-2.440105774	0.899068676
O478	10.747829914	-2.472049244	2.809773076
S479	-0.222317387	6.623498256	1.366021497
S480	1.176706859	4.323817358	-1.098445564
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S482	1.217069974	3.142781095	2.395061694
S483	1.314975973	0.301718472	-0.726640616
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C10	-2.909736418	-5.271958147	2.510161727
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C13	-2.890052056	-8.192335924	6.318976729
C14	-1.631956505	-7.536950710	6.904364052
C15	0.563175940	-6.532203692	6.434208214
C16	0.780805842	-5.022740346	6.291108370
C17	-0.124571374	-2.901229882	5.376459153
C18	-1.239388567	-2.180094567	6.156224824
C19	-0.107042973	-2.558847952	3.862332547
C20	-0.260066188	-1.054090429	3.616810121
C21	1.168167656	-3.100222064	3.205327305
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C29	10.337169635	-5.983635195	6.262867938

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C34	6.427843801	-1.218528346	5.717859203
C35	5.013518052	-1.311674819	5.145239168
C36	3.226911539	0.440751904	5.182029812
C37	9.821235288	0.131971950	8.584116030
C38	8.979471695	1.379514258	8.760044373
C39	-1.147280829	-4.626921161	-3.883004605
C40	-2.515921437	-3.957012554	-3.686647044
C41	-0.108097484	-3.796707241	-3.092563354
C42	1.269937769	-4.451907815	-2.874685761
C43	2.291516957	-4.203783982	-3.983190082
C44	-4.104177827	-2.395192620	-4.704579347
C45	-5.462444022	-3.076942041	-4.533276039
C46	-4.153622785	-1.413508370	-5.894902557
C47	-6.702934723	-5.164197349	-4.291258784
C48	-6.959975901	-5.239268105	-2.778156075
C49	-6.057736757	-4.870023149	-0.519553900
C50	-5.996139865	-3.518010758	0.189003297
C51	-5.933691411	-1.067871646	-0.010781748
C52	-7.326810355	-0.557639099	0.431098260
C53	-5.398244319	-0.010348438	-0.987606506
C54	-3.964680050	-0.120293683	-1.397907177
C55	-2.851017120	-0.703475860	-0.843109759
C56	-2.200203903	0.377923446	-2.671681187
C57	-9.720081012	-0.526268350	-0.156798940
C58	-10.262854118	-0.729445096	1.253215423
C59	-10.614978672	-1.272721297	-1.180371607
C60	-11.875321578	-0.567645670	-1.586302419
C61	-12.955371366	-0.156174458	-0.827878178
C62	-13.281141134	0.334747674	-2.963700273
C63	3.877863196	5.044973598	7.566081678
C64	5.351170253	4.754491721	7.782799323
C65	3.354015301	3.971429428	6.577851796
C66	1.880673445	4.109642240	6.276406543
C67	0.910494306	3.494362789	7.090090847
C68	1.438032297	4.848481649	5.164805451
C69	-0.454922025	3.604453116	6.803466128
C70	0.079780559	4.978150170	4.874097343
C71	-0.865381847	4.352032145	5.693083214
C72	-0.705943029	8.975127961	1.713895866
C73	-1.998781219	9.229005532	0.927998841
C74	-0.358953349	7.477326611	1.700809799
C75	-2.993694838	10.150088403	-1.118293788
C76	-3.583558574	8.937577684	-1.842423891
C77	-3.262528059	6.588830947	-2.522153015
C78	-4.040733408	5.703106523	-1.525498420
C79	-2.065814496	5.860015199	-3.161695809
C80	-2.354413078	4.558194401	-3.916495150
C81	-3.076774699	4.678026312	-5.272234939
C82	-5.480358383	5.358680721	-5.465369637
C83	-4.334622359	4.899467307	0.762108931
C84	-5.556959356	5.630378257	1.357060615
C85	-3.459455114	4.425173215	1.928260269
C86	-6.381484715	7.742222477	2.272656564
C87	-7.667897627	8.336652468	1.702791309
C88	-9.100827339	8.644966678	-0.280771731
C89	-10.436416262	7.872089408	-0.223629274
C90	-8.727341658	8.965067490	-1.747837812
C91	-8.392191984	7.698617168	-2.525906671
C92	-11.533822153	5.730348526	0.300816516
C93	-12.553857849	6.139990095	1.357968272
C94	-11.076714320	4.267078683	0.546886729
C95	-10.193807637	3.736931235	-0.561249317
C96	-10.762832543	3.165038111	-1.709382065
C97	-8.794262557	3.841490927	-0.498759713
C98	-9.969514999	2.734937010	-2.776233457
C99	-7.984990593	3.439797546	-1.566193213
C100	-8.585843427	2.895995127	-2.699473151
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C102	7.038785121	1.657241874	-6.383409756

C103	4.622648839	1.473011998	-5.845212944
C104	3.561072553	2.331910304	-6.541364316
C105	2.197225459	4.359105932	-6.359805396
C106	2.348238927	5.821506478	-5.949338555
C107	3.212488475	7.507205375	-4.429433456
C108	3.968215261	8.442007017	-5.352939565
C109	3.553886103	-1.244631180	-9.422223597
C110	2.032284303	-1.151874333	-9.599250409
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C112	5.346961752	-2.345872996	-7.989363445
C113	5.749297541	-2.682849878	-6.571402869
C114	-0.017334797	0.118638509	-9.171280857
C115	-0.360563442	1.551000355	-9.534685112
C116	-0.780701535	-0.435231961	-7.939850922
C117	-0.168970066	-0.018275355	-6.624336658
C118	-0.430492699	1.241893539	-6.057458823
C119	0.752562480	-0.864171974	-5.980298988
C120	0.238100839	1.651142781	-4.897278514
C121	1.420630777	-0.454830647	-4.820627284
C122	1.173363564	0.811082921	-4.280947125
C123	10.916365863	1.743152884	-0.750320149
C124	11.445928753	2.094787742	0.648431726
C125	10.156178668	0.406884332	-0.755367759
C126	9.444393385	0.064949801	-2.026776933
C127	10.010876230	-0.185522907	-3.261394463
C128	7.832830425	-0.576250006	-3.353622135
C129	12.593833046	1.409641557	2.678376950
C130	13.516953979	2.608772069	2.670943497
C131	5.275429361	-4.836921727	0.147888161
C132	5.907155555	-3.741433725	0.960689971
C133	7.049241836	-2.967318111	0.190578576
C134	8.108526815	-3.980785055	-0.326599927
C135	9.325048332	-3.282175768	-0.956686661
C136	10.479870049	-4.206149413	-1.220221088
C137	7.760053991	-2.064250581	1.247110249
C138	3.529656596	2.399658009	-0.325049902
Fe139	4.999454405	2.075847866	-1.643598143
Fe140	1.548921397	2.409442256	-0.280964240
Fe141	3.373895097	3.713784654	1.149144934
Fe142	3.389100500	4.052990806	-1.435754971
Fe143	1.359085556	5.049391564	0.091776920
Fe144	4.956843497	1.744924246	0.892033532
Fe145	3.571158821	0.098049496	-0.551640777
H146	0.829645562	-9.159360659	-2.797642894
H147	0.526723401	-8.163994932	-4.057478777
H148	-3.489293628	-9.497843312	-3.835601043
H149	-1.336894672	-9.466242008	-4.770642050
H150	-0.954911254	-10.658101853	-3.531165222
H151	-4.022565110	-7.295002958	-2.158219399
H152	-3.571706902	-10.698840226	-1.172426019
H153	-5.171016297	-8.596577035	-2.557288598
H154	-3.554593828	-11.634758910	0.955298249
H155	-1.499567476	-9.587346156	0.032835058
H156	-4.631035426	-10.333164936	1.517700473
H157	-1.062699995	-4.692174420	1.619987125
H158	-1.626675270	-7.125054074	0.170472070
H159	0.492271085	-8.832162347	0.973524654
H160	-5.276180350	-5.272342064	3.724257632
H161	-3.890957708	-6.958607891	1.821528603
H162	-0.055241967	-9.311023166	2.598756613
H163	-2.369304225	-4.955393192	0.434895609
H164	-3.188593774	-8.208780737	4.203281676
H165	-5.597308898	-6.993936597	3.386582767
H166	1.271998891	-4.183636252	3.361395996
H167	1.151543481	-2.914015272	2.120149386
H168	2.064801641	-2.605333986	3.611067467
H169	-0.974027836	-3.064662036	3.407371025
H170	-2.670373015	-9.261360562	6.184463259
H171	-3.810082651	-1.503725233	3.689540532
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H173	-6.400828396	-1.932891483	7.176267061
H174	-0.269139148	-0.852662607	2.534568722
H175	0.576015010	-0.483448848	4.046276353

H176	3.362041247	4.895791040	8.533764921
H177	-5.551061295	-1.175991575	3.606731715
H178	-7.014256953	-1.359206259	5.609696761
H179	-4.479936103	-0.049191924	4.475991073
H180	-5.981265153	-0.299530445	6.599480944
H181	-5.102574289	-2.947152825	5.296596551
H182	-3.393510500	-0.796992126	6.657924049
H183	-2.698665484	-3.117607926	5.021239600
H184	-1.198283679	-0.659578130	4.035191772
H185	-2.534775351	3.979405954	1.528878926
H186	-4.029020558	3.637563506	2.449800739
H187	-2.809365614	5.139113211	3.631931215
H188	-2.751112255	3.975247999	5.961661406
H189	-0.247667562	5.534754897	3.995952098
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H191	1.223378736	2.906916585	7.958044588
H192	-0.958801948	-4.872417237	5.229338065
H193	1.365808507	-7.025317353	5.865406678
H194	0.699702092	-6.779607980	7.495185802
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H199	-5.325464656	-4.199819273	9.550286504
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H203	4.288550757	-3.904731609	-4.301728323
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H206	6.010950374	-1.568164061	-8.393798472
H207	3.219114198	-2.729205323	-7.849570117
H208	0.401388813	2.052191058	-10.176414014
H209	3.863852571	-1.963560811	-10.196702817
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H211	1.163242825	-5.546049687	-2.772150936
H212	1.976793932	0.657848039	-8.586094610
H213	-0.336451306	-0.476392600	-10.050081773
H214	4.100471741	0.706022870	-8.964105657
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H216	3.678470939	-1.129929252	-7.259099598
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H219	-0.544137449	-3.597579890	-2.102688070
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H222	-5.321074323	-1.103196550	0.900665175
H223	-2.730478284	-1.305165555	0.049393378
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H226	-8.208518258	-1.855050178	-0.891479607
H227	-13.163035871	-0.196136113	0.235967685
H228	-9.949669490	-1.695371892	1.720258432
H229	-10.827778579	-2.284789962	-0.794478125
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H233	-6.030601666	-0.007588189	-1.890371373
H234	-14.732636679	0.833467485	-1.487876492
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H236	-5.943317914	-2.510831506	-1.615624200
H237	-5.284674619	-5.513521944	-0.074852971
H238	-7.595903729	-4.710673198	-4.741490913
H239	-1.566999242	0.797412220	-3.450023788
H240	-6.612609904	-6.186788118	-4.679563929
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H244	-4.733819385	4.006137029	0.262973167
H245	-4.624899753	7.444893885	1.136512677
H246	-4.149627841	1.108481925	-3.168913728
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H251	-7.881915908	9.668444388	-1.743132915
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H254	-6.813258026	6.457691521	-2.930425657
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H264	-2.694419022	10.884432381	-1.878607173
H265	-2.341485423	-3.379995807	-5.596927510
H266	-1.577576163	6.573456475	-3.846554444
H267	-6.904071350	3.587573789	-1.523300820
H268	-5.956902937	-0.945697249	-5.298791003
H269	-3.811237665	10.587724332	-0.528434017
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H283	-5.805801502	8.581854960	2.683985941
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H287	10.216087764	2.551963592	-1.006348477
H288	10.145730798	2.660812495	-7.001405241
H289	9.345527802	1.299899436	-7.440501603
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H316	4.875091016	0.504560083	4.041740271
H317	0.055704476	2.634473298	-4.457064749
H318	0.958495316	-1.854394024	-6.394042801
H319	12.169251160	-2.146812856	2.043670625
H320	10.871614424	-0.406600659	-0.537401469
H321	9.857667933	-2.020779342	2.823452964

H322	12.511585482	-2.803894754	0.687500615
H323	4.617435874	7.939426227	-6.109851717
H324	7.790945398	0.304730532	2.480446184
H325	6.317499083	-4.133041752	1.903331506
H326	5.981703505	2.951406826	-5.190005138
H327	8.440495170	-4.600530909	0.521583666
H328	9.057866502	-0.884353241	-5.049757813
H329	6.871658986	-0.876974459	-3.749718499
H330	11.420619040	-6.063856323	6.452967251
H331	3.215558429	1.912352093	3.750097160
H332	9.275632427	0.661886591	4.354414410
H333	7.272944815	1.679634766	2.988765191
H334	9.668494280	-0.327805030	6.485255064
H335	3.058361889	-0.660019416	6.915525825
H336	10.969797718	-5.763206702	-2.176044110
H337	9.015695063	-2.818868913	-1.904930244
H338	9.699534961	-2.487340394	-0.302630083
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H340	4.319621885	1.240773897	-4.812020329
H341	-1.144773889	1.908631713	-6.548323126
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H343	5.135475863	-2.993225925	1.185272882
H344	10.395784093	-0.408870073	4.277607157
H345	10.808248764	-2.583470524	3.921817053
H346	1.647071488	0.225513172	6.480236386
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C 35(3/2) dissociated Fe(139) 0.561 -2.498 Fe(140) 0.485 -0.891 Fe(141) 0.523 -2.351 Fe(142) 0.569 2.836 Fe(143) 0.560 2.956 Fe(144) 0.515 2.227 Fe(145) 0.303 0.340	bm22b6x2n2xd35tb.car_5 C1 -1.841389755 -8.122807057 -4.489621634 C2 -0.913959671 -8.586100188 -5.617143999 C3 -4.166919625 -7.753701075 -3.785477537 C4 -4.153697218 -8.473106743 -2.438318748 C5 -3.702484695 -10.536563218 -1.206307553 C6 -2.562757308 -10.073577190 -0.290203330 C7 -0.366210782 -8.995648315 -0.158137614 C8 -0.719993751 -7.644601351 0.468468397 C9 -1.881551031 -5.515299274 0.235314201 C10 -2.889986337 -5.669614670 1.383714963 C11 -4.790907811 -6.877494979 2.294607005 C12 -4.217857003 -7.504416602 3.572201827 C13 -2.870871572 -9.302660455 4.539436339 C14 -1.611768562 -8.765774497 5.233460142 C15 0.570221647 -7.666305245 4.952772104 C16 0.782567199 -6.158676158 5.115813838 C17 -0.120854556 -3.896966246 4.654078131 C18 -1.237179386 -3.341801707 5.560296893 C19 -0.090344275 -3.257011592 3.242189736 C20 -0.196403456 -1.730518857 3.316823310 C21 1.167741692 -3.688819664 2.481211734 C22 -3.662812252 -3.096124129 5.931281225 C23 -3.912761841 -3.973388882 7.173825608 C24 -4.917916735 -2.965425701 5.035302504 C25 -6.153157900 -2.596983219 5.863360058 C26 -4.687855365 -1.929971900 3.926251436 C27 -4.264741111 -6.193257052 8.089560177 C28 -3.268738865 -6.026979156 9.220456955 C29 10.358778017 -7.105510474 4.949923933 C30 10.092591739 -5.601501561 4.857226699 C31 8.503006158 -3.822506626 5.621257721 C32 8.770713189 -3.343318333 7.062373094 C33 7.008170109 -3.761025364 5.264459637 C34 6.397303965 -2.360509548 5.359453851 C35 5.007488540 -2.342970707 4.719896192 C36 3.192154753 -0.676148637 5.167013860 C37 9.813867767 -1.612822353 8.448123352 C38 8.990662026 -0.407508344 8.848233808 C39 -1.124290268 -3.728142089 -4.732395507 C40 -2.499403936 -3.122829684 -4.405972843 C41 -0.086792134 -3.076034326 -3.790346456 C42 1.294403293 -3.760586089 -3.715080818 C43 2.313419802 -3.300602258 -4.758510110 C44 -4.095419737 -1.393444438 -5.090827686 C45 -5.450762248 -2.102021514 -5.048193466 C46 -4.156926122 -0.202752003 -6.071204730 C47 -6.694805900 -4.192255777 -5.240969870 C48 -6.952514520 -4.573264004 -3.775885400 C49 -6.051639014 -4.678551305 -1.490641724 C50 -5.987806955 -3.496336043 -0.526601747

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H160	-5.255712947	-5.925457481	2.581246815
H161	-3.863796171	-7.194025911	0.380607199
H162	-0.067109354	-9.662194664	0.659647003
H163	-2.341978740	-4.937435814	-0.578725051
H164	-3.179273891	-8.908871334	2.461986796
H165	-5.569874949	-7.542191925	1.897608279
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H179	-4.519473273	-0.931389469	4.362864888
H180	-5.999518070	-1.641164270	6.387655232
H181	-5.096090706	-3.949129328	4.564056441
H182	-3.406107352	-2.107471626	6.339579921
H183	-2.692668047	-4.041895121	4.261947885
H184	-1.110068031	-1.398992473	3.832946870
H185	-2.514129443	3.715869076	2.406812591
H186	-3.998507478	3.113789116	3.201773861
H187	-2.873451131	4.375119944	4.693465047
H188	-2.739932080	2.725097103	6.703421416
H189	-0.242665383	4.608930879	5.029407774
H190	2.175572940	4.273043721	5.445952794
H191	1.247214802	1.254087792	8.387277167
H192	-0.963956407	-5.798037803	4.119140793
H193	1.369134178	-8.030606947	4.289176007
H194	0.720578939	-8.121333551	5.940573652
H195	-0.864897078	-8.052459706	3.432790183
H196	-3.649352914	-9.358010791	5.310417039

H197	-1.173260614	1.559145035	7.936585915
H198	0.815458061	-3.659351613	5.175651018
H199	-5.282847625	-6.054958201	8.488245932
H200	-4.179271198	-7.230649990	7.729627922
H201	-2.272879920	-5.630123471	8.912214201
H202	10.881869960	-1.346357238	8.466703534
H203	4.314825739	-2.971443414	-5.023713473
H204	6.416589130	-6.166450118	-0.205149782
H205	5.473093405	-1.420769307	-9.105818115
H206	6.022908045	0.180022937	-8.548355195
H207	3.231460669	-1.070422341	-8.263624025
H208	0.394226784	4.088371325	-9.536707975
H209	3.871912179	0.164871217	-10.398395574
H210	0.036413950	-2.020502450	-4.083683211
H211	1.186928142	-4.853549915	-3.827737501
H212	1.989454758	2.398125543	-8.284339003
H213	-0.326532893	1.584620472	-9.940134943
H214	4.113833164	2.522008894	-8.644025809
H215	3.869473469	-3.451768201	-3.385861920
H216	3.688946465	0.371966727	-7.354285010
H217	5.229071346	1.894590118	-9.679461797
H218	-1.044718755	-4.343937188	-6.702804000
H219	-0.521635672	-3.081455332	-2.780223921
H220	6.582841041	0.431513354	-6.498254794
H221	1.713899669	-3.603760920	-2.710573367
H222	-5.286879445	-1.274902994	0.645586645
H223	-2.719301236	-1.309174312	-0.194977552
H224	-7.025907959	-5.164463617	-1.341589881
H225	-5.013166585	-4.030260379	-3.236277638
H226	-8.191329253	-1.616945060	-1.245149040
H227	-13.165714593	-0.271586955	0.219065295
H228	-9.901197307	-1.924411589	1.399622029
H229	-10.811094272	-2.064210024	-1.165178681
H230	-9.656177178	0.652942617	-0.280100549
H231	-13.753986376	1.495845036	-3.583740433
H232	-5.517668746	1.037064943	-0.337422393
H233	-6.003670828	0.336148830	-1.881742987
H234	-14.726118057	1.103887157	-1.252951013
H235	-10.022245312	-0.970364421	-2.308840578
H236	-5.930194781	-2.150523915	-2.092761282
H237	-5.281294090	-5.400523565	-1.184637525
H238	-7.587051665	-3.657106644	-5.591796921
H239	-1.515554896	1.422242452	-3.214475885
H240	-6.604723911	-5.114410250	-5.828387232
H241	3.872166077	5.378949454	9.006031679
H242	2.765178021	5.026778603	7.856426296
H243	-2.678552930	5.947599844	1.239966299
H244	-4.739176887	3.891041292	1.146342661
H245	-4.650090429	7.098983784	2.659767856
H246	-4.100588512	1.672673834	-2.909444776
H247	-5.234429580	2.060236404	-4.605747987
H248	-6.151659046	2.692452488	-3.469397442
H249	-3.213273821	0.357444832	-6.020304527
H250	-4.292374770	-0.571599221	-7.101550462
H251	-7.884790289	9.828534278	0.222985762
H252	-9.590058357	9.699315929	-0.297709232
H253	-6.306791567	8.289850487	-0.628010346
H254	-6.796935791	6.877268648	-1.515880238
H255	-5.959880612	8.311934624	-4.569419501
H256	-2.700492986	5.022418630	-5.041459197
H257	-10.397321395	2.991843664	-3.150444980
H258	-8.269828177	4.002587973	1.234108259
H259	-7.027116657	5.069442802	-3.688252095
H260	-1.361377712	5.961569866	-1.170880759
H261	-1.911017530	7.922221739	0.188932421
H262	-2.936701179	4.415209230	-2.415579998
H263	-4.653468467	-3.810678617	-5.807426669
H264	-2.645586174	11.018329721	0.347437390
H265	-2.324509109	-2.167948721	-6.156811728
H266	-1.597262365	7.186242554	-2.420657502
H267	-6.864104197	3.745781273	-0.776210510
H268	-5.959501825	0.129337902	-5.387643534
H269	-3.764109553	10.489741595	1.624294628

