

Understanding non-reducible N₂ in the mechanism of Mo-nitrogenase

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1. Protein model

The quantum computed protein model is an extract from crystal 3U7Q, shown in Chart S1. The six principal chains surrounding FeMo-co are highlighted with different colours, and the connecting hydrogen bonds are marked. Homocitrate, the His442 ligation of Mo, and relevant nearby water molecules are included (485 atoms total). Details, and the rationale for inclusion of amino acids and for truncation of uninvolved sidechains, are provided in the caption for Chart S1. Investigations of the protonation state of homocitrate using crystal structures at various pH (summarised in ref ¹), vibrational circular dichroism spectroscopy,² QM/MM calculations,^{1, 3} and quantum refinement,³ indicate that the coordinated alcoholate O7 atom is protonated, and hydrogen bonded to O1. This proton is now included in the model, although it is not shown in Chart S1.

Experimental and computational studies are in general agreement that the redox level of the [CFe₇MoS₉] core of resting FeMo-co cluster is described by net charge -1,^{1,6-8} and so the net charge for the complete model in Chart S1 is -2 (-1 when the His195 side chain is protonated).

2. Computational constraints

Some constraints on the protein structure are required during optimization calculations because the modelled protein is incomplete and the bonding and dispersion influences of the complete protein outside the computational model are absent. The modelled protein must also maintain flexibility sufficient to accommodate the coordination of N₂ and of H₂, and the diffusion of these molecules to and from FeMo-co. The constraints used here involved the C α atoms at the ends of the modelled protein chains, allowing movement of the intermediate residues and all sidechains. The constraints maintained the crystallographic distances between C^c at the centre of FeMo-co and the C α atoms of residues 62, 95, 97, 191, 196, 229, 281, 355, 358, 380, 381, 443, and C^c-O distances for the included water molecules. The lengths of the hydrogen bonds between the backside water HOH531 and Arg277, Tyr281 and Ser192 (Chart S1) were also constrained.

As previously explained⁹ trial calculations on the modes of diffusion and coordination of N₂ / H₂ led to the conclusion that the front chain near Val70 should move away from FeMo-co. This is consistent with experimental data on mutation of amino acid 70 with smaller and larger side chains.¹⁰⁻¹² This expansion is controlled via the distance constraints C α (Val70) -- C^c and C α (Val70) -- CZ(Arg96), here set to the values used in prior calculations of the intermediates and reaction steps.^{13,14}

At the H₂ / N₂ exchange stage there are two unbound molecules, H₂ and reducible N₂, and therefore calculation of exo-Fe2 N₂ binding trajectories required additional constraints for stability of the computational model: the positions of H₂ and reducible N₂ were fixed.

There were no constraints on bond distances or bond angles, including during transition state searches.

This overall strategy for constraints provides a computationally stable model, able to adjust to non-bonding dispersion interactions in the vicinity of the active site and the N₂-pocket.

3. Density functional procedures

Density functional (DF) calculations use the DMol methodology of Delley,¹⁵⁻²⁰ with accurate DNP (double numerical plus polarisation) basis sets.¹⁸ The real-space cutoff in the calculation of atomic basis sets was 9 au (4.8 Å), which gives results within 0.1% of the limit for larger extensions of the basis sets. The gradient-corrected functional PBE²¹ was used because validation tests demonstrate that when used with the numerical basis sets of DMol it is more accurate than other commonly used functionals.²² The Supplementary Information of ref ¹⁴ contains details of the validation tests.

The DMol method uses numerical solutions of DFT-free atoms as part of its basis set, and thus gives highly accurate DFT solutions for the separated atoms limit.¹⁸ These numerical basis sets avoid the need for basis set superposition corrections, and provide reliable energies at long intermolecular distances. This advantage of the DMol methodology reduces the need for empirical treatment²³ of the long-range dispersion energies that are involved when the computational model is comprised of separate molecular units. This ability of the DMol methodology to incorporate long-range dispersion has been well demonstrated. Zhang *et al* reported very good agreement between the experimental interatomic potential energy curves and the DMol/PBE calculated potential energy curves for the inert-gas pairs He₂ Ne₂ and HeNe, and excellent agreement for the HeAr and NeAr pairs relevant to the nitrogenase active site.²⁴ Todorova and Delley used this DMol / DNP / PBE methodology to optimize the crystal structures of a comprehensive set over 40 molecular crystals in which dispersion and intermolecular interactions determine the crystal packing and crystal lattice parameters.²⁰ This set of molecular crystals ranged over amino acids, aliphatic and aromatic hydrocarbons, ice, H₂S, S₈, C₆₀, and the inert gases Ne, Ar, Kr and Xe. The PBE functional overestimates lattice parameters by about 4%, while the PBE_{sol} functional yields

lattice parameters with an average systematic error of less than 1%. Todorova and Delley emphasise that the DMol numerical basis sets have low BSSE because of the accurate tails of the molecular orbitals.

The calculations were all-electron, spin-unrestricted, with no imposed symmetry. The conductor-like screening model (COSMO)²⁵⁻²⁷ was used with a dielectric constant of 5. Constraints on interatomic distances used the Lagrange Multiplier Algorithm. Control of electronic states was via the input spin populations for Fe1, Fe3, Fe4, Fe5 and Fe7. Output spin populations are calculated by the Mulliken method.²⁸

4. Determination of transition states

The following procedure is used to map potential energy surfaces and locate transition states between minima.^{5, 8, 29, 30} A chemically reasonable geometry between energy minima is evaluated by observing the directions and extent of geometry change during an energy minimisation calculation that is restricted to small (ca 0.03 Å) atom displacements at each step. This reveals significant geometrical variables (i.e. which atoms are moving, which bond distances and angles are changing) and also the energy gradients involved. The trajectory of the structure in this calculation, towards one energy minimum, indicates that the energy saddle to the other energy minimum occurs in the opposite direction, towards the other energy minimum. Then, as illustrated in Figure S1, a point $\Delta 1$ that is a short distance along this first optimization trajectory is selected, and from this structure a new atomic arrangement (**2** on Figure S1) on the other side of the saddle is located manually, and similarly evaluated with small-displacement energy minimisation steps. A point $\Delta 2$ along the second optimisation trajectory is selected, and from this the key moving atoms are manually adjusted to be just back across the suspected saddle-point towards the opposite energy minimum. Repetition of this cycle, with subsequent short small-step energy minimisations, always starting from a point just on the other side of the barrier, allows the barrier to be straddled from opposing trial positions that progressively approach each other in geometry and energy as shown on Figure S1. The process involves choosing trial structures that in sequence are either side of the barrier, and progressively approaching each other. The requirement that trial structures oscillate across the barrier means that the energy minimisations are optimising all geometrical variables (including those that are not obviously part of the reaction step). The trial structures are moving down the ridge that they straddle, and approaching each other. The energy converges, and the gradients approach zero. Confirmation that this converged position is the transition state (TS) is obtained by calculating the complete energy minimisation trajectory of geometries from positions nudged just away from the TS, on either side, linking the TS with the connected reactant and product energy minima on the same potential energy surface. The electronic states are monitored throughout to confirm that reactant, TS and product are on the same potential energy surface. There can be substantial changes in the spin densities of Fe atoms that are changing coordination, and the continuity of these changes is checked.

This protocol requires human participation in choosing trial structures for each cycle of the calculation. An understanding and application of the relevant principles of coordination chemistry and stereochemistry improve the efficiency of the process. This methodology works well for complex reactions, such as those in the nitrogenase mechanism where multiple changes are occurring, sometimes in concert.

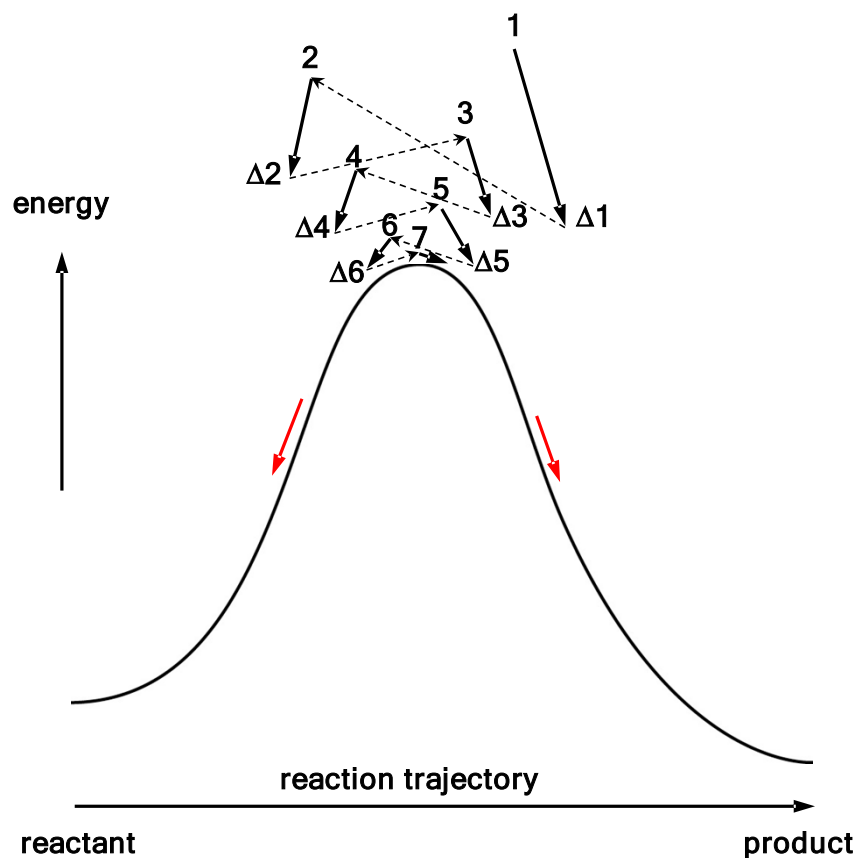


Figure S1. Generalised diagram of the procedure for locating a reaction transition state. The solid arrows represent the course of limited small-step energy reductions from the numbered positions, which are generated (broken arrows) from Δ positions partway along the previous energy reduction, chosen according to geometry and energy gradient. The postulated trials necessarily oscillate across the barrier, and therefore optimise all other variables and decrease the energy and gradient while approaching the top of the barrier. Confirmation that the transition state, reactant and product are on the same potential energy surface is obtained by complete energy minimisations (red arrows).

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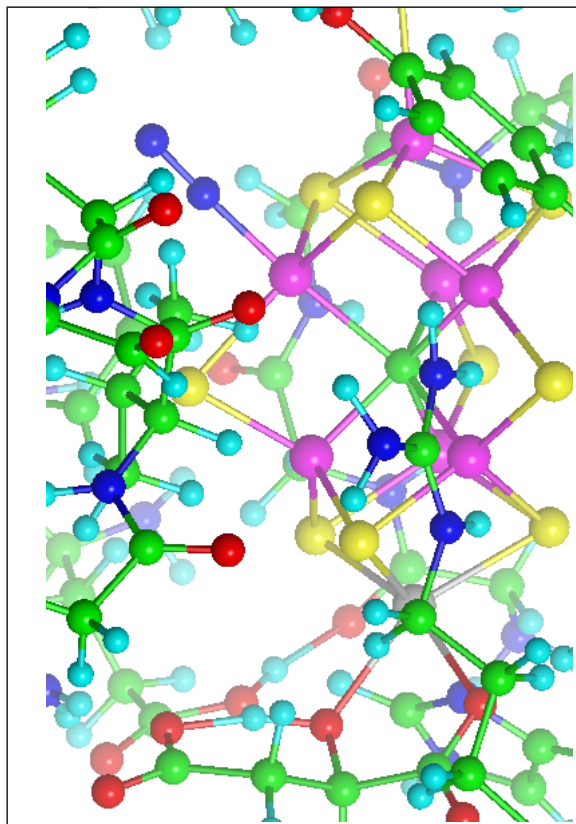
Atom coordinates, spin densities and pictures

Translation of Fe numbering

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

The pictures are sections of the complete model chosen to show key atoms in the reaction zone. Note that some bonds in transition states are arbitrarily drawn.

structure S, electronic state spin densities picture	filename coordinates			
resting 2N2 associated 35, S=3/2 Fe(139) -2.376 Fe(140) -1.534 Fe(141) -2.683 Fe(142) 2.881 Fe(143) 2.927 Fe(144) 1.692 Fe(145) 1.699	bm522n2xdtb.car_3			
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	2	-8.773296451	-5.761513368	-0.248142562 C
	3	-9.035957016	-2.631729551	1.923844823 C
	4	-8.469988143	-2.919034043	3.311947888 C
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	6	-6.769964023	-4.727242178	5.170925006 C
	7	-4.775739617	-5.278633910	3.875087528 C
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	9	-4.138921381	-1.587761271	3.151107677 C
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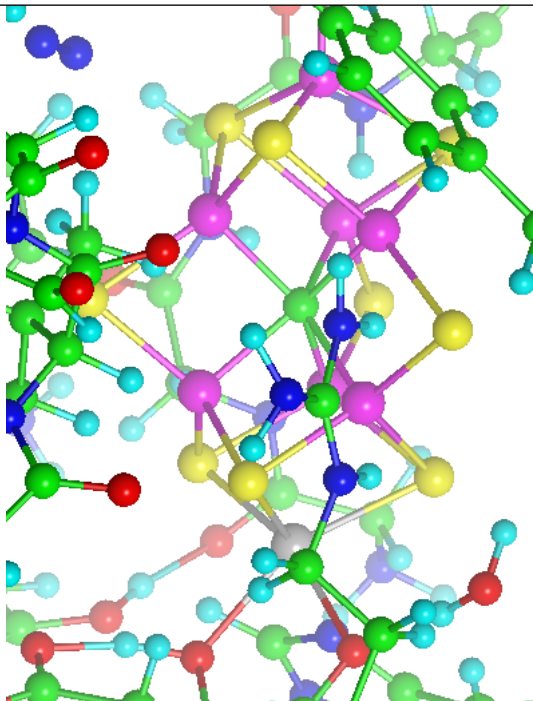
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134	2.134775402	-8.749990323	-1.405008834	C
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437	-5.733943246	3.564269313	-3.841711024	O
438	-9.729843237	2.428754926	1.469642624	O
439	-5.853462174	1.979704463	4.029969568	O

440	-4.142000927	5.430214860	3.502705257	O
441	-6.430872939	7.784693564	4.891891888	O
442	10.266003311	-1.172527422	5.228915859	O
443	3.486441064	4.198856787	4.309130054	O
444	4.344171877	8.033230988	-0.179009405	O
445	2.120508767	9.870635848	-3.377527274	O
446	-0.745410747	7.217578149	-1.569883061	O
447	-0.407809611	7.272403965	2.145498678	O
448	2.582701536	5.484893449	1.867751450	O
449	1.682628961	11.437457136	2.524179172	O
450	-1.270995610	13.775940469	0.573149007	O
451	-2.154538399	11.312600187	-1.512973582	O
452	-3.984560795	14.111969370	3.335075584	O
453	-4.732284020	7.304791754	-1.700590494	O
454	2.025363455	-4.664641901	-8.517679516	O
455	0.436357755	-0.732122596	-8.447842634	O
456	3.080828032	3.454213348	-8.049512016	O
457	6.853798503	3.900771082	-8.400913030	O
458	-4.400503751	-2.171111690	-9.271432155	O
459	-1.581808512	-6.484084342	-6.108834636	O
460	0.452935023	-5.777321222	-6.691042815	O
461	-2.947704643	2.666898608	-8.642686264	O
462	9.620034877	-6.357682927	-2.842923100	O
463	12.013241316	-8.118001565	-1.038264071	O
464	-0.291042417	-6.197421273	-1.279877903	O
465	-1.098157817	-7.106839785	0.625992453	O
466	4.249388197	-11.323528280	-2.883989691	O
467	2.008716958	-11.127848817	-3.116142203	O
468	4.457740149	-6.207336596	-0.850119482	O
469	4.167384665	-7.933923871	0.556226693	O
470	2.057486766	-6.323233145	-1.863369983	O
471	8.139989901	-7.437911565	1.746859195	O
472	6.521871780	-5.277700469	0.848317632	O
473	-3.746915482	5.105371962	-2.753444661	O
474	6.800619890	-11.145988740	-1.850500917	O
475	6.532740331	-9.361417561	0.543620183	O
476	4.020220835	4.618801967	-1.860384034	S
477	2.468360840	1.664948544	-3.256794313	S
478	1.990537977	-3.439020034	-3.467139709	S
479	3.526950857	1.395084045	0.294993301	S
480	0.451306596	-1.126449452	-1.011394999	S
481	4.507503887	-1.061661057	-5.105531052	S
482	2.901142914	-3.647514106	0.046081716	S
483	5.997937046	1.278283019	-2.300389181	S
484	5.567434953	-3.618232321	-2.533012709	S
485	6.029071172	-1.508786494	0.426392729	S
	end			
resting 2N2 dissociated 35, S=3/2		bm522n2xdta.car_4		
Fe(139) -2.419	1	-8.329836712	-4.651428980	0.721411370 C
Fe(140) -2.473	2	-8.761212528	-5.760320110	-0.245709318 C
Fe(141) -2.490	3	-9.036271481	-2.630567595	1.926570411 C
Fe(142) 2.803	4	-8.472091146	-2.918463091	3.314760536 C
Fe(143) 2.978	5	-8.284779209	-4.493241709	5.174152410 C
Fe(144) 2.186	6	-6.772037701	-4.730733605	5.172243544 C
Fe(145) 2.258	7	-4.778517010	-5.282745940	3.874567993 C
	8	-4.069706796	-3.926939509	3.862090772 C
	9	-4.133221914	-1.594257479	3.147546059 C
	10	-4.100119513	-0.954177829	4.545067237 C
	11	-5.264012728	-0.539864121	6.636120876 C
	12	-4.388906731	-1.225433958	7.694737996 C
	13	-3.789120905	-3.327593425	8.799361954 C
	14	-2.354570121	-3.790860474	8.505131308 C
	15	-0.796762568	-4.602594996	6.775526427 C
	16	0.167740556	-3.617269847	6.106007656 C
	17	0.430829064	-1.651755091	4.629620760 C
	18	0.770661768	-0.478851558	5.576926024 C
	19	-0.209459461	-1.194331469	3.301505057 C
	20	0.621430600	-0.075724891	2.664379454 C
	21	-0.368102693	-2.389453566	2.355206652 C
	22	-0.103294016	1.339706582	7.002477219 C
	23	0.087098197	0.931204268	8.479543236 C
	24	-1.247698005	2.366248282	6.814999160 C
	25	-1.128756082	3.517715667	7.820397376 C
	26	-1.257468320	2.906217058	5.378916504 C
	27	-0.795209906	-0.166076066	10.459353271 C
	28	0.541716602	-0.754707835	10.859941100 C
	29	4.478442022	-12.086173430	4.333933513 C
	30	5.206681569	-10.870848782	3.763116744 C
	31	5.644530617	-8.446309308	4.177555320 C
	32	6.812262049	-8.189369699	5.149314022 C
	33	4.575781112	-7.343467487	4.276553570 C