H270	-4.347767195	7.879342437	-4.990407594
H271	-7.524468305	6.653488370	-4.209220398
H272	0.219744197	-3.353663825	-6.241464323
H273	-1.202661447	-4.796381816	-4.453506923
H274	-11.814762539	3.370664850	-1.155298098
H275	-3.984866217	-0.983694268	-4.073691695
H276	-4.022575088	7.363775076	-1.821484347
H277	-2.866238025	6.672524188	-4.462977492
H278	-1.403692973	4.811701718	-3.169365792
H279	-4.841344249	4.432850933	-4.046692887
H280	-6.748705435	6.358631492	4.487694058
H281	-7.304700619	7.367724095	1.408432143
H282	-9.325716285	9.366796817	2.138096437
H283	-5.848064263	7.887799863	4.417249116
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H286	8.701598042	3.223551713	-4.651494999
H287	10.243746051	2.699766586	-0.466007991
H288	10.173527627	3.974852691	-6.350470915
H289	9.341346694	2.743213874	-7.043726395
H290	0.580983533	6.662697867	3.638064086
H291	-1.634942376	8.116429203	5.255377778
H292	-0.887453472	9.981488041	1.460354049
H293	-1.173424546	6.288281168	3.640594985
H294	-0.891391056	9.567005123	5.135418495
H295	3.858527556	8.080745844	-1.935685011
H296	0.151023917	8.992242843	3.099573609
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H298	9.071559770	-3.209974383	4.910795778
H299	3.674713331	6.196754714	-3.186872592
H300	1.867520433	0.867315895	5.263047020
H301	2.216707426	5.722101421	-6.417735986
H302	2.137739623	-0.246981420	-4.461057215
H303	1.174881414	5.218800752	-5.088019781
H304	4.327283919	-3.035624511	5.233365390
H305	3.499226562	4.383987210	-4.043272383
H306	5.079543692	-2.685147444	3.674547927
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H308	7.028308802	-1.629698866	4.830108951
H309	6.324301518	-2.034592917	6.409628753
H310	-0.755199836	0.120724355	-8.180573897
H311	8.501543725	-5.944124723	6.012843280
H312	10.174199068	-7.512419753	3.943861716
H313	1.676690204	1.771895880	-3.060081703
H314	9.960905102	-7.856545734	6.827053864
H315	9.318947235	-8.754103475	5.616052575
H316	4.808131546	-0.338703833	4.027936860
H317	0.049755889	3.450436519	-3.825437879
H318	0.972120677	-0.543904010	-6.633764557
H319	12.193809922	-2.525806297	1.581182694
H320	10.793466100	-0.314309552	-0.555697732
H321	9.872614110	-2.568303596	2.354348793
H322	12.533287470	-2.865360573	0.114887271
H323	4.552709865	9.056130959	-4.467910475
H324	7.764462372	-0.228484428	2.507749816
H325	6.283697990	-4.448603662	1.032256526
H326	6.004234724	3.962100244	-4.508593851
H327	8.398313257	-4.605279582	-0.430526604
H328	9.020955964	0.154223307	-5.099612067
H329	6.830005618	-0.097945169	-3.827758545
H330	11.438707933	-7.217193341	5.142577988
H331	3.112015250	1.048540829	4.057341808
H332	9.293451337	-0.249058233	4.397478848
H333	7.335680547	1.052850577	3.277630673
H334	9.693026916	-1.642182973	6.295687318
H335	3.091163362	-2.096602459	6.656727971
H336	10.960908017	-5.174929421	-3.262071157
H337	8.993599671	-2.346245233	-2.411381860
H338	9.654597085	-2.364544995	-0.762395130
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H340	4.335992336	2.196438655	-4.463045434
H341	-1.114832037	3.183097271	-6.034998965
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H343	5.099177247	-3.184036926	0.574553473
H344	10.418725644	-1.275339829	4.105477375
H345	10.818626657	-3.338256163	3.324961044
H346	1.639527738	-1.197594000	6.408326426
H347	10.996825722	0.616525215	-3.526208466
H348	9.368610309	0.426495915	0.171869520
H349	4.742352641	1.837571195	-6.165996249
H350	2.256387136	8.589829617	-2.511452605
H351	3.580513091	1.509056217	7.470748722
H352	3.951585159	2.823945715	6.328102470
H353	12.451589553	2.916643284	-1.194649965
H354	12.730505859	1.305483724	-1.196593967
H355	13.247053401	-0.061279817	3.056045190
H356	12.162090422	-0.072072419	1.044477280
H357	14.030148910	2.425975455	2.232217168
H358	11.829722572	0.818756922	3.673075334
H359	6.037795911	3.726744607	7.925612140
H360	-12.164469507	6.244304389	3.447451919
H361	9.641222249	-2.390799546	9.212169634
H362	7.991833410	-0.325971414	8.355627902
H363	-11.995355002	5.785462533	0.476770008
H364	-10.511303717	3.806698778	2.315519633
H365	-11.944648944	3.428524067	1.348702355
H366	3.243126585	-1.020127873	-1.023014878
H367	-8.274457629	2.970327178	-3.968250074
H368	0.965883839	-0.437034359	0.729300258
H369	-0.736069404	-0.239980295	-1.445115244
Mo370	6.158709920	-0.037504605	-0.563786477
N371	0.476080746	-8.176866037	-5.511679768
N372	-3.176542783	-8.232560295	-4.739220130
N373	-3.802809318	-9.782573157	-2.446647617
N374	-1.460251595	-9.586576007	-0.912464725
N375	-1.427331582	-6.785559108	-0.308391182
N376	-3.803367239	-6.660766898	1.251043637
N377	-3.363320135	-8.544882665	3.400315827
N378	-0.722615658	-8.095981527	4.446231543
N379	-0.183648845	-5.355144405	4.600084483
N380	-2.517834412	-3.574467615	5.154533258
N381	-3.978004246	-5.314170850	6.971184816
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N383	8.978973054	-5.196477597	5.496027490
N384	4.404960078	-1.004390068	4.696609320
N385	2.561671245	-1.458799110	6.071808930
N386	2.570283915	0.410546708	4.683992792
N387	9.440465190	-2.167776145	7.161020467
N388	-0.799430889	-3.521047782	-6.148011210
N389	3.594241769	-3.243380395	-4.347834307
N390	-2.967136064	-2.263944367	-5.353116541
N391	-5.508843286	-3.382742576	-5.458816257
N392	-5.927181172	-4.359573730	-2.901433295
N393	-5.948958404	-2.243445308	-1.078038454
N394	-3.483797331	0.990208922	-2.397777933
N395	-1.746940750	-0.082176397	-1.682072033
N396	-8.346994113	-0.992546814	-0.458084552
N397	-12.071064345	0.355806495	-2.866084033
N398	-13.823490333	0.753130160	-1.562412814
N399	3.730319216	4.844503911	8.145455302
N400	-0.776627898	8.570865540	4.926561728
N401	-1.824666116	9.693922855	1.728084220
N402	-2.804663856	8.059488805	-0.306410279
N403	-4.542202074	5.414057617	-4.183719825
N404	-5.201497891	7.640654184	-4.497060496
N405	-6.769883061	6.018346845	-3.966237289
N406	-3.629681719	5.642518155	0.963336219
N407	-5.542900418	6.612876610	2.793905819
N408	-7.998433998	7.786386454	2.031120099
N409	-7.067534112	7.678861930	-0.948185415
N410	-10.357903967	6.414982062	1.609922653
N411	9.250996901	3.702686577	-6.696780524
N412	5.932801254	3.285837251	-5.276259370
N413	3.165241776	4.518506716	-5.018996011
N414	3.195620087	7.015715214	-3.586170387
N415	4.225449180	2.019341172	-9.532933886

N416	1.438878663	1.824532002	-8.931218651
N417	12.002680105	2.009968441	-1.353580716
N418	8.032388402	0.248730794	-2.077250771
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N420	12.103500300	0.807818331	1.558040771
N421	-2.247820843	2.877961261	-0.183000055
N422	-1.919214911	2.117160900	0.556117280
O423	-1.414147018	-7.729629726	-3.387720473
O424	-4.464861039	-7.870139416	-1.398190611
O425	-2.660204532	-10.177118446	0.943085231
O426	-0.379647810	-7.359627649	1.627142547
O427	-2.864957343	-4.914287096	2.368617012
O428	-4.558656830	-7.093644047	4.694723333
O429	-1.431576096	-8.990729120	6.437892031
O430	1.811281017	-5.746345888	5.671764638
O431	-0.963582366	-2.717023671	6.596788523
O432	-4.049760832	-3.480859173	8.305525367
O433	-3.503469123	-6.354611448	10.373612630
O434	10.874593881	-4.875614754	4.206410089
O435	8.393428625	-4.020776815	8.034500472
O436	9.367781703	0.419937405	9.662279758
O437	-3.123276264	-3.387759045	-3.358660178
O438	1.976931539	-3.013868202	-5.929957498
O439	-6.443852311	-1.479750708	-4.607471329
O440	-5.220869658	0.696959170	-5.723664726
O441	-8.048929978	-5.048870554	-3.458254565
O442	-5.994199238	-3.688721515	0.692358431
O443	-7.390573336	0.069753538	1.322240526
O444	-10.950375810	-0.223094478	1.815031486
O445	5.820433699	2.234138358	9.303832169
O446	-2.189124507	3.338330140	6.182926813
O447	-3.100397336	8.411996285	3.110733770
O448	-4.727860437	9.311500927	-0.429775709
O449	-5.060685859	5.343337075	-0.799321055
O450	-6.528476979	4.544527546	2.830598907
O451	-3.242442486	4.911317724	3.960497227
O452	-8.389552176	8.483508568	4.180428453
O453	-11.480124192	8.317608606	1.030195557
O454	-9.247588379	7.461112816	-1.599890625
O455	-13.681162866	5.318304781	2.444228818
O456	-7.718669276	3.229130677	-3.207400229
O457	7.096099077	1.986009190	-6.772377321
O458	3.149911523	3.580045507	-7.111400413
O459	1.713377636	7.878774280	-5.082156354
O460	3.804722973	10.561256834	-3.308879681
O461	1.404019288	0.053825552	-10.369848258
O462	5.480943823	-2.440144891	-6.679485381
O463	6.424284939	-0.496046336	-6.137073285
O464	-1.399150598	3.938186668	-8.584810240
O465	11.366529120	2.941261559	1.749871877
O466	13.754598319	2.506000110	4.251725065
O467	4.355062148	-4.460742045	-1.613283805
O468	5.727421746	-6.052668173	-0.887461144
O469	11.583072256	-3.818581811	-1.525941786
O470	10.147208082	-4.669449247	-3.051041887
O471	7.626849178	-0.987758892	0.866066143
O472	8.340421310	-2.981405590	1.641614058
O473	6.456521960	-1.999068180	-1.253898242
O474	10.085611780	-0.668861540	4.818686060
O475	7.780992615	0.193553433	3.405961192
O476	-5.223128094	2.655641352	-3.807637612
O477	12.924137817	-2.457651519	0.914980845
O478	10.762448028	-2.495043066	2.804301675
S479	-0.324192881	6.502806820	1.372872427
S480	1.023942633	4.023986471	-1.116949600
S481	4.655402639	0.485050885	-2.383766310
S482	1.050623062	2.809671108	2.175340306
S483	1.211260969	0.212650399	-0.450582238
S484	4.852419034	4.392411872	-2.198876753
S485	4.521877741	-0.662907382	1.100087462
S486	3.375171776	5.486659604	1.350365504
S487	6.804269081	2.138542005	0.173418047
S488	4.685758329	2.400243045	3.284799979

Structure D 47(1)

D 47(1) associated	bm2cnx2b6x2hn2n2xd1td.car_3			
Fe(139) 0.546 2.404	C1	-2.339904736	-1.801171039	-8.960994760
Fe(140) 0.277 0.161	C2	-1.283774871	-1.555374425	-10.042926180
Fe(141) 0.521 1.789	C3	-4.685511427	-1.497449152	-8.300708847
Fe(142) 0.543 -2.624	C4	-5.028482854	-2.913289193	-7.840370661
Fe(143) 0.605 3.126	C5	-5.130932691	-5.290769015	-8.387320444
Fe(144) 0.487 -2.198	C6	-4.143475538	-5.853851823	-7.361174740
Fe(145) 0.353 -1.066	C7	-1.873507343	-5.748703412	-6.446192588
	C8	-2.122611476	-5.109870243	-5.076445961
	C9	-2.802207939	-3.124367718	-3.830986679
	C10	-4.022520232	-3.709657166	-3.104256749
	C11	-6.236492475	-4.700216155	-3.278138444
	C12	-6.044178260	-6.146793228	-2.800949032
	C13	-5.378820482	-8.421699591	-3.423995441
	C14	-4.183682505	-8.931036168	-2.610926774
	C15	-1.794140698	-8.687859399	-2.099129050
	C16	-1.352768816	-7.895379247	-0.866050970
	C17	-1.720493747	-5.829016681	0.456385615
	C18	-2.836144389	-5.754027485	1.514428673
	C19	-1.312573130	-4.444830422	-0.116537185
	C20	-1.115825403	-3.390895901	0.977724377
	C21	-0.052074208	-4.567882603	-0.980910077
	C22	-5.196482047	-5.234500049	2.004840622
	C23	-5.836777696	-6.614435550	2.253866303
	C24	-6.220222485	-4.179095079	1.521560112
	C25	-7.468877497	-4.176742647	2.411019380
	C26	-5.584143085	-2.782175919	1.487106088
	C27	-6.811717684	-8.636598061	1.333154310
	C28	-6.031507148	-9.556242093	2.254860031
	C29	7.459133277	-11.001880539	-1.893736926
	C30	7.517009784	-9.880046172	-0.855554812
	C31	6.222070493	-8.856945239	1.025926998
	C32	6.263407079	-9.640204058	2.352770511
	C33	4.879251043	-8.125112387	0.841603901
	C34	4.590247249	-7.082999246	1.925889324
	C35	3.400885772	-6.203909159	1.539053692
	C36	1.999971373	-4.794629205	3.064070524
	C37	7.234351013	-9.754805141	4.598557755
	C38	6.555746403	-9.006104537	5.725867828
	C39	-0.982894422	1.072907797	-5.831098666
	C40	-2.222926176	1.669058902	-5.145466254
	C41	0.006428662	0.648228929	-4.719364534
	C42	1.186565261	-0.238773766	-5.168861558
	C43	2.439718780	0.521575815	-5.602435868
	C44	-3.293574578	3.777452830	-4.491709855
	C45	-4.716099619	3.725804386	-5.065500192
	C46	-2.855706891	5.237510760	-4.257484498
	C47	-6.216682954	2.669744468	-6.688065155
	C48	-6.811748720	1.427757103	-6.006188025
	C49	-6.405146222	-0.492457042	-4.521462098
	C50	-6.447159794	-0.383314334	-2.996685276
	C51	-5.825905065	0.831111541	-0.959880149
	C52	-7.245452301	1.117060269	-0.407418378
	C53	-4.975616174	2.022897669	-0.491958907
	C54	-3.503829065	1.994411112	-0.754633443
	C55	-2.573743487	0.997365887	-0.924752356
	C56	-1.481118393	2.929158312	-0.890582518
	C57	-9.260096841	2.509239897	-0.787270636
	C58	-10.285039594	1.419786015	-0.479694127
	C59	-9.752818888	3.407379241	-1.945930022
	C60	-10.763604443	4.463082228	-1.605638474
	C61	-11.872578446	4.435579436	-0.782415131
	C62	-11.671899533	6.424164648	-1.740499184
	C63	2.365140022	-4.616627941	8.278937187
	C64	3.662959817	-5.397922698	8.197738761
	C65	1.939221485	-4.299409575	6.822096944
	C66	0.626767922	-3.555726959	6.743987336
	C67	-0.602179330	-4.236103188	6.658593929
	C68	0.598146810	-2.149207805	6.772471187
	C69	-1.815206006	-3.541376510	6.602087309

C70	-0.603561179	-1.442284367	6.727481200
C71	-1.810496493	-2.140210983	6.640191653
C72	0.170408425	3.529565488	8.448883358
C73	-0.873081213	4.632586709	8.225977197
C74	0.289646980	2.653677818	7.192419224
C75	-1.256128886	7.042834093	7.909982733
C76	-1.800318221	7.189945958	6.487931834
C77	-1.619165999	6.452272606	4.133729888
C78	-2.668141504	5.351392835	3.861944798
C79	-0.376697416	6.343434550	3.228926697
C80	-0.588239118	6.368864757	1.712045871
C81	-1.066732995	7.694565214	1.096134823
C82	-3.291550424	8.777312147	1.389940481
C83	-3.487403878	3.103242474	4.343120984
C84	-4.734219448	3.227422281	5.238250945
C85	-2.878751137	1.710803246	4.564793042
C86	-5.532380814	3.717967585	7.494232375
C87	-6.536770963	4.835715553	7.756308445
C88	-7.357845843	7.070875483	7.143865534
C89	-8.785691300	6.981236424	6.563684741
C90	-6.647020979	8.362693817	6.686018177
C91	-6.443220018	8.406930454	5.176402148
C92	-10.276594363	5.834959883	4.981859931
C93	-11.402094948	5.494793636	5.952970130
C94	-10.158485305	4.729655169	3.899537341
C95	-9.146746310	5.090407597	2.835721085
C96	-9.504172760	5.939122391	1.775779149
C97	-7.814134853	4.652082428	2.912831805
C98	-8.560983478	6.365798730	0.838022405
C99	-6.850389827	5.086378773	1.996047463
C100	-7.236328581	5.947444528	0.970930624
C101	9.732443308	4.268682596	-1.047030105
C102	8.469657950	4.288154612	-1.890197251
C103	5.988045251	4.355841108	-1.815656766
C104	5.175904204	5.614145274	-1.490106859
C105	3.915743719	6.790674696	0.249129851
C106	4.038573045	7.173223025	1.721805052
C107	4.883930931	6.672751146	3.966505333
C108	6.197540614	7.305404396	4.376191032
C109	5.477405225	6.077271478	-6.012860758
C110	4.055629727	6.645513882	-6.079046829
C111	5.396540762	4.546428706	-5.810296082
C112	6.746540702	3.868502347	-6.104216949
C113	6.731515899	2.433903463	-5.625013533
C114	2.083581604	7.396178966	-4.844417850
C115	1.953215876	8.516517434	-3.831777231
C116	1.012507919	6.284401377	-4.729117043
C117	1.317010878	5.310633769	-3.621542609
C118	0.983482728	5.602185939	-2.288919190
C119	2.050198716	4.141979237	-3.893159516
C120	1.419886185	4.766923635	-1.254531227
C121	2.484319921	3.308122953	-2.858009260
C122	2.187888325	3.632834515	-1.532353633
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C126	9.671032560	-0.953030565	-0.892836315
C127	10.481005947	-0.197856003	-1.716811508
C128	8.362651828	0.337344755	-2.075183851
C129	11.610717099	-5.128851384	2.684281735
C130	12.682693120	-4.812204993	3.703147465
C131	4.320127218	-3.846177911	-3.866863445
C132	4.933175294	-4.236046989	-2.551759660
C133	6.341807328	-3.563987543	-2.293083753
C134	7.324372794	-3.954949780	-3.433326497
C135	8.763888651	-3.493321217	-3.148067296
C136	9.772582859	-4.062906038	-4.104147574
C137	6.889252530	-4.194911433	-0.975781345
C138	3.891252672	0.524700163	1.905034922
Fe139	5.563045740	1.079078781	0.969257182
Fe140	1.666602140	0.495216450	1.960942710
Fe141	3.733985249	0.218297851	3.812338792
Fe142	3.983539465	2.392523272	2.504451530

Fe143	1.954307278	2.325989879	4.219182829
Fe144	4.986177604	-1.145353939	2.108314526
Fe145	3.671334261	-0.437286020	-0.011417558
H146	0.235597577	-2.599472131	-9.169522315
H147	0.332832002	-0.988206504	-8.927839939
H148	-3.767198030	-0.899194767	-10.135975632
H149	-1.438706712	-0.552288579	-10.471193686
H150	-1.490197103	-2.266412621	-10.862131854
H151	-4.430956252	-0.931205412	-7.393930783
H152	-4.537310948	-3.677109175	-9.682523607
H153	-5.584043825	-1.049283407	-8.746603009
H154	-5.084586634	-5.903285134	-9.297269806
H155	-2.673434097	-4.601244777	-8.057688569
H156	-6.134172970	-5.394141658	-7.953723123
H157	-1.958679684	-3.188388822	-3.130427383
H158	-2.492595779	-3.275343759	-5.957246715
H159	-0.887377452	-5.439944256	-6.818046631
H160	-6.541858668	-4.105149286	-2.408540797
H161	-5.031700619	-3.947060984	-4.896386188
H162	-1.865049459	-6.835254643	-6.296510234
H163	-2.980425931	-2.062317304	-4.054253042
H164	-5.165779536	-6.657089901	-4.604503142
H165	-7.050054374	-4.682114467	-4.016189394
H166	-0.193096063	-5.275894275	-1.809595434
H167	0.213791150	-3.590441216	-1.412526769
H168	0.806229181	-4.904253065	-0.378221448
H169	-2.140450388	-4.108911686	-0.761726935
H170	-5.360722615	-8.938941985	-4.394794382
H171	-4.712547250	-2.738943742	0.818351441
H172	-6.052291729	-6.981882493	0.212850807
H173	-7.994668296	-5.142999697	2.394628657
H174	-0.940978353	-2.404859560	0.522215449
H175	-0.235040331	-3.606848139	1.598397589
H176	1.600781244	-5.284731999	8.720116583
H177	-6.320591103	-2.043161659	1.137872312
H178	-8.169984325	-3.401063178	2.070464129
H179	-5.260170605	-2.484848589	2.498153557
H180	-7.199498549	-3.956222481	3.456618977
H181	-6.526491583	-4.452572584	0.494967362
H182	-4.804659628	-4.927464714	2.985859520
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H184	-1.990460576	-3.297233127	1.639449549
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H190	1.535724145	-1.590031353	6.795956139
H191	-0.616308068	-5.328997246	6.630067810
H192	-2.785214999	-6.508550522	-1.276864426
H193	-0.962390672	-8.653500367	-2.817859126
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H200	-6.856432635	-9.129062784	0.348220941
H201	-4.932775018	-9.367044362	2.287508167
H202	8.297747386	-9.898642718	4.841463253
H203	4.486396327	0.427587046	-5.534519967
H204	5.106346498	-5.434872312	-4.624465331
H205	6.924542143	3.868429162	-7.189695182
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H207	4.629700832	4.113439893	-6.471075290
H208	2.889991407	9.105396741	-3.682229637
H209	5.882867974	6.256990364	-7.021125798
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H217	7.297713781	6.568119468	-5.201090742
H218	-0.697617622	1.874746778	-7.714352540
H219	-0.571848105	0.090800556	-3.968328939
H220	7.727933038	3.022534009	-4.035001594
H221	1.445715247	-0.932535963	-4.355868232
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H223	-2.684987192	-0.079090191	-0.982299513
H224	-7.429701825	-0.715070697	-4.845795289
H225	-4.963195213	0.930420865	-5.192753138
H226	-7.668025410	2.087374945	-2.156854055
H227	-12.289733156	3.670085111	-0.137642687
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H232	-5.129583820	2.099880061	0.597076956
H233	-5.394159977	2.943496407	-0.930811900
H234	-13.264652876	6.011180693	-0.388427830
H235	-8.873763230	3.941583775	-2.338243525
H236	-5.147993708	1.222531970	-2.965026184
H237	-5.789507427	-1.364331838	-4.790342160
H238	-6.919567855	3.494451456	-6.514034763
H239	-0.670970183	3.651397930	-0.920636169
H240	-6.177358231	2.485811192	-7.769887930
H241	2.655544973	-3.599634161	10.034596640
H242	1.791308952	-2.761782474	8.929413648
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H245	-3.621555586	4.139382582	6.698160217
H246	-3.199503533	4.151925707	-0.625173311
H247	-3.748044132	5.916893625	-1.626756046
H248	-4.759772679	5.823667235	-0.405361571
H249	-1.864045874	5.244494826	-3.785235748
H250	-2.795057285	5.772250006	-5.220477003
H251	-5.691984952	8.441807548	7.226274842
H252	-7.282712926	9.211547554	6.971563941
H253	-4.384977326	7.972726060	5.353574419
H254	-5.053751004	8.007359580	3.735368391
H255	-3.380855797	10.645419525	2.221477011
H256	-0.626584690	7.823272548	0.095371500
H257	-8.860332475	7.014377102	0.010800110
H258	-7.499541206	3.957305165	3.697044458
H259	-5.069617198	7.796735389	1.025417143
H260	0.150832493	5.407691478	3.472328725
H261	-0.448303744	5.801527226	5.799223193
H262	-1.250052506	5.548358431	1.394002490
H263	-4.070331481	2.690660736	-6.691001851
H264	-0.705089505	7.960240336	8.156989854
H265	-1.552228842	3.435448119	-5.804729445
H266	0.300310950	7.167275865	3.509662542
H267	-5.805476256	4.789800355	2.109950900
H268	-4.670479266	5.579824429	-3.633498248
H269	-2.130939770	6.989033063	8.573762304
H270	-1.823321054	10.195157535	1.631809440
H271	-5.209161767	9.476759852	1.380812765
H272	0.641703848	1.978954263	-6.715823909
H273	-1.333286885	0.151357553	-6.332551114
H274	-10.537092727	6.281687846	1.678365213
H275	-3.395263502	3.301938259	-3.500862047
H276	-2.144270187	7.399438305	3.952043736
H277	-0.707696936	8.531703939	1.708706739
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H280	-6.123766306	2.811378982	7.298197424
H281	-5.786784796	5.933583167	6.194525793
H282	-7.504176345	7.132262161	8.232335012
H283	-4.981890599	3.562739736	8.432300307
H284	-8.229873057	5.376957215	5.434083331
H285	9.558692489	4.787522822	-0.093340235
H286	9.910189071	3.200693255	-0.800715678
H287	10.283749475	-0.885591634	1.817079889
H288	11.711322710	4.691237024	-1.292741733

H289	10.896358678	4.498062064	-2.700488648
H290	1.082423433	1.913884306	7.360511689
H291	-1.142483621	2.352478637	9.473957186
H292	0.615812362	6.051359160	8.194464605
H293	-0.665699333	2.138586021	7.020115570
H294	-0.156090648	3.214690414	10.452970546
H295	4.728525294	5.746242674	4.541729308
H296	1.149999396	3.990834018	8.652104639
H297	4.069937114	-8.873804442	0.803684052
H298	7.040539096	-8.127760726	0.993325479
H299	5.191424732	5.509394130	2.213793842
H300	1.071960841	-3.371500085	4.206002954
H301	4.193496735	7.674403439	-0.339962002
H302	3.064648580	2.409728611	-3.078965803
H303	2.842900179	6.619820357	0.064293366
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C128	8.384364649	0.327431860	-2.095072215
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C132	4.943203248	-4.238327849	-2.572620543
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Fe145	3.659641015	-0.438633719	-0.042067321
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O429	-6.417174424	-6.492173678	-1.663007034
O430	-4.275944777	-9.946356412	-1.920883356
O431	-0.371662040	-8.272653605	-0.189988781
O432	-2.590099735	-6.029379571	2.721629115
O433	-6.038609758	-7.034892468	3.439459944
O434	-6.518919058	-10.490556073	2.900877471
O435	8.508450962	-9.122674509	-0.818937423
O436	5.577501759	-10.674926718	2.489898829
O437	6.915251947	-9.106731488	6.880884505
O438	-3.082901449	0.954703472	-4.527049227
O439	2.363483055	1.591810251	-6.233367703
O440	-5.662430884	4.275808128	-4.452227443
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O443	-7.102538616	-1.204531293	-2.335157706
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O445	-11.122739855	1.525984886	0.376058236
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O447	-2.992310988	-1.385986081	6.565129755
O448	-2.101031367	4.398704351	8.146973435
O449	-2.739451198	7.983876653	6.310858793
O450	-3.587987486	5.575043438	3.102642433
O451	-5.763150057	2.697566980	4.875671073
O452	-2.763639515	1.450422369	6.020868955
O453	-7.331771615	4.726913647	8.681372637
O454	-9.657810900	7.763859736	6.929879850

	O455 -7.368695191 8.630358928 4.388887988
	O456 -12.566392909 5.691054891 5.715866267
	O457 -6.243650880 6.384086656 0.080157988
	O458 8.528546626 4.206714475 -3.143675014
	O459 4.951655407 6.499739004 -2.325987415
	O460 3.388471934 8.155823320 2.121653075
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	O463 6.176259406 1.515170378 -6.194987712
	O464 7.349026911 2.207235249 -4.428169545
	O465 0.897392227 8.774288571 -3.268974475
	O466 11.059287658 -2.605857694 3.496867636
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	O470 10.755136226 -4.748318437 -3.789981322
	O471 9.553591713 -3.718726110 -5.401777578
	O472 7.127663081 -3.330088388 -0.038604968
	O473 7.118317807 -5.403975242 -0.921496248
	O474 6.211298919 -2.187438799 -2.220132515
	O475 8.471491038 -6.684197260 2.859352861
	O476 6.771972284 -4.436670589 2.553789195
	O477 -3.790587254 5.765180096 -0.638405524
	O478 11.719053867 -5.930999177 -1.103703739
	O479 9.247071495 -6.641353082 0.176167843
	S480 0.671544601 3.610831658 5.688101033
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	S489 4.552231932 -1.877279258 4.120322289
D 47(1) dissociated	bm2cnx2b6x2hn2n2xd1te 2 53125.96
Fe(139) 0.548 2.417	C1 -2.326451552 -1.787246142 -8.942496029
Fe(140) 0.349 -0.884	C2 -1.272217034 -1.540492327 -10.027434171
Fe(141) 0.551 2.646	C3 -4.679201925 -1.499333194 -8.298493605
Fe(142) 0.553 -2.708	C4 -5.018265067 -2.916364232 -7.839280361
Fe(143) 0.607 3.183	C5 -5.116578682 -5.294644489 -8.385817547
Fe(144) 0.521 -2.216	C6 -4.132474816 -5.854337012 -7.356555177
Fe(145) 0.323 -1.018	C7 -1.864654089 -5.744297258 -6.433503146
	C8 -2.116524813 -5.099805382 -5.066834521
	C9 -2.795766696 -3.106893881 -3.835167382
	C10 -4.015863113 -3.688927297 -3.102588546
	C11 -6.225232187 -4.694183195 -3.271398741
	C12 -6.028004350 -6.138754119 -2.790972723
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	C14 -4.174089560 -8.923592945 -2.603500750
	C15 -1.784669863 -8.672236621 -2.092777672
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	C17 -1.703664795 -5.812568413 0.465330339
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	C22 -5.183029547 -5.228033621 2.022375347
	C23 -5.816976918 -6.609302590 2.272127499
	C24 -6.213144210 -4.180300926 1.539234210
	C25 -7.459163315 -4.177572383 2.431710926
	C26 -5.582826090 -2.781916989 1.497379509
	C27 -6.783404860 -8.632586615 1.352052094
	C28 -6.007483698 -9.554307779 2.273648680
	C29 7.457816885 -10.994525993 -1.902038758
	C30 7.515590306 -9.874984139 -0.860216151
	C31 6.217791320 -8.857475159 1.021266128
	C32 6.259481428 -9.639871407 2.347300992
	C33 4.875600057 -8.125118223 0.837980090
	C34 4.587927012 -7.085820795 1.924887040
	C35 3.403651555 -6.199202622 1.541207056
	C36 1.993717329 -4.792992940 3.060001600

C37	7.236871463	-9.759180354	4.590645148
C38	6.560336118	-9.010257203	5.719121893
C39	-0.981237831	1.065233131	-5.804409776
C40	-2.227566824	1.660160294	-5.126281420
C41	0.010650640	0.648491672	-4.694359055
C42	1.191196608	-0.237185824	-5.144917726
C43	2.441395805	0.524804783	-5.582093380
C44	-3.302547172	3.771477960	-4.490619982
C45	-4.724355333	3.725557340	-5.071011648
C46	-2.862104771	5.230113479	-4.255619293
C47	-6.224066998	2.663501212	-6.691515456
C48	-6.819192824	1.421081264	-6.011969744
C49	-6.414293525	-0.498212698	-4.526359321
C50	-6.458018703	-0.386665538	-3.002239608
C51	-5.819097089	0.820342995	-0.968921049
C52	-7.237957420	1.105964639	-0.418495612
C53	-4.980103873	2.021850836	-0.506709213
C54	-3.513552406	1.997002613	-0.783676599
C55	-2.594965368	1.000282817	-1.002653083
C56	-1.487763811	2.920126444	-0.922285225
C57	-9.232570023	2.517688761	-0.786900614
C58	-10.262261765	1.433722353	-0.475391058
C59	-9.731517255	3.413886233	-1.945771199
C60	-10.743550592	4.469281798	-1.606093494
C61	-11.844468556	4.445949065	-0.771549739
C62	-11.661896906	6.424939700	-1.752171595
C63	2.350138322	-4.612070081	8.279297768
C64	3.645203904	-5.400212263	8.201996933
C65	1.928591241	-4.300433746	6.819917197
C66	0.620349735	-3.550464406	6.732413499
C67	-0.611223482	-4.228428287	6.659574291
C68	0.596735100	-2.142696231	6.742488316
C69	-1.822069734	-3.530480729	6.599650869
C70	-0.604258137	-1.433309964	6.696293722
C71	-1.813557873	-2.129707113	6.624165999
C72	0.157397895	3.520469342	8.465743743
C73	-0.877924949	4.629008706	8.237139423
C74	0.270589792	2.641697535	7.210399274
C75	-1.250877645	7.040169014	7.926428018
C76	-1.792043309	7.193534971	6.503113766
C77	-1.605975992	6.460631538	4.148115984
C78	-2.654081345	5.357732501	3.878438461
C79	-0.363414726	6.353525890	3.244369705
C80	-0.573812850	6.375950223	1.726426769
C81	-1.057431446	7.699298695	1.109246672
C82	-3.287600795	8.776648483	1.373584648
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C90	-6.642282739	8.360759221	6.680749651
C91	-6.436708896	8.395465703	5.171225427
C92	-10.260285955	5.829166778	4.979774473
C93	-11.385038265	5.493159047	5.953382930
C94	-10.150899273	4.725384478	3.896774884
C95	-9.141137491	5.086045096	2.832044339
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C97	-7.812746135	4.637250003	2.903755600
C98	-8.551343706	6.368384567	0.841041837
C99	-6.848052609	5.067077114	1.986891687
C100	-7.230535244	5.935202648	0.966687717
C101	9.740248890	4.284660321	-1.057910169
C102	8.472753832	4.304626576	-1.895775836
C103	5.991396571	4.355265589	-1.817025394
C104	5.167400708	5.603954633	-1.484052110
C105	3.907037096	6.773727296	0.259022359
C106	4.028370849	7.165260276	1.729531919
C107	4.881534427	6.687095202	3.974722283
C108	6.193304089	7.323012909	4.383350470
C109	5.484867401	6.079834534	-6.007274191

C110	4.065501581	6.653595609	-6.081931064
C111	5.397881602	4.548219588	-5.806412431
C112	6.745480798	3.864543462	-6.101025059
C113	6.734409331	2.433989042	-5.611640829
C114	2.078140625	7.375429792	-4.852642987
C115	1.943843702	8.495980766	-3.839501238
C116	1.007682289	6.263741886	-4.737120744
C117	1.304241497	5.297838464	-3.619492343
C118	0.955542090	5.597692807	-2.292364729
C119	2.041559623	4.127672839	-3.874418802
C120	1.379104954	4.769451479	-1.247252551
C121	2.461008359	3.299520784	-2.828301618
C122	2.147457993	3.630579673	-1.508306062
C123	10.866974511	-1.650444939	1.272594696
C124	11.079722226	-2.802938476	2.269157671
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C126	9.668013495	-0.964099018	-0.894800798
C127	10.483167986	-0.208990506	-1.713490558
C128	8.368051198	0.326618047	-2.087873370
C129	11.621972080	-5.141256194	2.681333538
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C136	9.781987478	-4.061643539	-4.108738292
C137	6.889343290	-4.178963567	-0.988239562
C138	3.916149557	0.533059261	1.918153774
Fe139	5.572574285	1.098073392	0.933769230
Fe140	2.060192982	0.595173795	1.788955358
Fe141	3.579863953	0.158066545	3.846780899
Fe142	4.069629731	2.409316554	2.598268489
Fe143	1.933389293	2.356888840	4.163119949
Fe144	4.947957177	-1.139091913	2.079231554
Fe145	3.653858567	-0.424183163	-0.024901180
H146	0.250766920	-2.592252667	-9.168563460
H147	0.348756074	-0.981512544	-8.913684021
H148	-3.755537638	-0.905799064	-10.130102657
H149	-1.428095997	-0.536275838	-10.454691842
H150	-1.485131780	-2.251016191	-10.845754984
H151	-4.431688586	-0.932514320	-7.390603758
H152	-4.527839648	-3.676848871	-9.681997003
H153	-5.578227221	-1.057253154	-8.749078738
H154	-5.065956366	-5.904899069	-9.296491128
H155	-2.660015619	-4.605990668	-8.054755286
H156	-6.122451972	-5.401284558	-7.958950285
H157	-1.952441298	-3.168182951	-3.133438227
H158	-2.483347421	-3.268402821	-5.958597038
H159	-0.877484998	-5.436141808	-6.804822200
H160	-6.528890837	-4.098472237	-2.402556674
H161	-5.021385334	-3.947798064	-4.891009165
H162	-1.857434773	-6.830449907	-6.279978239
H163	-2.976675515	-2.046017897	-4.064129033
H164	-5.165534670	-6.653371986	-4.601326487
H165	-7.039791276	-4.676824131	-4.008276311
H166	-0.181282687	-5.277040678	-1.806769039
H167	0.219560096	-3.588516625	-1.421373185
H168	0.815958228	-4.888870614	-0.371609434
H169	-2.134693848	-4.105823993	-0.765688166
H170	-5.356963603	-8.934012392	-4.384151597
H171	-4.714663629	-2.738161384	0.824625493
H172	-6.032123173	-6.974745920	0.228767614
H173	-7.981941579	-5.144734526	2.422724439
H174	-0.930685443	-2.394959920	0.503339587
H175	-0.245204128	-3.593855743	1.604995837
H176	1.583105946	-5.278332339	8.719144457
H177	-6.322096021	-2.044948912	1.149515247
H178	-8.164660725	-3.406726331	2.089099372
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H180	-7.188250327	-3.952693791	3.475542429
H181	-6.521838544	-4.458532378	0.515154342
H182	-4.791226710	-4.918301389	3.001752252

H183	-4.163816778	-4.974628544	0.147673252
H184	-1.999140896	-3.268900608	1.613887559
H185	-1.837930225	1.692976084	4.159684684
H186	-3.477246550	0.977047011	4.107005658
H187	-2.870693989	0.481766730	6.138470893
H188	-3.743804044	-1.977100951	6.473456198
H189	-0.602697461	-0.342767671	6.683874823
H190	1.536987244	-1.585686216	6.758349940
H191	-0.628787128	-5.321898149	6.644372065
H192	-2.778370922	-6.500832358	-1.256747798
H193	-0.953067490	-8.633660638	-2.812654519
H194	-1.913922566	-9.717533283	-1.781631426
H195	-2.941081097	-7.442412184	-3.390201153
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H197	-2.768790494	-4.072464741	6.528684218
H198	-0.843914037	-6.252195779	0.987225522
H199	-7.814589099	-8.535104900	1.731039820
H200	-6.828962618	-9.125652447	0.367907979
H201	-4.909157429	-9.365827339	2.310905966
H202	8.300450375	-9.903543351	4.833414561
H203	4.489164017	0.431503479	-5.523714701
H204	5.117676212	-5.449765421	-4.638816286
H205	6.917684161	3.856318450	-7.186775662
H206	7.564869892	4.422384316	-5.626125304
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H208	2.879088046	9.086901755	-3.688370844
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H210	0.390313387	1.560260548	-4.205665016
H211	0.885504643	-0.871762997	-5.995270890
H212	3.927346954	6.690940799	-4.005999084
H213	1.922169198	7.874165058	-5.829424864
H214	6.067742401	6.604470550	-4.084977564
H215	3.673846184	-0.887109490	-4.686083193
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H217	7.300798558	6.554841695	-5.176310703
H218	-0.699275740	1.854873408	-7.693312485
H219	-0.564845705	0.093369780	-3.938991865
H220	7.735801911	3.036868759	-4.029557479
H221	1.453179634	-0.927760435	-4.330669497
H222	-5.481809794	-0.111538154	-0.489342180
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H224	-7.438755417	-0.721958793	-4.849690092
H225	-4.971489690	0.926925509	-5.197387998
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H227	-12.249372835	3.686051926	-0.112977043
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H230	-9.066649248	3.119775926	0.120035003
H231	-11.898781665	7.451730346	-2.017948102
H232	-5.126624528	2.101569936	0.583586063
H233	-5.408638391	2.940151157	-0.943041789
H234	-13.235738864	6.024976706	-0.376576428
H235	-8.855614480	3.948484490	-2.345448010
H236	-5.123699769	1.192107202	-2.970838116
H237	-5.797298617	-1.368589454	-4.795026708
H238	-6.924798403	3.489596540	-6.517192154
H239	-0.673654987	3.639450459	-0.940342467
H240	-6.183128302	2.481601118	-7.773089902
H241	2.644915831	-3.595441075	10.031979819
H242	1.778480282	-2.757900604	8.929114771
H243	-1.581975389	3.972825040	4.998338313
H244	-3.806998908	3.138699926	3.316349527
H245	-3.614258180	4.140776814	6.707518704
H246	-3.196397022	4.150711187	-0.609287333
H247	-3.734684687	5.905046466	-1.617299397
H248	-4.744615324	5.817366555	-0.400779670
H249	-1.869896917	5.235628913	-3.784705306
H250	-2.803389583	5.768673236	-5.216966012
H251	-5.689435760	8.447233374	7.222954407
H252	-7.279418332	9.210357060	6.959868296
H253	-4.371466892	7.987635782	5.354342451
H254	-5.039651980	8.011498485	3.734614830
H255	-3.388054849	10.655278466	2.176644221

H256	-0.610252756	7.831159052	0.111951685
H257	-8.847632534	7.027625150	0.021246395
H258	-7.503354762	3.937952552	3.684734943
H259	-5.060815733	7.781145772	1.022680029
H260	0.171942013	5.423134838	3.492036347
H261	-0.443195448	5.800019732	5.814284607
H262	-1.231342289	5.550968337	1.408814334
H263	-4.077431329	2.679692317	-6.688546593
H264	-0.698031198	7.954997337	8.178024695
H265	-1.558619174	3.420335856	-5.798609646
H266	0.308070959	7.182600134	3.521039721
H267	-5.806005097	4.761049497	2.098684390
H268	-4.675917586	5.581736849	-3.628277702
H269	-2.128569970	6.986996551	8.586326753
H270	-1.826341716	10.205202338	1.594577702
H271	-5.208592024	9.469901831	1.343919947
H272	0.637875203	1.973727742	-6.695044031
H273	-1.330515770	0.141185598	-6.301838590
H274	-10.524450590	6.298483982	1.689538812
H275	-3.414964605	3.296434183	-3.500245356
H276	-2.130147438	7.407696618	3.963422594
H277	-0.709751953	8.536032958	1.728671389
H278	0.414108245	6.166585759	1.291633746
H279	-2.975039582	6.994382744	0.457379453
H280	-6.117068274	2.807084361	7.285840692
H281	-5.773483554	5.936993736	6.201726911
H282	-7.494052623	7.135804084	8.234661057
H283	-4.983111564	3.559173655	8.428932753
H284	-8.205259238	5.387747602	5.417434058
H285	9.566083586	4.793092160	-0.098605816
H286	9.922421796	3.214943758	-0.822121513
H287	10.277464944	-0.900354884	1.820084747
H288	11.716225733	4.712411821	-1.294982289
H289	10.905766154	4.529485285	-2.707426474
H290	1.068280636	1.905457137	7.370123143
H291	-1.159748171	2.350792057	9.497809881
H292	0.618229831	6.039772744	8.209834987
H293	-0.682344244	2.118824107	7.050811396
H294	-0.186739351	3.231658554	10.471577644
H295	4.722357200	5.765302890	4.555645134
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H300	1.058200961	-3.372900612	4.190083180
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H302	3.044932592	2.399881573	-3.033870681
H303	2.836096118	6.586464833	0.079128693
H304	2.487517470	-6.791434571	1.431129474
H305	4.828296001	4.803425335	0.362071838
H306	3.593718592	-5.729296822	0.562183842
H307	4.915274168	-7.630463458	-0.145818543
H308	5.465428686	-6.439637646	2.074215410
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H311	5.739047871	-10.542936385	-0.230344349
H312	7.309841743	-10.499106794	-2.873953675
H313	2.489868521	3.013091855	-0.676382379
H314	6.690435432	-12.727613071	-1.096847813
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H316	3.897917445	-4.398866029	2.548142003
H317	1.126424248	5.001898631	-0.211025393
H318	2.294088679	3.859326262	-4.902621223
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H320	10.693510315	-2.784846108	-0.558847062
H321	8.490472353	-6.093629981	-0.165100251
H322	11.428835298	-5.553899899	-1.962625817
H323	6.806103226	7.725190585	3.539821805
H324	6.929559577	-4.061114359	1.655634353
H325	5.056010255	-5.334079092	-2.490710616
H326	7.335418313	4.333117089	-0.187570754
H327	7.316090825	-5.052551843	-3.559565946
H328	9.924579348	1.243802819	-3.186831109