34	5.116591566	-5.946832945	3.961312294	C
35	3.983310691	-4.933567447	3.798419335	C
36	4.243232221	-2.437968949	3.958837535	C
37	9.173658170	-7.561774115	5.334410057	C
38	9.561926418	-6.098809070	5.348130126	C
39	-5.458092339	-2.212468840	-1.968432880	C
40	-5.712423145	-0.745115560	-1.576472466	C
41	-3.959476160	-2.520474179	-1.763264728	C
42	-3.575115294	-4.014968810	-1.824111738	C
43	-3.214220270	-4.543526342	-3.211961547	C
44	-5.861172996	1.520378851	-2.533440104	C
45	-6.974443960	2.105509506	-1.653860089	C
46	-5.844782527	2.126440651	-3.943200520	C
47	-9.253288528	1.832177446	-0.796200158	C
48	-8.976006904	1.808815278	0.711266636	C
49	-7.498896336	1.079247356	2.525866099	C
50	-6.273792380	1.925632503	2.866120363	C
51	-4.523416436	3.454103629	2.104701084	C
52	-4.907702786	4.806773303	2.758041410	C
53	-3.761399221	3.798035371	0.817998535	C
54	-3.174910731	2.660253673	0.047997786	C
55	-2.704301033	1.413505791	0.387472755	C
56	-2.281118419	1.719400360	-1.770575297	C
57	-6.575455087	6.626857403	2.750202937	C
58	-6.627923530	6.751720666	4.271291376	C
59	-7.983081932	6.823774659	2.140749549	C
60	-8.470096038	8.236680665	2.009801812	C
61	-8.378825124	9.313136959	2.870905089	C
62	-9.486769254	9.883219128	1.037652018	C
63	8.942631321	0.669495497	4.358770511	C
64	9.871804076	-0.525578596	4.263976878	C
65	7.519555741	0.162995832	4.008441857	C
66	6.467840202	1.242709589	4.113057245	C
67	5.806176289	1.495087535	5.328582220	C
68	6.111704368	2.017684016	2.995830246	C
69	4.812490411	2.474164421	5.427784227	C
70	5.131379428	3.007078669	3.082772066	C
71	4.477407319	3.227029189	4.297836973	C
72	5.966752960	6.313316597	-0.773524944	C
73	5.063605893	7.526816540	-1.056583058	C
74	5.109439329	5.093526906	-0.455248459	C
75	4.324422368	9.170744603	-2.745319400	C
76	2.854078239	8.906004119	-3.080316271	C
77	1.074152977	7.162946526	-3.164012503	C
78	0.433374027	6.850832493	-1.784910973	C
79	1.098906617	5.928770350	-4.100525630	C
80	-0.196414169	5.154299731	-4.372484407	C
81	-1.206071604	5.800185234	-5.333783394	C
82	-2.577336157	7.851279250	-4.963995395	C
83	0.676523237	5.915722290	0.465581141	C
84	0.531815026	7.171173436	1.330938075	C
85	1.546856016	4.912791925	1.262945121	C
86	1.784293901	9.078738041	2.193910671	C
87	1.332376736	10.484426555	1.843429631	C
88	0.213347158	11.881559739	0.196590222	C
89	-1.048191008	12.562159450	0.783923393	C
90	0.184376162	11.917209087	-1.333803018	C
91	-1.000654663	11.189035928	-1.957699871	C
92	-3.166267032	12.269717083	1.979008365	C
93	-3.050911881	13.355911511	3.040065016	C
94	-4.013319753	11.084168700	2.520918317	C
95	-4.254969010	10.026142834	1.468691520	C
96	-5.364977840	10.109544555	0.613740051	C
97	-3.350403650	8.967923832	1.276360606	C
98	-5.553781543	9.185475752	-0.417311528	C
99	-3.505342470	8.053880294	0.230444514	C
100	-4.606037619	8.180654020	-0.613143991	C
101	4.409919922	-4.325503820	-8.570543935	C
102	2.989999896	-3.928957344	-8.202093629	C
103	1.604259248	-2.282645642	-6.963824344	C
104	1.286456962	-0.895665760	-7.532086499	C
105	1.867929695	1.488836432	-7.435280489	C
106	3.135314858	2.334954083	-7.499159849	C
107	5.443196906	2.721591576	-6.857058724	C
108	6.059783817	2.998302564	-8.213262866	C
109	-2.226355467	-3.241396788	-9.368444493	C
110	-3.165123828	-2.050694455	-9.143972902	C
111	-1.974842420	-3.965371970	-8.024527360	C
112	-1.376607513	-5.367120110	-8.244806933	C
113	-0.862666227	-5.935479235	-6.939825302	C
114	-3.411390496	0.291958457	-8.498230994	C
115	-2.759217214	1.534439200	-9.069595584	C

116	-3.905848622	0.428394675	-7.038614004	C
117	-2.799187668	0.251159276	-6.032060092	C
118	-1.920623548	1.304338763	-5.722789743	C
119	-2.564921614	-1.011674581	-5.463891109	C
120	-0.811902324	1.081140553	-4.899300746	C
121	-1.458193333	-1.233325681	-4.638224772	C
122	-0.568057528	-0.190155816	-4.367555343	C
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130	11.054756938	-8.395024694	-1.740653804	C
131	-0.161274543	-6.796989380	-0.122142330	C
132	1.291867211	-7.065562657	0.325757090	C
133	2.296477844	-7.333154099	-0.823316868	C
134	2.130193966	-8.764460254	-1.392525672	C
135	3.228356621	-9.203589786	-2.368358148	C
136	3.143714591	-10.680630652	-2.813506210	C
137	3.736238164	-7.176128013	-0.310277858	C
138	3.628492319	-1.065014578	-1.817012958	C
139	3.958237426	-2.342822622	-3.375999118	Fe
140	2.288022890	0.295117833	-1.448507344	Fe
141	4.843143339	0.067373340	-0.734683459	Fe
142	4.179334494	0.202354712	-3.276801989	Fe
143	3.939215213	2.372181724	-1.666666661	Fe
144	4.608121971	-2.521843084	-0.872645641	Fe
145	2.123792745	-2.349565961	-1.525270740	Fe
146	-7.075682985	-6.909666695	-0.161983811	H
147	-7.111267293	-5.900781439	-1.444058487	H
148	-10.238979839	-3.880599373	0.684325889	H
149	-9.404635634	-5.314285318	-1.021603394	H
150	-9.406309571	-6.450368698	0.324364249	H
151	-8.300460190	-1.989940417	1.418696594	H
152	-9.430453535	-4.726931702	3.368083800	H
153	-9.964932623	-2.056159473	2.043901036	H
154	-8.784717215	-5.419348125	5.488241779	H
155	-6.789372115	-5.192234454	3.160577386	H
156	-8.481988691	-3.722912210	5.931685184	H
157	-3.102746502	-1.592752062	2.772692450	H
158	-5.518174802	-3.150009532	2.625023976	H
159	-4.558717414	-5.816535318	2.940274090	H
160	-4.940535144	0.507507644	6.583489371	H
161	-6.022325106	-1.602277792	4.924503446	H
162	-4.364892759	-5.860722414	4.709618706	H
163	-4.748240807	-0.986161744	2.470085063	H
164	-5.100355091	-3.084417832	7.126154157	H
165	-6.310625277	-0.563738857	6.969498583	H
166	-0.957055590	-3.200276419	2.807966295	H
167	-0.858797692	-2.077160835	1.421564918	H
168	0.612680975	-2.794501394	2.062516402	H
169	-1.207109192	-0.787609490	3.543764369	H
170	-4.384853865	-4.224040919	9.025224980	H
171	-1.383651827	2.103260146	4.639086929	H
172	-1.725838140	-0.106754583	8.546725818	H
173	-1.176328636	3.172819160	8.863378015	H
174	0.184933634	0.224466137	1.702646010	H
175	1.647619052	-0.406484630	2.447946629	H
176	8.936461432	1.003437817	5.414033110	H
177	-2.083634132	3.620919299	5.246180802	H
178	-1.948779524	4.234088541	7.662770981	H
179	-0.314282078	3.433675782	5.160149163	H
180	-0.176536115	4.055075460	7.683922445	H
181	-2.204061198	1.842801739	6.996264533	H
182	0.851107346	1.810198991	6.725110592	H
183	-1.232242755	-0.076187655	5.841143953	H
184	0.676426700	0.813704296	3.310004974	H
185	1.950307113	4.149039526	0.581166861	H
186	0.880653150	4.418877636	1.987946068	H
187	2.851965452	5.032623924	2.721913273	H
188	3.097912647	4.247573532	5.210024046	H
189	4.847606729	3.582414730	2.201796908	H
190	6.580628756	1.823870558	2.028314604	H
191	6.053983464	0.900858087	6.212104306	H
192	-1.386699547	-2.694057806	5.129511907	H
193	-0.970885862	-5.430738932	6.071133414	H
194	-0.278599343	-5.000798105	7.654772017	H
195	-2.793938086	-3.939424123	6.488810961	H
196	-3.740719885	-2.713347906	9.706742306	H
197	4.290039508	2.635999812	6.374115351	H

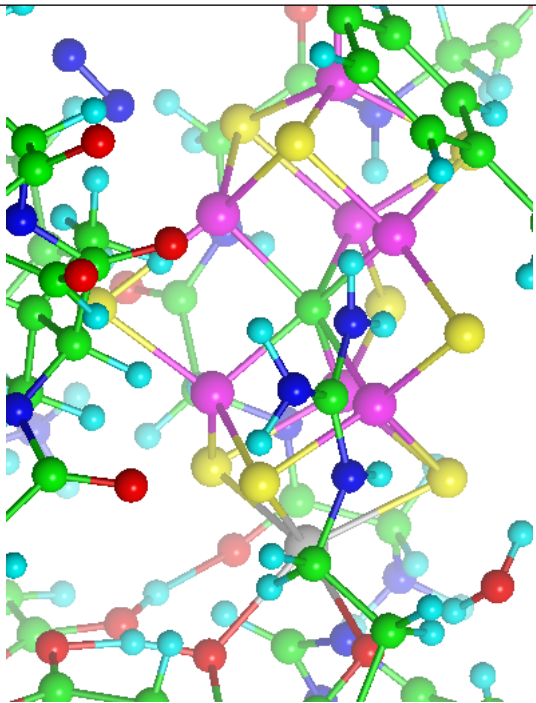
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199	-1.003404910	0.714147704	11.089808395	H
200	-1.560619878	-0.928595957	10.671468150	H
201	1.067242843	-1.320973350	10.057474750	H
202	10.024515054	-8.163439881	4.979104861	H
203	-1.964166215	-5.833426983	-4.171421424	H
204	0.995848085	-6.144773757	-1.741428147	H
205	-2.155211200	-6.039490522	-8.631001113	H
206	-0.560299611	-5.321394538	-8.979861389	H
207	-2.916927144	-4.064298019	-7.463292036	H
208	-2.118484803	1.346498736	-9.962902383	H
209	-2.815872642	-3.920662197	-10.003321749	H
210	-3.378273716	-1.954378390	-2.509427864	H
211	-4.413897398	-4.631531055	-1.456198299	H
212	-1.578361674	-0.825060258	-8.590769385	H
213	-4.312059467	0.150926680	-9.130541761	H
214	-0.367705053	-2.334133714	-9.552608391	H
215	-1.647141479	-5.704028112	-2.434700090	H
216	-1.304753930	-3.346823338	-7.406579042	H
217	-0.551485396	-3.690620339	-10.463514890	H
218	-6.822319418	-2.839251537	-3.387233735	H
219	-3.675523248	-2.134126436	-0.773199174	H
220	0.932336173	-5.315489213	-7.451235127	H
221	-2.739113024	-4.202505686	-1.134712696	H
222	-3.870721900	2.950561317	2.832005864	H
223	-2.683663482	0.902960004	1.344580374	H
224	-8.333843978	1.470808368	3.123238820	H
225	-7.309295975	0.588861192	0.458051608	H
226	-6.737398374	4.694579888	1.837930409	H
227	-7.906961094	9.441036942	3.838826515	H
228	-6.925099781	5.808267567	4.789698730	H
229	-8.706555972	6.210313865	2.707242488	H
230	-5.878690843	7.383957157	2.357834709	H
231	-10.036464704	10.505860704	0.335821296	H
232	-2.946949284	4.483555604	1.102998580	H
233	-4.433222974	4.358752912	0.152095311	H
234	-9.136487311	11.295066296	2.594064873	H
235	-7.962394847	6.405681627	1.122296602	H
236	-6.065057388	2.565520496	0.895291484	H
237	-7.309207914	0.055045832	2.879208296	H
238	-9.567555576	2.857893156	-1.033266405	H
239	-1.901095341	1.562886528	-2.777534979	H
240	-10.101592814	1.165296806	-0.997986112	H
241	10.194383231	2.187715062	3.782657261	H
242	8.649285321	2.387517662	3.284038392	H
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244	-0.334853506	5.498886911	0.363434167	H
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250	-4.983869710	1.707226628	-4.489246920	H
251	-6.768429860	1.854587485	-4.476719470	H
252	1.142368953	11.553092196	-1.731192308	H
253	0.089053437	12.975180617	-1.625018861	H
254	0.271430531	10.192544724	-3.263653442	H
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259	-2.503024718	8.826257095	1.952681343	H
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261	1.817877439	5.212506792	-3.673260557	H
262	3.155761682	6.907513290	-2.784808147	H
263	-0.697825898	4.874788085	-3.432737475	H
264	-8.203081034	0.560396264	-2.171964068	H
265	4.793936974	9.625129558	-3.627490374	H
266	-5.871745273	-0.444075384	-3.540162456	H
267	1.531154857	6.259157015	-5.059647515	H
268	-2.753752847	7.282826179	0.058182128	H
269	4.323918938	9.919240398	-1.940218020	H
270	-1.770716607	7.916481163	-6.859159950	H
271	-3.901286381	9.335231159	-4.477480778	H
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277	-0.670063366	6.426636955	-6.058591913	H
278	0.114570702	4.207014451	-4.837103567	H
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289	3.730814757	-5.809896725	-9.782876537	H
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292	5.700585962	7.561080866	-3.011863092	H
293	4.489805955	5.293616516	0.431100631	H
294	7.499274179	7.354539847	0.119743820	H
295	6.199742992	2.206731782	-6.243403615	H
296	6.578277707	6.096882544	-1.663647824	H
297	4.133648003	-7.363567495	5.287139821	H
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322	5.867739757	-11.162578965	-2.219953195	H
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326	3.710359590	-2.323248659	-7.144932074	H
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332	7.680830664	-6.627305093	1.433418679	H
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446	-0.736318655	7.200556612	-1.556953019	O
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450	-1.266241709	13.764329123	0.573976056	O
451	-2.154211629	11.316954116	-1.520397712	O
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453	-4.721866762	7.292653941	-1.702346932	O
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457	6.842773806	3.913680179	-8.413240670	O
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459	-1.581039788	-6.476259797	-6.105693935	O
460	0.453613774	-5.774646242	-6.693636538	O
461	-2.935891639	2.668984808	-8.646905011	O
462	9.622985961	-6.367639615	-2.846645876	O
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476	4.004762086	4.658299937	-1.874308485	S
477	2.419617849	1.649996544	-3.237655175	S
478	1.997973532	-3.439427769	-3.464122957	S
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481	4.555130960	-1.051769360	-5.087353722	S
482	2.932474041	-3.677387221	0.081587404	S
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resting 2N2 transition state 35, S=3/2		bm522n2xdta 2 53008.75				
		1	-8.345050006	-4.659285578	0.711383181	C
Fe(139) -2.365		2	-8.789899697	-5.761687791	-0.256308908	C
		3	-9.027801633	-2.631863751	1.916947255	C
Fe(140) -2.589		4	-8.459391277	-2.920169058	3.303387082	C
		5	-8.277337153	-4.488714799	5.169279229	C
Fe(141) -2.555		6	-6.763860152	-4.721112909	5.167102906	C
		7	-4.768559374	-5.270778385	3.872744015	C
Fe(142) 2.831		8	-4.064322290	-3.912229852	3.865287940	C
		9	-4.154531613	-1.574627069	3.155458129	C
Fe(143) 3.018		10	-4.106133330	-0.939424372	4.554108376	C
		11	-5.257968846	-0.524623936	6.649596763	C
Fe(144) 2.125		12	-4.381493085	-1.212131263	7.704762195	C
		13	-3.785932314	-3.313133626	8.810168326	C
Fe(145) 2.279		14	-2.351672168	-3.771452483	8.511024932	C
		15	-0.803994357	-4.599504414	6.781481678	C
		16	0.165856443	-3.624653588	6.104762349	C
		17	0.432636894	-1.643269507	4.645617398	C
		18	0.777999541	-0.471766812	5.594116243	C
		19	-0.234303865	-1.181390444	3.335339874	C
		20	0.580387586	-0.062673063	2.677728043	C
		21	-0.424999937	-2.370884296	2.386829695	C
		22	-0.095951040	1.353522055	7.014543204	C
		23	0.093326106	0.947153677	8.492450891	C
		24	-1.240948723	2.380738642	6.828118869	C
		25	-1.124835266	3.528873941	7.838081111	C
		26	-1.251984999	2.927077470	5.394997808	C
		27	-0.789411907	-0.156531628	10.472052417	C
		28	0.554523274	-0.732607429	10.871106548	C
		29	4.495575396	-12.094908889	4.339428327	C
		30	5.212020110	-10.875443205	3.765351143	C
		31	5.641039156	-8.451357177	4.184851945	C
		32	6.807937512	-8.193601830	5.157408787	C
		33	4.567702873	-7.353846217	4.282233823	C
		34	5.106822896	-5.955403375	3.975043871	C
		35	3.973833530	-4.943335451	3.805367548	C
		36	4.239739763	-2.446533724	3.965004096	C
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38	9.562098205	-6.106313387	5.364160478	C
39	-5.470132919	-2.212885865	-1.959844523	C
40	-5.708074599	-0.745080890	-1.556790766	C
41	-3.968763093	-2.526426125	-1.769132083	C
42	-3.577800038	-4.017001031	-1.856438396	C
43	-3.239652221	-4.532939770	-3.254829650	C
44	-5.835452644	1.528153653	-2.503013315	C
45	-6.960726779	2.106677365	-1.634802098	C
46	-5.809795824	2.135343697	-3.912364168	C
47	-9.243616374	1.807246307	-0.795514147	C
48	-8.971695294	1.794191862	0.712817851	C
49	-7.492619330	1.088807906	2.536338003	C
50	-6.255271477	1.920869952	2.870574921	C
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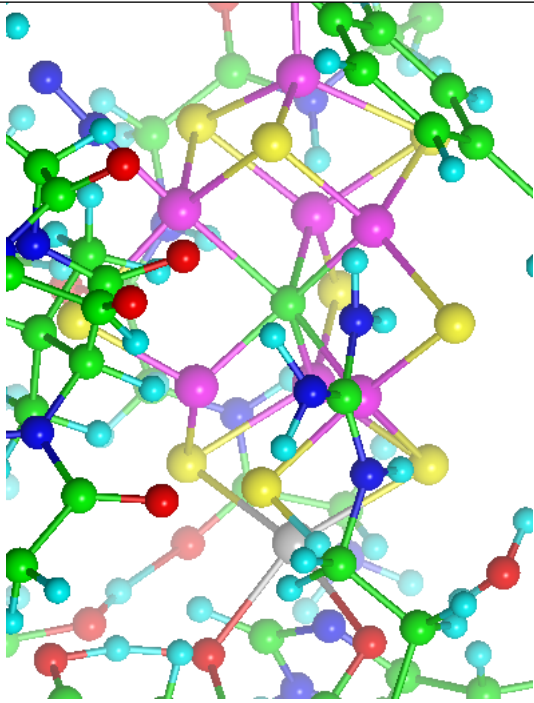
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451	-2.150381780	11.279335708	-1.499445191	O
452	-3.989398046	14.120378544	3.294157229	O
453	-4.747438504	7.309456744	-1.708577658	O
454	2.030653611	-4.665989098	-8.517196741	O
455	0.427525673	-0.736754378	-8.446917529	O
456	3.063636030	3.470653467	-8.041783017	O
457	6.882292610	3.865153494	-8.383489950	O
458	-4.421117694	-2.184016034	-9.250633884	O
459	-1.583169969	-6.487675590	-6.112576749	O
460	0.451723712	-5.779567543	-6.692752075	O
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462	9.613111139	-6.344632025	-2.821469812	O
463	12.022583690	-8.148410007	-1.036741635	O
464	-0.251009145	-6.164553712	-1.269390645	O
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469	4.189382484	-7.941710676	0.542230524	O
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471	8.139412026	-7.447169160	1.759043433	O
472	6.549302524	-5.268844605	0.856689691	O
473	-3.725223089	5.117172274	-2.740984976	O
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475	6.545929720	-9.374613065	0.541613357	O
476	4.004202744	4.638738918	-1.848857062	S
477	2.444993574	1.684709495	-3.246115766	S
478	2.000468891	-3.443664914	-3.468351762	S
479	3.485898451	1.401455680	0.312937329	S
480	0.432588574	-1.075124016	-1.012066645	S
481	4.509998539	-1.024336103	-5.092029549	S
482	2.938352939	-3.704925279	0.071664047	S
483	5.957135372	1.281994050	-2.279458068	S
484	5.585534948	-3.621979146	-2.554953249	S
485	6.029938604	-1.474133929	0.433294028	S
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rest-3b5 2N2 associated 35, S=1/2 Fe(139) -2.117 Fe(140) -1.543 Fe(141) -2.746 Fe(142) 2.306 Fe(143) 2.803 Fe(144) 2.088 Fe(145) 0.118	bm522n2x3b5dtb.car_3			
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	C4	-8.471718797	-2.910262086	3.304720067
	C5	-8.288938131	-4.476821679	5.172262408
	C6	-6.776577259	-4.713225795	5.167689714
	C7	-4.786993209	-5.273857954	3.870475182
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	C9	-4.154893073	-1.582727762	3.145635687
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	C15	-0.810329062	-4.592196632	6.773320828
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	C17	0.418982116	-1.639358270	4.632410899
	C18	0.757166753	-0.461124953	5.574980969
	C19	-0.230855444	-1.183634433	3.309818628
	C20	0.588760182	-0.063065796	2.660748985
	C21	-0.400147009	-2.376069018	2.360979801
	C22	-0.112473696	1.355484698	7.002891135
	C23	0.082158044	0.947243610	8.480038088
	C24	-1.256098611	2.382789904	6.816271212
	C25	-1.136397073	3.532711901	7.823010590
	C26	-1.266443953	2.924543992	5.380810104
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	C35	4.008079311	-4.916350339	3.893814679
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	C38	9.550971687	-6.086075864	5.348571345
	C39	-5.476268812	-2.196101769	-1.970321174
	C40	-5.713138343	-0.726796910	-1.573239580
	C41	-3.977469170	-2.513488776	-1.780087477



C42	-3.596479444	-4.005836148	-1.869303765
C43	-3.250163935	-4.514008526	-3.268485860
C44	-5.861359371	1.540512904	-2.527841139
C45	-6.975556374	2.121871415	-1.646473966
C46	-5.848731305	2.144282263	-3.938318535
C47	-9.256897590	1.841553324	-0.794729457
C48	-8.981504496	1.819270137	0.712857467
C49	-7.501449207	1.094035828	2.527776531
C50	-6.268035727	1.930855825	2.863892309
C51	-4.526360493	3.473799342	2.113615795
C52	-4.922328614	4.815043393	2.777915363
C53	-3.770932178	3.847263270	0.829266223
C54	-3.162355715	2.724920777	0.054232712
C55	-2.742981386	1.457670504	0.376736864
C56	-2.299202735	1.781303194	-1.776862262
C57	-6.583139154	6.638393857	2.749713283
C58	-6.634725975	6.769993918	4.270674473
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C61	-8.389270543	9.319640266	2.864611417
C62	-9.489365208	9.891409660	1.027369640
C63	8.927725527	0.683251023	4.353414545
C64	9.855343296	-0.513063510	4.255322051
C65	7.502879708	0.177077887	4.012017780
C66	6.453168294	1.258611938	4.113549064
C67	5.782552258	1.507187744	5.325166075
C68	6.107065627	2.040466510	2.997994827
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C71	4.462478697	3.245808999	4.292950692
C72	5.967376599	6.309004730	-0.779499174
C73	5.050990186	7.510329618	-1.064918459
C74	5.126824120	5.076170383	-0.448406192
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C76	2.848186926	8.906644070	-3.079645727
C77	1.063957006	7.163661191	-3.172963259
C78	0.409574890	6.848374903	-1.802167968
C79	1.094109895	5.930022498	-4.106658837
C80	-0.201153686	5.156602507	-4.381875104
C81	-1.211172819	5.807298634	-5.341244999
C82	-2.576867522	7.861511162	-4.968947309
C83	0.625792932	5.906931008	0.449006950
C84	0.504216718	7.158913280	1.328822169
C85	1.458441863	4.869206013	1.233236564
C86	1.771635843	9.066521621	2.191486018
C87	1.329796958	10.475585026	1.836959907
C88	0.207157747	11.884410224	0.196370126
C89	-1.054053557	12.566308343	0.783495932
C90	0.175155655	11.915633357	-1.334461489
C91	-1.008929241	11.183554718	-1.955727984
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C93	-3.060456214	13.365693797	3.036151513
C94	-4.015424055	11.087591864	2.521674688
C95	-4.259916380	10.031122711	1.467644680
C96	-5.369483071	10.121031869	0.612387381
C97	-3.360285182	8.968909875	1.273677541
C98	-5.562802103	9.200383642	-0.420695920
C99	-3.519712608	8.057475858	0.225775863
C100	-4.619285958	8.192131793	-0.617852379
C101	4.406803618	-4.311076662	-8.576295556
C102	2.985448287	-3.921421353	-8.208230362
C103	1.596981889	-2.261374178	-6.982029118
C104	1.274355098	-0.879372756	-7.558734905
C105	1.848696216	1.509309684	-7.465441143
C106	3.112851347	2.362688222	-7.507371689
C107	5.423901915	2.733294306	-6.850010693
C108	6.067749804	2.999783263	-8.196492570
C109	-2.246061488	-3.237215637	-9.367291207
C110	-3.187610061	-2.049364750	-9.134769792
C111	-1.987242473	-3.960340568	-8.025496843
C112	-1.388028305	-5.362324432	-8.246986062
C113	-0.875865834	-5.924019162	-6.940328851
C114	-3.429052312	0.297227985	-8.496099820
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C116	-3.920756537	0.436716788	-7.035170911
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C118	-1.935959751	1.321130989	-5.723404698
C119	-2.564497831	-1.000597511	-5.471570849
C120	-0.819327066	1.099834674	-4.909092831
C121	-1.449103478	-1.220431528	-4.656961194
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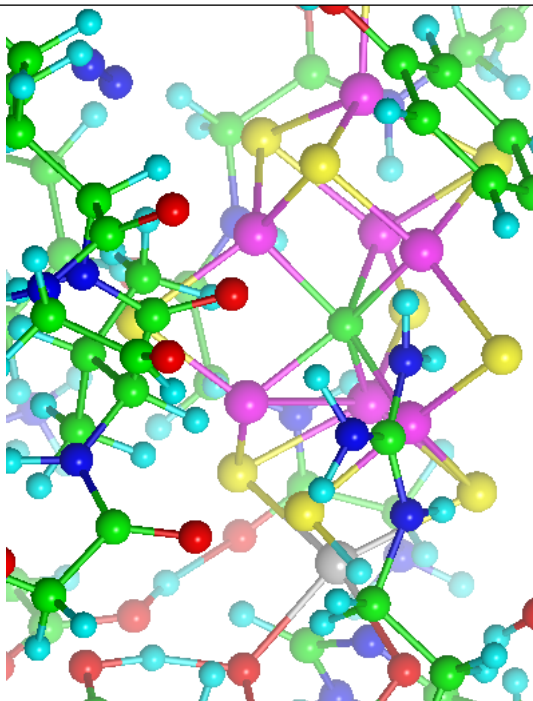
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C130	11.045456878	-8.387928855	-1.751057690
C131	-0.126249349	-6.814266531	-0.101585717
C132	1.321706186	-7.051681421	0.317120604
C133	2.319304561	-7.267735582	-0.860672664
C134	2.142462185	-8.693684046	-1.447992817
C135	3.244671359	-9.150716528	-2.406711549
C136	3.148075201	-10.635839982	-2.825938577
C137	3.755348926	-7.144747408	-0.323629580
C138	3.612311918	-1.064759582	-1.817463646
Fe139	3.947590707	-2.325375188	-3.342474696
Fe140	2.072903516	0.454534149	-1.334930280
Fe141	4.927662734	0.027594853	-0.746531406
Fe142	4.099619664	0.226220058	-3.185579563
Fe143	3.972904731	2.329676205	-1.637376806
Fe144	4.573159152	-2.515453201	-0.862874154
Fe145	2.158351090	-2.220616323	-1.597079296
H146	-7.100774911	-6.903207366	-0.162735659
H147	-7.132779858	-5.892910246	-1.444376546
H148	-10.260541036	-3.876130870	0.692147443
H149	-9.427055075	-5.306938615	-1.025236210
H150	-9.430067560	-6.441902030	0.320367185
H151	-8.314639531	-1.981880362	1.407187537
H152	-9.455222882	-4.704511766	3.378959490
H153	-9.975019317	-2.047361283	2.045358574
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	O469	4.488346356	-6.198344502	-0.851354771	
	O470	4.172620801	-7.921308426	0.555485354	
	O471	2.083990870	-6.247017376	-1.836846214	
	O472	8.137011225	-7.433543673	1.753780615	
	O473	6.515910776	-5.254367868	0.886088884	
	O474	-3.747218400	5.106324225	-2.754234572	
	O475	6.807329216	-11.150690878	-1.864943782	
	O476	6.545203343	-9.360076602	0.544307616	
	S477	4.019864557	4.595989123	-1.852731336	
	S478	2.444118617	1.686337696	-3.213940782	
	S479	1.979976376	-3.383010289	-3.410762793	
	S480	3.479215752	-1.391394965	0.310625817	
	S481	0.434632928	-1.099814118	-1.103029266	
	S482	4.430633463	-0.973002400	-5.006324619	
	S483	3.001399638	-3.759522289	0.205959343	
	S484	5.902963456	1.300962017	-2.287769941	
	S485	5.568316960	-3.624493087	-2.516810101	
	S486	6.034118002	-1.487289819	0.415158015	
	end				
	rest-3b5		bm522n2x3b5dtd.car_4		
	2N2 dissociated				
	35, S=1/2				
	Fe(139) -2.197	C1	-8.343983227	-4.640884878	0.719941210
	Fe(140) -2.422	C2	-8.772623650	-5.752341980	-0.243058569
	Fe(141) -2.606	C3	-9.051419243	-2.622894020	1.924578898
	Fe(142) 2.804	C4	-8.475014712	-2.911699997	3.308830087
	Fe(143) 2.920	C5	-8.290181872	-4.478889407	5.175701228
	Fe(144) 2.236	C6	-6.778231310	-4.718231283	5.170232468
	Fe(145) -0.072	C7	-4.790456787	-5.283455025	3.869832621
		C8	-4.076540702	-3.930614359	3.848543378
		C9	-4.152637335	-1.595632479	3.137620881
		C10	-4.105495625	-0.955649940	4.535074728
		C11	-5.262078806	-0.530446381	6.628681206
		C12	-4.387000720	-1.217721561	7.685235533
		C13	-3.795372789	-3.318410091	8.795375454
		C14	-2.360797268	-3.775999557	8.497244539
		C15	-0.810377141	-4.593076893	6.765611457
		C16	0.156049902	-3.611733614	6.093114009
		C17	0.423814353	-1.644984504	4.618827875
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		C19	-0.221719137	-1.190295075	3.293050658
		C20	0.600162145	-0.067491109	2.652095134
		C21	-0.383190634	-2.385057246	2.346235870
		C22	-0.116019636	1.349407210	6.988907777
		C23	0.082040761	0.939753611	8.463658576
		C24	-1.260882956	2.376133559	6.805198339
		C25	-1.138271642	3.526214447	7.811540927
		C26	-1.274928681	2.917708714	5.369808355
		C27	-0.794977688	-0.156802712	10.447681544
		C28	0.538998967	-0.757021596	10.843247782
		C29	4.477199766	-12.087991440	4.334030440
		C30	5.200278827	-10.869646593	3.762255405
		C31	5.645262743	-8.452309640	4.195024297
		C32	6.818771682	-8.199590856	5.161336746
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		C34	5.140879172	-5.950296099	4.029137009
		C35	4.025963387	-4.912240627	3.926323400
		C36	4.259083735	-2.409013577	4.062526804
		C37	9.174960098	-7.548275729	5.332844366
		C38	9.553910795	-6.083706471	5.341565656
		C39	-5.472382376	-2.193309598	-1.979567915
		C40	-5.717909066	-0.724212159	-1.586638558
		C41	-3.971997643	-2.510101340	-1.789235306
		C42	-3.594667531	-4.003499540	-1.873152883
		C43	-3.247353541	-4.514847036	-3.271303873
		C44	-5.885467867	1.539296655	-2.546196309



C45	-6.992872423	2.120134283	-1.657206627
C46	-5.880542833	2.142178661	-3.957069471
C47	-9.269127054	1.848046218	-0.793202793
C48	-8.988203890	1.823772449	0.713888803
C49	-7.507989793	1.085329638	2.523412144
C50	-6.276318433	1.923351657	2.859914263
C51	-4.531461188	3.459319591	2.099563410
C52	-4.906570999	4.808205662	2.759949717
C53	-3.781858100	3.813746324	0.807224101
C54	-3.210780138	2.676509995	0.026865748
C55	-2.777713437	1.414511824	0.357621552
C56	-2.346881972	1.724768512	-1.800392077
C57	-6.564604274	6.637005693	2.749084118
C58	-6.611262523	6.771181537	4.269914696
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C60	-8.461932274	8.244659625	2.007978844
C61	-8.374084775	9.321069720	2.869508432
C62	-9.482824909	9.888584525	1.036177720
C63	8.934630738	0.684500347	4.335272930
C64	9.862057709	-0.511600493	4.235995954
C65	7.509147255	0.179285397	3.995423073
C66	6.458709481	1.259006426	4.105689720
C67	5.793981628	1.500915590	5.321468401
C68	6.106083019	2.043514717	2.994403095
C69	4.800230535	2.479059541	5.426459353
C70	5.125753850	3.031827476	3.086792846
C71	4.466958584	3.241460568	4.301884468
C72	5.966202442	6.299485256	-0.786305958
C73	5.056628965	7.508461959	-1.068816761
C74	5.114245675	5.077456082	-0.457974633
C75	4.321155613	9.164308846	-2.748207470
C76	2.850199586	8.900723696	-3.082824366
C77	1.066289058	7.156198851	-3.160331657
C78	0.424558873	6.847351806	-1.781090008
C79	1.089849358	5.921527326	-4.095196708
C80	-0.205887615	5.148665804	-4.371777782
C81	-1.212024076	5.798337881	-5.334311171
C82	-2.582922860	7.849642731	-4.962789348
C83	0.687428387	5.944082350	0.483410039
C84	0.556649223	7.198560789	1.362413206
C85	1.542952278	4.926635697	1.268362565
C86	1.807980993	9.113673743	2.221710557
C87	1.344021642	10.508129435	1.849444591
C88	0.214660240	11.873874466	0.184675975
C89	-1.047776160	12.553496844	0.772216884
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C91	-1.008503015	11.170811463	-1.965956746
C92	-3.163681441	12.264083105	1.971408933
C93	-3.048969356	13.350533403	3.032387191
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C95	-4.254048955	10.020356846	1.459745831
C96	-5.363142160	10.106324664	0.603749749
C97	-3.352517147	8.959198705	1.269246456
C98	-5.554736772	9.181954768	-0.426493325
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C100	-4.610136960	8.173936023	-0.619977986
C101	4.405219789	-4.318281769	-8.592468423
C102	2.987359009	-3.925550375	-8.217696783
C103	1.608022262	-2.266388746	-6.981468932
C104	1.287251597	-0.882926721	-7.554772318
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C113	-0.878983700	-5.919497237	-6.944531029
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C120	-0.827100612	1.090698688	-4.904138519
C121	-1.466869393	-1.226517676	-4.653073221
C122	-0.580528303	-0.181785353	-4.375353392
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C124	8.675228940	-7.172029361	-2.993330696
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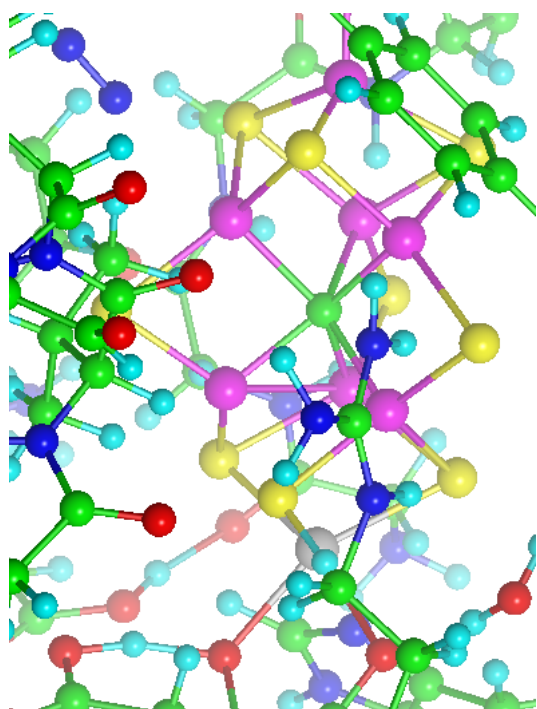
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C130	11.046966396	-8.396919731	-1.755445206
C131	-0.126702853	-6.814293189	-0.090701520
C132	1.320757539	-7.054575779	0.324656672
C133	2.317519614	-7.269306946	-0.855021201
C134	2.139416342	-8.693300733	-1.445703146
C135	3.241978952	-9.150565647	-2.404305830
C136	3.146180028	-10.635269284	-2.825782794
C137	3.752605156	-7.149937589	-0.316574419
C138	3.617943583	-1.075484544	-1.831103021
Fe13	3.964811773	-2.338381889	-3.355605150
Fe14	2.277659452	0.315927056	-1.374305181
Fe14	4.765543746	0.110863084	-0.683696660
Fe14	4.143978123	0.222951120	-3.268907852
Fe14	3.872010640	2.388558399	-1.613742392
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H146	-7.083120270	-6.894600862	-0.155708917
H147	-7.120556545	-5.886111846	-1.439036779
H148	-10.257523618	-3.881866686	0.693351044
H149	-9.418072742	-5.311353290	-1.019993633
H150	-9.414438179	-6.444466341	0.328107325
H151	-8.320776469	-1.978677109	1.413313640
H152	-9.456279380	-4.707380902	3.382596655
H153	-9.981863112	-2.052756504	2.049378747
H154	-8.789642727	-5.404293112	5.491733323
H155	-6.803756167	-5.196227118	3.161301154
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H159	-4.576690221	-5.815750618	2.933221265
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H168	0.597741702	-2.781198719	2.041936354
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H170	-4.388913922	-4.217138228	9.018434079
H171	-1.405575710	2.115640669	4.630133006
H172	-1.732239633	-0.095127961	8.539396676
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H177	-2.099696354	3.634316350	5.240314689
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H181	-2.217228743	1.853853260	6.989313385
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H186	0.884243156	4.464703999	2.019893212
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rest-3b5 2N2 TS 35, S=1/2 Fe(139) -2.088 Fe(140) -2.632 Fe(141) -2.570 Fe(142) 2.800 Fe(143) 2.951 Fe(144) 2.275 Fe(145) -0.111	bm522n2x3b5dtd_1_52967.435			
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C92	-3.167416281	12.265667132	1.977331221
C93	-3.064864534	13.364519174	3.027221412
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C98	-5.564002313	9.206726229	-0.419796785
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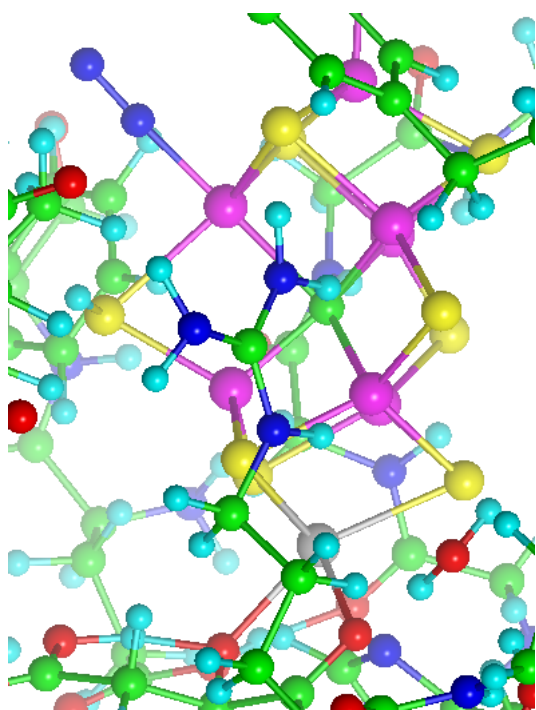
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	S479	1.986864254	-3.384020503	-3.440313674
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	S485	5.570445097	-3.631967688	-2.529111253
	S486	6.012332647	-1.460957432	0.402221897
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rest-S2BH 2N2 associated 35, S=1/2 Fe(139) -2.108 Fe(140) -1.639 Fe(141) -2.770 Fe(142) 2.698 Fe(143) 2.887 Fe(144) 2.254 Fe(145) -0.733			bm522n2x2bhdtb.car_3	
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	C4	-7.419981938	-2.707274532	5.350991423
	C5	-6.760815726	-3.760528373	7.454505909
	C6	-5.248921955	-3.874072460	7.235864505
	C7	-3.431603071	-4.562939741	5.757651998
	C8	-2.905600823	-3.199325906	5.304755924
	C9	-3.394818091	-1.118391900	4.120653092
	C10	-3.192082769	-0.162039831	5.306426075
	C11	-4.027541491	0.656537076	7.436582491
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	C14	-0.499254339	-1.818784218	9.417296402
	C15	0.851427461	-2.904061287	7.665319324
	C16	1.575044599	-2.045629539	6.622661869
	C17	1.359636150	-0.462489089	4.731934691
	C18	1.712075935	0.922660597	5.327951278
	C19	0.432729200	-0.375501566	3.506509446
	C20	0.988029031	0.623042161	2.485452972
	C21	0.234181531	-1.771190451	2.903825174
	C22	0.866205030	2.965046128	6.436787448
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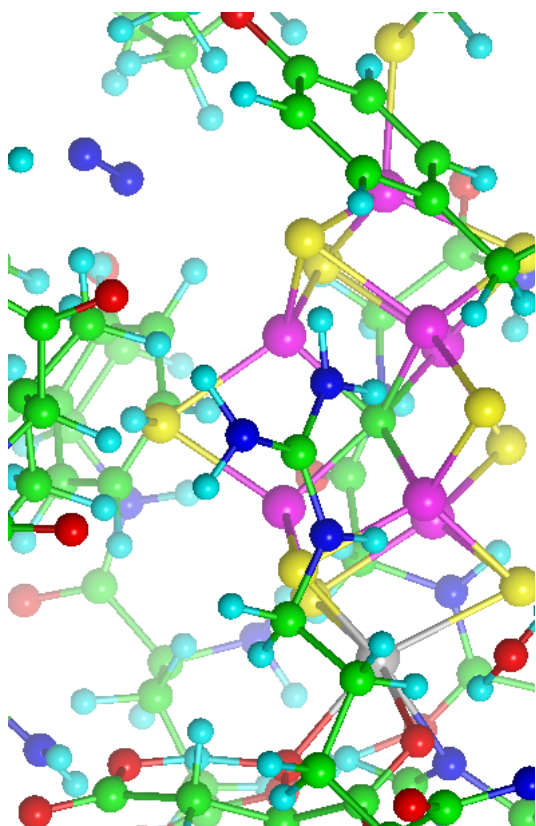
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H225	-7.156411071	0.107431496	1.650112740
H226	-6.868907255	4.458707863	1.946621125
H227	-8.253465990	9.417545791	3.044727289
H228	-6.728198117	6.230313564	4.575207281
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H230	-6.269859521	7.248699023	1.703734932
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H232	-3.275400114	4.453269925	0.614441346
H233	-4.860984550	3.957306503	0.004864951
H234	-9.860677540	10.841249377	1.664617147
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H236	-6.108670716	2.248008167	1.396666805
H237	-6.724698012	0.182384446	4.104946388
H238	-9.881702805	1.767894438	0.137159844
H239	-2.555225761	0.772272833	-2.691499035
H240	-10.197933688	0.095751166	0.638978575
H241	10.334614680	3.777053900	1.255234472
H242	8.709856530	3.797516000	1.075636723
H243	1.181772903	5.472328488	-2.748236669
H244	-0.979491830	5.382763587	-0.837488908
H245	1.440232776	7.874590330	-1.564170396
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H260	-5.066515854	6.837580739	-4.235303768
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H265	2.991714893	8.808133521	-6.474599527
H266	-6.290120999	-1.719300718	-2.214189197
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O425	-2.242043515	0.637672495	5.326624387
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O434	12.061494321	-3.370524406	4.626481322
O435	-5.604854106	-0.867349953	0.739972594
O436	-3.976337258	-5.317989817	-2.493278113
O437	-7.176290639	2.273172493	-0.374766590
O438	-6.639023361	2.097887929	-3.424024557
O439	-9.583959348	1.940434100	2.660178557
O440	-5.290474987	2.381727623	4.483772512
O441	-4.145480724	5.768084648	2.924349819
O442	-6.419483989	8.198572182	4.131578803
O443	11.028746830	0.912530904	3.382792736
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O446	0.376037271	8.921981483	-5.787852061
O447	-1.844106119	6.511981907	-2.961730867
O448	-0.893322360	7.497301880	0.559693909
O449	2.210646392	5.897577761	0.061976682
O450	0.685155415	11.808809638	-0.401919941
O451	-2.776763224	13.361909677	-2.274339729
O452	-3.686011925	10.408033613	-3.534107576
O453	-5.064096001	14.129846261	0.793991802
O454	-5.798937396	6.297143782	-2.384671905
O455	1.191243429	-6.380612785	-7.486944390
O456	-0.846982656	-2.680510464	-7.993465928
O457	1.304550401	1.690764720	-9.026959901
O458	4.920016658	2.327602787	-10.149708646
O459	-5.554050182	-4.657172720	-7.581226167
O460	-1.770203457	-7.865724453	-4.148236682