H329	7.501753646	0.796195167	-2.535319070
H330	8.463376213	-11.447741502	-1.926677863
H331	2.598393290	-2.878113235	3.543225263
H332	7.904370034	-5.877625032	2.890531316
H333	6.547493686	-3.661608743	3.108831353
H334	7.587876806	-8.230576064	3.114038885
H335	1.170789831	-6.681381436	3.028704319
H336	10.260869022	-4.126747754	-5.937116571
H337	8.799644378	-2.392631892	-3.211478508
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H339	6.982227906	-3.504045888	-4.385027799
H340	5.477282574	3.443770738	-1.471890438
H341	0.371399020	6.497340691	-2.083598660
H342	0.037000502	6.762584314	-4.590853198
H343	4.276353665	-3.892227707	-1.769275881
H344	8.843484619	-6.674375506	1.942312245
H345	9.017144759	-7.553792536	-0.135866124
H346	0.076433747	-5.427387565	3.482695946
H347	11.560195165	-0.192450514	-1.834057441
H348	9.177571728	-2.615194949	0.335079480
H349	6.117131424	4.310183062	-2.901388110
H350	4.074020084	7.392343859	4.230827107
H351	1.850309933	-5.260705675	6.287024507
H352	2.729653884	-3.713577390	6.342907597
H353	12.612578692	-0.688169820	1.761699196
H354	12.781443177	-1.738513733	0.519233471
H355	11.987165681	-5.992507103	2.085199389
H356	11.375625988	-4.233430850	0.770255727
H357	13.432842144	-4.051877020	3.379994271
H358	10.697938551	-5.463045506	3.188089062
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H361	6.760369847	-10.753648081	4.534296819
H362	5.688373548	-8.382246943	5.414620491
H363	-10.525496230	6.782934754	4.493869902
H364	-9.877443800	3.773299224	4.377699304
H365	-11.151045467	4.599264214	3.456533685
H366	3.223903489	-1.142076058	-1.273576635
H367	-6.666102572	6.890902112	-0.637062255
H368	1.974640567	-0.913516556	1.754148715
H369	0.933419324	-0.909302316	-0.470422227
H370	-0.412020880	1.133666982	-1.081214478
Mo371	6.177984388	-1.288401757	-0.328213530
N372	0.115975663	-1.683749393	-9.620582514
N373	-3.598475797	-1.423041586	-9.269343907
N374	-4.855682873	-3.909755152	-8.747567154
N375	-2.860073577	-5.388739533	-7.434270068
N376	-2.481837922	-3.791310714	-5.080854378
N377	-5.043080326	-4.108760172	-3.882036311
N378	-5.431615137	-6.984873552	-3.670280339
N379	-3.010083937	-8.226791369	-2.734560489
N380	-2.050949238	-6.755544647	-0.592653656
N381	-4.046228869	-5.317192571	1.101465921
N382	-6.129755443	-7.348794482	1.176149573
N383	6.366457670	-11.950149330	-1.676549774
N384	6.426941141	-9.798107448	-0.071578578
N385	3.174753433	-5.123360389	2.512946573
N386	0.980277862	-5.687666611	3.098129709
N387	1.800377738	-3.549302590	3.515610505
N388	7.070526624	-9.117706425	3.299986338
N389	-0.395893813	2.035418014	-6.734480157
N390	3.619311515	-0.027093698	-5.235498256
N391	-2.320754817	3.010463108	-5.233408782
N392	-4.904689268	3.039845054	-6.218962517
N393	-5.964698683	0.677654741	-5.250579845
N394	-5.817639521	0.682801409	-2.424379713
N395	-2.790637288	3.184294332	-0.745324493
N396	-1.355538641	1.602113966	-1.091212121
N397	-7.989305709	1.900901580	-1.223369599
N398	-10.641926260	5.711601795	-2.213663382
N399	-12.411715963	5.699470574	-0.875706891
N400	2.585009162	-3.379690870	9.033853448
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N403	-1.165521864	6.484350802	5.540384265
N404	-2.516396842	7.773930485	0.961751721
N405	-2.763211218	9.920423922	1.860129984
N406	-4.634390179	8.632041004	1.394656644
N407	-2.495175643	4.184935769	4.547585139
N408	-4.568941613	3.912755892	6.412621555
N409	-6.525228287	5.893784865	6.890562976
N410	-5.193628563	8.054857052	4.740962152
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N413	7.316751859	4.414344121	-1.210530226
N414	4.701384076	5.655771201	-0.218836961
N415	4.801224343	6.405503149	2.551190968
N416	6.321330620	6.822861154	-5.056611862
N417	3.449293383	6.899116503	-4.889827663
N418	12.155368493	-1.026609229	0.909963599
N419	8.341644533	-0.605362525	-1.139925988
N420	9.645184119	0.592120058	-2.459327594
N421	11.391567859	-4.031508152	1.769489717
N422	-1.793824236	-0.180602775	1.881131695
N423	-1.185989437	0.747929419	1.934164267
O424	-2.059716317	-2.326839338	-7.852789816
O425	-5.435360629	-3.125756055	-6.688532703
O426	-4.492623335	-6.704160003	-6.526557375
O427	-2.002858721	-5.745452641	-4.012650596
O428	-4.048434015	-3.750405894	-1.863461820
O429	-6.440613497	-6.501410049	-1.675876894
O430	-4.288884333	-9.943868558	-1.911547247
O431	-0.375338806	-8.277569597	-0.188906191
O432	-2.596872579	-6.052368153	2.704851029
O433	-6.040029152	-7.024091193	3.421852836
O434	-6.522395431	-10.480080904	2.882219278
O435	8.508572083	-9.117367677	-0.822771264
O436	5.585443528	-10.674860072	2.493708440
O437	6.916003331	-9.085027929	6.884495739
O438	-3.073583563	0.962437991	-4.524597495
O439	2.372464222	1.586621247	-6.242702327
O440	-5.655548303	4.268017652	-4.440304095
O441	-3.772700331	5.901617617	-3.368426144
O442	-8.011992727	1.145084554	-6.186496063
O443	-7.074501233	-1.220262271	-2.334397416
O444	-7.581657998	0.752385263	0.711381604
O445	-11.118378771	1.524001268	0.387099566
O446	3.709698246	-6.621191166	8.200851457
O447	-2.975573939	-1.384217311	6.567411190
O448	-2.096199853	4.391539185	8.142375775
O449	-2.743233877	7.976672770	6.300444415
O450	-3.593811915	5.572327769	3.091674016
O451	-5.774004757	2.692226558	4.888628305
O452	-2.773204719	1.448690085	6.016427916
O453	-7.329622373	4.737337085	8.694041840
O454	-9.660242473	7.769143660	6.918751188
O455	-7.367924558	8.661154056	4.394335923
O456	-12.562702018	5.689881503	5.701275799
O457	-6.235907872	6.391067813	0.083237579
O458	8.535994132	4.188563409	-3.146634093
O459	4.974322412	6.507546060	-2.327612535
O460	3.398650305	8.163239786	2.118021117
O461	6.567376013	7.402935536	5.542390573
O462	3.496168119	6.839185708	-7.170510807
O463	6.178556165	1.516857400	-6.207991993
O464	7.342293324	2.200542761	-4.432854139
O465	0.910530270	8.787426360	-3.253696826
O466	11.055036760	-2.606018772	3.498626884
O467	12.796482144	-5.397445952	4.776841202
O468	3.640672134	-2.866274618	-4.091759160
O469	4.570139514	-4.699775742	-4.941990503
O470	10.728002401	-4.781456624	-3.796152068
O471	9.557796853	-3.703538452	-5.399634589
O472	7.118534519	-3.335494189	-0.035830003
O473	7.118006142	-5.409408021	-0.920447967
O474	6.205471442	-2.192900352	-2.216573953

O475	8.476877230	-6.684241478	2.866010793
O476	6.774593422	-4.437982481	2.559202224
O477	-3.785466844	5.758312378	-0.632205998
O478	11.719263595	-5.938386335	-1.109750402
O479	9.252291209	-6.643138328	0.180373327
S480	0.648546358	3.613591590	5.676578817
S481	1.971719334	3.060086533	2.028906974
S482	5.160994654	0.679041410	-1.237783144
S483	1.312530124	0.141668238	3.884345881
S484	1.456244640	0.341158099	-0.374133445
S485	5.915191107	3.211544236	1.611927921
S486	4.246027944	-2.482934498	0.438710146
S487	4.138444278	2.160127459	4.810354811
S488	7.043638673	-0.435932932	1.727604105
S489	4.528458894	-1.859218101	4.122536680

Structure D 35(1)

D 35(1)		bm2cnx2b6x2hn2n2xd135tf.car 2	
associated		C1	-2.331627540 -1.789287460 -8.963776554
Fe(139)	0.558 -2.516	C2	-1.272068000 -1.532810939 -10.040852260
Fe(140)	0.287 -0.041	C3	-4.681225353 -1.503973385 -8.308892282
Fe(141)	0.551 -2.622	C4	-5.013193864 -2.920703907 -7.845253825
Fe(142)	0.579 2.853	C5	-5.104973711 -5.299148089 -8.388770889
Fe(143)	0.614 3.209	C6	-4.123212126 -5.855238170 -7.353272905
Fe(144)	0.512 2.252	C7	-1.858673385 -5.741672473 -6.425032997
Fe(145)	0.365 -1.824	C8	-2.112221280 -5.091632212 -5.061114449
		C9	-2.793473044 -3.093759356 -3.836220288
		C10	-4.011672063 -3.674709782 -3.102536371
		C11	-6.217506296 -4.687833535 -3.265399151
		C12	-6.015552225 -6.131568154 -2.782134902
		C13	-5.366316463 -8.411025184 -3.407329210
		C14	-4.163632607 -8.922467831 -2.608009079
		C15	-1.774552326 -8.667552761 -2.099112613
		C16	-1.341714475 -7.883180865 -0.858153165
		C17	-1.722402730 -5.826256265 0.470567781
		C18	-2.825246287 -5.738449006 1.538836472
		C19	-1.318490068 -4.442623704 -0.114396696
		C20	-1.138218369 -3.372262866 0.965855253
		C21	-0.050968172 -4.568545712 -0.969428715
		C22	-5.191346838 -5.240618763 2.036937475
		C23	-5.827287035 -6.622164032 2.289349999
		C24	-6.218356186 -4.188203019 1.555335672
		C25	-7.461510442 -4.180463797 2.451446300
		C26	-5.581425936 -2.792569339 1.508462388
		C27	-6.798907148 -8.649021386 1.371394451
		C28	-6.013719854 -9.563094942 2.292491553
		C29	7.459385539 -10.996452947 -1.908223899
		C30	7.514740207 -9.878967865 -0.864114689
		C31	6.212241719 -8.861021985 1.013961086
		C32	6.253545161 -9.641521039 2.341723078
		C33	4.869375841 -8.131611894 0.826349658
		C34	4.579905910 -7.094921084 1.915008434
		C35	3.397946903 -6.206327228 1.527963279
		C36	1.989928051 -4.797723415 3.049147436
		C37	7.237250027 -9.759246973 4.581446194
		C38	6.567185666 -9.010852317 5.715227440
		C39	-0.997978802 1.058321542 -5.818121623
		C40	-2.241730145 1.652723100 -5.136262139
		C41	-0.004653871 0.651481488 -4.701243734
		C42	1.183151573 -0.231698712 -5.138924263
		C43	2.432511549 0.531526018 -5.575456845
		C44	-3.313004761 3.766765917 -4.495981406
		C45	-4.733077356 3.725945075 -5.078160553
		C46	-2.865646114 5.222683777 -4.261131334
		C47	-6.234024643 2.657464135 -6.695618000
		C48	-6.829933736 1.415645894 -6.014629815
		C49	-6.424115824 -0.501295717 -4.526330398
		C50	-6.471416466 -0.382633630 -3.001795882
		C51	-5.829242103 0.824755642 -0.967065684
		C52	-7.250203082 1.113953080 -0.423632017
		C53	-4.984952775 2.022404556 -0.504248101
		C54	-3.517335177 1.994757442 -0.779534100

C55	-2.601254263	0.993804189	-0.991729603
C56	-1.487915145	2.913626366	-0.914556170
C57	-9.250414600	2.524269999	-0.805241448
C58	-10.273923360	1.436005946	-0.489237447
C59	-9.741234461	3.417954428	-1.966766198
C60	-10.744841723	4.478774024	-1.622790073
C61	-11.828434274	4.462866915	-0.765756130
C62	-11.662844394	6.434260498	-1.765328872
C63	2.338897655	-4.609477624	8.279324188
C64	3.633160821	-5.397354565	8.197557862
C65	1.908136121	-4.306528760	6.821239864
C66	0.599069885	-3.557614322	6.738467627
C67	-0.632012630	-4.235091537	6.656929434
C68	0.574524974	-2.150728986	6.760248884
C69	-1.842767073	-3.537090962	6.596147603
C70	-0.625430941	-1.440913710	6.712860708
C71	-1.834149230	-2.136191538	6.629290008
C72	0.158352209	3.525590543	8.461318747
C73	-0.877853917	4.634014442	8.235538163
C74	0.289244095	2.655851999	7.201368730
C75	-1.250007686	7.047233942	7.935195623
C76	-1.789634148	7.200963965	6.511747187
C77	-1.600914243	6.465711930	4.157194788
C78	-2.646242884	5.361634291	3.886290756
C79	-0.356202712	6.359098999	3.256186338
C80	-0.565943577	6.381123938	1.739381795
C81	-1.051598812	7.702353583	1.119743353
C82	-3.285591659	8.776534228	1.355085742
C83	-3.440493274	3.103064373	4.355525363
C84	-4.702478033	3.234216038	5.228223114
C85	-2.826587531	1.715552661	4.610637823
C86	-5.523853786	3.712801009	7.478604391
C87	-6.535394640	4.824426684	7.738686125
C88	-7.347403414	7.067132960	7.141655735
C89	-8.777539414	6.973350475	6.568246867
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C91	-6.432840525	8.389250512	5.166614043
C92	-10.272236189	5.837809119	4.985442395
C93	-11.390610913	5.495764417	5.962626150
C94	-10.161761372	4.732485996	3.901837848
C95	-9.150234774	5.089160162	2.835984785
C96	-9.500802428	5.955575311	1.788126449
C97	-7.824784450	4.628055734	2.900369773
C98	-8.557617962	6.375379362	0.848188494
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C100	-7.240213207	5.931197856	0.965944080
C101	9.727396979	4.277789139	-1.050630538
C102	8.462946522	4.306050325	-1.890150070
C103	5.983073639	4.354269304	-1.816855578
C104	5.159256725	5.601181859	-1.480257631
C105	3.894226017	6.759872040	0.264123760
C106	4.021267790	7.154101817	1.732333344
C107	4.874891269	6.673442706	3.975149866
C108	6.182274435	7.318949758	4.384959131
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C112	6.742946476	3.864738683	-6.101762926
C113	6.734812799	2.436491384	-5.604772564
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C116	1.001654143	6.251954701	-4.753513251
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C119	2.040658962	4.134855113	-3.850370996
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C138	3.894588399	0.525497434	1.907451803
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Fe140	1.678069756	0.524541537	1.838244568
Fe141	3.633273490	0.186659961	3.859604980
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H191	-0.664364561	-5.329575652	6.633593144
H192	-2.790755780	-6.511018826	-1.249772503
H193	-0.934180740	-8.605184448	-2.815515910
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H197	-2.801871617	-4.078039246	6.513483510
H198	-0.857826691	-6.263592811	0.990766429
H199	-7.823512534	-8.558249041	1.762905135
H200	-6.835395901	-9.144121906	0.398131057
H201	-4.909848234	-9.370227199	2.335004093
H202	8.303470111	-9.917340672	4.803478410
H203	4.477207537	0.448925562	-5.508136049
H204	5.144794811	-5.473205734	-4.618092517
H205	6.907150405	3.850019567	-7.192126875
H206	7.564649457	4.426709925	-5.638501398
H207	4.624140968	4.124142232	-6.460962200
H208	2.854592218	9.062438649	-3.694947799
H209	5.904046173	6.260491829	-7.005099874
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H310	0.979414462	5.727508890	-5.702173925
H311	5.741044366	-10.546611864	-0.231802936
H312	7.312272980	-10.502446088	-2.875627188
H313	2.474309991	3.031038045	-0.656915504

H314	6.693323714	-12.730075877	-1.099910593
H315	6.065872197	-12.358562382	-2.565599263
H316	3.896884763	-4.396193348	2.536125952
H317	1.099178188	5.003339259	-0.209063521
H318	2.297034116	3.853206209	-4.892656424
H319	10.873879758	-6.229076234	-0.694857345
H320	10.700604114	-2.794407273	-0.554839372
H321	8.494228002	-6.091372667	-0.166221332
H322	11.437843651	-5.550061229	-1.962217293
H323	6.802279917	7.730126590	3.540360140
H324	6.930542610	-4.060023203	1.648218988
H325	5.051379282	-5.334497629	-2.496992700
H326	7.335229990	4.320772443	-0.185591468
H327	7.321202209	-5.057298072	-3.555216045
H328	9.955667086	1.230629329	-3.189996433
H329	7.530200621	0.780049547	-2.565799561
H330	8.463113971	-11.452238985	-1.926416323
H331	2.607257824	-2.886499565	3.555080334
H332	7.907972069	-5.876899197	2.884067704
H333	6.579871638	-3.664008250	3.108508368
H334	7.592160871	-8.236755645	3.110878291
H335	1.168950834	-6.678539577	3.013044063
H336	10.267391801	-4.132464236	-5.940378481
H337	8.803961457	-2.395799943	-3.215212171
H338	9.081283344	-3.794724550	-2.156424265
H339	6.990111925	-3.516012410	-4.397382788
H340	5.478198591	3.444038142	-1.475114068
H341	0.357408846	6.500703448	-2.095355052
H342	0.036631779	6.756834340	-4.595413806
H343	4.278453610	-3.888264101	-1.774983174
H344	8.846318616	-6.677751668	1.939666153
H345	9.013380996	-7.554153023	-0.140553586
H346	0.080052032	-5.427137771	3.480544257
H347	11.581297755	-0.199596843	-1.815286466
H348	9.182973960	-2.621130280	0.336699676
H349	6.123259147	4.316101392	-2.899541289
H350	4.073482951	7.388908767	4.225831560
H351	1.848045089	-5.259889591	6.286297266
H352	2.727899576	-3.712377117	6.345200177
H353	12.614016785	-0.691130252	1.770135166
H354	12.790521361	-1.740777838	0.527720750
H355	11.988382530	-5.993120615	2.088038106
H356	11.385941602	-4.234869790	0.771619435
H357	13.434892106	-4.055802187	3.384432210
H358	10.698870676	-5.466862156	3.192108934
H359	4.553877375	-4.763530262	8.123580739
H360	-11.052881227	5.020538938	6.910366045
H361	6.759920985	-10.756636815	4.532522942
H362	5.687641471	-8.386929130	5.409708858
H363	-10.522997126	6.783516462	4.493709157
H364	-9.879377723	3.771549924	4.378039287
H365	-11.149114021	4.599450255	3.456079646
H366	3.395864450	-0.888296531	-1.427889054
H367	-6.666225053	6.890626651	-0.639826585
H368	1.697735870	-0.830614708	1.745949173
H369	0.993378931	-0.879757137	-0.454096082
H370	-0.418188376	1.122089665	-1.068116431
Mo371	6.187682225	-1.292672883	-0.329244270
N372	0.116741879	-1.681226816	-9.618426764
N373	-3.598429542	-1.423328142	-9.270258937
N374	-4.853584036	-3.910776280	-8.747463796
N375	-2.857329165	-5.387714021	-7.431307239
N376	-2.479488557	-3.787974063	-5.080602818
N377	-5.042024257	-4.104921405	-3.881206767
N378	-5.431500987	-6.984018581	-3.668500195
N379	-3.006317776	-8.223071778	-2.731677570
N380	-2.052273087	-6.755479755	-0.591285248
N381	-4.043418308	-5.315504318	1.105861362
N382	-6.129701386	-7.350531563	1.183451572
N383	6.367462168	-11.952657940	-1.678496058
N384	6.427446979	-9.800786223	-0.073152064
N385	3.176855086	-5.124049752	2.506908897
N386	0.980406081	-5.684570603	3.085761845

N387	1.807143900	-3.552219210	3.520732902
N388	7.071764124	-9.122120610	3.297218631
N389	-0.398654697	2.032446507	-6.732363520
N390	3.618907120	-0.023705537	-5.228247680
N391	-2.324541774	3.006724972	-5.230448937
N392	-4.907588877	3.037418539	-6.217469726
N393	-5.967944743	0.674966369	-5.253400202
N394	-5.814573137	0.677053073	-2.424950596
N395	-2.789311832	3.181313123	-0.734975395
N396	-1.360348513	1.594714566	-1.085061993
N397	-7.988253508	1.901417883	-1.224620712
N398	-10.640782942	5.712090283	-2.220483485
N399	-12.403941347	5.702118203	-0.873587212
N400	2.580189339	-3.378551709	9.031417460
N401	-0.187999996	2.664224008	9.587227490
N402	-0.385611727	5.903709138	8.153203269
N403	-1.163435480	6.490210801	5.540968993
N404	-2.513056790	7.773552202	0.965293712
N405	-2.765798494	9.926085360	1.845930935
N406	-4.633333407	8.630234760	1.390973865
N407	-2.489126642	4.193277365	4.553984701
N408	-4.566849465	3.915688045	6.414157461
N409	-6.518569350	5.894691193	6.893025978
N410	-5.191234896	8.060404797	4.739335952
N411	-8.992784014	5.965220142	5.683292042
N412	10.835891330	4.945778041	-1.771790799
N413	7.317282486	4.410425140	-1.207792141
N414	4.703901151	5.647493829	-0.214594632
N415	4.805809853	6.402516520	2.552306503
N416	6.321915838	6.822290808	-5.054487934
N417	3.447702185	6.892963192	-4.890394389
N418	12.161359460	-1.030455373	0.916316255
N419	8.356065293	-0.615788460	-1.151694598
N420	9.670481264	0.576520314	-2.466700991
N421	11.393468979	-4.035293561	1.771496359
N422	-1.956036351	-0.314328470	1.962612054
N423	-1.613433874	0.738356015	1.957799317
O424	-2.058686069	-2.325118769	-7.853735264
O425	-5.432187561	-3.128305579	-6.686877271
O426	-4.488702025	-6.705840064	-6.525246927
O427	-2.002035480	-5.740779811	-4.010424418
O428	-4.044967883	-3.745276309	-1.862996959
O429	-6.431408641	-6.499003317	-1.670591457
O430	-4.284764665	-9.940355684	-1.907986914
O431	-0.372777751	-8.274554610	-0.187166850
O432	-2.589724767	-6.047054162	2.709518483
O433	-6.031064261	-7.026226221	3.428494649
O434	-6.513453683	-10.481848208	2.889835878
O435	8.507268554	-9.118743687	-0.825886790
O436	5.581562280	-10.676450727	2.492050711
O437	6.916434395	-9.084573983	6.880357794
O438	-3.076779642	0.956998480	-4.524794441
O439	2.371567904	1.586129657	-6.241948365
O440	-5.658644727	4.270200141	-4.441887550
O441	-3.771852035	5.897390913	-3.365404069
O442	-8.015709301	1.142212526	-6.189415809
O443	-7.083125126	-1.217556340	-2.338466027
O444	-7.582465589	0.744436099	0.707852462
O445	-11.110664635	1.524160623	0.394220392
O446	3.705126307	-6.620376221	8.199386559
O447	-2.978479989	-1.382619994	6.562508241
O448	-2.094537698	4.397518809	8.138188541
O449	-2.744321189	7.979002877	6.300850348
O450	-3.595346770	5.575900032	3.099882783
O451	-5.767562110	2.694969422	4.885706545
O452	-2.774905971	1.457343128	6.038104031
O453	-7.330448663	4.733090020	8.691017715
O454	-9.658338598	7.761843906	6.917906434
O455	-7.370730081	8.645585127	4.390854033
O456	-12.559172755	5.688207028	5.702577145
O457	-6.236633299	6.391129457	0.081179975
O458	8.535541734	4.203216682	-3.146042323
O459	4.975442096	6.508940106	-2.320234017

O460	3.394118719	8.150680322	2.120825622
O461	6.570100726	7.404612426	5.542228267
O462	3.506683629	6.855723310	-7.171092590
O463	6.179444082	1.516215431	-6.197815189
O464	7.347751656	2.207637990	-4.427687675
O465	0.908206811	8.784671026	-3.260577048
O466	11.057496096	-2.609411712	3.499512019
O467	12.797570455	-5.402795036	4.779423566
O468	3.635645035	-2.867294298	-4.096476866
O469	4.565385644	-4.699369859	-4.948611429
O470	10.739868303	-4.771064240	-3.795540929
O471	9.558072851	-3.715961331	-5.405549315
O472	7.111249348	-3.332755370	-0.041550392
O473	7.121483847	-5.405039481	-0.927707835
O474	6.204863742	-2.190205209	-2.227551668
O475	8.480192649	-6.684848914	2.863654365
O476	6.775822805	-4.440921889	2.549589919
O477	-3.784338752	5.759518066	-0.628903478
O478	11.724391169	-5.935072885	-1.108289473
O479	9.252123085	-6.645116460	0.178276872
S480	0.706843913	3.646666457	5.671844687
S481	1.814402525	3.025289902	2.045983540
S482	5.265582408	0.726527839	-1.226100698
S483	1.330229472	0.121957427	3.921879847
S484	1.459322537	0.397447208	-0.380643660
S485	5.868386960	3.199791280	1.578986878
S486	4.214576522	-2.444547615	0.412064483
S487	4.183928502	2.097490414	4.774301918
S488	7.045303470	-0.501286269	1.755207399
S489	4.535689419	-1.831219335	4.179096558

Structure D 47(2)

D 47(2) associated		bm2cnx2b6x2hn2n2xd2tg.car_3	
Fe(139)	0.551 2.420	C1	-2.398024928 -2.395509051 -8.794960133
Fe(140)	0.276 0.104	C2	-1.338046315 -2.247606993 -9.892113810
Fe(141)	0.564 2.671	C3	-4.730296838 -1.971801797 -8.153396744
Fe(142)	0.554 -2.684	C4	-5.124592272 -3.337150701 -7.592815614
Fe(143)	0.618 3.209	C5	-5.308527896 -5.743817764 -7.957260339
Fe(144)	0.497 -2.029	C6	-4.342773567 -6.261365509 -6.887048978
Fe(145)	0.300 -0.116	C7	-2.075224967 -6.161932783 -5.967015460
		C8	-2.311456111 -5.401999520 -4.657116274
		C9	-2.914735508 -3.298232524 -3.582597638
		C10	-4.150743084 -3.782087349 -2.808656599
		C11	-6.393231836 -4.720775324 -2.899857611
		C12	-6.238748130 -6.132346195 -2.314738673
		C13	-5.660960121 -8.468782397 -2.773053093
		C14	-4.471390795 -8.967462334 -1.944106135
		C15	-2.080062415 -8.731432266 -1.429767877
		C16	-1.618251741 -7.872162662 -0.249323235
		C17	-1.920480013 -5.701830871 0.914206169
		C18	-3.022996909 -5.497302983 1.967043741
		C19	-1.464374706 -4.385048269 0.224534477
		C20	-1.235069291 -3.251583590 1.229186570
		C21	-0.208235416 -4.631923943 -0.620303097
		C22	-5.368270242 -4.879968969 2.420304337
		C23	-6.049662818 -6.218417582 2.771940842
		C24	-6.361471845 -3.834260435 1.862969501
		C25	-7.607573288 -3.724935225 2.751567196
		C26	-5.686175210 -2.464818186 1.715194961
		C27	-7.085260018 -8.276625045 2.009279679
		C28	-6.333328835 -9.141336634 3.001463705
		C29	7.071763811 -11.358969932 -1.041152576
		C30	7.166533578 -10.167615482 -0.086535697
		C31	5.906778096 -8.961492937 1.704722972
		C32	5.924431463 -9.639743756 3.088728378
		C33	4.595313701 -8.191681964 1.461277873
		C34	4.345137810 -7.072722393 2.475122480
		C35	3.186559031 -6.178701812 2.034552745
		C36	1.829336099 -4.603770601 3.431630578
		C37	6.903912875 -9.619228391 5.333464820
		C38	6.266557078 -8.782436255 6.422333715
		C39	-0.955640665 0.650224776 -5.882368083

C40	-2.181229325	1.333168302	-5.251112057
C41	0.014065501	0.278461804	-4.735840655
C42	1.171902363	-0.672984930	-5.108313019
C43	2.446320713	0.007110212	-5.607615977
C44	-3.184892555	3.528392376	-4.786224219
C45	-4.603647816	3.501065948	-5.373174945
C46	-2.674405521	4.976806962	-4.657868212
C47	-6.150249073	2.340779792	-6.881278353
C48	-6.785942277	1.177426906	-6.103025754
C49	-6.440525571	-0.628082107	-4.463047276
C50	-6.473264657	-0.390115327	-2.952398992
C51	-5.790702370	0.961844641	-1.024938524
C52	-7.201489911	1.349367612	-0.517079783
C53	-4.903467978	2.163393698	-0.663127861
C54	-3.437303149	2.057483136	-0.933485255
C55	-2.559599652	1.008651308	-1.054463813
C56	-1.379857802	2.889689785	-1.165547256
C57	-9.150136592	2.781570318	-1.017546021
C58	-10.193142473	1.755232377	-0.578737269
C59	-9.640162523	3.576598381	-2.250705699
C60	-10.602771927	4.696487723	-1.979615753
C61	-11.672301316	4.777832856	-1.109260191
C62	-11.456243860	6.667731371	-2.244648687
C63	2.199719991	-4.043196164	8.613453649
C64	3.452745266	-4.897514874	8.594448972
C65	1.774512643	-3.833397323	7.135536332
C66	0.493598178	-3.044331560	7.004158033
C67	-0.760820159	-3.682729404	6.977241306
C68	0.521234592	-1.641594336	6.916003425
C69	-1.946411923	-2.947903847	6.867937253
C70	-0.652809582	-0.894429427	6.817524960
C71	-1.886280458	-1.550577176	6.788124914
C72	0.285342158	4.161363836	8.179824711
C73	-0.719124950	5.279733489	7.869601667
C74	0.381220684	3.192382971	6.992150902
C75	-1.018748319	7.672027866	7.377906750
C76	-1.542801325	7.737106531	5.942323647
C77	-1.377410515	6.818470425	3.653652181
C78	-2.463081015	5.737001038	3.467950003
C79	-0.142841429	6.589012542	2.761220341
C80	-0.368262503	6.483810116	1.249070960
C81	-0.784818365	7.769396580	0.513297919
C82	-2.972671221	8.954145797	0.666776692
C83	-3.339070743	3.548330581	4.086254381
C84	-4.590635676	3.801053397	4.949402773
C85	-2.791778366	2.154257996	4.431796718
C86	-5.388444555	4.463642864	7.162341559
C87	-6.337319793	5.643365016	7.348373558
C88	-7.079059338	7.856218551	6.570985194
C89	-8.516214973	7.756142970	6.016335816
C90	-6.342123598	9.080103435	5.985525697
C91	-6.138621541	8.964367207	4.478771196
C92	-10.050092926	6.565479960	4.516867532
C93	-11.171164519	6.318789840	5.519305967
C94	-9.986567776	5.388790567	3.507955177
C95	-8.961881219	5.626674360	2.423213473
C96	-9.283049365	6.409044190	1.303829285
C97	-7.655047210	5.125647891	2.532971998
C98	-8.325933589	6.703557182	0.329959371
C99	-6.676600723	5.429736842	1.580065213
C100	-7.025548747	6.222148431	0.489640207
C101	9.871580824	3.840352249	-1.368551510
C102	8.608555131	3.846151789	-2.210497648
C103	6.128664155	3.981222745	-2.136259252
C104	5.360264658	5.289153432	-1.910540347
C105	4.156420398	6.654836951	-0.276412288
C106	4.276194468	7.142602171	1.164529898
C107	5.104673447	6.797084218	3.444917910
C108	6.434884922	7.425010398	3.804884724
C109	5.678578379	5.399155569	-6.453217752
C110	4.280680084	6.015185847	-6.572263687
C111	5.546301319	3.893498754	-6.130908840
C112	6.866693370	3.143638154	-6.384642199

C113	6.808476959	1.760518398	-5.775509723
C114	2.323906550	6.903718577	-5.407203615
C115	2.221581622	8.100919537	-4.483756043
C116	1.212690715	5.842611221	-5.226397931
C117	1.469496357	4.971908786	-4.026148457
C118	1.125303240	5.402104139	-2.733509797
C119	2.175710490	3.764286163	-4.171539170
C120	1.533691627	4.666104413	-1.617368653
C121	2.579228802	3.028967637	-3.054406272
C122	2.283302440	3.495512035	-1.769777272
C123	10.783791859	-1.917516654	1.409284088
C124	10.955270395	-3.002932112	2.482349062
C125	9.983270347	-2.411096234	0.193133388
C126	9.603052389	-1.364458488	-0.808948805
C127	10.436207812	-0.717617628	-1.699233051
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C138	3.917544878	0.539820549	1.872983376
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	S480	0.814354401	4.029992783	5.399106505
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	S483	1.471077855	0.311257825	4.155271033
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	S486	4.211333027	-2.628914022	0.751880328
	S487	4.255333794	2.465901358	4.562514793
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D 47(2)	bm2cnx2b6x2hn2n2xd2ti 1 53120.671			
TS	C1	-2.396513505	-2.387605422	-8.795899674
Fe(139) 0.547 2.398	C2	-1.333455792	-2.242093487	-9.889628599
Fe(140) 0.352 0.480	C3	-4.735662645	-1.979942170	-8.167967242
Fe(141) 0.563 2.725	C4	-5.119974180	-3.345672411	-7.602810222
Fe(142) 0.547 -2.615	C5	-5.290160759	-5.752551982	-7.961242939
Fe(143) 0.609 3.185	C6	-4.328735415	-6.262736995	-6.882798308
Fe(144) 0.511 -2.212	C7	-2.064073504	-6.155758366	-5.954793615
Fe(145) 0.316 -0.470	C8	-2.302828099	-5.388890795	-4.650093284
	C9	-2.903142885	-3.278589025	-3.588637597
	C10	-4.139595309	-3.758061623	-2.811312524
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	C15	-2.068101506	-8.725263874	-1.425099109
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	C17	-1.921178037	-5.701577382	0.922505305
	C18	-3.016893094	-5.493547258	1.981130897
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	C20	-1.258229170	-3.236611830	1.218511883
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	C22	-5.364301926	-4.882218956	2.441748128
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	C53	-4.902438125	2.144240333	-0.667019890
	C54	-3.437129936	2.041465930	-0.940720290
	C55	-2.559290498	0.994771488	-1.079546915
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Fe(140) 0.344 0.684		C2 -1.333458527	-2.245011246 -9.879437935
Fe(141) 0.544 2.567		C3 -4.725740148	-1.970309240 -8.141028512
		C4 -5.125547786	-3.334907932 -7.584555787
		C5 -5.311962850	-5.739454405 -7.955782410
		C6 -4.346513118	-6.261975521 -6.886505870

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Fe(143)	0.601	3.171	C8	-2.312793589	-5.404622617	-4.658188468
Fe(144)	0.522	-2.276	C9	-2.915825545	-3.302947292	-3.583055934
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			C64	3.447929816	-4.902398949	8.597569250
			C65	1.789413878	-3.826201158	7.128248754
			C66	0.512437922	-3.032996783	6.986583704
			C67	-0.743572578	-3.669133369	6.974696257
			C68	0.542125430	-1.631455226	6.877013499
			C69	-1.929030018	-2.934353347	6.865414230
			C70	-0.632171078	-0.883547810	6.779135940
			C71	-1.867266729	-1.538310411	6.770982675
			C72	0.289142442	4.151829049	8.165184992
			C73	-0.715236881	5.269643749	7.854683527
			C74	0.372970715	3.171116228	6.987294075
			C75	-1.016524262	7.664467901	7.376692512
			C76	-1.540455510	7.735702984	5.940953463
			C77	-1.375392146	6.821763708	3.650089773
			C78	-2.466126210	5.743120004	3.471041179
			C79	-0.143195031	6.586609718	2.756648110

C80	-0.370885830	6.479002118	1.245421225
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C82	-2.972956029	8.951218818	0.668813238
C83	-3.343447279	3.559587391	4.107262572
C84	-4.598064907	3.813688691	4.962476639
C85	-2.789093757	2.175073735	4.480725705
C86	-5.394905652	4.468025463	7.175902361
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C88	-7.074324018	7.861878606	6.575618021
C89	-8.507603091	7.748560589	6.016826274
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C92	-10.030227990	6.554587220	4.515628391
C93	-11.154886727	6.313102555	5.516166663
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C127	10.459553384	-0.722598510	-1.703199028
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N375	-3.057393400	-5.854551425	-6.997788366
N376	-2.626148785	-4.087967922	-4.774082861
N377	-5.198144009	-4.220347829	-3.553009811
N378	-5.675138873	-7.062110598	-3.132826046
N379	-3.297899986	-8.292028847	-2.090684149
N380	-2.290556126	-6.702076814	-0.064356748
N381	-4.223666212	-5.059078062	1.507702875
N382	-6.371859631	-7.019408074	1.730689532
N383	5.953648162	-12.266500515	-0.738279446
N384	6.081127863	-9.990002374	0.687224366
N385	3.010136859	-5.019776574	2.926408972
N386	0.798330270	-5.450674110	3.555837650
N387	1.688975306	-3.309546930	3.767427446
N388	6.746151815	-9.066646382	4.006106550
N389	-0.323289111	1.539244006	-6.854686387
N390	3.612955614	-0.551962653	-5.202699275
N391	-2.228216115	2.673519769	-5.456018482
N392	-4.812015727	2.705814428	-6.438855543
N393	-5.951035374	0.469577078	-5.282651229
N394	-5.773879605	0.686606789	-2.466678463
N395	-2.655454426	3.214316100	-1.007125750
N396	-1.284159317	1.561975182	-1.253842138
N397	-7.901223768	2.094493424	-1.390004198
N398	-10.468143423	5.880758877	-2.671816274
N399	-12.197626280	6.027289312	-1.289235903
N400	2.499025121	-2.767076163	9.260110111
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N402	-0.188323381	6.516838747	7.688770833
N403	-0.930319422	6.940270998	5.036124384
N404	-2.238767620	7.891566473	0.340664194
N405	-2.410562960	10.115364063	1.046683701
N406	-4.324463298	8.855336818	0.706090749
N407	-2.337500256	4.611300486	4.213253652
N408	-4.419897893	4.549772751	6.097824330
N409	-6.281594458	6.644049999	6.428069770
N410	-4.893037736	8.602967978	4.078484705
N411	-8.757233625	6.694194283	5.203252376
N412	10.997361455	4.432048156	-2.137000583
N413	7.467828352	4.036008939	-1.542464245
N414	4.907802913	5.467480211	-0.657448105
N415	5.022775018	6.424350154	2.041009082
N416	6.546160084	6.187491186	-5.572291972
N417	3.679520596	6.373048007	-5.398670974
N418	12.099752145	-1.369035783	1.011249438
N419	8.310157034	-0.978135680	-1.080595559
N420	9.647432048	0.052407710	-2.503762752
N421	11.267586836	-4.271607594	2.068614279
N422	-2.064853275	-0.186714063	1.954285193
N423	-1.668853344	0.846679700	1.895094652
O424	-2.134924817	-2.866739068	-7.658457649
O425	-5.556128869	-3.443025956	-6.424563817
O426	-4.739516370	-7.032688086	-5.995696698
O427	-2.233509478	-5.969161857	-3.556038519
O428	-4.180839407	-3.757302621	-1.566934178
O429	-6.661698334	-6.407921494	-1.177993132
O430	-4.607499995	-9.962598825	-1.218778469
O431	-0.657377065	-8.239456378	0.446566826
O432	-2.787220382	-5.691860591	3.168094316
O433	-6.266380873	-6.530010501	3.943791059
O434	-6.860810938	-9.996854860	3.668967449
O435	8.192845810	-9.457500775	-0.094501481
O436	5.231876673	-10.648685927	3.306368968
O437	6.627644327	-8.818161716	7.588900424
O438	-3.039583034	0.712239262	-4.583703729
O439	2.421936455	0.997682252	-6.362548755
O440	-5.501965600	4.162727040	-4.812850678
O441	-3.552827575	5.763202213	-3.835953159
O442	-7.982842846	0.926814145	-6.259554436
O443	-7.111317621	-1.144828656	-2.221309858
O444	-7.540558388	1.101936134	0.638501855

O445	-11.015738491	1.966111074	0.288185838
O446	3.445671509	-6.121511765	8.691624973
O447	-2.999901773	-0.755731756	6.652491818
O448	-1.939931662	5.062269179	7.776719196
O449	-2.461947092	8.532781108	5.668969755
O450	-3.411015623	5.937408511	2.684864886
O451	-5.684146418	3.312393776	4.638559071
O452	-2.735527538	2.018492993	5.898733004
O453	-7.125227800	5.668515309	8.318943651
O454	-9.372137991	8.582317095	6.321974799
O455	-7.077191640	9.133798143	3.679290226
O456	-12.328737766	6.525203098	5.260113696
O457	-6.008191779	6.560654126	-0.435088667
O458	8.678260358	3.656148342	-3.459752780
O459	5.207913883	6.119849376	-2.831959985
O460	3.677236577	8.185306851	1.469500622
O461	6.839077482	7.537206324	4.951882777
O462	3.715579815	6.141289772	-7.667292830
O463	6.212486550	0.818930925	-6.285205427
O464	7.434598744	1.602012197	-4.591852654
O465	1.187710110	8.490248518	-3.958817911
O466	10.905645016	-2.737752307	3.695641000
O467	12.565737156	-5.480451477	5.191040086
O468	3.571355396	-3.327711176	-3.907605756
O469	4.403783071	-5.290339713	-4.536607957
O470	10.598593054	-5.350215068	-3.375885954
O471	9.407866314	-4.470085381	-5.081739272
O472	6.988295650	-3.594488609	0.241373948
O473	6.937076322	-5.721582545	-0.501980253
O474	6.122901793	-2.577953585	-2.021244921
O475	8.253987143	-6.735299458	3.384361328
O476	6.627118853	-4.463908255	2.900712587
O477	-3.577625089	5.804382848	-1.096374847
O478	11.518565670	-6.408748653	-0.624584877
O479	9.022791472	-6.930699815	0.706146744
S480	0.792959099	4.000168666	5.385998868
S481	1.999993348	3.088328131	1.800846444
S482	5.171525066	0.377491991	-1.261728101
S483	1.266045551	0.356073997	3.868276437
S484	1.601548589	0.390376107	-0.406413364
S485	5.956858050	3.133495956	1.305640278
S486	4.134615352	-2.562906776	0.661209856
S487	4.217843029	2.391439438	4.575334468
S488	7.046084032	-0.554974928	1.781779422
S489	4.468327894	-1.639745088	4.302081082

Structure D 35(2)

D 35(2)		bm2cnx2b6x2hn2n2xd235tf 2 53135.362	
associated		C1	-2.403560352 -1.860999197 -8.925882758
Fe(139)	0.554 -2.430	C2	-1.351622923 -1.618669777 -10.014717415
Fe(140)	0.284 0.070	C3	-4.745369125 -1.549408846 -8.256185021
Fe(141)	0.547 -2.665	C4	-5.087001094 -2.959401989 -7.779307769
Fe(142)	0.573 2.825	C5	-5.199100258 -5.341339184 -8.305274509
Fe(143)	0.618 3.237	C6	-4.210212714 -5.897024814 -7.275913864
Fe(144)	0.508 2.227	C7	-1.937181661 -5.788654819 -6.366434726
Fe(145)	0.292 0.158	C8	-2.178497907 -5.133456648 -5.003300145
		C9	-2.841025151 -3.126325890 -3.782856717
		C10	-4.058707697 -3.697491678 -3.040412465
		C11	-6.273256849 -4.693255960 -3.186889875
		C12	-6.079137203 -6.134506660 -2.696293146
		C13	-5.438810386 -8.419109382 -3.307666576
		C14	-4.236295239 -8.928766032 -2.506530773
		C15	-1.843232285 -8.681933810 -2.007480743
		C16	-1.398792048 -7.887972683 -0.776109254
		C17	-1.749242904 -5.809454167 0.528912511
		C18	-2.850916685 -5.715895826 1.599015099
		C19	-1.335752718 -4.435474144 -0.067916597
		C20	-1.133845273 -3.364166510 1.007708365
		C21	-0.077008114 -4.581361619 -0.932107034
		C22	-5.209299688 -5.191229696 2.107147722
		C23	-5.849441919 -6.568027816 2.373359752
		C24	-6.233814787 -4.135983384 1.624229383