O461	0.052665149	-7.145820612	-5.213795177
O462	-4.543151929	0.297239665	-8.311450785
O463	9.696908211	-6.032417758	-3.035467557
O464	12.570681935	-7.163828782	-1.366525571
O465	0.274435981	-6.261693769	0.185938107
O466	-0.107843695	-6.833568758	2.326927385
O467	5.035036812	-11.272674121	-1.065849863
O468	2.782218197	-11.292388475	-0.863630273
O469	5.012215213	-5.812261517	-0.254189091
O470	5.124351589	-7.185959795	1.520972501
O471	2.506658411	-6.296864571	-0.774103961
O472	9.137999166	-6.153343337	1.830811144
O473	7.171631843	-4.353123234	0.817132030
O474	-4.704643471	4.005834130	-3.069742084
O475	7.698118204	-10.711524284	-0.573097602
O476	7.605956704	-8.429340655	1.393903022
S477	3.098164590	4.325620176	-3.520616545
S478	1.707400731	1.043294770	-3.903528080
S479	1.818939187	-3.915364704	-2.929016580
S480	3.327642238	1.682590181	-0.645309226
S481	0.335807313	-1.429224055	-0.832507132
S482	3.755774677	-1.859623814	-5.443084403
S483	3.322599399	-3.248187348	0.345340251
S484	5.305848527	1.149265838	-3.572650505
S485	5.527572518	-3.674583614	-2.639541153
S486	6.223421269	-0.849348064	-0.415738848
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rest-S2BH		bm522n2x2bhdtf.car_5			
2N2 dissociated		C1	-7.498586784	-4.979202838	3.233111909
35, S=1/2		C2	-7.933425331	-6.322025644	2.632291252
Fe (139) -2.194		C3	-8.259249142	-2.803774570	4.085462723
Fe (140) -1.878		C4	-7.427547531	-2.713079430	5.360162861
Fe (141) -2.431		C5	-6.762687387	-3.766801787	7.462245166
Fe (142) 2.830		C6	-5.250165311	-3.885031848	7.249816731
Fe (143) 2.869		C7	-3.428967704	-4.580058994	5.779278840
Fe (144) 2.302		C8	-2.903921822	-3.221413775	5.311051567
Fe (145) -0.958		C9	-3.396672050	-1.151601147	4.110850183
		C10	-3.193333150	-0.189371769	5.292156010
		C11	-4.025992007	0.638313620	7.419396620
		C12	-2.916100033	0.295992986	8.421270562
		C13	-1.911142473	-1.424086338	9.847304140
		C14	-0.494982920	-1.825339675	9.413406458
		C15	0.863372658	-2.910140450	7.666102185
		C16	1.585057137	-2.056252091	6.617360579
		C17	1.364898219	-0.487511804	4.714246865
		C18	1.715700961	0.896722934	5.315361681
		C19	0.432047464	-0.394319020	3.494177440
		C20	0.977263485	0.619498035	2.483103379
		C21	0.239550416	-1.785778348	2.879700760
		C22	0.865873413	2.937892114	6.421679146
		C23	1.335264904	2.909902577	7.892234931
		C24	-0.412264724	3.792304095	6.224352725
		C25	-0.275116157	5.157295470	6.908962836
		C26	-0.723672619	3.971468930	4.733524517
		C27	0.909997291	2.251854223	10.193427879
		C28	2.345497061	1.846376804	10.461481147
		C29	6.508741069	-10.321193837	5.999621971
		C30	6.999297891	-9.221865177	5.061404409
		C31	7.214854072	-6.743781537	4.855960386
		C32	8.491202618	-6.174184449	5.504129871
		C33	6.056877455	-5.733776144	4.919310885
		C34	6.370359557	-4.409039308	4.221094866
		C35	5.105922017	-3.575210291	4.017516692
		C36	5.099552503	-1.098718655	3.582308476
		C37	10.749412842	-5.326855488	5.090832215
		C38	10.968109644	-3.877560050	4.715673386
		C39	-5.404772289	-3.032907887	-0.420988966
		C40	-5.764603779	-1.537856550	-0.323754308
		C41	-3.867475497	-3.167621496	-0.448192082
		C42	-3.320874000	-4.599888993	-0.271600648
		C43	-3.149417828	-5.404255614	-1.560621674
		C44	-6.373770169	0.409114838	-1.705918007
		C45	-7.387601946	1.093835953	-0.779309154
		C46	-6.656388840	0.660829955	-3.191827166
		C47	-9.436627907	0.867830007	0.539017981
		C48	-8.907487591	1.228670916	1.931092041
		C49	-7.076749770	1.054143790	3.551309329
		C50	-5.907986335	2.033078170	3.455303914
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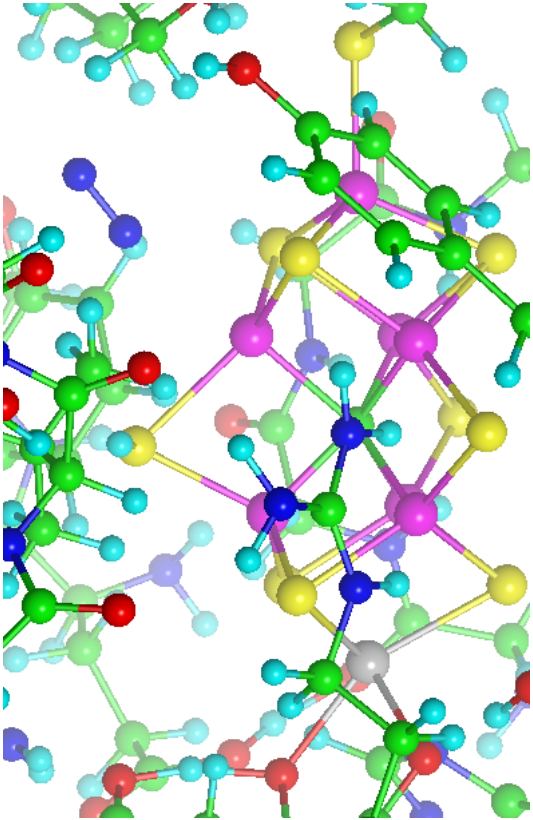
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C65	7.992020897	1.690136882	2.438279805
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C67	6.347449209	3.146258163	3.717036850
C68	6.246116065	3.143072938	1.309350017
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C70	5.189103505	4.053779051	1.343975668
C71	4.704478462	4.502933218	2.575453186
C72	4.991102930	6.381858816	-3.249488246
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C74	4.360236601	5.198408603	-2.512762446
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H354	7.836361801	-9.136715128	-4.170478756
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	O464	12.564735106	-7.156737765	-1.342810808
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	O472	9.135801584	-6.161227608	1.830260419
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	O476	7.593837502	-8.433751784	1.404396804
	S477	3.059265096	4.354420197	-3.523619619
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	S479	1.795210319	-3.963680768	-2.947447666
	S480	3.032122735	1.677969295	-0.616345958
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	S482	3.809460527	-1.842604201	-5.458037406
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	S485	5.502643779	-3.666877375	-2.634098619
	S486	6.146396089	-0.757302061	-0.406361842
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rest-S2BH 2N2 TS 35, S=1/2 Fe(139) -2.093 Fe(140) -2.612 Fe(141) -2.601 Fe(142) 2.817 Fe(143) 2.962 Fe(144) 2.281 Fe(145) -0.140			bm522n2x2bhdtd 2 52985.815	
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	C2	-7.965806940	-6.324832368	2.630875441
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	C6	-5.246734432	-3.873752966	7.232929463
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	C9	-3.393260038	-1.114229648	4.121784744
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	C11	-4.027140055	0.658241025	7.439050922
	C12	-2.916304504	0.311694935	8.438596828
	C13	-1.911305764	-1.413127534	9.857799374
	C14	-0.498538700	-1.816415137	9.414983070
	C15	0.849102545	-2.900335023	7.659647510
	C16	1.574359462	-2.044345768	6.615550276
	C17	1.359786091	-0.460310470	4.724219619
	C18	1.713433726	0.925001530	5.319675180
	C19	0.432268694	-0.373318322	3.499686580
	C20	0.989719905	0.625731581	2.480477288
	C21	0.232549583	-1.769901676	2.899318092
	C22	0.868442837	2.966032717	6.431886177
	C23	1.338108748	2.935831090	7.902334593
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	C25	-0.273490189	5.184792827	6.926909777
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	C31	7.201747226	-6.748340941	4.847020843
	C32	8.472574447	-6.175356444	5.504023152
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C41	-3.873020104	-3.177174744	-0.421152328	
C42	-3.326749943	-4.609461724	-0.249861537	
C43	-3.159544688	-5.411179945	-1.540785630	
C44	-6.323189692	0.425830151	-1.682313216	
C45	-7.349277384	1.103106531	-0.764178134	
C46	-6.594315380	0.680940661	-3.170110163	
C47	-9.410803645	0.850002437	0.532316488	
C48	-8.896364548	1.209949235	1.930325081	
C49	-7.067243134	1.068970276	3.555964785	
C50	-5.893874800	2.042799668	3.462349301	
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C52	-4.945494161	4.923446070	2.504287306	
C53	-4.026375825	3.625483685	0.628619227	
C54	-3.433536942	2.399985769	0.017269176	
C55	-2.844205722	1.268525556	0.526457157	

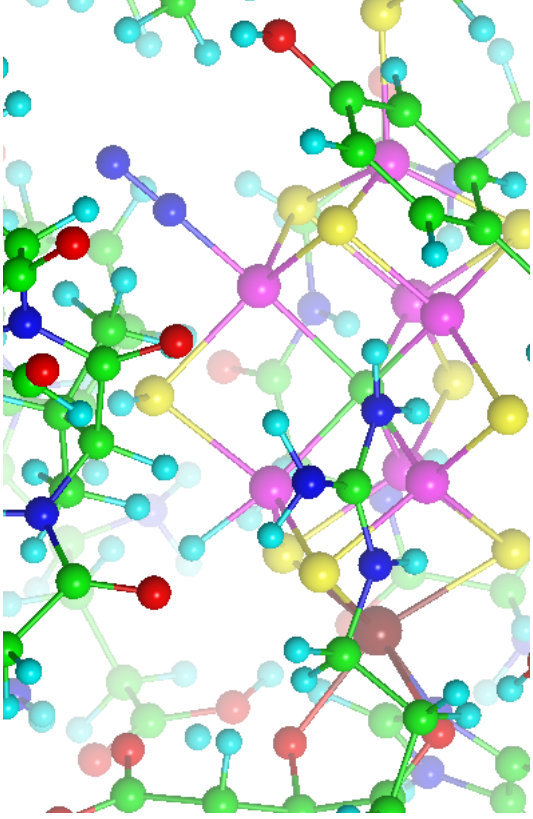
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C61	-8.852070177	9.032715933	2.221595518
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C63	9.364430248	2.380371772	2.403183115
C64	10.405157642	1.276526624	2.400169666
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C67	6.333679414	3.167655486	3.718554528
C68	6.231516915	3.142201275	1.310963343
C69	5.260029620	4.063931058	3.761837662
C70	5.170997037	4.048995467	1.338553116
C71	4.682754600	4.503635196	2.565831493
C72	4.992655924	6.371832540	-3.224520433
C73	3.910280577	7.402233746	-3.594652360
C74	4.354549103	5.199564194	-2.486244157
C75	2.727584865	8.543776783	-5.440980210
C76	1.261064554	8.102449111	-5.430642862
C77	-0.293333081	6.250051010	-4.813146657
C78	-0.680944269	6.225434936	-3.311599812
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C80	-1.490830267	3.921455266	-5.295538865
C81	-2.710807969	4.245561991	-6.170925257
C82	-4.233929137	6.216156571	-6.018533992
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C84	-0.119755032	7.296669900	-0.388922287
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C86	1.030814598	9.445425282	-0.211698662
C87	0.364153644	10.684587107	-0.781806927
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C90	-1.438221208	11.210041871	-3.936879699
C91	-2.613000868	10.263974437	-4.149733984
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C93	-4.100664694	13.412238265	0.516002137
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C98	-6.601531557	8.373301441	-1.410184106
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Fe142	3.464012601	-0.223586982	-3.928419578
Fe143	3.288817442	2.225050650	-2.794698691
Fe144	4.700344182	-2.265717215	-1.096261290
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	O469	5.007608147	-5.811562361	-0.254942300
	O470	5.129428884	-7.197513556	1.510535330
	O471	2.506981844	-6.303083759	-0.777521688
	O472	9.145367052	-6.162042832	1.835025227
	O473	7.179450279	-4.366920223	0.814282582
	O474	-4.691419920	4.000862646	-3.065326051
	O475	7.702139739	-10.725349436	-0.566334720
	O476	7.614365678	-8.440174682	1.395971043
	S477	3.070376890	4.369367059	-3.526248803
	S478	1.600361258	1.059786592	-3.853858900
	S479	1.830733526	-3.910014250	-2.955915879
	S480	3.181366401	1.731457491	-0.608369671
	S481	0.365718006	-1.355404826	-0.821958158
	S482	3.764689982	-1.809454973	-5.450468985
	S483	3.293868177	-3.248944661	0.342850993
	S484	5.205914815	1.207457105	-3.526460442
	S485	5.522203916	-3.666377780	-2.629728227
	S486	6.143736359	-0.769571124	-0.395388865
	end			
rest-S2BH-6Hx 2N2 associated 35, S=1				
Fe (139) -2.278				
Fe (140) -1.093				
Fe (141) -2.731				
Fe (142) 2.734				
Fe (143) 2.695				
Fe (144) 2.005				
Fe (145) 0.321				
				
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	C1	-8.140429240	-5.159439932	0.145678781
	C2	-8.510999831	-6.283566527	-0.828792626
	C3	-8.922252439	-3.137403263	1.293083813
	C4	-8.421357488	-3.390991496	2.710888494
	C5	-8.314110697	-4.910859415	4.619546733
	C6	-6.793100544	-5.043567680	4.732538670
	C7	-4.680693839	-5.520767205	3.611952348
	C8	-4.046876183	-4.127653942	3.621421810
	C9	-4.201320832	-1.809725835	2.852500282
	C10	-4.282214652	-1.134516018	4.230866624
	C11	-5.562839756	-0.756095932	6.254006288
	C12	-4.711134729	-1.394569108	7.358831373
	C13	-4.089455697	-3.458678420	8.515807006
	C14	-2.607657970	-3.822284644	8.362544549
	C15	-0.842926329	-4.586121323	6.829439215
	C16	0.121126687	-3.583680112	6.190581836
	C17	0.314276993	-1.529984983	4.785981015
	C18	0.504773724	-0.337081334	5.751035347
	C19	-0.356719032	-1.132097610	3.453872996
	C20	0.295439934	0.108905543	2.824654208
	C21	-0.352878837	-2.320440198	2.484532555
	C22	-0.596469043	1.457417074	7.046420552
	C23	-0.490485505	1.069381174	8.536405875
	C24	-1.804194778	2.387190283	6.767153418
	C25	-1.857640941	3.540757997	7.776450743
	C26	-1.759464431	2.927793375	5.332151372
	C27	-1.439223040	-0.087007455	10.449640087
	C28	-0.077665709	-0.443737402	11.009568331
	C29	4.930776794	-11.789735184	4.740142956
	C30	5.606512072	-10.525965632	4.207978960
	C31	5.861591386	-8.082455902	4.651205439
	C32	6.944505097	-7.735491229	5.691140287
	C33	4.707658733	-7.064671334	4.676307209
	C34	5.161370234	-5.635199705	4.376164519
	C35	3.971358203	-4.701248702	4.155958659
	C36	4.131184380	-2.188156098	4.293879336
	C37	9.237012341	-6.935805729	6.018974568
	C38	9.547861026	-5.455794833	6.050062758
	C39	-5.234793755	-2.551175331	-2.296069714
	C40	-5.608346701	-1.108631927	-1.907071882
	C41	-3.727516376	-2.742921601	-2.010042251
	C42	-3.213932602	-4.196117975	-2.048957779
	C43	-2.741966570	-4.689585076	-3.416117188
	C44	-5.867026388	1.154093881	-2.853655873
	C45	-7.089000529	1.640006879	-2.062207052
	C46	-5.781471683	1.771080061	-4.256796232
	C47	-9.379483683	1.157958382	-1.336751933
	C48	-9.180261358	1.215034277	0.181935644
	C49	-7.739045168	0.658777123	2.089209626
	C50	-6.571204019	1.572512568	2.459115905
	C51	-4.896076232	3.207509139	1.754482210
	C52	-5.412985153	4.526586124	2.376322117
	C53	-4.110730045	3.617444575	0.501070543
	C54	-3.388599182	2.531395300	-0.225286547
	C55	-2.991678834	1.259324413	0.102777790
	C56	-2.306407231	1.665556664	-1.976936154
	C57	-7.197239080	6.223543111	2.235172589
	C58	-7.368396714	6.371590848	3.746848399

C59	-8.564545482	6.320894711	1.518875285
C60	-9.117333192	7.701250819	1.312861300
C61	-9.110178516	8.811093960	2.134871982
C62	-10.146580965	9.268229223	0.231066875
C63	8.587209410	1.287504169	4.882975839
C64	9.592627855	0.153648958	4.859714606
C65	7.214617991	0.685911281	4.490885594
C66	6.100203671	1.709573899	4.515996901
C67	5.346872213	1.945717298	5.681186723
C68	5.784963515	2.469168108	3.373695936
C69	4.314863939	2.892596157	5.709934473
C70	4.771600216	3.430983409	3.390089668
C71	4.027699787	3.633900670	4.557378386
C72	5.671930363	6.621705315	-0.485976591
C73	4.707727400	7.755589230	-0.876813316
C74	4.892717925	5.342471906	-0.196353284
C75	4.026931484	9.352564856	-2.629009988
C76	2.571250808	9.029833563	-2.972988319
C77	0.894876756	7.202937273	-3.196522824
C78	0.195038278	6.889724025	-1.848430506
C79	1.016052985	5.947563052	-4.093445812
C80	-0.237402806	5.116763649	-4.392379516
C81	-1.220672925	5.690957805	-5.425391637
C82	-2.732066576	7.667074769	-5.162148202
C83	0.331451378	5.984261536	0.420756721
C84	0.097636585	7.237172986	1.277313533
C85	1.162207887	4.998475152	1.267390441
C86	1.179288835	9.258398740	2.133247139
C87	0.592452328	10.603242303	1.737582731
C88	-0.557812210	11.874808133	0.014090459
C89	-1.894941406	12.484236394	0.506755433
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C91	-1.583687627	11.022442748	-2.165541171
C92	-4.040860557	12.083396306	1.633602110
C93	-4.083724974	13.184574179	2.685218202
C94	-4.813172759	10.830558209	2.135725409
C95	-4.936729886	9.759999993	1.073112982
C96	-6.009650942	9.779194323	0.167119120
C97	-3.965229698	8.756980619	0.922409985
C98	-6.102127734	8.844090481	-0.866800926
C99	-4.024415474	7.831311199	-0.124920110
C100	-5.095227713	7.889566925	-1.012213484
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C102	3.745090814	-3.796911305	-7.974519068
C103	2.133413657	-2.248009103	-6.891500628
C104	1.753875651	-0.880048283	-7.470512613
C105	2.216160991	1.530886820	-7.367813900
C106	3.423875029	2.464864487	-7.336268661
C107	5.618955143	3.044162619	-6.451899082
C108	6.494931569	3.121686103	-7.688648279
C109	-1.524010912	-3.443203825	-9.394052796
C110	-2.563119268	-2.330671085	-9.211536923
C111	-1.259377164	-4.140395922	-8.039891235
C112	-0.546656163	-5.491168215	-8.239298247
C113	-0.043995706	-6.026431174	-6.918073908
C114	-2.992155314	0.003304465	-8.606296494
C115	-2.398073674	1.278482877	-9.172414262
C116	-3.527370733	0.128743458	-7.157421374
C117	-2.420410176	0.066504973	-6.138253845
C118	-1.672854180	1.210563568	-5.811640715
C119	-2.0411111632	-1.169488757	-5.583543989
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C121	-0.907981287	-1.271522484	-4.770660706
C122	-0.142095904	-0.135151739	-4.493622900
C123	8.262313332	-6.470117429	-3.495909331
C124	9.294492955	-6.612866706	-2.365914172
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C126	5.727641939	-6.548342973	-3.953083616
C127	5.537132069	-7.125869429	-5.191065123
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C129	10.204326178	-7.893378615	-0.516157869
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C131	0.339094010	-6.947374295	-0.073390520
C132	1.768017073	-7.052125480	0.449132884
C133	2.853574564	-7.198563863	-0.656480360
C134	2.816491989	-8.634411824	-1.244968233
C135	3.991669414	-9.006450050	-2.153391825
C136	4.012053903	-10.493790137	-2.569866854
C137	4.238252089	-6.969896859	-0.028528264
C138	3.737843255	-0.871739681	-1.536542788
Fe139	4.165447303	-2.124304785	-3.043422843
Fe140	2.162835813	0.654820857	-1.051590140

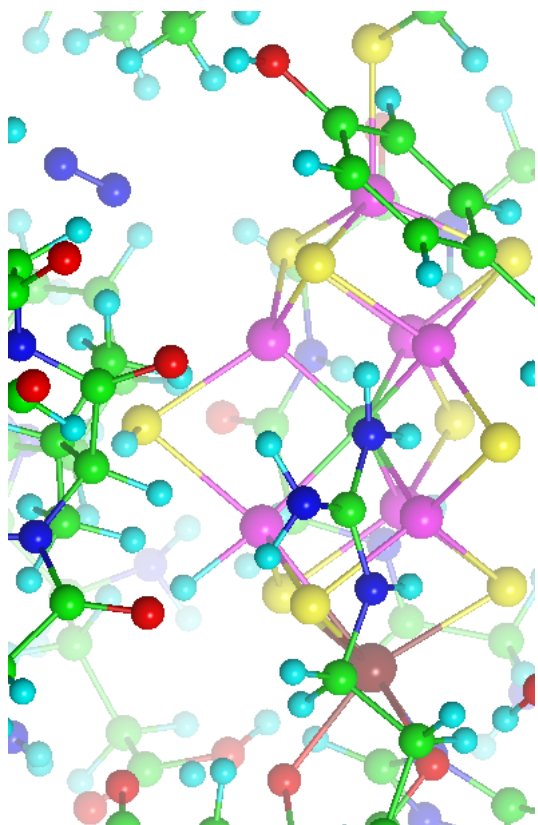
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	Fe142	4.301205655	0.395349562	-2.939002223
	Fe143	4.062351816	2.524148653	-1.380551935
	Fe144	4.755429549	-2.243075987	-0.561339122
	Fe145	2.345201766	-2.364403584	-1.223409157
	H146	-6.797820943	-7.380720533	-0.689417104
	H147	-6.815006807	-6.362781757	-1.963740905
	H148	-10.062777031	-4.425484042	0.032547671
	H149	-9.144185211	-5.859475288	-1.625107717
	H150	-9.150915572	-6.996094460	-0.280368845
	H151	-8.167653668	-2.502853757	0.804683058
	H152	-9.353986651	-5.212113486	2.757896896
	H153	-9.857510082	-2.565149769	1.355013060
	H154	-8.776921781	-5.863587505	4.909489707
	H155	-6.640744678	-5.604074364	2.751063116
	H156	-8.620693856	-4.147366581	5.346902993
	H157	-3.153831381	-1.756002756	2.531989666
	H158	-5.501685183	-3.433373365	2.345641409
	H159	-4.352522742	-6.060497633	2.713569592
	H160	-5.279888600	0.302582619	6.201799364
	H161	-6.174164316	-1.898702516	4.530634894
	H162	-4.301604625	-6.053400533	4.492165754
	H163	-4.816332607	-1.258160974	2.127040340
	H164	-5.286500729	-3.287183212	6.752244731
	H165	-6.620782487	-0.823381864	6.542801498
	H166	-0.811070256	-3.215813472	2.927182635
	H167	-0.926899396	-2.081662013	1.574938336
	H168	0.673797900	-2.573147320	2.174858380
	H169	-1.400801186	-0.874314443	3.694909874
	H170	-4.638399013	-4.397787447	8.678475031
	H171	-1.776602223	2.122709400	4.584662084
	H172	-2.199789711	-0.125867105	8.464513559
	H173	-1.972945833	3.184442569	8.810198409
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	H175	0.592782004	0.860435690	3.569916633
	H176	8.499416385	1.634519114	5.928826660
	H177	-2.626956844	3.578237597	5.147100877
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	H179	-0.847428384	3.525856961	5.172173092
	H180	-0.939794998	4.147625805	7.727712899
	H181	-2.723547957	1.785127694	6.885383964
	H182	0.337005778	1.999390656	6.836914086
	H183	-1.530295322	-0.004335295	5.782628448
	H184	-0.414043346	0.605917977	2.145473842
	H185	1.538513868	4.195822672	0.616974472
	H186	0.476098333	4.556774050	2.006024977
	H187	2.387513257	5.231568216	2.791098465
	H188	2.557231506	4.608613984	5.369301246
	H189	4.529182741	4.004562983	2.494450620
	H190	6.326275890	2.299850496	2.440374764
	H191	5.557745395	1.367293401	6.583567645
	H192	-1.451182780	-2.607781443	5.327137255
	H193	-0.885377735	-5.465329816	6.167571275
	H194	-0.389385601	-4.897733601	7.778078616
	H195	-2.850236824	-4.093864815	6.321459886
	H196	-4.168388387	-2.852232212	9.426294095
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	H198	1.319640839	-1.917010350	4.587882904
	H199	-1.851463366	0.757414725	11.027048738
	H200	-2.090692065	-0.961501367	10.605348797
	H201	0.607638426	-0.961602984	10.300236413
	H202	10.140176621	-7.491086459	5.720911830
	H203	-1.385644066	-5.943974667	-4.297622995
	H204	1.227404235	-6.119522108	-1.573529807
	H205	-1.254893629	-6.218943537	-8.659524366
	H206	0.289195924	-5.375254521	-8.944965659
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	H208	-1.707679377	1.119707293	-10.032978274
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	H212	-1.089054367	-0.984513845	-8.639647456
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	H215	-1.209022409	-5.815003207	-2.552368881
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	H217	0.194979912	-3.766139679	-10.469755638
	H218	-6.461136159	-3.263552577	-3.802503294
	H219	-3.538855223	-2.343963409	-1.002371662
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	H221	-2.393651594	-4.307375647	-1.324687623
	H222	-4.233129749	2.758395707	2.507639624

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H226	-7.183849504	4.266520689	1.372196670
H227	-8.690997061	8.988833399	3.119657114
H228	-7.654800283	5.422934127	4.262557309
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H230	-6.520908574	7.016814203	1.880731550
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H235	-8.438673909	5.882982649	0.515897378
H236	-6.331027053	2.213615610	0.491074781
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H238	-9.799449559	2.128381065	-1.634704760
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H240	-10.132621368	0.389097915	-1.553148893
H241	9.801085711	2.828559603	4.302994422
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H244	-0.657862505	5.536307743	0.249532261
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H251	-6.644530774	1.450871613	-4.860367310
H252	0.501335216	11.596803054	-1.850644471
H253	-0.686804106	12.918119627	-1.833394442
H254	-0.141955038	10.047680979	-3.286308676
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H258	-6.952276584	8.864385699	-1.553993853
H259	-3.137220355	8.669530704	1.631639250
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H261	1.747717353	5.276451390	-3.614868387
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H264	-8.140431508	-0.012163437	-2.643194558
H265	4.499567028	9.761813190	-3.531685527
H266	-5.682497214	-0.795552547	-3.874015525
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H271	-4.179163485	9.067132437	-4.804790568
H272	-4.826776665	-3.397113991	-4.128896678
H273	-5.795754967	-3.200605625	-1.599056206
H274	-6.794303429	10.531896538	0.271569050
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H289	4.784982157	-5.636906373	-9.433042102
H290	5.612813624	4.563649320	0.086791024
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H327	2.799507455	-9.323429720	-0.386039151
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H329	2.754833256	-5.514264208	-4.733402711
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O454	-5.089366660	13.833576748	2.923781147
O455	-5.120116791	6.980684311	-2.092255793
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O457	0.917693595	-0.759047183	-8.389554512
O458	3.361897614	3.541344647	-7.953087455
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	O471	4.645680264	-7.714468942	0.883131369
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	S484	3.234761078	-3.581639499	0.365562303
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rest-S2BH-6Hx 2N2 dissociated 35, S=1			bm522bh6x1a2n2xdtb.car_3	
Fe(139) -2.366	C1	-2.489434593	-5.874671727	-7.185842125
Fe(140) -2.357	C2	-1.764739869	-6.006034018	-8.529398064
Fe(141) -2.529	C3	-4.674914552	-5.721823334	-6.077799572
Fe(142) 2.709	C4	-4.496811437	-6.741927515	-4.955895586
Fe(143) 2.872	C5	-3.891991211	-9.020409919	-4.319227571
Fe(144) 2.204	C6	-2.729086995	-8.712691165	-3.372608300
Fe(145) 1.455	C7	-0.628286892	-7.532272390	-3.004414968
	C8	-1.071585439	-6.472406769	-1.994975550
	C9	-2.500033392	-4.539898040	-1.553363976
	C10	-3.331181771	-5.148119680	-0.412046313
	C11	-5.010547362	-6.763187381	0.263661880
	C12	-4.246609520	-7.670803846	1.235620233
	C13	-2.730964531	-9.578855649	1.473101500
	C14	-1.406674886	-9.192229646	2.144234234
	C15	0.725138829	-7.992229589	1.902469323
	C16	0.909259259	-6.612476884	2.536845987
	C17	0.069159977	-4.267082975	2.640328154
	C18	-0.811513993	-4.154793080	3.906036125
	C19	-0.322621777	-3.267046015	1.531059925
	C20	-0.454365253	-1.850680301	2.095889260
	C21	0.687822622	-3.344345129	0.380854712
	C22	-3.095136522	-4.347504540	4.842950820
	C23	-3.135070895	-5.622807801	5.709138563
	C24	-4.496680990	-3.953717190	4.310125387
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	C28	-2.424159056	-8.223922117	6.892905742
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	C30	9.855693757	-7.737650172	1.623086025
	C31	8.346801569	-6.469809650	3.153602126
	C32	8.653098823	-6.659560676	4.651437461
	C33	6.846642809	-6.221723347	2.912152083
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	C35	4.909322226	-4.612198244	3.158983112
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	C43	1.952794634	-1.313891377	-5.968716229
	C44	-4.258322250	0.913434577	-5.027633251
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	C46	-4.263363435	2.325944218	-5.629148967
	C47	-7.165545328	-1.289513931	-6.182540744
	C48	-7.408413974	-2.315749126	-5.070854505
	C49	-6.470059925	-3.569072780	-3.180468886
	C50	-6.329424954	-2.903792373	-1.810836786
	C51	-6.030125731	-0.846221444	-0.517380432
	C52	-7.400631912	-0.625785493	0.165333749
	C53	-5.422393722	0.551029712	-0.694532813
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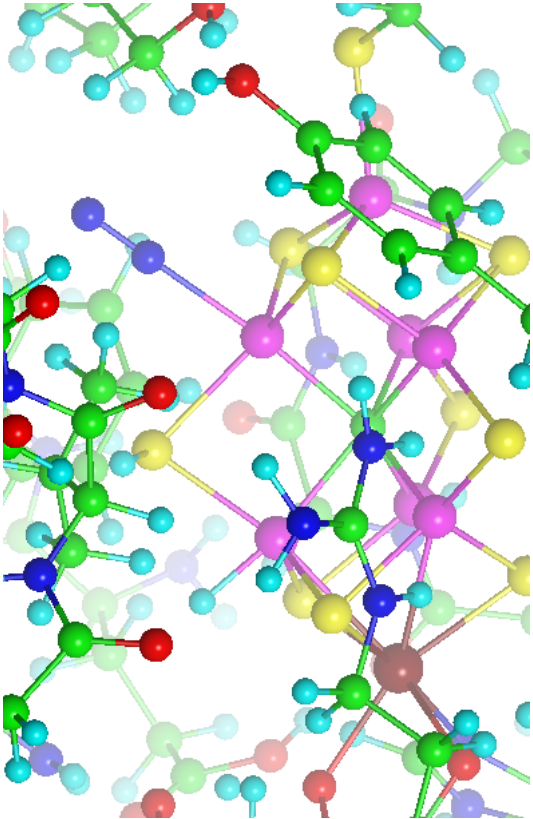
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C71	-0.588130377	0.246669055	7.048128210
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C79	-2.165182992	6.938504754	0.568095473
C80	-2.428774270	6.250332188	-0.775843748
C81	-3.250163531	7.038239133	-1.805378361
C82	-5.688197875	7.594166973	-1.731478704
C83	-3.763045927	3.522195453	3.168680330
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C86	-5.759352404	4.558407912	6.207985770
C87	-6.963566092	5.483172295	6.159806405
C88	-8.161569228	7.155189469	4.861816665
C89	-9.638091618	6.758873578	4.607344354
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C92	-11.185857009	5.019531798	3.824894116
C93	-12.191056413	4.925779967	4.964710180
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C96	-10.719429183	4.005505478	0.640084417
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C98	-9.916263149	4.133385472	-0.495732044
C99	-7.951946475	3.655426654	0.850740125
C100	-8.535350317	3.977942586	-0.372053842
C101	8.421839354	5.033807494	-3.880124088
C102	7.122361483	4.558161922	-4.506110497
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C106	2.645915765	7.890808988	-1.567800617
C107	3.661730713	8.330586573	0.604873111
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C109	3.473596875	4.150057774	-8.556269337
C110	1.956528377	4.372979638	-8.591713378
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C113	5.591858466	1.220118917	-7.170029831
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C115	-0.292634463	6.631118709	-6.896788847
C116	-0.846175167	4.112622602	-6.795018493
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C118	-0.543356727	4.382213513	-4.290304709
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C120	0.124582331	4.061701990	-3.103654005
C121	1.324254874	2.294190336	-4.238991478
C122	1.071408144	3.031275865	-3.078972411
C123	11.007463541	1.130841115	0.025920667
C124	11.548778093	0.558505825	1.344504768
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C126	9.354654953	0.602207650	-1.874881452
C127	9.902629418	1.071444012	-3.051163244
C128	7.720522955	0.822313635	-3.313723302
C129	12.598312783	-1.264571375	2.545328232
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C132	5.728810811	-4.133360030	-1.662996520
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N409	-9.881076898	5.457929692	4.307157943
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N415	1.406347548	5.005991681	-7.515363803
N416	12.086955934	1.586200564	-0.870769159
N417	7.976890557	0.467808485	-2.054786188
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O426	-3.233574567	-4.720457642	0.750550112
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O437	1.584614443	-0.492726279	-6.840405415
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O458	2.019134705	8.962377025	-1.526706356
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O461	5.250638764	0.059891018	-7.374860395
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	O471	8.121613660	-3.914583422	0.118217066
	O472	6.302532131	-1.837217663	-2.170165996
	O473	9.977167474	-3.275270456	3.780547002
	O474	7.650034039	-1.845806350	2.957097640
	O475	-5.195343194	3.947099277	-2.282850511
	O476	12.772515531	-3.250751550	-0.816435441
	O477	10.650570604	-4.025986737	1.193613680
	S478	0.019359928	5.388841882	3.443411106
	S479	1.333004279	3.993233966	0.379557438
	S480	4.723882612	1.008975443	-2.153338561
	S481	1.193428470	1.608708949	3.023030516
	S482	1.183357706	0.345415386	-0.760193587
	S483	5.123755678	4.451090452	-0.460690110
	S484	4.524599642	-1.440142695	0.617770441
	S485	3.650764881	4.260620927	3.173390739
	S486	6.889341073	1.400440537	0.780467102
	S487	4.893395444	0.648051330	3.785327927
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rest-S2BH-6Hx 2N2 TS 35, S=1 Fe(139) -2.293 Fe(140) -2.079 Fe(141) -2.537 Fe(142) 2.507 Fe(143) 2.840 Fe(144) 2.158 Fe(145) 1.329	bm522bh6x1a2n2xdtf_orig			
	C1	-2.492218614	-5.887777754	-7.211658206
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	C3	-4.656191879	-5.712241445	-6.069733943
	C4	-4.479630526	-6.729021430	-4.946397086
	C5	-3.876621116	-9.005217558	-4.299888248
	C6	-2.725396474	-8.686219179	-3.343173253
	C7	-0.627691812	-7.503144718	-2.968742355
	C8	-1.085130839	-6.446555413	-1.961168769
	C9	-2.520869020	-4.511780770	-1.542006823
	C10	-3.356608731	-5.111435419	-0.400651573
	C11	-5.020583400	-6.736083248	0.285017812
	C12	-4.261716380	-7.650203688	1.256276044
	C13	-2.749958770	-9.563063638	1.492529166
	C14	-1.413479026	-9.203754716	2.153699197
	C15	0.723812012	-8.009108447	1.919600671
	C16	0.913805185	-6.624153623	2.540841982
	C17	0.052830825	-4.285180964	2.645197267
	C18	-0.825006465	-4.178968427	3.912548773
	C19	-0.358544280	-3.294045579	1.534113826
	C20	-0.539016793	-1.867097823	2.074279301
	C21	0.656807044	-3.334876092	0.386239002
	C22	-3.105589909	-4.354458517	4.853281855
	C23	-3.140196717	-5.629227730	5.720979487
	C24	-4.508629632	-3.962208997	4.326952299
	C25	-5.549066269	-3.989202436	5.453793104
	C26	-4.475425070	-2.581094238	3.657900441
	C27	-3.532550231	-8.021777197	5.873469241
	C28	-2.458422701	-8.211482846	6.924474724
	C29	10.075296264	-9.121163652	1.003145956
	C30	9.865714714	-7.743479146	1.627705374
	C31	8.342739902	-6.471740901	3.143109826
	C32	6.636612364	-6.659239829	4.643540591
	C33	6.845047639	-6.226822532	2.887260558
	C34	6.310007772	-4.982447738	3.598020072
	C35	4.900989564	-4.624360036	3.126575590
	C36	3.337748374	-3.121091397	4.411376734
	C37	9.674036521	-5.667187759	6.628489520
	C38	8.918675245	-4.678172306	7.488667248
	C39	-1.516796941	-1.593751158	-5.860473361
	C40	-2.824055470	-1.102782044	-5.211012641
	C41	-0.383694718	-1.440049813	-4.820917974
	C42	0.944277600	-2.147801853	-5.162057007
C43	1.939777512	-1.319395498	-5.973688914	
C44	-4.255364031	0.896680496	-4.999807761	
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C46	-4.252335630	2.312306094	-5.592828892	
C47	-7.147106078	-1.309091772	-6.189716022	
C48	-7.409896479	-2.305625330	-5.055310636	
C49	-6.481645728	-3.558623132	-3.158676534	
C50	-6.334423963	-2.888240667	-1.793233119	
C51	-6.034205571	-0.838258864	-0.497037182	
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C53	-5.430525723	0.563657726	-0.652807650	
C54	-4.031893281	0.642212356	-1.167000237	
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C56	-2.263505552	1.708852208	-2.019200361	
C57	-9.772171696	-0.051624879	-0.295945372	
C58	-10.359569462	-1.098039801	0.648951343	
C59	-10.637934788	0.087279111	-1.569547577	
C60	-11.884882978	0.912242711	-1.442840055	
C61	-12.806311739	1.010849261	-0.418439254	
C62	-13.379959734	2.330870647	-2.103771157	