C25	-7.473707546	-4.119899317	2.523869724
C26	-5.591254419	-2.743138602	1.566997739
C27	-6.836582033	-8.596536850	1.476507299
C28	-6.053331691	-9.508161045	2.401642636
C29	7.386168580	-11.048056543	-1.854826402
C30	7.454656194	-9.920808501	-0.823234844
C31	6.174815526	-8.881746765	1.057541370
C32	6.221377939	-9.650591535	2.391526571
C33	4.834567843	-8.147289830	0.873240310
C34	4.561219406	-7.098768027	1.953648584
C35	3.377221430	-6.211099931	1.573471147
C36	2.004275746	-4.773607028	3.098205495
C37	7.216788772	-9.750359945	4.626502227
C38	6.556922340	-8.990336893	5.757561094
C39	-1.026331246	1.014351310	-5.821690253
C40	-2.262604047	1.621486342	-5.135814850
C41	-0.028595018	0.603549650	-4.712281431
C42	1.147384198	-0.291232536	-5.156243866
C43	2.398385366	0.462479423	-5.602568083
C44	-3.318087249	3.749456037	-4.512416136
C45	-4.741604561	3.717987122	-5.086792292
C46	-2.854360916	5.202893928	-4.292368594
C47	-6.265248885	2.635582312	-6.672573592
C48	-6.859829568	1.400796542	-5.974751609
C49	-6.449378363	-0.502324927	-4.469295205
C50	-6.480017792	-0.370363558	-2.945258658
C51	-5.823481255	0.858447548	-0.930648508
C52	-7.241459903	1.159098863	-0.379661927
C53	-4.968903579	2.054771185	-0.482786800
C54	-3.501519017	2.019019240	-0.767244835
C55	-2.591583871	1.013545726	-0.983025844
C56	-1.470277567	2.932980070	-0.925323137
C57	-9.246353356	2.564639227	-0.761078400
C58	-10.262633558	1.480710728	-0.414624739
C59	-9.755648109	3.434695399	-1.934155797
C60	-10.745307141	4.507915630	-1.589718432
C61	-11.823114772	4.506927352	-0.724536566
C62	-11.643674477	6.472430757	-1.734160256
C63	2.379703052	-4.550038179	8.306554708
C64	3.664038319	-5.353868417	8.222903644
C65	1.944261038	-4.251745542	6.848551637
C66	0.638875268	-3.497209301	6.769708336
C67	-0.596012911	-4.169613075	6.703754212
C68	0.621477877	-2.090179828	6.777586900
C69	-1.804102525	-3.466451943	6.644457542
C70	-0.575482308	-1.374654648	6.733245067
C71	-1.788647541	-2.064845361	6.664659259
C72	0.233773256	3.601463130	8.435007936
C73	-0.799665544	4.710569718	8.203721835
C74	0.341581613	2.713473358	7.185239846
C75	-1.162836670	7.121646007	7.876239356
C76	-1.709192507	7.265919986	6.453759381
C77	-1.542362867	6.507229370	4.105839287
C78	-2.599944627	5.409493551	3.853638271
C79	-0.308859708	6.375966768	3.193344739
C80	-0.536522612	6.384094697	1.678293897
C81	-1.006461309	7.706543209	1.050487897
C82	-3.228762222	8.803555958	1.308507663
C83	-3.409607292	3.162509077	4.342470661
C84	-4.659809879	3.307195396	5.233291828
C85	-2.805325938	1.769051235	4.585608231
C86	-5.454160135	3.813634405	7.488954206
C87	-6.448784246	4.941464547	7.747973705
C88	-7.261388880	7.174950257	7.123596143
C89	-8.697846102	7.082814153	6.566486390
C90	-6.554954613	8.456336272	6.633182473
C91	-6.356229357	8.460483781	5.122427386
C92	-10.210780451	5.941856907	5.003934562
C93	-11.324742000	5.611276131	5.991128814
C94	-10.113167793	4.829694366	3.926948766
C95	-9.104525338	5.171780108	2.854251154
C96	-9.458953087	6.020467054	1.793079781
C97	-7.779724244	4.709322615	2.917782952

C98	-8.518800867	6.425240485	0.841856259
C99	-6.818559343	5.123887783	1.989029977
C100	-7.200642695	5.983435812	0.961532360
C101	9.744278352	4.212781185	-1.149894637
C102	8.476858775	4.235081877	-1.985123606
C103	5.995178694	4.301184234	-1.895181737
C104	5.188363858	5.564173739	-1.573803694
C105	3.946666913	6.761122543	0.163591829
C106	4.088697549	7.169683823	1.626287640
C107	4.936448269	6.690655542	3.873984688
C108	6.253038921	7.327074659	4.272317453
C109	5.474513288	5.989034273	-6.102789335
C110	4.056633847	6.567893126	-6.173034608
C111	5.383034514	4.459325886	-5.884237769
C112	6.722438620	3.764629991	-6.186020884
C113	6.704064052	2.344122271	-5.668907065
C114	2.084201440	7.323698676	-4.938965593
C115	1.961906548	8.450819211	-3.933197147
C116	1.006199301	6.219885321	-4.815955617
C117	1.298891240	5.277200160	-3.680471730
C118	0.941684727	5.604772689	-2.362520986
C119	2.046395480	4.106909393	-3.908922892
C120	1.376936694	4.808942330	-1.297424674
C121	2.478381816	3.312974802	-2.841349504
C122	2.166167050	3.678494031	-1.528723070
C123	10.854699792	-1.693346626	1.209008590
C124	11.066702690	-2.837276301	2.216299491
C125	10.060663084	-2.132984876	-0.031954761
C126	9.630714724	-1.032455760	-0.952471149
C127	10.436446590	-0.283477467	-1.785341382
C128	8.316689837	0.248929425	-2.141253157
C129	11.592910566	-5.174704509	2.646697948
C130	12.664512857	-4.855107491	3.664987916
C131	4.271822182	-3.936317554	-3.878584849
C132	4.883296645	-4.305794180	-2.555314222
C133	6.287962979	-3.620922767	-2.309422021
C134	7.272439240	-4.018092430	-3.449647750
C135	8.715596908	-3.560973432	-3.176193291
C136	9.722713053	-4.144127866	-4.126892345
C137	6.856812133	-4.233693455	-0.995070974
C138	3.906946340	0.526130463	1.880907573
Fe139	5.563966135	1.067102844	0.920478544
Fe140	1.822176138	0.499827878	1.733653023
Fe141	3.741639573	0.221895414	3.883979965
Fe142	3.956649578	2.385905610	2.452785730
Fe143	2.003395360	2.221434461	4.273848063
Fe144	5.004400656	-1.119201246	2.131976666
Fe145	3.600965071	-0.559053738	0.055679705
H146	0.166697368	-2.677413575	-9.155523774
H147	0.277395070	-1.068870912	-8.907806296
H148	-3.834818879	-0.966416733	-10.100429603
H149	-1.503208234	-0.612445322	-10.437714197
H150	-1.570112769	-2.326440805	-10.833026239
H151	-4.486180476	-0.975775101	-7.356024521
H152	-4.608387942	-3.739485745	-9.615807681
H153	-5.646102464	-1.105553742	-8.700629142
H154	-5.156157006	-5.961434261	-9.210162712
H155	-2.737598551	-4.657457826	-7.989887222
H156	-6.201285682	-5.439615817	-7.868447338
H157	-1.994033516	-3.186125489	-3.086542550
H158	-2.544355376	-3.310024777	-5.908244834
H159	-0.950884238	-5.489126988	-6.745608471
H160	-6.572024008	-4.090633482	-2.320303950
H161	-5.078389052	-3.963530356	-4.822973236
H162	-1.933689229	-6.873301489	-6.206112776
H163	-3.014957010	-2.065846453	-4.019237104
H164	-5.235462092	-6.668432242	-4.509317767
H165	-7.092095428	-4.679770395	-3.919232052
H166	-0.223867544	-5.304275258	-1.746956456
H167	0.193790302	-3.613356093	-1.381753738
H168	0.779069747	-4.909889847	-0.322118752
H169	-2.163774560	-4.105705490	-0.715888916
H170	-5.437567171	-8.946935742	-4.272527769

H171	-4.727503765	-2.711037896	0.888042761
H172	-6.079413306	-6.951043070	0.337843227
H173	-8.001210036	-5.084814562	2.524569678
H174	-0.938465627	-2.391127158	0.533615844
H175	-0.265260489	-3.582983356	1.644518304
H176	1.610509746	-5.200939684	8.763405954
H177	-6.327979815	-2.004737029	1.218643118
H178	-8.174545081	-3.347183721	2.178769330
H179	-5.252933675	-2.437830836	2.570231263
H180	-7.194852579	-3.885718600	3.563146778
H181	-6.550470674	-4.420395806	0.604324402
H182	-4.808423477	-4.880059114	3.082510339
H183	-4.206025740	-4.965285707	0.220711688
H184	-2.015414622	-3.240785539	1.655042367
H185	-1.823939463	1.718534258	4.083666653
H186	-3.474976890	1.032239745	4.116388588
H187	-2.814921351	0.559379442	6.134165646
H188	-3.717811306	-1.898692269	6.509790670
H189	-0.567058631	-0.284206951	6.713988843
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Fe(144) 0.510 2.168	C6	-4.198579886	-5.901542901	-7.273763430
Fe(145) 0.320 0.630	C7	-1.930763410	-5.788842924	-6.355956563
	C8	-2.176602380	-5.126383115	-4.997107358
	C9	-2.834964104	-3.114973859	-3.783971371
	C10	-4.053112812	-3.680445058	-3.037938866
	C11	-6.265077784	-4.683323315	-3.177916766
	C12	-6.063348429	-6.123824832	-2.684945477
	C13	-5.429545182	-8.410643260	-3.297609702
	C14	-4.219636040	-8.930244628	-2.514131362
	C15	-1.831223502	-8.668710703	-2.005562135
	C16	-1.393164842	-7.881597644	-0.767707904
	C17	-1.748973067	-5.805402974	0.539685546
	C18	-2.842636049	-5.698401031	1.615704375
	C19	-1.340502932	-4.433241523	-0.066404849
	C20	-1.151376459	-3.350583379	0.999938029
	C21	-0.076237540	-4.577477276	-0.921890647
	C22	-5.204542043	-5.192241585	2.127066554
	C23	-5.844171748	-6.569177713	2.393440218
	C24	-6.230542135	-4.139530464	1.644156194
	C25	-7.468797596	-4.119679923	2.547062080
	C26	-5.590222070	-2.745663082	1.580351775
	C27	-6.825674782	-8.600267847	1.498570511
	C28	-6.040776686	-9.506543688	2.428827320
	C29	7.385704999	-11.054856891	-1.859504240
	C30	7.452520822	-9.931611764	-0.824692010
	C31	6.168662528	-8.887504283	1.048267158
	C32	6.213256889	-9.654734526	2.383865247
	C33	4.832349670	-8.147307889	0.861600174
	C34	4.555704127	-7.103216462	1.946211059
	C35	3.374692756	-6.213301468	1.561086128
	C36	1.979679168	-4.782294188	3.071205463
	C37	7.215290420	-9.762650916	4.614132665
	C38	6.573864484	-9.010009332	5.761004585
	C39	-1.030083336	1.008624728	-5.811286428
	C40	-2.268438141	1.614012287	-5.127668289
	C41	-0.034499285	0.601883055	-4.698015917
	C42	1.148741093	-0.286772618	-5.135921453
	C43	2.396365791	0.469962175	-5.591320182
	C44	-3.328809046	3.744374746	-4.514654051

C45	-4.750522883	3.717124623	-5.095118960
C46	-2.859492547	5.195564057	-4.291010122
C47	-6.273296076	2.622800336	-6.675362046
C48	-6.870952186	1.390972966	-5.977665181
C49	-6.462355028	-0.511671817	-4.469803730
C50	-6.495534068	-0.376294812	-2.946361015
C51	-5.821163881	0.847272822	-0.932471787
C52	-7.239682748	1.156299615	-0.390018837
C53	-4.964930430	2.043981062	-0.491187459
C54	-3.498602911	2.005552079	-0.778487482
C55	-2.590124058	0.998585608	-0.997993487
C56	-1.467099322	2.915380812	-0.949187591
C57	-9.228603653	2.576690344	-0.774873791
C58	-10.245859925	1.494376605	-0.420805862
C59	-9.736996058	3.448227014	-1.947404393
C60	-10.728182560	4.519522854	-1.600488357
C61	-11.792102839	4.519237713	-0.719060742
C62	-11.637013193	6.479242978	-1.742450224
C63	2.366705085	-4.546205187	8.307190543
C64	3.652722157	-5.346928390	8.220624555
C65	1.923400349	-4.258810396	6.848745027
C66	0.620506676	-3.498731934	6.767149667
C67	-0.615694263	-4.168780907	6.701839021
C68	0.605976664	-2.091395345	6.771345604
C69	-1.822062527	-3.463987063	6.640801838
C70	-0.590023809	-1.374206202	6.724462930
C71	-1.804051092	-2.062951872	6.656762485
C72	0.226953623	3.603346528	8.438444087
C73	-0.804718199	4.714575536	8.208317128
C74	0.346760153	2.718605595	7.187693755
C75	-1.167897634	7.126709651	7.891201288
C76	-1.705418067	7.274279270	6.466712015
C77	-1.531747272	6.515709065	4.120358765
C78	-2.585297670	5.415010718	3.864968014
C79	-0.296378346	6.392557090	3.209348856
C80	-0.528475134	6.389811411	1.695699347
C81	-0.998560876	7.708854716	1.057953958
C82	-3.225415718	8.803320285	1.286430920
C83	-3.391286675	3.166719541	4.352113490
C84	-4.648705347	3.318601786	5.227955578
C85	-2.792963928	1.775185245	4.624040285
C86	-5.447978832	3.808771760	7.483314053
C87	-6.446317101	4.932018590	7.741574609
C88	-7.250952239	7.170169020	7.125971528
C89	-8.686953156	7.070197786	6.570551908
C90	-6.550010188	8.454632375	6.635535494
C91	-6.350336548	8.461404707	5.124688281
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C94	-10.108044017	4.830471191	3.921108583
C95	-9.099888811	5.168232510	2.846494021
C96	-9.448278529	6.028158966	1.792804381
C97	-7.779743336	4.691675356	2.905594446
C98	-8.507021357	6.426466594	0.840848753
C99	-6.817144533	5.097640639	1.974613394
C100	-7.194337657	5.967811325	0.953790174
C101	9.744707752	4.220321452	-1.158042980
C102	8.473660437	4.244262383	-1.988628661
C103	5.993731958	4.301238687	-1.892873902
C104	5.179153793	5.558250901	-1.569424013
C105	3.933168094	6.746380382	0.170150231
C106	4.074069413	7.158408320	1.632922607
C107	4.930240697	6.687680698	3.878888125
C108	6.245495495	7.326461860	4.270911593
C109	5.476747627	5.995295666	-6.097263019
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C116	1.000231669	6.198557704	-4.834604994
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C119	2.034088446	4.098561219	-3.893334907
C120	1.336341445	4.826869488	-1.296878871
C121	2.456761381	3.316988120	-2.813435315
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C124	11.073335317	-2.849166835	2.213805344
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C126	9.661758019	-1.033984395	-0.959679065
C127	10.474961970	-0.303329635	-1.802599082
C128	8.361520634	0.260611428	-2.146686335
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C130	12.664177229	-4.859781034	3.665784371
C131	4.294895417	-3.941557087	-3.894970575
C132	4.897944003	-4.285508635	-2.561599928
C133	6.311220619	-3.617800586	-2.319451886
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C136	9.746541830	-4.135155938	-4.130623870
C137	6.868191120	-4.234795528	-0.999845121
C138	3.919313507	0.521625759	1.881041106
Fe139	5.584630159	1.063491581	0.903558366
Fe140	1.991201139	0.617880277	1.772146881
Fe141	3.691644764	0.174465654	3.864426496
Fe142	3.979590530	2.386375656	2.468496545
Fe143	2.003026576	2.224197430	4.262505931
Fe144	4.981161701	-1.142093885	2.078483409
Fe145	3.648204228	-0.480889302	-0.020841529
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H148	-3.834033251	-0.969894151	-10.103774810
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H150	-1.562897020	-2.307174625	-10.834911111
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H158	-2.537178050	-3.303157840	-5.908208510
H159	-0.941774065	-5.492938158	-6.731275095
H160	-6.563107510	-4.080146349	-2.311530600
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H165	-7.085679441	-4.674936931	-3.907965980
H166	-0.202639939	-5.328641329	-1.714068566
H167	0.171312206	-3.618831197	-1.403194665
H168	0.787710397	-4.865612199	-0.302193407
H169	-2.167553218	-4.114116624	-0.721334731
H170	-5.449150586	-8.938785966	-4.262124643
H171	-4.725769597	-2.717706899	0.901970384
H172	-6.075017552	-6.953999093	0.356843017
H173	-7.995429049	-5.085390510	2.553688464
H174	-0.946837099	-2.385768313	0.512727069
H175	-0.292787807	-3.560542707	1.652895426
H176	1.600917239	-5.193838620	8.775817945
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H180	-7.189060530	-3.880965333	3.585983787
H181	-6.549139748	-4.425557968	0.625221178
H182	-4.798985724	-4.877752373	3.099710355
H183	-4.212475021	-4.989988577	0.232030561
H184	-2.041883220	-3.216844147	1.632361250
H185	-1.790481046	1.730217232	4.167140739
H186	-3.441485769	1.035297555	4.130138851
H187	-2.842933474	0.561848744	6.167037875
H188	-3.733966729	-1.895793898	6.506130606
H189	-0.580723666	-0.283759758	6.706820081
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H191	-0.639634197	-5.261830034	6.690836151
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H205	6.880013522	3.746032617	-7.276381208
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H207	4.603602794	4.034721219	-6.524175989
H208	2.886373095	8.992554946	-3.755455908
H209	5.884121955	6.164051854	-7.106057042
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H211	0.842703905	-0.940800721	-5.971037315
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H213	1.926118522	7.800258810	-5.928392416
H214	6.071768967	6.541639439	-4.183930226
H215	3.637568139	-0.934368530	-4.693116224
H216	5.078675028	4.276734856	-4.839696354
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H219	-0.610415749	0.052189679	-3.939116053
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H257	-8.797600447	7.087075732	0.019991817
H258	-7.471999715	3.992237401	3.687673219
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H262	-1.206327439	5.571636214	1.405260435
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H267	-5.781016465	4.768653887	2.074153652
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H287	10.270818151	-0.948295463	1.756516574
H288	11.718947085	4.659719589	-1.414993761
H289	10.892944982	4.482526453	-2.818316407
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H291	-1.102509160	2.444860617	9.462397096
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H294	-0.121789052	3.312259140	10.441901286
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H299	5.224243203	5.498771165	2.140755252
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H302	3.049278642	2.414711582	-2.981684567
H303	2.861624144	6.544419150	0.010862181
H304	2.453332065	-6.799582279	1.458199547
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H306	3.565758130	-5.746188961	0.580240757
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H312	7.224127621	-10.565080956	-2.831562428
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Fe(141) 0.527 -2.449	C3	-4.742350271	-1.827724097	-8.181193776
Fe(142) 0.565 2.786	C4	-5.094362553	-3.219168751	-7.660759614
Fe(143) 0.606 3.217	C5	-5.221252817	-5.616113784	-8.104361628
Fe(144) 0.517 2.125	C6	-4.223052751	-6.148240655	-7.071868297
Fe(145) 0.314 0.498	C7	-1.943120152	-6.005245266	-6.180724606
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C137	6.834203396	-4.257827093	-0.840218896

C138	3.939328631	0.600648934	1.870073227
Fe139	5.596250325	1.110348461	0.856284348
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Fe141	3.541621141	0.306195749	3.808519459
Fe142	3.957028655	2.494398116	2.386175497
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Fe144	4.927342003	-1.075663605	2.088098281
Fe145	3.619041167	-0.400929906	-0.030839860
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O440	-5.638009233	4.180061949	-4.634533779
O441	-3.723429876	5.779607596	-3.600021002
O442	-8.041819433	0.907960518	-6.165635097
O443	-7.081318255	-1.265493360	-2.218500420
O444	-7.550731496	0.827868059	0.731110111
O445	-11.059528068	1.600503675	0.465650331
O446	3.707077354	-6.298524636	8.519476780
O447	-2.910228993	-1.079202141	6.626026414
O448	-2.018598023	4.759019591	7.955205632
O449	-2.647202510	8.270262828	5.938117594
O450	-3.566295870	5.746449098	2.880678350
O451	-5.749575333	2.951218891	4.821006353
O452	-2.709694357	1.731748913	5.931986478
O453	-7.203196935	5.219855041	8.578319295
O454	-9.574095561	8.095743279	6.659550848
O455	-7.304560346	8.800281198	4.021269982
O456	-12.481820484	6.007153519	5.554549694
O457	-6.194807324	6.431388217	-0.159021472
O458	8.565148328	3.989510066	-3.385083510
O459	5.013922387	6.348769277	-2.673351540
O460	3.533557472	8.285671626	1.691753183
O461	6.657725648	7.559067612	5.165425610
O462	3.471964038	6.496170371	-7.487329408
O463	6.117994204	1.195251451	-6.281952490
O464	7.334960323	1.962296672	-4.578166931
O465	0.982229347	8.660444677	-3.619902929
O466	11.013761540	-2.536426979	3.530170738
O467	12.752739671	-5.256974513	4.933417960
O468	3.561072142	-3.108557281	-4.000882053
O469	4.530675465	-4.964302852	-4.749537104
O470	10.711982068	-4.923438336	-3.601783645
O471	9.466170264	-4.063191980	-5.278670717
O472	7.054238944	-3.379464327	0.081374127
O473	7.078339226	-5.482614380	-0.725694870
O474	6.146790174	-2.325610846	-2.150149270
O475	8.473638193	-6.590395270	3.101747444
O476	6.763981309	-4.360574678	2.707030557
O477	-3.754590728	5.745604817	-0.860409167
O478	11.694878176	-6.039307776	-0.904602633
O479	9.217653388	-6.679483092	0.410256135
S480	0.730695025	3.898868117	5.494836533
S481	1.801127251	3.057521736	1.863650944
S482	5.131646754	0.608667933	-1.288773913
S483	1.305148426	0.281994096	3.870069613
S484	1.497683672	0.332091542	-0.367644572
S485	5.840236356	3.272355259	1.421629227
S486	4.156859550	-2.450514584	0.515767295
S487	4.152388510	2.270830550	4.678920673
S488	7.034373596	-0.415276341	1.713098209
S489	4.520851134	-1.654184832	4.195531733

Atomic coordinates and electronic state for the structure with promotional N₂ at *exo*-Fe2 and reactive N₂ at *endo*-Fe6, shown in Fig 7, together with the transition state for dissociation, and the dissociated form.

structure, S, spin densities	filename, coordinates
associated	bm22b2n2x6x6n2ncnxdtr.car_3