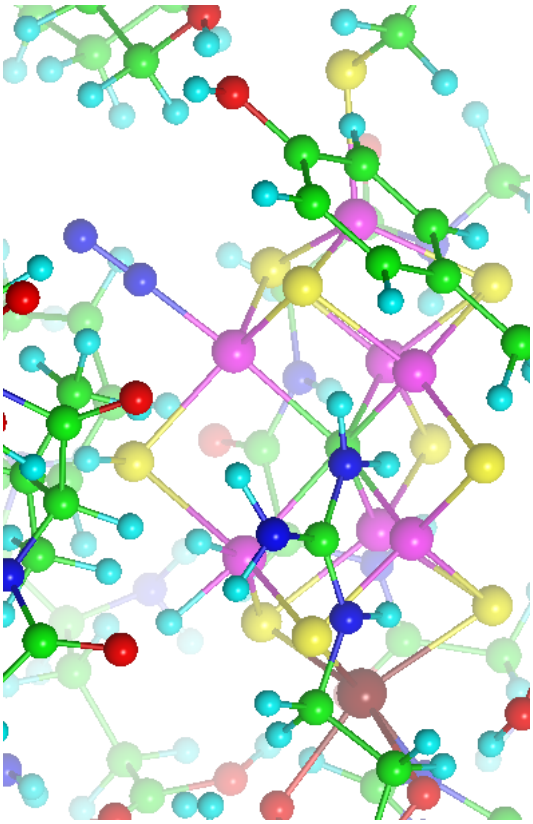
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C64	5.579242943	-0.336619541	9.184342550
C65	3.613369549	-0.499181122	7.702525125
C66	2.142761237	-0.240295975	7.474458878
C67	1.168151229	-1.175432846	7.870626779
C68	1.704098410	0.951215010	6.869779149
C69	-0.194355743	-0.941527671	7.656871099
C70	0.348081514	1.206021387	6.665685901
C71	-0.600276043	0.254386775	7.053087514
C72	-0.146739012	6.254671800	6.099655384
C73	-1.484522289	6.927036309	5.740869768
C74	0.054457790	5.008908883	5.246249317
C75	-2.585871274	8.957120578	4.870643932
C76	-3.333231707	8.541738741	3.600635578
C77	-3.287251835	7.037377012	1.619160297
C78	-3.911183502	5.649506768	1.923364988
C79	-2.160522727	6.943491971	0.561551981
C80	-2.438826427	6.245086402	-0.775355421
C81	-3.265519453	7.028423279	-1.809038243
C82	-5.702519955	7.583085354	-1.716700397
C83	-3.774695947	3.505143128	3.096024795
C84	-4.971122434	3.589218862	4.053711426
C85	-2.741992849	2.553775466	3.738535138
C86	-5.731114384	4.566480968	6.161807182
C87	-6.935810813	5.492792556	6.127695179
C88	-8.167665274	7.155622781	4.849070237
C89	-9.644206492	6.753398078	4.601171227
C90	-7.755007302	8.272818615	3.885907886
C91	-7.806365834	7.866220526	2.419636371
C92	-11.195347433	5.012699390	3.827464941
C93	-12.199889024	4.922502661	4.967267732
C94	-11.050631276	3.631033593	3.128132415
C95	-10.177305656	3.693357944	1.893539838
C96	-10.735646799	4.010926344	0.644886793
C97	-8.788013907	3.490967368	1.962956177
C98	-9.937150458	4.145822411	-0.494094608
C99	-7.967938735	3.651169093	0.840350293
C100	-8.556111447	3.983960637	-0.377103023
C101	8.412955452	5.025871418	-3.872135263
C102	7.116951486	4.571121400	-4.518217085
C103	4.685329130	4.241326416	-4.141651619
C104	3.661749237	5.382156049	-4.157201894
C105	2.394023867	6.947189526	-2.751605980
C106	2.640310845	7.888257956	-1.574657907
C107	3.619457420	8.309164044	0.616568525
C108	4.490666188	9.530256051	0.387601352
C109	3.461542787	4.135927598	-8.562103027
C110	1.945976952	4.362228005	-8.601424989
C111	3.774898028	2.815743930	-7.820632235
C112	5.217976884	2.353245223	-8.096345078
C113	5.603113745	1.228208003	-7.162674841
C114	-0.035041844	5.232654638	-7.459227004
C115	-0.303961204	6.618051629	-6.903230728
C116	-0.854316076	4.098598465	-6.794889786
C117	-0.272076625	3.679461811	-5.470347368
C118	-0.564787728	4.391652330	-4.294248705
C119	0.669617725	2.636448697	-5.412036405
C120	0.112878696	4.099869756	-3.105783260
C121	1.350400270	2.347852441	-4.224781910
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C127	9.897920421	1.086823497	-3.053067931
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C130	13.580531574	-0.352327957	3.255703213
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C132	5.762069599	-4.123916706	-1.683593796
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Fe141	3.485708109	2.069080769	2.905175728
Fe142	3.510146639	3.716573970	0.908946880
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	H148	-4.319021043	-5.971145304	-8.160154101
	H149	-2.313963575	-5.373225939	-9.295331866
	H150	-1.911984862	-7.043329049	-8.910873403
	H151	-4.415328496	-4.728448789	-5.640874516
	H152	-3.966622184	-8.187542202	-6.289258837
	H153	-5.714446112	-5.706631431	-6.363717332
	H154	-3.656511290	-9.950126823	-4.813918810
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	H156	-4.769406919	-9.155616652	-3.678387209
	H157	-1.729019676	-3.914126654	-1.073957224
	H158	-2.267749524	-5.562125316	-3.391455367
	H159	0.181244458	-7.089446296	-3.585962703
	H160	-5.501909085	-5.954168389	0.885800054
	H161	-4.289816261	-6.396277903	-1.715462102
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	H163	-3.145817258	-3.843727766	-2.150912806
	H164	-3.291618545	-8.570476450	-0.322444167
	H165	-5.800442521	-7.326077519	-0.215903055
	H166	0.804954289	-4.352652877	0.000275265
	H167	0.313529463	-2.716982481	-0.459162788
	H168	1.633303062	-2.941400987	0.709928462
	H169	-1.335479350	-3.634605585	1.154605594
	H170	-2.572537735	-10.433935519	0.845051068
	H171	-3.779685849	-2.549988553	2.807567968
	H172	-3.563373464	-6.861177711	4.090031691
	H173	-5.660511103	-4.988752583	5.898950020
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	H175	-1.039720750	-1.842040466	3.053312895
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	H178	-6.528240575	-3.683244359	5.057744346
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	H188	-2.488581401	-0.198756187	7.092807990
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	H190	2.438057644	1.682914883	6.525533656
	H191	1.477926647	-2.114573026	8.338361893
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	H204	5.267288921	-2.264809454	-2.922782768
	H205	5.289545124	1.981564382	-9.128465297
	H206	5.915869931	3.195562474	-7.981992527
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	H226	-8.268877123	-0.635886904	-1.702835720

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	O477	10.655373897	-4.023779458	1.202732745
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	S479	1.348202279	4.082873327	0.462875685
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rest-S2BH-6Hx-6Hn 2N2 associated 35, S=3/2 Fe (139) -2.268 Fe (140) -0.962 Fe (141) -2.601 Fe (142) 2.757 Fe (143) 2.713 Fe (144) 2.295 Fe (145) 0.892	bm522bh6x6hn2n2xt3g.car_2			
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	C21	0.988669212	-2.783412625	1.731376346
	C22	-2.456819033	-2.022857031	6.493792891
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	C40	-2.888555316	-3.484210838	-3.981560337
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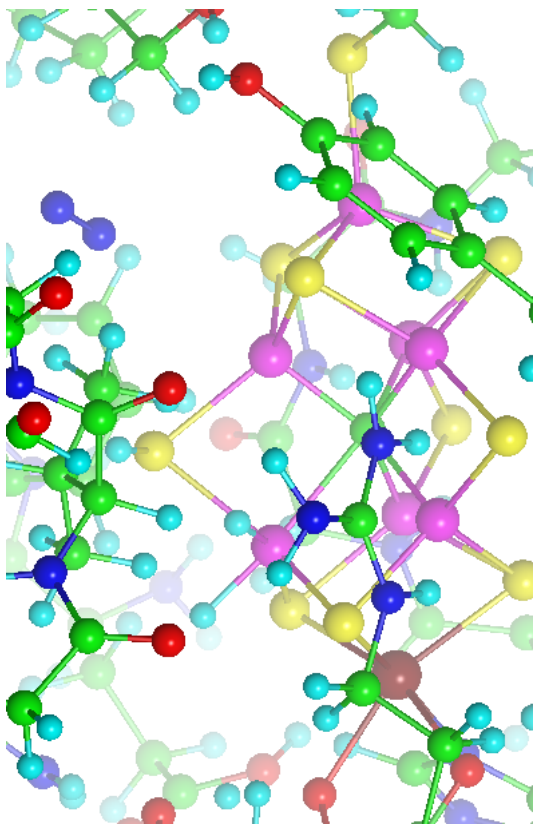
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H151	-4.102573748	-7.029014899	-2.673750402
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H158	-1.794902338	-6.631071354	-0.472139705
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H160	-4.827165181	-5.388426258	3.790682311
H161	-3.652418254	-6.819280902	1.556311809
H162	0.549507480	-8.536065316	1.478106183
H163	-2.808617555	-4.623366190	-0.027820439
H164	-2.402617028	-8.090365526	3.682379119
H165	-5.005103832	-7.124657826	3.418087206
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H167	0.567478381	-2.582876411	0.733370131
H168	1.945162531	-2.244085606	1.797800961
H169	-0.927088619	-2.870538679	2.717439894
H170	-1.441662443	-9.172685814	5.490369956
H171	-3.406836346	-1.373180428	3.917522646
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H349	1.753353727	8.385746935	-3.052966019
H350	4.248636252	2.240173478	7.279436434
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H353	12.531028590	1.306062974	-2.348359939
H354	13.344273038	0.065745086	1.968835699
H355	12.177769086	0.019692732	0.009441690
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H359	-11.982362837	6.081839397	4.211528606
H360	10.324709287	-2.190047624	8.434019565
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H366	-8.735558121	2.082893370	-3.197104754
H367	0.707202773	-0.544882482	-0.289776351
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O423	-1.506440156	-7.987328751	-2.872584296
O424	-4.103582239	-7.728100961	-0.246997956
O425	-1.871895219	-9.317058838	2.193058048
O426	-0.053430551	-6.176148681	2.145648498
O427	-2.774055016	-4.092401612	2.942375843
O428	-3.567364101	-6.056571351	5.853021396
O429	0.039977211	-7.375435178	7.193269293
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O433	-1.431565771	-4.661623566	11.189604404
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O435	9.223383026	-3.960317186	7.368986499
O436	10.042954451	0.651963197	8.771124552
O437	-3.397017145	-3.730221533	-2.869795836
O438	1.352790312	-3.325526969	-6.061435288
O439	-6.608095636	-1.913959160	-3.355459584
O440	-5.691040159	0.264549591	-5.342462611
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O442	-6.049816787	-4.023152741	1.360309516
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O453	-11.114233897	8.061492504	1.821843058
O454	-9.442951285	6.699716074	-0.722817990
O455	-13.664158917	5.410809305	3.267720127
O456	-8.158444320	2.494443374	-2.524750519
O457	6.429511435	1.722333242	-7.413634859
O458	2.375237405	3.222997900	-7.483775319
O459	1.020308928	7.522492010	-5.425464027
O460	3.464326955	10.238067915	-3.812389128
O461	0.472286607	-0.530078000	-10.361519933
O462	4.957954753	-2.742464067	-7.022555544
O463	5.887660902	-0.754913694	-6.622453495
O464	-2.284593014	3.364421886	-8.561555691
O465	11.456637109	3.065113567	0.677083794
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O470	10.184376546	-4.757537124	-3.590771005
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	O477	12.982582940	-2.279657062	-0.343814780
	O478	11.049750310	-2.241292052	1.968920400
	S479	-0.360501078	6.357806217	0.749594833
	S480	0.906449106	3.954171105	-1.440524403
	S481	4.422792672	0.146996011	-2.600968901
	S482	1.238875761	3.016769437	2.062320154
	S483	1.309893462	0.218932446	-1.250558989
	S484	4.535369108	4.038707735	-2.781909210
	S485	4.915694261	-0.567019087	0.963149933
	S486	3.402178191	5.498590357	0.648924306
	S487	6.709586606	2.170077126	-0.559559136
	S488	5.002240653	2.708543532	2.748978363
	end			
rest-S2BH-6Hx-6Hn 2N2 dissociated 35, S=3/2			bm522bh6x6hn2n2xt3c_3_53067.67	
Fe(139) -2.388	C1	-2.128655055	-8.588998414	-3.739763933
Fe(140) -0.801	C2	-1.462289557	-9.234437871	-4.959763317
Fe(141) -2.265	C3	-4.257416484	-8.111631521	-2.616565251
Fe(142) 2.695	C4	-3.930945171	-8.524644427	-1.184610740
Fe(143) 2.769	C5	-3.074469987	-10.248795225	0.319463008
Fe(144) 2.374	C6	-1.933495426	-9.453777399	0.959280121
Fe(145) 0.393	C7	0.043964469	-8.065344847	0.626396744
	C8	-0.486512582	-6.715929024	1.112186684
	C9	-2.097071553	-4.908799478	0.762111448
	C10	-2.829609274	-5.011963622	2.108353050
	C11	-4.279388202	-6.311363919	3.554454964
	C12	-3.394201167	-6.634533812	4.764668305
	C13	-1.686786499	-8.120161253	5.699700298
	C14	-0.373876142	-7.397689129	6.025863895
	C15	1.617369952	-6.274333592	5.121920425
	C16	1.690112577	-4.745819604	5.063872723
	C17	0.595201074	-2.669245111	4.206924198
	C18	-0.239544845	-2.090327888	5.374968492
	C19	0.029492833	-2.311961811	2.818046674
	C20	-0.281117518	-0.813434731	2.694534558
	C21	0.989928918	-2.781914166	1.721015312
	C22	-2.449475514	-2.014065066	6.484812925
	C23	-2.317885208	-2.779745840	7.817511004
	C24	-3.906904267	-2.007974849	5.958168412
	C25	-4.898075086	-1.614739634	7.060177097
	C26	-4.047530876	-1.069208888	4.752534714
	C27	-2.448300763	-4.891453244	9.011038901
	C28	-1.333830142	-4.521897665	9.966726141
	C29	10.995412604	-6.947389690	4.022830222
	C30	10.659018671	-5.457495379	4.007626665
	C31	9.076695640	-3.777750533	4.954920970
	C32	9.447733711	-3.267859047	6.361022233
	C33	7.553612812	-3.786320496	4.740585988
	C34	6.921615748	-2.401609556	4.883179956
	C35	5.463557160	-2.395391630	4.424020534
	C36	3.807470713	-0.597626470	5.048827072
	C37	10.453701158	-1.435818033	7.636714406
	C38	9.631876021	-0.229237298	8.032316855
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	C40	-2.882428228	-3.473236230	-3.976932132
	C41	-0.400547965	-3.401086624	-3.670584002
	C42	0.979756470	-4.081788414	-3.775808770
	C43	1.848762443	-3.635911936	-4.951545300
	C44	-4.519069699	-1.715738488	-4.549789103
	C45	-5.828563253	-2.424868005	-4.180178538
	C46	-4.687371258	-0.706686769	-5.694215302
	C47	-7.209992313	-4.432578713	-4.429394876
	C48	-7.317355758	-4.848790992	-2.957125220
	C49	-6.188274434	-5.076749374	-0.790194439
	C50	-6.067134850	-3.865949898	0.134372694
	C51	-5.923705689	-1.437431452	0.381943462
	C52	-7.293352136	-1.066453753	0.999314093
	C53	-5.478844128	-0.207614617	-0.421334827
	C54	-4.119731704	-0.264034997	-1.036297591
	C55	-3.009145881	-1.047883518	-0.831620634
	C56	-2.507105171	0.433037050	-2.417925561
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	C58	-10.147754699	-1.500690416	1.873152323
	C59	-10.638848336	-1.426167783	-0.602391910
	C60	-11.961689018	-0.731291414	-0.745094575
	C61	-12.851268661	-0.258755333	0.200148781
	C62	-13.621789427	0.122193479	-1.842457358
	C63	4.417351202	4.313370067	7.839461626
	C64	5.919173578	4.147342725	7.988275495
	C65	3.932648124	3.209999348	6.865232231



C66	2.436527457	3.223971944	6.662175372
C67	1.579812707	2.480971879	7.493893767
C68	1.855007169	3.982055962	5.629005607
C69	0.193483610	2.484161085	7.302024285
C70	0.473419334	4.009254398	5.436287066
C71	-0.355718117	3.250760747	6.266571058
C72	-0.594282294	8.272155489	2.797314201
C73	-2.004984745	8.617384331	2.292789126
C74	-0.280687928	6.796237294	2.548008853
C75	-3.340603760	9.965116723	0.718418115
C76	-4.079379513	8.985491274	-0.196424193
C77	-3.943845582	6.769845938	-1.321112599
C78	-4.406291913	5.616811512	-0.392494332
C79	-2.854513076	6.306169401	-2.318615302
C80	-3.116738172	5.069610266	-3.188429389
C81	-4.051471124	5.256886557	-4.395865326
C82	-6.525553102	5.602319381	-4.354465432
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C85	-2.836627504	3.779947631	2.505942395
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C91	-8.506438293	7.507619763	-0.606365338
C92	-11.507556922	5.299998355	2.160732837
C93	-12.453259059	5.634485587	3.306387752
C94	-11.254912716	3.766005826	2.110254096
C95	-10.436206079	3.353423548	0.907581021
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C97	-9.032586099	3.306802831	0.956627209
C98	-10.320342982	2.728546657	-1.449166395
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C101	7.685621335	3.467067080	-6.315582450
C102	6.422289242	2.676124095	-6.604626933
C103	4.051138233	2.354052249	-5.940336163
C104	2.915582146	3.296226557	-6.356435637
C105	1.543769207	5.208454789	-5.665929770
C106	1.730968708	6.586391884	-5.037260465
C107	2.742133379	8.006695310	-3.335087491
C108	3.487268796	9.068441813	-4.121165218
C109	2.687026177	0.230319284	-9.734065847
C110	1.155275473	0.299600733	-9.737473594
C111	3.169081252	-0.607874772	-8.528029058
C112	4.641540608	-1.029744639	-8.695547713
C113	5.179308007	-1.596419342	-7.401346182
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C115	-1.244238362	2.898322633	-9.008790504
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C119	0.180035398	0.065052029	-6.069157058
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C121	0.942856911	0.397820528	-4.946974267
C122	0.639930339	1.549162147	-4.214811761
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C131	5.102637212	-4.610053827	-1.179546409
C132	6.107313908	-4.006876597	-0.202169649
C133	7.131992588	-3.028620807	-0.846973575
C134	8.188919297	-3.824951961	-1.658721223
C135	9.402728104	-3.015980826	-2.124825551
C136	10.525449544	-3.869438933	-2.756883589
C137	7.867722575	-2.257045041	0.261712312
C138	3.454740968	2.296699601	-0.185207948
Fe139	4.770825162	2.131346651	-1.679045388
Fe140	1.622321991	2.211941207	-0.175333230
Fe141	3.258471537	3.335632965	1.451404381
Fe142	3.205040378	4.080950945	-1.053062656
Fe143	1.190930733	4.674480545	0.637540430
Fe144	5.039251593	1.580973160	0.831607026
Fe145	3.460238504	0.064329985	-0.566721925
H146	0.485088541	-9.006238671	-4.400017575
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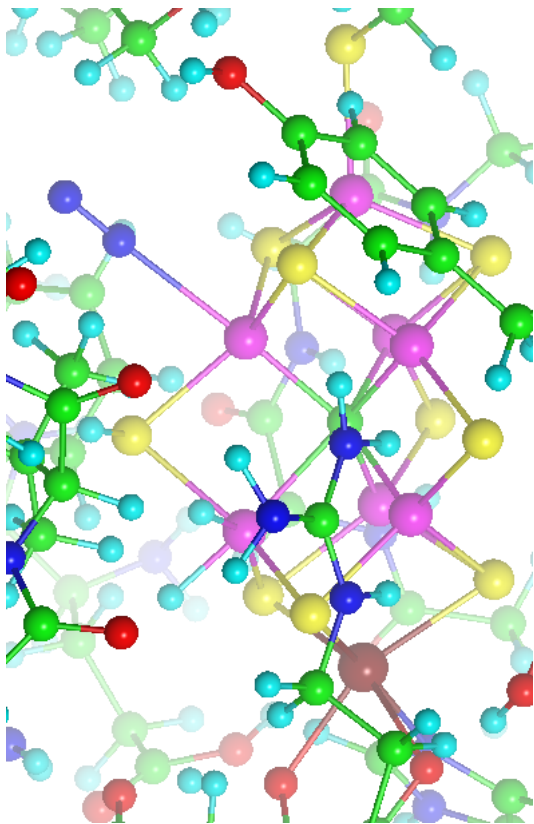
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H158	-1.792378377	-6.630501390	-0.474729647
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O461	0.471927187	-0.529343595	-10.361491540
O462	4.959104610	-2.742750020	-7.024266506
O463	5.889533575	-0.755540466	-6.623035847
O464	-2.281988290	3.365040333	-8.561966760
O465	11.459939153	3.061314260	0.680263308
O466	13.946621090	2.660272754	3.068020783
O467	4.740031078	-3.806906295	-2.186830089
O468	4.616086811	-5.728928356	-1.027555489
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O470	10.185224233	-4.757851573	-3.588107918
O471	7.773293474	-0.953937549	0.223014939
O472	8.533943864	-2.871435819	1.116472289
O473	6.404534188	-2.111461777	-1.668487158
O474	10.395711542	-0.508717277	4.026758853
O475	7.919416683	0.212428187	2.817355027

	O476	-5.668240365	2.126813191	-3.326043901
	O477	12.989887594	-2.285092118	-0.341935968
	O478	11.054020687	-2.242156567	1.969283555
	S479	-0.368619529	6.336333574	0.755692950
	S480	0.977889960	3.867753375	-1.488841891
	S481	4.399663586	0.142375278	-2.625496792
	S482	1.123483593	2.822407785	1.921538025
	S483	1.208981842	0.186719695	-1.089430751
	S484	4.589522138	4.060091821	-2.783910107
	S485	4.886497223	-0.639414042	0.924782810
	S486	3.333986907	5.443192885	0.762489505
	S487	6.707936282	2.157333258	-0.526538242
	S488	4.924407650	2.663633443	2.743468169
	end			
rest-S2BH-6Hx-6Hn 2N2 TS 35, S=3/2			bm522bh6x6hn2n2xt3g_orig	
Fe(139) -2.291	C1	-7.243096966	-5.885086551	-2.315323398
Fe(140) -1.029	C2	-7.280278125	-6.850707645	-3.504106792
Fe(141) -2.486	C3	-8.483070566	-4.187104981	-1.050046077
Fe(142) 2.754	C4	-8.225744449	-4.641974756	0.383327549
Fe(143) 2.806	C5	-8.280967308	-6.462178330	2.010717472
Fe(144) 2.306	C6	-6.805321281	-6.453868280	2.417610095
Fe(145) 0.760	C7	-4.473982942	-6.500921993	1.705934864
	C8	-4.052782993	-5.072632135	2.054208957
	C9	-4.376960588	-2.686296760	1.624333658
	C10	-4.805093956	-2.273039871	3.040209094
	C11	-6.473722498	-2.405014516	4.794307306
	C12	-5.757365119	-3.131261896	5.940243705
	C13	-5.090410401	-5.294004211	6.879595538
	C14	-3.570148972	-5.477215465	6.972542889
	C15	-1.467821354	-5.778951379	5.732751959
	C16	-0.543524847	-4.588389358	5.460745234
	C17	-0.378707890	-2.307305088	4.452210002
	C18	-0.531057545	-1.293312396	5.611578780
	C19	-0.855158924	-1.756618535	3.091540818
	C20	-0.293192420	-0.352931664	2.803078268
	C21	-0.505401072	-2.743508799	1.972774748
	C22	-2.079967599	0.124326593	6.918301931
	C23	-2.198305207	-0.504361214	8.321383101
	C24	-3.329846823	0.96338351	6.550374007
	C25	-3.720207430	1.915383689	7.687792067
	C26	-3.096303341	1.746996551	5.252369399
	C27	-3.321496610	-2.069637488	9.800521341
	C28	-2.057673579	-2.373362355	10.577434528
	C29	5.502492086	-11.867737162	3.777727409
	C30	6.086962785	-10.468998288	3.596991547
	C31	5.927609840	-8.134622282	4.459281676
	C32	6.743588359	-7.865655966	5.738501574
	C33	4.661504812	-7.263994064	4.399189517
	C34	4.964749971	-5.765982572	4.415008342
	C35	3.721285450	-4.933202539	4.103101705
	C36	3.533434297	-2.476834918	4.652475802
	C37	8.812335355	-6.921334512	6.644870053
	C38	8.912002494	-5.446791687	6.965114637
	C39	-4.311512225	-2.612127411	-3.673955121
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	C41	-2.870360042	-2.695151870	-3.118146122
	C42	-2.169735789	-4.060776349	-3.272033000
	C43	-1.406760078	-4.267176080	-4.579882767
	C44	-5.349148009	1.040585137	-3.779492750
	C45	-6.750737529	1.251652590	-3.191501444
	C46	-5.085729433	1.900847094	-5.023208746
	C47	-9.047712329	0.413244855	-3.032639162
	C48	-9.136317934	0.217170724	-1.514309633
	C49	-8.011068671	-0.509731862	0.541507574
	C50	-7.072445961	0.444454729	1.278527100
	C51	-5.526914862	2.336256643	1.182821303
	C52	-6.320426011	3.466065773	1.880455267
	C53	-4.597960346	3.031951420	0.179554781
	C54	-3.645551413	2.155579724	-0.563243089
	C55	-3.159971811	0.887410454	-0.357452346
	C56	-2.162277192	1.708137236	-2.174566356
	C57	-8.258407172	4.968018749	1.637371029
	C58	-8.727850727	4.825316009	3.084157599
	C59	-9.473250767	5.051290718	0.685290378
	C60	-10.157170263	6.383554676	0.587725487
	C61	-10.447311518	7.333304783	1.548170661
	C62	-11.171022377	7.998265461	-0.438327716
	C63	7.285569138	1.279450699	6.699784783
	C64	8.419432344	0.269672741	6.707387366
	C65	6.102543979	0.623750181	5.943859096
	C66	4.877977015	1.505447433	5.893526534



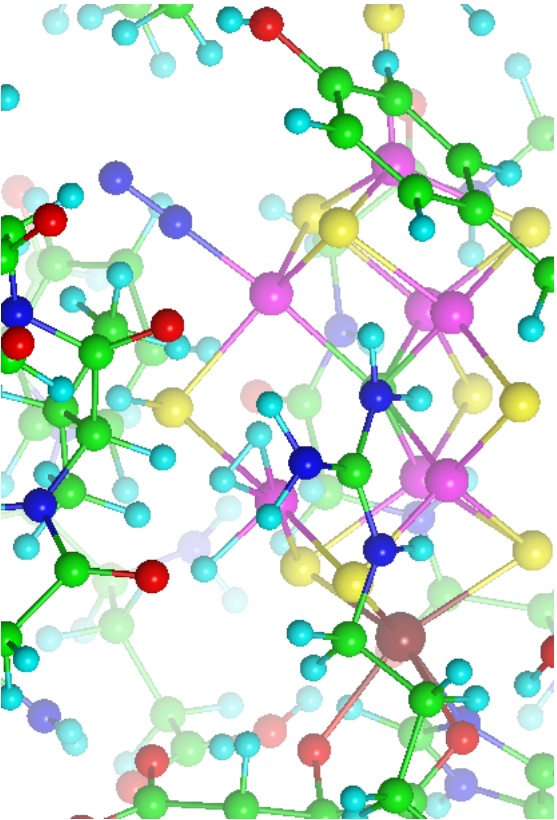
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C68	4.682141654	2.406746365	4.830639712
C69	2.757827578	2.265601452	6.851143737
C70	3.560881868	3.235046483	4.777335801
C71	2.592343750	3.153423600	5.780718506
C72	4.720881272	7.172908058	1.711513969
C73	3.700978386	8.249773504	1.306893888
C74	4.090755760	5.783677356	1.616688590
C75	3.148109930	10.046125384	-0.288805327
C76	1.840196203	9.641872324	-0.972320174
C77	0.496976515	7.724109887	-1.807791410
C78	-0.386811876	7.109923929	-0.690465873
C79	0.943139309	6.658291554	-2.839166535
C80	-0.118659897	5.769985548	-3.500310190
C81	-0.959039525	6.409683393	-4.619231840
C82	-2.742782526	8.143797586	-4.370139919
C83	-0.537491711	5.846631316	1.401559025
C84	-1.100732410	6.899625528	2.365929472
C85	0.260260374	4.829690703	2.246794254
C86	-0.490515913	8.837902757	3.722438430
C87	-1.168746820	10.162394522	3.418768242
C88	-2.149483072	11.584591595	1.711623437
C89	-3.623883692	11.954368881	2.014945944
C90	-1.826001558	11.866073372	0.241784911
C91	-2.635210616	11.023550171	-0.733561918
C92	-5.865894920	11.143607137	2.603578521
C93	-6.246504506	12.020951731	3.786492527
C94	-6.544817375	9.749260916	2.732108432
C95	-6.319184030	8.879116650	1.515963896
C96	-7.198983360	8.941461643	0.422801385
C97	-5.208969809	8.022266190	1.422119398
C98	-6.972171828	8.190773915	-0.732584583
C99	-4.948482967	7.287224925	0.262235225
C100	-5.834715447	7.386122088	-0.806275584
C101	7.132435258	-2.012317680	-7.469946487
C102	5.618556301	-1.925211563	-7.529395586
C103	3.634240487	-0.763884817	-6.588393709
C104	3.194067749	0.644017050	-7.006754200
C105	3.304521224	3.028575700	-6.441676868
C106	4.345016454	4.063164649	-6.022091573
C107	6.244009689	4.700891296	-4.632959588
C108	7.332080224	5.070528368	-5.624058433
C109	0.714432354	-1.866174108	-9.895489744
C110	-0.477383470	-0.912374686	-9.752184055
C111	0.815991544	-2.767900414	-8.643994966
C112	1.727281564	-3.982107006	-8.906269812
C113	2.049964037	-4.690982950	-7.610906899
C114	-1.322094675	1.220895813	-8.911875130
C115	-0.804815383	2.629434409	-9.133950326
C116	-2.155284319	1.036687815	-7.618822666
C117	-1.267346929	0.914918941	-6.411048700
C118	-0.757944615	2.058422993	-5.773753620
C119	-0.806292794	-0.349595764	-6.005279286
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C124	10.376468910	-5.116545896	-1.412593377
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C131	1.274881577	-6.771190160	-1.078055596
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C133	3.865144348	-6.677935505	-1.169314788
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C137	5.074778518	-6.427608534	-0.255226224
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Fe139	4.774048327	-1.142883526	-2.421780176
Fe140	2.434872060	0.890877267	-0.559732101
Fe141	4.854994998	0.863347987	0.623885108
Fe142	4.720563580	1.342026110	-1.931485749
Fe143	3.787468845	3.126346829	-0.134590970
Fe144	5.109362797	-1.605053589	0.077332064
Fe145	2.710020924	-1.966543037	-0.914864295
H146	-5.494320664	-7.786493980	-3.195131086
H147	-5.410717041	-6.572908116	-4.283603115
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H149	-7.810195402	-6.361902099	-4.337334463
H150	-7.911645225	-7.703886767	-3.201684981
H151	-7.742697325	-3.401591445	-1.262927877
H152	-8.908226683	-6.522878778	-0.048305382
H153	-9.482663067	-3.734279073	-1.092443317
H154	-8.648936596	-7.496092680	2.039607614
H155	-6.204993599	-6.638057679	0.449805177
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H157	-3.305992375	-2.464062434	1.540454379
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H159	-3.909388517	-6.840638469	0.827093850
H160	-6.339586496	-1.329029150	4.959478465
H161	-6.587732239	-3.286288013	2.829536103
H162	-4.202642845	-7.134422023	2.559119318
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H166	-0.929732191	-3.740908519	2.152542262
H167	-0.893628262	-2.391653146	1.003290009
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H175	-0.125222039	0.239180355	3.714173484
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H238	-9.535846255	1.372773872	-3.250238620
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H251	-5.769765078	1.609164389	-5.833972518
H252	-0.745507048	11.757915369	0.075062011
H253	-2.093443577	12.918147071	0.058153544
H254	-0.885650114	10.391574013	-1.644313022
H255	-2.401497368	9.731530333	-2.261388912
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H261	1.654929172	5.989671358	-2.328015040
H262	2.476837441	7.703729742	-1.013835514
H263	-0.783764486	5.321653671	-2.745052238
H264	-7.439089392	-0.371735525	-4.219870428
H265	3.722746090	10.658355980	-0.996491442
H266	-4.707736753	-0.672075578	-5.020152149
H267	1.519426028	7.179518947	-3.621266594
H268	-4.044616575	6.678634694	0.187944068
H269	2.866051932	10.686309577	0.559839772
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H288	8.639338475	-2.788454225	-8.602756755
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H291	4.390541863	7.460598513	3.706075371
H292	4.844865092	8.746869397	-0.330501131
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	O478	7.912397478	-8.197448567	1.110434665
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	C22	-2.935864253	-2.316450278	6.217271113
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	C46	-4.401117495	-0.087826768	-5.985804828
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	C48	-7.380048355	-4.249924571	-3.666105921
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	C50	-6.254524873	-3.523400073	-0.450520412
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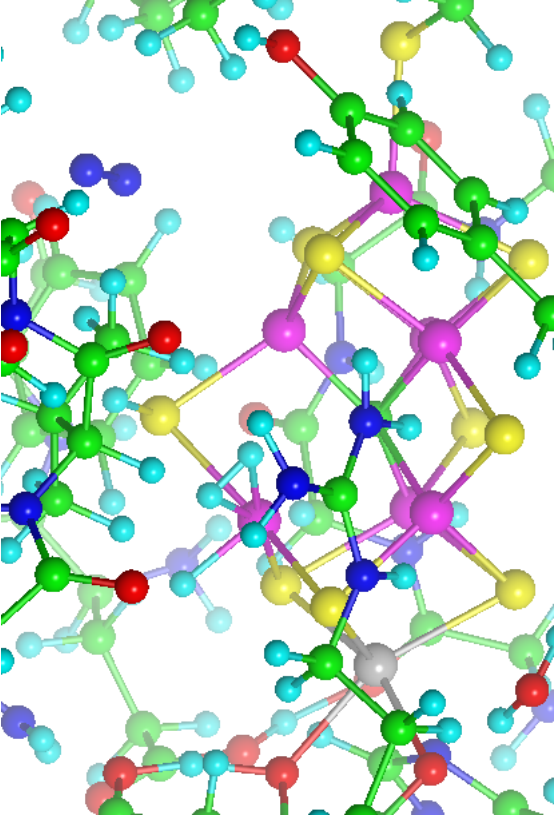
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C73	-1.702066194	8.534486611	2.754833616
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C76	-3.626196320	9.178334089	0.205694957
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C85	-2.789013951	3.706160713	2.546673341
C86	-5.872354128	6.360501107	4.116587033
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C89	-9.865116772	7.708163454	1.938469090
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C91	-8.079109220	7.969316714	-0.540572269
C92	-11.359372128	5.756310995	1.918586181
C93	-12.338666537	6.057257238	3.043992686
C94	-11.168466740	4.218934628	1.780979130
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C96	-10.887509450	3.658162126	-0.671417465
C97	-8.915814979	3.713689036	0.705931340
C98	-10.104987254	3.371555775	-1.792467190
C99	-8.112422298	3.456089941	-0.409254118
C100	-8.718799817	3.293055614	-1.651277845
C101	8.181520128	3.447020693	-5.621749800
C102	6.899675133	2.744841923	-6.031558885
C103	4.479308926	2.512684201	-5.524620238
C104	3.419864676	3.538871571	-5.948596609
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C106	2.343911517	6.802250897	-4.471808542
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C108	4.169832153	9.094838503	-3.281732911
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C112	5.063781516	-0.689762138	-8.483321027
C113	5.488069611	-1.385193962	-7.210070276
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C117	-0.508082390	1.357127838	-6.460358864
C118	-0.836685236	2.450963058	-5.642952612
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C124	11.538136883	1.393170151	0.761845539
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C126	9.311835373	0.149231400	-2.188690413
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N394	-6.088076937	-2.257108726	-0.944447884
N395	-3.629074328	1.004927390	-2.144807543