	S=3/2	C1	2.011406082	0.661737048	-9.263681736
Fe(139)	0.545 2.517	C2	3.375613270	0.178647804	-9.762176575
Fe(140)	0.411 -1.171	C3	0.289225886	2.403860015	-9.378453855
Fe(141)	0.570 2.748	C4	-0.941426594	1.536051043	-9.641130574
Fe(142)	0.519 -2.337	C5	-2.013873167	-0.151848772	-11.044403555
Fe(143)	0.557 2.861	C6	-2.196768292	-1.278397570	-10.021166314
Fe(144)	0.488 -2.041	C7	-1.123283955	-2.730747979	-8.367406365
Fe(145)	0.259 -0.012	C8	-1.646950946	-2.162218011	-7.045906598
		C9	-1.700971417	-0.275939558	-5.501155101
		C10	-3.203263372	0.043746755	-5.560990813
		C11	-5.117474228	0.681319986	-6.912005061
		C12	-5.989232237	-0.582073972	-6.948702279
		C13	-6.393569096	-2.742795166	-8.030706975
		C14	-6.280900686	-3.937738110	-7.077422678
		C15	-4.820535210	-5.260698862	-5.602528709
		C16	-4.710796254	-4.968688723	-4.102288624
		C17	-4.656111004	-3.156202647	-2.393869713
		C18	-5.969514810	-2.485499685	-1.956867412
		C19	-3.413206402	-2.248050716	-2.227440714
		C20	-3.454181950	-1.500873977	-0.889321747
		C21	-2.129987456	-3.066029570	-2.410087338
		C22	-7.453610158	-0.538964877	-2.166311675
		C23	-8.750250792	-1.170131965	-2.703338460
		C24	-7.297893817	0.949353309	-2.562654620
		C25	-8.572449717	1.743567584	-2.257082438
		C26	-6.095162904	1.579980350	-1.845832719
		C27	-9.933052375	-2.144138347	-4.581753560
		C28	-10.426955018	-3.345375647	-3.797634565
		C29	-0.050497448	-13.175602408	-2.938378496
		C30	0.061265276	-12.404801214	-1.622278228
		C31	-1.183634558	-10.820831026	-0.145827912
		C32	-2.282760882	-11.478661676	0.710149449
		C33	-1.538694102	-9.372178103	-0.520991682
		C34	-1.770739203	-8.472511397	0.694520256
		C35	-1.819646162	-6.998473827	0.295087177
		C36	-2.923504929	-5.221016389	1.682772830
		C37	-2.864215099	-12.331859339	2.932741889
		C38	-3.441978498	-11.397318174	3.973631319
		C39	2.995113651	1.758421630	-5.020847812
		C40	2.134820567	2.981385473	-4.669087858
		C41	2.832825127	0.734906875	-3.871318985
		C42	3.357526453	-0.689173822	-4.143525217
		C43	4.824274096	-0.922184963	-3.786234707
		C44	2.216952394	5.233609983	-3.697169516
		C45	1.518866950	6.158230774	-4.703415529
		C46	3.181407342	6.037657706	-2.801296542
		C47	0.730190639	6.432233348	-7.003774792
		C48	-0.697979816	5.866767292	-7.042613424
		C49	-2.225676479	4.077596660	-6.324430355
		C50	-2.971498142	4.101492705	-4.990112105
		C51	-2.921035558	4.567722853	-2.579141653
		C52	-3.995859809	5.677022781	-2.468436981
		C53	-1.913858731	4.857319038	-1.456016122
		C54	-0.787926801	3.890751305	-1.270845766
		C55	-0.596148510	2.569565295	-1.592194528
		C56	1.189195441	3.250913794	-0.451298746
		C57	-4.473793313	8.035536723	-3.043650328
		C58	-5.923012219	7.803664959	-3.467147864
		C59	-3.804288645	9.100465402	-3.942670711
		C60	-4.091429801	10.533101320	-3.598104237
		C61	-5.260181078	11.148583741	-3.193709661
		C62	-3.614623872	12.626635428	-3.327342974
		C63	-5.007686909	-5.462722231	6.576714124
		C64	-4.520782877	-6.895807752	6.692906904
		C65	-4.421888271	-4.902607799	5.260576375
		C66	-4.872182588	-3.492274310	4.957261992
		C67	-6.057485181	-3.244564816	4.239612560
		C68	-4.106868999	-2.385983376	5.365143091
		C69	-6.465290913	-1.940615844	3.937279530
		C70	-4.504016052	-1.079503521	5.077654943
		C71	-5.685177225	-0.858053404	4.362606248
		C72	-2.331853787	2.107817504	8.605644055
		C73	-2.269175917	3.631904340	8.443838952

C74	-2.068928871	1.419471900	7.258180799
C75	-1.010014379	5.687195990	8.910660022
C76	-0.575135170	6.217750584	7.543841293
C77	0.281466325	5.660339882	5.297583690
C78	-0.901692772	5.555833105	4.311091982
C79	1.490995598	4.806477077	4.878037362
C80	2.086632835	5.055110141	3.488577071
C81	2.863421882	6.368155095	3.279650578
C82	1.805980778	8.637840192	3.271487562
C83	-2.948650847	4.419955068	3.628341339
C84	-4.132131205	5.317325346	4.041481832
C85	-3.466546868	2.980217713	3.508900002
C86	-5.490909728	6.086200658	5.922946646
C87	-5.670652790	7.577683693	6.189701556
C88	-4.681745522	9.830311880	6.107937619
C89	-5.375669885	10.729253365	5.061507202
C90	-3.256779916	10.346887356	6.410600014
C91	-2.347952501	10.242019311	5.192022573
C92	-6.198832944	10.913810266	2.755424132
C93	-7.628082570	11.371032013	3.028283290
C94	-6.153470077	10.065424367	1.456586549
C95	-4.738119110	9.726468814	1.046548012
C96	-3.967356056	10.652618399	0.325778205
C97	-4.139262069	8.510895293	1.419645492
C98	-2.635073407	10.388365396	0.002962514
C99	-2.799873145	8.237725800	1.124661305
C100	-2.061278378	9.188388600	0.423926608
C101	9.280499674	-3.217484564	4.098013628
C102	8.906496143	-2.308093887	2.940244446
C103	7.293802481	-0.587351693	2.162599632
C104	7.300592094	0.864085003	2.659227038
C105	6.304817141	2.442854005	4.242372570
C106	5.853542808	2.518100665	5.698252494
C107	4.869675501	1.437066099	7.658585872
C108	5.903015170	1.129590934	8.726006925
C109	10.020390430	1.345072720	-0.938073771
C110	9.428413348	2.726610571	-1.248322192
C111	9.020003376	0.243504693	-1.354706444
C112	9.698271834	-1.138049083	-1.421530585
C113	8.662141147	-2.230446677	-1.563050946
C114	7.915731122	4.518582664	-0.555305744
C115	7.908377929	5.348874225	0.713160900
C116	6.546358268	4.419007959	-1.271929278
C117	5.659958639	3.394075451	-0.618347391
C118	4.917312778	3.710892025	0.531266223
C119	5.677309004	2.061177252	-1.065462595
C120	4.269613155	2.701247394	1.249936587
C121	5.028851644	1.052978713	-0.346776492
C122	4.348828812	1.369703240	0.833105758
C123	5.775655322	-8.419107522	4.414016169
C124	4.769064180	-9.460360676	4.932789989
C125	5.612534947	-8.152476364	2.909755318
C126	6.383646030	-6.992531103	2.355198478
C127	7.753416465	-6.885160810	2.219100759
C128	6.786043455	-5.132978928	1.269652108
C129	3.597896882	-11.570710444	4.634229297
C130	3.923145530	-12.054750866	6.029753523
C131	2.868370622	-5.665287619	-3.291476589
C132	2.387979692	-6.356537247	-2.044960666
C133	3.564578617	-6.751930981	-1.065858967
C134	4.607212833	-7.629116624	-1.822186929
C135	5.673529614	-8.214754405	-0.880129957
C136	6.506061195	-9.294173288	-1.511316430
C137	2.958979944	-7.667978220	0.040213521
C138	1.864918149	-2.247592757	3.138815659
Fe139	3.771323357	-2.869549091	3.108875271
Fe140	0.817366630	-0.305071763	2.678231879
Fe141	0.500534936	-2.464234146	4.542454389
Fe142	2.666889038	-1.090008606	4.527463825
Fe143	0.460303624	0.203841988	5.260787841
Fe144	1.644498331	-4.225137954	3.171177801
Fe145	1.785653851	-2.879711450	0.855156783
H146	3.387824911	-1.590822037	-8.748521932

H147	4.276154055	-0.425883697	-8.027438677
H148	2.162030264	2.364844707	-10.411475235
H149	4.043879349	1.042981511	-9.899261840
H150	3.208178245	-0.239020751	-10.770414207
H151	0.301043838	2.595033868	-8.295649333
H152	-0.087621868	0.762142075	-11.341301889
H153	0.154449987	3.362504056	-9.897187135
H154	-1.839118859	-0.597796310	-12.032623934
H155	-0.191365707	-1.242829657	-9.581436020
H156	-2.961169865	0.401955103	-11.078183725
H157	-1.551787151	-0.916685390	-4.622055779
H158	-0.479618967	-0.468587867	-7.265347490
H159	-0.115778916	-3.141188096	-8.213824436
H160	-5.468586396	1.295098982	-6.072899915
H161	-3.063990082	0.581899656	-7.554919773
H162	-1.790868290	-3.552644370	-8.653211915
H163	-1.131560283	0.652760883	-5.350351550
H164	-4.712858911	-1.460480206	-8.322009173
H165	-5.271901034	1.238905389	-7.846072756
H166	-2.106159913	-3.546862293	-3.399082573
H167	-1.244950448	-2.415787056	-2.327692169
H168	-2.037988130	-3.846702751	-1.641137918
H169	-3.444310145	-1.496018060	-3.031185279
H170	-6.155724493	-3.106032940	-9.040914128
H171	-5.146265781	1.093910018	-2.112875218
H172	-7.950636738	-1.349212555	-4.616410009
H173	-9.441460438	1.368654043	-2.816030947
H174	-2.520760663	-0.939893252	-0.738611418
H175	-3.552855792	-2.193029965	-0.042389206
H176	-6.109498187	-5.501077134	6.467570566
H177	-6.010176656	2.642274437	-2.117962713
H178	-8.422408740	2.799429651	-2.527906613
H179	-6.221957295	1.517566716	-0.752721408
H180	-8.813490851	1.699358984	-1.183055011
H181	-7.119091554	0.987475494	-3.652671834
H182	-7.543894502	-0.608810913	-1.070947597
H183	-5.608687368	-0.878952881	-3.213600055
H184	-4.287693214	-0.785716891	-0.849010847
H185	-2.611315875	2.304667363	3.346744799
H186	-4.116101705	2.945371336	2.618925687
H187	-4.796272099	1.884614023	4.443497462
H188	-6.835080300	0.478548182	3.547053608
H189	-3.882818162	-0.235081603	5.378332078
H190	-3.158553524	-2.545417350	5.883061466
H191	-6.669808236	-4.083886898	3.896974205
H192	-4.868964008	-2.985681331	-4.517687648
H193	-3.881765627	-5.747639456	-5.906483532
H194	-5.637738276	-5.981706002	-5.737899454
H195	-4.280765919	-3.517001428	-6.695452157
H196	-7.447967621	-2.438076455	-8.020197588
H197	-7.379692805	-1.768903596	3.363432687
H198	-4.552863997	-4.040528439	-1.751063993
H199	-10.756895474	-1.416625797	-4.671888894
H200	-9.683888065	-2.494636234	-5.595532609
H201	-9.646374178	-3.874101264	-3.202254010
H202	-2.377968718	-13.183880101	3.431280923
H203	6.098389777	-2.340047398	-3.038246447
H204	2.788289088	-7.375130054	-4.180656283
H205	10.359247704	-1.174290433	-2.299997134
H206	10.308873117	-1.306925641	-0.522769908
H207	8.589648935	0.474658738	-2.341781809
H208	8.762178347	5.145018954	1.400909528
H209	10.886365401	1.279541513	-1.614867741
H210	3.313418315	1.145635673	-2.968098863
H211	3.234140839	-0.941391974	-5.211031433
H212	8.330903296	2.702714190	0.514092221
H213	8.596452042	5.074009001	-1.231386426
H214	9.780807191	1.198679639	1.118067941
H215	4.412166891	-2.845586821	-3.108413848
H216	8.181702925	0.234405294	-0.641913115
H217	11.134481021	0.456654665	0.539484524
H218	4.599691789	2.281671468	-6.211543847
H219	1.755398041	0.659487973	-3.664585512

H220	8.845317626	-2.577235422	0.366458588
H221	2.733967992	-1.408615345	-3.593181178
H222	-3.441696702	3.615278029	-2.405373885
H223	-1.223358132	1.864764803	-2.125444002
H224	-2.862880999	4.591814282	-7.055955300
H225	-0.139436911	4.225789398	-5.887658863
H226	-2.938187501	6.768925791	-3.837754294
H227	-6.257869539	10.769432297	-3.000287839
H228	-6.039608973	7.080407771	-4.310584715
H229	-4.058584181	8.892416681	-4.997635461
H230	-4.465503572	8.361077582	-1.991296302
H231	-3.105417575	13.586131628	-3.278490467
H232	-2.491771708	4.903410055	-0.518755245
H233	-1.490197602	5.863133249	-1.611088547
H234	-5.570892167	13.211910119	-2.724689300
H235	-2.713961009	8.971894674	-3.857806328
H236	-1.281080706	4.708036526	-3.971582376
H237	-2.150011665	3.029287093	-6.649213187
H238	0.643846350	7.509869609	-6.817798065
H239	2.152092146	3.242038460	0.055472946
H240	1.179164119	6.296240116	-7.996872646
H241	-5.108068138	-4.922755915	8.549774246
H242	-4.682461135	-3.697094293	7.556734189
H243	-1.533521458	3.753631641	5.129060664
H244	-2.650717850	4.754091063	2.624428635
H245	-3.599672631	5.155317256	6.016444781
H246	0.523412170	5.260681180	-0.204613323
H247	1.580788581	7.018073035	-0.630574391
H248	0.223166475	7.535917944	0.023855921
H249	3.609387231	5.372129595	-2.038829335
H250	4.006668236	6.446527224	-3.408470524
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	O476	0.543616523	-10.734859312	3.046248542
	O477	0.918797308	-7.937656142	2.994125827
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C66	-4.869300900	-3.487163238	4.930518180
C67	-6.052727416	-3.239415804	4.209581253
C68	-4.108837748	-2.381123412	5.347004377
C69	-6.465136483	-1.935389218	3.915084896
C70	-4.509949015	-1.074784035	5.066843069
C71	-5.690330185	-0.853148567	4.350663715
C72	-2.328488378	2.110374233	8.604805472
C73	-2.262926724	3.633618429	8.434626025
C74	-2.064820876	1.409050533	7.263031311
C75	-1.006202084	5.688852418	8.909882435
C76	-0.568377854	6.220256912	7.543914941
C77	0.287716326	5.662303700	5.297844404
C78	-0.895372098	5.556761932	4.310990357
C79	1.497740616	4.809951623	4.877208645
C80	2.084491710	5.057284077	3.484439455
C81	2.858795582	6.372094034	3.272435675
C82	1.809038949	8.644467332	3.265348701
C83	-2.940851587	4.418444683	3.627722538
C84	-4.127086676	5.313582882	4.038423172
C85	-3.451434228	2.975241268	3.506238962
C86	-5.492594399	6.082862667	5.916872056
C87	-5.663334782	7.572001148	6.199914026
C88	-4.679538692	9.825894315	6.114070012
C89	-5.381402871	10.723358967	5.071766937
C90	-3.256384941	10.347772148	6.409374793
C91	-2.351992083	10.242146823	5.186778993
C92	-6.201650052	10.910751796	2.760916961

C93	-7.628231870	11.377250439	3.029876814
C94	-6.157634118	10.057340914	1.466963633
C95	-4.742187012	9.721189780	1.054003406
C96	-3.976570055	10.651236586	0.332354010
C97	-4.139975293	8.504292303	1.416185771
C98	-2.645062127	10.390945837	0.001152392
C99	-2.801748841	8.234798110	1.111918045
C100	-2.067015235	9.189231622	0.412152286
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C102	8.916566519	-2.300224342	2.941091827
C103	7.301069007	-0.578052511	2.167844427
C104	7.305495000	0.873534786	2.662292664
C105	6.321261708	2.452078863	4.251741883
C106	5.851916422	2.531666359	5.700012883
C107	4.872706130	1.451085275	7.664319272
C108	5.910240752	1.120037585	8.721776749
C109	10.021928174	1.356499326	-0.948587513
C110	9.427277895	2.735241633	-1.263991387
C111	9.019984104	0.251746460	-1.357588108
C112	9.700933334	-1.127450854	-1.415839906
C113	8.669727665	-2.224973957	-1.564782356
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C115	7.906007891	5.346298209	0.716882890
C116	6.545537573	4.423602954	-1.273136068
C117	5.660650503	3.395680439	-0.622286189
C118	4.905419823	3.712990044	0.519269374
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C124	4.764169021	-9.461908232	4.934085731
C125	5.624340918	-8.156450262	2.911179073
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C127	7.776474122	-6.909922418	2.215821524
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Fe141	0.497400408	-2.473044720	4.548018460
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Fe144	1.612596895	-4.264493354	3.149553332
Fe145	1.928056900	-2.834302424	0.949528922
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H149	4.041373022	1.046934882	-9.876949047
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H151	0.295680210	2.596155438	-8.288372519
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H182	-7.522479274	-0.627778151	-1.051121835
H183	-5.589734191	-0.896615781	-3.190681072
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H245	-3.603553468	5.145538717	6.016147678
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	O461	5.885373978	3.640146132	6.261892662
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	O465	8.335433655	-2.894956612	-0.445139050
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	O476	0.540060243	-10.726140645	3.043839394
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	O478	0.943967643	6.878638427	0.132247884
	O479	5.154752151	-12.099199294	1.140433232
	O480	2.468729654	-11.087738494	1.050857806
	S481	-0.478111766	1.928150561	6.459920446
	S482	2.089489564	1.007080075	3.923684323
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	S485	1.723813484	-0.584020887	0.557043139
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	S488	1.501644414	-1.478541286	6.368072530
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	C5	-2.017682969	-0.145004268	-11.049330360
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	C9	-1.715531916	-0.262362708	-5.514927048
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	C11	-5.130900193	0.681510228	-6.936774189
	C12	-5.999946581	-0.584019592	-6.966158578
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	C14	-6.278695583	-3.946955219	-7.075372648
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	C20	-3.486632999	-1.450483374	-0.934034586
	C21	-2.141705708	-3.019053046	-2.459528267
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	C23	-8.756706503	-1.155195382	-2.717682394
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C78	-0.905993926	5.559437637	4.312113361
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C103	7.301876857	-0.593665962	2.170466392
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H152	-0.092056907	0.768050902	-11.351136556
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H154	-1.845459180	-0.590615370	-12.038139648
H155	-0.190986157	-1.233307207	-9.589435915
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H162	-1.779936578	-3.548598761	-8.658737176
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H181	-7.136220628	1.005820602	-3.673012246
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H185	-2.618217667	2.312861745	3.345833156
H186	-4.126030742	2.952292343	2.624337694
H187	-4.798150122	1.885962839	4.449520957
H188	-6.835421860	0.466916541	3.549571085
H189	-3.887733877	-0.229481789	5.392610990
H190	-3.155729874	-2.534569613	5.906795601
H191	-6.670743582	-4.092793018	3.943297327
H192	-4.899776151	-2.988021721	-4.515184546
H193	-3.880503624	-5.747603583	-5.892927676
H194	-5.636455079	-5.982909489	-5.726425004
H195	-4.282090947	-3.516842184	-6.685633414
H196	-7.449129080	-2.452818375	-8.022778167
H197	-7.386882512	-1.782142414	3.396848621
H198	-4.545202239	-4.009858980	-1.739311714
H199	-10.749448699	-1.428110475	-4.696255007
H200	-9.668428657	-2.513582943	-5.601414865
H201	-9.650739630	-3.871404427	-3.195155175
H202	-2.379395068	-13.180015149	3.448623848
H203	6.101723475	-2.339721566	-3.029519522
H204	2.809866349	-7.347560149	-4.192700872
H205	10.369334498	-1.169511188	-2.309394242
H206	10.323164083	-1.304943216	-0.532489380
H207	8.602775188	0.484665516	-2.342669088
H208	8.773027213	5.140975660	1.397849699
H209	10.907995537	1.282056638	-1.609393844
H210	3.314220656	1.142228451	-2.982472676
H211	3.258185729	-0.940540638	-5.228319746
H212	8.332580423	2.699273505	0.504942582
H213	8.616662799	5.070940028	-1.237814650
H214	9.782883052	1.197273455	1.115889930
H215	4.415041842	-2.843435089	-3.106214294
H216	8.199628143	0.239987828	-0.642649378
H217	11.136229411	0.450390861	0.546958896
H218	4.628159012	2.282152976	-6.209873826
H219	1.761543499	0.656982609	-3.687592070
H220	8.855823400	-2.575835670	0.359805413
H221	2.740969186	-1.412786789	-3.617392445
H222	-3.427696637	3.622676033	-2.413054189
H223	-1.234472553	1.841587246	-2.068574685
H224	-2.861222695	4.600981711	-7.057493708
H225	-0.135690414	4.222668604	-5.897487470
H226	-2.951303063	6.779284840	-3.846176244
H227	-6.284060243	10.774544219	-2.998967740
H228	-6.058154874	7.072746809	-4.279643012
H229	-4.087584268	8.893559609	-4.993552589
H230	-4.464891958	8.366375300	-1.981894471
H231	-3.136531366	13.594982995	-3.290082818
H232	-2.471744928	4.922547972	-0.530027879
H233	-1.458638330	5.860278382	-1.631330207
H234	-5.600222563	13.218044506	-2.730827326
H235	-2.735593311	8.983917484	-3.862961665
H236	-1.280664353	4.743006759	-3.988953532
H237	-2.150890062	3.034028401	-6.663107553
H238	0.648077530	7.510170082	-6.819180656
H239	2.136796086	3.227390646	0.110740250
H240	1.184123520	6.299290770	-8.000400421
H241	-5.028628194	-4.898365275	8.603559615
H242	-4.625316044	-3.676262799	7.598598125
H243	-1.540811152	3.759688590	5.129970144
H244	-2.662341479	4.762436880	2.628070271
H245	-3.606722322	5.155453969	6.023043872
H246	0.537943176	5.260453352	-0.212426775
H247	1.594658377	7.022053460	-0.637913669
H248	0.236404835	7.537141658	0.018252060
H249	3.617852816	5.373596211	-2.047584417
H250	4.010136684	6.443708270	-3.421968472
H251	-2.863659208	9.777424869	7.265879827
H252	-3.337884764	11.404870365	6.696437853
H253	-1.381714045	8.523488539	5.948794205
H254	-1.016860640	8.976687636	4.301761494
H255	2.179392712	9.924434774	4.825157860
H256	3.697369911	6.195292783	2.590395129
H257	-2.038695455	11.107532375	-0.571831375

H258	-4.712625292	7.748242283	1.946411906
H259	0.329111150	9.143157110	1.927727642
H260	1.194194338	3.738349125	4.924157985
H261	-0.132546633	4.309430565	6.904026677
H262	1.311541541	4.953455184	2.708210170
H263	2.201317159	5.047924585	-6.270155912
H264	-0.258110578	6.000359795	9.646465996
H265	3.880129306	3.914482806	-4.328391270
H266	2.269058981	4.945739331	5.637317830
H267	-2.327790409	7.315493121	1.482924254
H268	1.844335292	7.450653355	-2.795501008
H269	-1.953272029	6.200937008	9.157856333
H270	3.312287779	8.620995313	4.683116908
H271	0.884492482	10.424090271	2.940028215
H272	5.028373668	1.417628363	-4.835382557
H273	2.553265670	1.323455262	-5.944770392
H274	-4.403341764	11.594581698	-0.004081238
H275	1.397202231	4.869618449	-3.061758779
H276	0.553937895	6.722598325	5.304105131
H277	3.307061744	6.682916346	4.235691689
H278	2.788623542	4.226955229	3.319465479
H279	1.610788540	7.253032410	1.805269215
H280	-6.316462534	5.783606585	5.267527264
H281	-3.815167805	7.982612082	5.420038586
H282	-5.288365487	9.947345176	7.014932435
H283	-5.645465750	5.591187396	6.899609458
H284	-5.408716349	9.173038149	3.737051863
H285	8.958856358	-2.790424052	5.050777519
H286	8.697873324	-4.159784252	3.950292856
H287	5.546452962	-7.492844694	4.958708009
H288	10.948333667	-4.221564936	4.750115204
H289	11.040042618	-3.727954579	3.190637061
H290	-2.048042974	0.338266962	7.411153127
H291	-4.363783075	2.071874748	8.530867846
H292	-0.474817079	3.690350327	9.450431198
H293	-2.883994605	1.671799492	6.556605687
H294	-3.771977753	2.033473657	10.055462703
H295	4.051929005	0.686112124	7.759353642
H296	-1.551480362	1.785673519	9.313080519
H297	-2.418671457	-9.401316167	-1.170684239
H298	-0.222589907	-10.848123715	0.404208031
H299	5.283133829	0.497775637	5.799793075
H300	-3.577212469	-3.771549332	2.950442851
H301	7.273271517	2.929103718	4.181599461
H302	5.070700364	0.026737212	-0.672278315
H303	5.588996620	3.059873281	3.680627866
H304	-2.625202024	-6.818609962	-0.400554930
H305	5.734234346	0.361227452	3.868077698
H306	-0.874993031	-6.735460295	-0.185035284
H307	-0.687795104	-9.000831323	-1.108698776
H308	-0.961856566	-8.632228952	1.433375308
H309	-2.715828754	-8.775402408	1.201231016
H310	6.754006119	4.148699196	-2.328507144
H311	-1.752238220	-11.720922768	-2.023016149
H312	0.677425029	-12.699901489	-3.632997542
H313	3.921455561	0.615179850	1.469702272
H314	-1.925885325	-13.947299177	-3.204001824
H315	-1.321316809	-13.227017339	-4.545132789
H316	-1.137268145	-6.053951052	2.078583776
H317	3.755245921	2.954438859	2.177217376
H318	6.215681927	1.806571153	-1.981476881
H319	4.233267406	-11.790781081	1.061039714
H320	5.885748972	-9.053828663	2.343722126
H321	2.457698109	-10.174501790	0.652951636
H322	5.639554264	-11.592998849	0.451079692
H323	6.944357153	0.988858608	8.356594180
H324	1.613504530	-7.699881259	2.381046710
H325	1.800651796	-7.238083247	-2.308690520
H326	7.298006361	-1.631900227	4.008886679
H327	4.036150881	-8.486596809	-2.302606464
H328	8.974803410	-5.434636916	1.264072662
H329	6.794786849	-4.222446031	0.743721876
H330	0.359761620	-14.196893934	-2.750379367

H331	-1.911337499	-4.314173141	3.206730730
H332	0.602975563	-9.750799767	3.153623693
H333	0.828169451	-7.190644057	3.620807730
H334	-1.025133680	-11.352613936	2.372751337
H335	-4.350940151	-6.131260479	0.473251644
H336	7.689119250	-9.627953576	-2.924016288
H337	6.293695221	-7.406559032	-0.532913936
H338	5.183416784	-8.678929928	0.017460877
H339	5.067068631	-7.056640085	-2.595501090
H340	6.277730527	-0.917025579	1.926329804
H341	4.915455035	4.764617673	0.873093622
H342	6.113819059	5.427625165	-1.265638554
H343	1.755442619	-5.641582904	-1.494403583
H344	1.274212542	-10.926775946	2.396339250
H345	1.981571056	-11.630493340	0.371505821
H346	-4.835393428	-4.666606484	1.213826909
H347	8.572840789	-7.622329289	2.543373585
H348	4.551680738	-7.948412059	2.679249090
H349	7.921994815	-0.644561099	1.273480505
H350	4.433810117	2.419102252	7.858352112
H351	-4.736406442	-5.580265818	4.501409008
H352	-3.311328180	-4.931229205	5.344703640
H353	7.237365516	-8.906844459	5.750870231
H354	7.345234209	-9.738440448	4.345469074
H355	3.690086193	-12.442863224	3.962957643
H356	4.930090761	-10.670580861	3.223346356
H357	5.008344351	-11.957780682	6.311802808
H358	2.557064121	-11.224828907	4.589223889
H359	-3.472539686	-6.997085880	7.200571506
H360	-8.170850685	10.765507047	3.791532764
H361	-3.710899162	-12.712499835	2.353143108
H362	-3.512412479	-10.316193632	3.652410768
H363	-5.589606617	11.820603329	2.604064467
H364	-6.737067618	9.146631649	1.593963229
H365	-6.642215888	10.653101416	0.661779494
H366	2.203959846	-2.866099526	-0.513033901
H367	-0.339227087	9.624850635	-0.392867861
H368	0.700229853	-0.819532302	-0.210912488
H369	1.009708371	1.236687694	-0.944709298
Mo370	3.632106804	-5.046384375	1.417422629
N371	-1.198489476	-3.064088964	0.681786460
N372	-1.115367954	-1.965821635	0.835136287
N373	4.037200410	-0.818193782	-8.951629993
N374	1.546255368	1.818043551	-9.834911483
N375	-0.911523066	0.749883413	-10.748982229
N376	-1.063547597	-1.740032520	-9.445899767
N377	-1.203171155	-0.917830444	-6.710115683
N378	-3.708700696	0.414971248	-6.791905085
N379	-5.557580409	-1.596866996	-7.757921722
N380	-5.079717362	-4.115644483	-6.448644283
N381	-4.797443623	-3.654473257	-3.752668332
N382	-6.285729287	-1.288639059	-2.584609358
N383	-8.734449544	-1.569033667	-4.010346608
N384	-1.376096685	-13.148929316	-3.528782293
N385	-0.985262886	-11.639867779	-1.346673955
N386	-1.965182319	-6.155111299	1.483809286
N387	-4.069067773	-5.272834536	0.936244676
N388	-2.803082107	-4.365237661	2.666482988
N389	-1.948325968	-11.682586160	2.017272350
N390	4.409292878	2.155318851	-5.219952909
N391	5.128274433	-2.131172986	-3.274719301
N392	2.859114531	4.067538593	-4.289342422
N393	1.600893409	5.827504790	-6.012415740
N394	-0.913523281	4.710528594	-6.357048991
N395	-2.275950708	4.554109711	-3.900536887
N396	0.350142445	4.278003115	-0.553781990
N397	0.617481139	2.187187586	-1.015088387
N398	-3.724750799	6.801802895	-3.186050380
N399	-3.098930528	11.474439680	-3.682757351
N400	-4.964244134	12.484275558	-3.031073857
N401	-4.475011509	-4.673540208	7.773307742
N402	-3.629650615	1.656011659	9.113997754
N403	-1.194902005	4.254089244	9.006266313

N404	-0.096284751	5.313382098	6.665358173
N405	2.045846287	7.447216839	2.723979608
N406	2.440745611	9.046553775	4.388296601
N407	0.822108199	9.422125188	2.778633210
N408	-1.791899391	4.545122336	4.504789334
N409	-4.227974900	5.646774847	5.372160514
N410	-4.674211574	8.413160658	5.767252048
N411	-1.590721456	9.112213965	5.133101282
N412	-5.666102141	10.148247857	3.867149903
N413	10.739706190	-3.438741955	4.126049787
N414	7.863653272	-1.498668250	3.163527607
N415	6.414004908	1.117128458	3.644716274
N416	5.398827017	1.379222679	6.315363588
N417	10.550022827	1.280454998	0.437645131
N418	8.584093998	3.244311477	-0.327056555
N419	7.152907940	-8.809872862	4.734962021
N420	5.864616082	-5.869503653	1.769777097
N421	8.059405683	-5.769174995	1.551074866
N422	4.539374050	-10.561654427	4.159147275
N423	-1.053916098	1.602173198	1.510147961
N424	-0.390905402	0.798205455	1.958188782
O425	1.330957202	0.021045468	-8.457132547
O426	-1.912488613	1.583007361	-8.877942344
O427	-3.323934649	-1.734375563	-9.783371498
O428	-2.448949370	-2.787051140	-6.347140340
O429	-3.932335934	-0.019314802	-4.569858537
O430	-7.065621207	-0.640309175	-6.329541477
O431	-7.240249871	-4.715573315	-6.937326020
O432	-4.542595271	-5.893588533	-3.287940811
O433	-6.709268761	-2.968817448	-1.100221592
O434	-9.765592418	-1.287557417	-2.005906723
O435	-11.574876664	-3.755675797	-3.865693582
O436	1.105203918	-12.533801213	-0.921115115
O437	-3.362478465	-11.824647952	0.209798646
O438	-3.799047729	-11.738234645	5.085239625
O439	0.898007772	2.967538967	-4.739120829
O440	5.706073861	-0.043496016	-3.969934291
O441	0.849403960	7.115654584	-4.279783365
O442	2.497358391	7.098862446	-2.135818992
O443	-1.560293370	6.463084510	-7.698237822
O444	-4.135868839	3.721932553	-4.927380951
O445	-4.930886260	5.573891401	-1.677716004
O446	-6.892010967	8.362010308	-2.936194716
O447	-5.126375725	-7.849604751	6.361113678
O448	-6.031405964	0.445741277	4.100389007
O449	-3.154612271	4.274505503	7.849568614
O450	-0.657251978	7.444529985	7.318842458
O451	-1.024082121	6.397783150	3.401252539
O452	-4.979400513	5.673763862	3.207246821
O453	-4.201753380	2.625113283	4.689389097
O454	-6.707361831	7.997439317	6.734702514
O455	-5.632834257	11.915757974	5.307607309
O456	-2.366824406	11.088427722	4.287129280
O457	-8.154101525	12.286127622	2.425305973
O458	-0.693660159	8.918439567	0.181249200
O459	9.548614379	-2.362390425	1.860910060
O460	8.084466057	1.714774590	2.197552181
O461	5.881930781	3.612048388	6.269840733
O462	5.642813280	1.098807208	9.924338913
O463	9.729959671	3.327761856	-2.299346505
O464	8.112005294	-2.491215666	-2.629145330
O465	8.342281230	-2.891913689	-0.448106425
O466	7.102274156	6.220378170	0.959724777
O467	4.228065167	-9.337987951	6.038564077
O468	3.111080365	-12.544534979	6.780680349
O469	3.126343190	-4.452077644	-3.382804422
O470	3.057116207	-6.426374426	-4.401732778
O471	6.594400022	-10.458845575	-1.093486775
O472	7.176502546	-8.863388850	-2.585004676
O473	3.021739712	-7.221666771	1.250310985
O474	2.350510045	-8.740181074	-0.272033454
O475	4.162080836	-5.654858501	-0.520795365
O476	0.547347201	-10.733146298	3.045349073

O477	0.853146354	-7.923544914	2.973824992
O478	0.969782961	6.882003104	0.128487863
O479	5.169643758	-12.103809140	1.141942406
O480	2.475377965	-11.096285379	1.044790704
S481	-0.477388114	1.947181396	6.459508267
S482	2.048422391	0.946223529	3.823414035
S483	4.503584384	-2.861883968	1.022883796
S484	-1.058637190	-0.956945883	4.084748008
S485	1.783823546	-0.561679921	0.572868625
S486	4.842378260	-1.574439350	4.620795122
S487	1.330138405	-4.723965259	0.888918472
S488	1.515204882	-1.484285378	6.378755621
S489	3.551606084	-5.038381353	3.803603229
S490	-0.086865875	-4.654148429	4.396777198

Atomic coordinates and electronic state for the structure with promotional N₂ at exo-Fe2 and reactive N₂ within the N₂ channel, shown in Fig7(b).

S, spin densities	filename, coordinates
S=3/2	bm22b2n2x6x6n2ncnxdisd 1 53315.23
Fe(139) 0.541 2.397	C1 -2.379492949 -9.022593629 -1.692399375
Fe(140) 0.413 1.111	C2 -1.371055473 -9.929417135 -2.407261593
Fe(141) 0.577 2.782	C3 -4.724015750 -8.311764924 -1.524995901
Fe(142) 0.517 -2.427	C4 -4.932861563 -8.467114695 -0.020028958
Fe(143) 0.521 2.354	C5 -4.862589185 -9.931112236 1.934870013
Fe(144) 0.501 -2.267	C6 -3.818521097 -9.195642385 2.782589627
Fe(145) 0.364 -1.224	C7 -1.556682657 -8.256431254 2.870701625
	C8 -1.834684335 -6.748651637 2.858836584
	C9 -2.683301558 -4.831233329 1.604500825
	C10 -3.852837522 -4.432040443 2.514944184
	C11 -5.933600514 -5.068466983 3.590724518
	C12 -5.570987683 -5.194031610 5.080438989
	C13 -4.658019226 -6.646212478 6.834148035
	C14 -3.404860167 -6.076962750 7.515599211
	C15 -1.046173340 -5.420802435 7.265118492
	C16 -0.655723662 -3.974291738 6.943888449
	C17 -1.298080623 -1.959193207 5.624907188
	C18 -2.414717159 -1.029526461 6.143244860
	C19 -1.120147317 -1.938612600 4.090343248
	C20 -1.205708927 -0.511637921 3.547834130
	C21 0.205627901 -2.586968912 3.677885299
	C22 -4.783500085 -0.371685319 6.034943135
	C23 -5.296428997 -0.701857382 7.447744484
	C24 -5.903941550 -0.416300968 4.966083763
	C25 -7.141129894 0.374822096 5.406310270
	C26 -5.391528583 0.113634712 3.620080192
	C27 -6.045399113 -2.394940312 9.016916623
	C28 -5.231668426 -1.844731799 10.171589223
	C29 8.412258201 -5.943854058 8.694468911
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	C32 7.085122724 -1.544811560 9.214983221
	C33 5.612362817 -2.439164435 7.329801028
	C34 5.221993299 -1.044106767 6.848049945
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	C37 8.106122536 0.483951034 10.136724890
	C38 7.409960257 1.815413926 9.952155028
	C39 -1.153647780 -5.001733010 -3.257397515
	C40 -2.428800200 -4.157044221 -3.422854744
	C41 -0.115720904 -4.145519615 -2.493901578
	C42 1.125675455 -4.895447129 -1.963315771
	C43 2.300923098 -4.964549437 -2.933450138
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	C48 -7.021365004 -5.046170559 -3.118165227
	C49 -6.421223739 -4.437684462 -0.809480781
	C50 -6.446575189 -2.993262786 -0.305263324

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C52	-7.321432392	-0.004550376	-0.626843427
C53	-5.121943827	0.254621485	-1.680380600
C54	-3.673329697	-0.045190698	-1.891241479
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C56	-1.731474901	0.139983165	-2.976577728
C57	-9.493880057	0.135155121	-1.803896934
C58	-10.354370179	0.038614821	-0.541936563
C59	-10.153314857	-0.619286942	-2.981247679
C60	-11.233600162	0.116476855	-3.718113450
C61	-12.260598132	0.918837118	-3.261377688
C62	-12.324803870	0.767284977	-5.471762656
C63	3.098240681	6.058891546	7.180160516
C64	4.454903416	5.704147393	7.764934538
C65	2.614575502	4.810192660	6.407483363
C66	1.223175960	4.962507874	5.832557533
C67	0.078621038	4.615878265	6.574914612
C68	1.037740396	5.470116702	4.533886298
C69	-1.204322619	4.757979237	6.036439092
C70	-0.235239855	5.629087036	3.990841825
C71	-1.356150732	5.282190538	4.747710922
C72	0.035064303	9.117745901	0.105668861
C73	-1.081395577	9.338185510	-0.925860462
C74	0.241352491	7.613677411	0.347036574
C75	-1.632484410	9.982362541	-3.233319627
C76	-2.229797627	8.719814075	-3.855153421
C77	-2.073338464	6.264162734	-4.080973923
C78	-3.052325180	5.603582737	-3.087363197
C79	-0.865893944	5.368770852	-4.415072562
C80	-1.150920717	3.978278496	-4.996768464
C81	-1.707295973	3.918961902	-6.430207042
C82	-3.981195596	4.704863741	-7.117145032
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C89	-9.224462390	8.629368849	-3.099793737
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C94	-10.451287547	5.281001631	-1.959934851
C95	-9.488446531	4.465693313	-2.798246251
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C101	9.357558314	0.812874854	-5.043034147
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C106	3.663774051	4.536961775	-6.223454588
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C116	0.370049764	-1.731593930	-7.805455391
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C118	0.534441527	0.171810486	-6.141561306
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C120	1.129081369	0.747373655	-5.014774953
C121	2.208457682	-1.352800966	-4.495133117
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C126	9.701650089	-1.042955860	-0.295864423
C127	10.435998688	-1.500795003	-1.371766890
C128	8.273570427	-1.668775888	-1.825165340
C129	12.050624216	0.674541943	4.749322801
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C131	4.646821806	-5.112356625	1.621075234
C132	5.275504783	-4.011729950	2.431374347
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C138	3.834884531	1.976001554	-0.043153249
Fe139	5.457985162	1.326700924	-1.044803515
Fe140	1.694268745	2.347565177	-0.347560268
Fe141	3.776067924	3.667566896	1.000209454
Fe142	4.005466663	3.322473561	-1.525951601
Fe143	2.105914302	5.000330522	-0.912507602
Fe144	5.037314248	1.517973080	1.486610933
Fe145	3.657679026	-0.172912739	0.080226396
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H147	0.201283487	-8.663028059	-2.724835135
H148	-3.895154215	-9.742240322	-2.883451939
H149	-1.632773111	-9.989357717	-3.475876419
H150	-1.522382273	-10.943692066	-1.998754341
H151	-4.496096702	-7.250734726	-1.693765763
H152	-4.455549462	-10.464209000	-0.112070999
H153	-5.667007733	-8.549412670	-2.034755581
H154	-4.772764827	-11.008463683	2.123378045
H155	-2.470883734	-9.273082156	1.234510551
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H157	-1.834250078	-4.195783472	1.891503582
H158	-2.400926174	-6.837864298	0.871958902
H159	-0.601871236	-8.449054332	2.363579873
H160	-6.289364198	-4.043686888	3.430469498
H161	-4.829977465	-6.218608652	2.145164758
H162	-1.458941278	-8.557348473	3.920713915
H163	-2.939115549	-4.613638285	0.557069415
H164	-4.654810360	-7.019550675	4.733740991
H165	-6.756234918	-5.763682310	3.369848216
H166	0.289116534	-3.615912610	4.052560069
H167	0.286417289	-2.618688704	2.578906116
H168	1.064815558	-2.005733394	4.051174097
H169	-1.941858073	-2.525444899	3.645952784
H170	-4.603178190	-7.742391273	6.912319507
H171	-4.541547207	-0.468754660	3.237733480
H172	-5.420327677	-2.734082195	7.004528305
H173	-7.575146064	-0.004946631	6.342609729
H174	-0.952606130	-0.487417642	2.475321779
H175	-0.500241204	0.152470467	4.073635855
H176	2.405730983	6.216887143	8.030825610
H177	-6.193186676	0.067704187	2.868101641
H178	-7.913675143	0.313737188	4.625309842
H179	-5.078817077	1.166455584	3.715175652
H180	-6.893419389	1.438103587	5.556254806
H181	-6.198990097	-1.473390472	4.837223317
H182	-4.401600490	0.656338327	6.114508695
H183	-3.815018014	-1.916602518	4.898537933
H184	-2.215037451	-0.093038786	3.659940402
H185	-2.079388227	4.322094399	0.358816929
H186	-3.692431080	4.180185596	1.103283493
H187	-2.724898948	5.796820068	2.255928204
H188	-3.291116793	5.100470251	4.738013200
H189	-0.356485330	5.999535788	2.973983221
H190	1.908466312	5.703461452	3.918355724
H191	0.186645869	4.216101883	7.587142755
H192	-2.308942058	-3.841560675	5.775171866
H193	-0.234125577	-6.060359091	6.891430219
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H218	-0.974309762	-6.390765910	-4.774050654
H219	-0.636904778	-3.701684427	-1.632593498
H220	7.364595368	-2.423683134	-5.021354345
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H222	-5.487650569	-0.563907460	0.312897519
H223	-2.752064530	-1.174895298	-0.191469251
H224	-7.424325963	-4.850680429	-0.639720181
H225	-5.112192591	-4.493812540	-2.495883973
H226	-7.924598997	-1.292856411	-2.099151038
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H229	-10.514144418	-1.599520627	-2.624154693
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H233	-5.634000733	0.235137470	-2.657507233
H234	-13.753832609	1.935194962	-4.409958926
H235	-9.364334810	-0.829120632	-3.718944727
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H237	-5.727181850	-5.007846973	-0.173917462
H238	-7.302405010	-4.765254147	-5.214016010
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H260	-0.266527308	5.226684614	-3.500912007
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H262	-1.801779935	3.400375329	-4.322011895
H263	-4.403326696	-5.199051668	-4.767717810
H264	-1.135745813	10.550136902	-4.031718437
H265	-1.924337212	-4.055242652	-5.356802235
H266	-0.230410316	5.926480112	-5.123199053
H267	-6.156654498	3.678935639	-3.058476037
H268	-5.168911730	-1.269585910	-6.214183055
H269	-2.479578103	10.584699663	-2.874665222

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H306	4.249650634	-1.724779110	5.030643043
H307	5.647882221	-3.138648026	6.479843945
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H309	4.991335495	-0.391208105	7.705095629
H310	0.310107595	-2.828955071	-7.757379662
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O457	-12.929270908	7.239694939	-1.918277541
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O459	8.134402910	-1.144490415	-5.746989975
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O461	3.037834389	5.315262655	-6.962371281
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