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N397	-8.449904280	-0.953893536	-0.302944380
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N404	-4.960176035	5.422491350	-4.050414989
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N418	12.016064665	1.578191882	-1.687434505
N419	7.937962107	-0.089079011	-2.238785714
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N422	-1.563657606	1.834634390	0.221655426
N423	-0.441099701	1.960575561	0.164256635
O424	-1.742741976	-7.726828799	-3.472047105
O425	-4.486063556	-7.481317879	-0.994510415
O426	-2.447311783	-9.339940752	1.443723798
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O434	-2.260858552	-5.312486635	10.753557651
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O436	8.590863368	-4.916796832	7.552662772
O437	9.543131857	-0.452725242	9.312473790
O438	-3.419737537	-3.350809230	-3.309248773
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O440	-6.489258179	-1.315430598	-3.817029097
O441	-5.342674787	0.933128350	-5.600968802
O442	-8.509653816	-4.615487073	-3.316107975
O443	-6.303674761	-3.761729587	0.761057618
O444	-7.526389442	-0.159059427	1.630805912
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O450	-5.202746084	5.365077433	-0.564745301
O451	-5.942705424	3.866934304	2.797214861
O452	-2.625913891	4.483849624	3.736647799
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O454	-10.794300466	8.509488830	1.765653778
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O457	-7.894065920	3.082957052	-2.776818466
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O460	1.713964062	7.807548105	-4.838093812
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O463	5.182989720	-2.541314944	-6.939204412
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O471	10.119087400	-5.043232562	-3.384839059
O472	7.766782382	-1.366971968	0.526691475
O473	8.319634375	-3.380320291	1.353952146
O474	6.365558587	-2.317841134	-1.453155504
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O476	7.774043755	-0.367473100	3.206637330
O477	-5.393227806	2.650252402	-3.466365796

	O478	12.853520824	-2.924591282	0.172688485
	O479	10.797874080	-2.939881017	2.390996905
	S480	-0.087525432	6.295871035	1.155302268
	S481	1.214618670	4.021056414	-1.156988447
	S482	4.540380426	0.061463403	-2.235844785
	S483	1.295971048	2.796522767	2.283506779
	S484	1.444024023	0.259774044	-1.302761298
	S485	4.917813157	3.985681477	-2.257227207
	S486	4.937366497	-0.920834772	1.240729448
	S487	3.649652295	5.263810811	1.169339391
	S488	6.869010597	1.843529302	0.008802464
	S489	4.970956902	2.255273806	3.190326776
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Fe6-H2n 2N2 dissociated 35, S=1				
Fe (139) -2.601				
Fe (140) -1.032				
Fe (141) -2.385				
Fe (142) 2.667				
Fe (143) 2.789				
Fe (144) 2.207				
Fe (145) 0.145				
				
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	C1	-2.346952370	-8.224161588	-4.403693820
	C2	-1.626776162	-8.819914642	-5.619215811
	C3	-4.527084179	-7.719291911	-3.390554097
	C4	-4.307060621	-8.242767412	-1.975109795
	C5	-3.606635278	-10.102191925	-0.551839448
	C6	-2.459654435	-9.412967763	0.192413667
	C7	-0.396482549	-8.118492132	0.050479158
	C8	-0.884195587	-6.779013666	0.604866374
	C9	-2.379279714	-4.866623971	0.302357770
	C10	-3.179793213	-5.019776401	1.603963284
	C11	-4.774098326	-6.324696341	2.880774353
	C12	-3.970546975	-6.767076710	4.110445295
	C13	-2.377012976	-8.386242448	5.024146500
	C14	-1.053139727	-7.753609849	5.470574190
	C15	1.032641570	-6.666048061	4.754234579
	C16	1.153515981	-5.140859870	4.827838311
	C17	0.210318268	-2.963450968	4.048404207
	C18	-0.661099355	-2.409827578	5.200542806
	C19	-0.245752242	-2.482812783	2.658009474
	C20	-0.379174574	-0.958084147	2.629682111
	C21	0.723280324	-2.996027348	1.587905511
	C22	-2.923884435	-2.310946196	6.196765401
	C23	-2.915427459	-3.171303011	7.476273846
	C24	-4.341177986	-2.182355984	5.583615611
	C25	-5.375995893	-1.808886619	6.651887181
	C26	-4.352624040	-1.153209986	4.446370359
	C27	-3.189318253	-5.348308122	8.513997412
	C28	-2.097135958	-5.104813021	9.534978761
	C29	10.407682612	-7.752866441	4.122866441
	C30	10.147212721	-6.247089651	4.199097171
	C31	8.584987219	-4.552099575	5.152122444
	C32	8.915239118	-4.163596593	6.605985424
	C33	7.073974839	-4.454219572	4.878260079
	C34	6.504396609	-3.052686406	5.111457068
	C35	5.076667779	-2.933151441	4.577255376
	C36	3.450329325	-1.107385251	5.206703965
	C37	9.929032447	-2.465751706	8.055482928
	C38	9.126226276	-1.257094615	8.485353480
	C39	-1.503160425	-3.693305394	-4.818760282
	C40	-2.828886906	-3.038197632	-4.385255907
	C41	-0.366808601	-3.135936114	-3.933836993
	C42	0.974431908	-3.894125377	-4.012890433
	C43	1.945366662	-3.392824821	-5.081166429
	C44	-4.335686742	-1.160656161	-4.923645755
	C45	-5.696825911	-1.811314398	-4.646105927
	C46	-4.410098557	-0.085224992	-6.016665364
	C47	-7.188698156	-3.704937347	-5.088351895
	C48	-7.385339282	-4.240824925	-3.665865091
	C49	-6.376390543	-4.663478321	-1.468324735
	C50	-6.246054237	-3.523350600	-0.460815086
	C51	-6.014433718	-1.129016774	-0.041525724
	C52	-7.387814028	-0.712268230	0.536186042
	C53	-5.452931903	0.120000750	-0.735034849
	C54	-4.083049231	0.004337689	-1.317149494
	C55	-3.045682312	-0.879477167	-1.144979621
	C56	-2.361105920	0.700725966	-2.559394615
	C57	-9.773732860	-0.435758911	-0.026053314
	C58	-10.307072242	-1.067004086	1.259077489
	C59	-10.666122570	-0.809686966	-1.233362034
	C60	-11.939044772	-0.032022335	-1.398537048
	C61	-12.844703654	0.437099288	-0.466867701
	C62	-13.500000847	0.968546696	-2.515249355
	C63	4.189331964	3.561703872	8.325067472
	C64	5.676158551	3.324617133	8.512408978
	C65	3.706279768	2.553913004	7.248993171
	C66	2.226313716	2.659035047	6.967142690
	C67	1.287997721	1.923987436	7.714762073

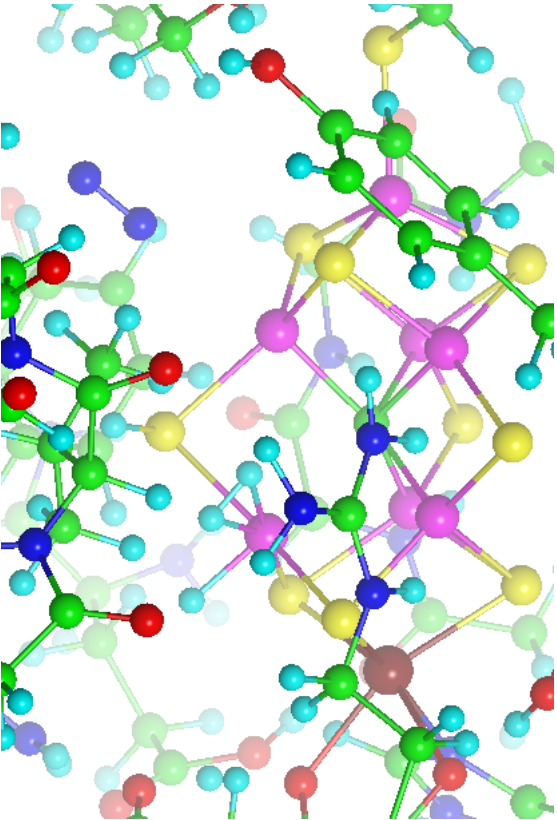
C68	1.742058465	3.496546695	5.945782322
C69	-0.083411190	2.011658298	7.450021512
C70	0.376677724	3.606058484	5.680599979
C71	-0.534730491	2.857198939	6.430275949
C72	-0.339693912	8.105183992	3.289738491
C73	-1.711329039	8.550787278	2.753525411
C74	-0.089362782	6.632136779	2.970810117
C75	-2.911511019	10.058899143	1.211986402
C76	-3.636401693	9.184477351	0.185666817
C77	-3.541819999	7.029760639	-1.063005473
C78	-4.102478618	5.845933871	-0.231679675
C79	-2.417498619	6.585070233	-2.029447548
C80	-2.679045991	5.425518534	-2.997552387
C81	-3.536460740	5.732381531	-4.235980994
C82	-5.986925660	6.216216101	-4.325548216
C83	-3.853753218	4.330951663	1.672091202
C84	-5.060734260	4.703735298	2.542136068
C85	-2.764653059	3.764447008	2.611065986
C86	-5.884934371	6.355169909	4.145676551
C87	-7.103834053	7.188690293	3.786869566
C88	-8.387902223	8.216041591	1.994757523
C89	-9.851105676	7.708514870	1.946728521
C90	-8.009504983	8.898547107	0.678799949
C91	-8.066982855	7.978978195	-0.532212210
C92	-11.343546344	5.756649237	1.918309083
C93	-12.326267057	6.061123015	3.040103974
C94	-11.158097109	4.219144672	1.781579709
C95	-10.297675248	3.844975910	0.595302061
C96	-10.871228453	3.665735938	-0.672068464
C97	-8.904873546	3.710816475	0.712945619
C98	-10.084542084	3.381600970	-1.791320728
C99	-8.096899017	3.456720439	-0.399391116
C100	-8.698684166	3.300608479	-1.644015955
C101	8.202586749	3.442397115	-5.637761055
C102	6.912534786	2.743013154	-6.030386837
C103	4.495640768	2.513758635	-5.499438001
C104	3.439780186	3.541563505	-5.925994314
C105	2.129705390	5.483615750	-5.193079803
C106	2.367993981	6.808821737	-4.473159830
C107	3.358533020	8.050167614	-2.626560390
C108	4.147993041	9.138186893	-3.329241879
C109	3.247175480	0.742002500	-9.551990362
C110	1.723292625	0.885798782	-9.641463581
C111	3.613131633	-0.198050594	-8.380707927
C112	5.071409289	-0.681719903	-8.482172375
C113	5.484792834	-1.382853998	-7.208183781
C114	-0.282177602	2.053785420	-8.870239953
C115	-0.602405457	3.535662515	-8.872707554
C116	-1.082327720	1.220018410	-7.841053704
C117	-0.496280972	1.353971241	-6.463649809
C118	-0.823021129	2.448735606	-5.646747265
C119	0.502321834	0.459750151	-6.039021586
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C121	1.214531207	0.694714738	-4.859428270
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C123	10.966993256	1.403785448	-0.675165459
C124	11.541066339	1.387652967	0.751552463
C125	10.084999869	0.170042543	-0.918242761
C126	9.286722855	0.151932658	-2.183486889
C127	9.762362668	0.177167717	-3.478149265
C128	7.592128616	-0.253456536	-3.511259052
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C130	13.617003648	1.302019847	2.845142604
C131	4.926374807	-4.809051413	-1.184891610
C132	5.911492159	-4.316505336	-0.128173840
C133	6.999764740	-3.341748812	-0.670759056
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C136	10.447086223	-4.236085473	-2.460360784
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Fe139	5.029324837	2.048655785	-1.223534892
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Fe141	3.311983468	3.071336226	1.835386381
Fe142	3.442188216	3.947244125	-0.598039807
Fe143	1.334261781	4.537600038	0.977723779
Fe144	5.044646824	1.281496439	1.212668702
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H147	-0.132563520	-7.453441301	-5.904952740
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H154	-3.349691237	-11.160385541	-0.694699121
H155	-1.556011160	-8.865639462	-1.583358354
H156	-4.486372582	-10.049653562	0.104122364
H157	-1.605953589	-4.111205139	0.488907047
H158	-2.081659523	-6.504100372	-1.046701563
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H160	-5.287635601	-5.393676699	3.150929740
H161	-4.074434657	-6.730337072	0.881905816
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H163	-3.038948792	-4.501468118	-0.497652241
H164	-2.968450329	-8.176824288	2.978254250
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H167	0.430515218	-2.638139833	0.588476511
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H173	-5.467881327	-2.574850040	7.434463931
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H176	3.688390161	3.303316893	9.277789234
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H184	-0.788585791	-0.629081800	1.662344163
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H186	-3.062664612	2.734902656	2.863320156
H187	-2.430242667	3.943440494	4.540629010
H188	-2.408870265	2.423394823	6.705318883
H189	0.019336647	4.242948644	4.871595229
H190	2.448608153	4.051759219	5.325483225
H191	1.629427132	1.254168727	8.508488369
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H193	1.733107227	-7.008544048	3.977220749
H194	1.377476214	-7.057764447	5.718520471
H195	-0.607603610	-7.221748910	3.514908202
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H197	-0.795053781	1.409101734	8.021193683
H198	1.227476179	-2.605751029	4.240928263
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	C23	-2.918520654	-3.165466792	7.497880930
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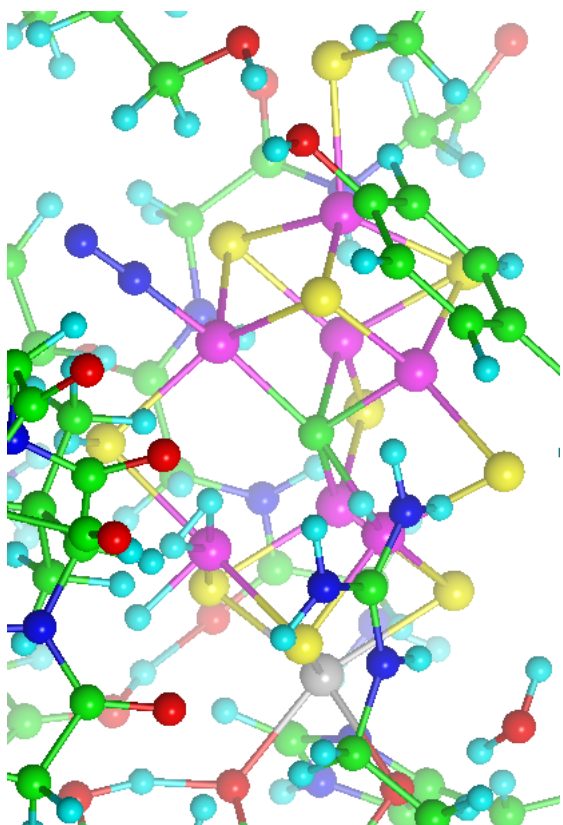
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H173	-5.444657092	-2.540633871	7.482312603
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H181	-4.630176456	-3.169806148	5.194653249
H182	-2.588595119	-1.317546849	6.543053859
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H184	-1.321430901	-0.755617723	1.922040110
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H325	6.370467534	-5.168821099	0.330673204
H326	5.886373208	3.770196474	-4.580283167
H327	8.346849638	-5.015666016	-0.909869458
H328	8.776590970	-0.147598013	-5.324955079
H329	6.664762755	-0.433905410	-3.956105062
H330	11.486364899	-7.908346492	4.208351716
H331	3.651152637	0.774780810	4.357025826
H332	9.307092422	-0.885769725	4.137373181
H333	7.517673845	0.558012154	3.094077509
H334	9.755056159	-2.404627877	5.916939859
H335	2.832331546	-2.899619772	5.973451987
H336	9.134286545	-2.566687368	-2.575378218
H337	9.773586403	-2.885077526	-0.957763072
H338	7.605456609	-4.501250235	-2.435087204
H339	4.189818491	2.023622340	-4.583538657
H340	-1.624418961	3.130510723	-5.948388475
H341	-2.142265658	1.580873394	-7.868438362
H342	5.326081086	-3.758891338	0.598075750
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H344	10.877738796	-3.833087481	2.825102919
H345	1.766062287	-1.602862800	6.179794687
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H347	9.429182873	0.007767164	-0.084938480
H348	4.550349160	1.758066599	-6.316626638
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H351	4.257635809	2.708698834	6.339093863
H352	12.517385351	2.465657126	-1.482306154
H353	12.703561796	0.844889827	-1.601531686
H354	13.185842266	-0.766617735	2.664979452
H355	12.153746285	-0.610675738	0.638641380
H356	14.165762320	1.686381503	1.957099805
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H368	2.487627375	-0.147140586	1.029886759
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N382	-3.071443246	-4.506458226	7.357362146
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N388	9.531857396	-2.981721989	6.757420596
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N393	-6.280880934	-4.301971884	-2.854462001
N394	-6.073554275	-2.265274220	-0.938320044
N395	-3.631546844	0.999780061	-2.145835351

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N397	-8.439451099	-0.948135546	-0.317278471
N398	-12.346725391	0.307939637	-2.708104169
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N405	-5.856280814	7.408524964	-4.905989135
N406	-7.236317045	5.835041112	-3.922249473
N407	-3.375449459	5.425072958	0.811619964
N408	-5.034678142	5.986341606	2.993977504
N409	-7.411829863	7.255071772	2.426893588
N410	-7.016950328	8.065159765	-1.394544524
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N417	1.139446324	1.830880750	-8.836053513
N418	12.011790819	1.597029709	-1.676482178
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N421	12.126479299	0.243484034	1.199923904
N422	-2.174071584	1.865152758	0.325500531
N423	-1.074531678	1.960675575	0.206179863
O424	-1.733309097	-7.706069743	-3.485457197
O425	-4.469279531	-7.462388384	-0.989313780
O426	-2.440362533	-9.328728261	1.452510883
O427	-0.505765669	-6.279480958	1.722614677
O428	-3.143526635	-4.123486870	2.513827401
O429	-4.202020973	-6.246610111	5.242950745
O430	-0.717272827	-7.843380495	6.663886415
O431	2.095024988	-4.652547407	5.484581689
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O433	-2.793912510	-2.635501910	8.614276832
O434	-2.271439182	-5.300082698	10.756650979
O435	10.885978728	-5.478679755	3.584113305
O436	8.569647613	-4.911692143	7.556417230
O437	9.557696202	-0.464397074	9.326449079
O438	-3.413513899	-3.349879037	-3.291420447
O439	1.518237814	-3.012766468	-6.205567362
O440	-6.498386520	-1.329965334	-3.818206908
O441	-5.352509400	0.923454837	-5.588391305
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O443	-6.303152559	-3.767547460	0.766498992
O444	-7.531828383	-0.195318049	1.640768941
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O446	6.123208905	2.598409784	9.421908772
O447	-1.889835216	2.992526768	6.121375176
O448	-2.769422356	8.060603734	3.170059466
O449	-4.763497122	9.493348281	-0.166823101
O450	-5.199740881	5.368803304	-0.567083341
O451	-5.943794506	3.885259273	2.809217795
O452	-2.627092991	4.474036032	3.734746721
O453	-7.738162794	7.791947164	4.631612726
O454	-10.793793917	8.503985843	1.752296021
O455	-9.031056276	7.193167120	-0.753370358
O456	-13.541386041	5.943852261	2.918909112
O457	-7.894057926	3.078911106	-2.786808041
O458	6.914840820	1.845764589	-6.909580946
O459	2.923467802	3.547845645	-7.092513775
O460	1.692660021	7.798252898	-4.831886493
O461	4.287324823	10.222648038	-2.860512704
O462	1.024993052	0.134747342	-10.357168959
O463	5.189162472	-2.542697929	-6.931807936
O464	6.209781985	-0.648859788	-6.337008035
O465	-1.646331931	4.026107896	-8.450254303
O466	11.517795851	2.405517807	1.493424748
O467	13.866115070	1.703801449	3.974899643
O468	4.670340068	-3.889520587	-2.187869818
O469	4.349143129	-5.851710537	-1.137870862
O470	11.664066956	-4.069887693	-2.044483154
O471	10.131532981	-5.067209174	-3.374326082
O472	7.775489396	-1.372337860	0.511516738
O473	8.321249531	-3.384780652	1.346330860
O474	6.388530016	-2.325710455	-1.479789976
O475	10.108395705	-1.319458613	4.521727428
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O477	-5.388233309	2.646091200	-3.457934149

	O478	12.852155492	-2.931887779	0.170882615
	O479	10.795641090	-2.947715144	2.389219419
	S480	-0.070160094	6.322086126	1.152446368
	S481	1.205769793	3.991228279	-1.155872952
	S482	4.548773351	0.071654584	-2.268835462
	S483	1.289311478	2.809517592	2.271052148
	S484	1.401982164	0.310477018	-1.271276127
	S485	4.944473857	3.974451352	-2.277978648
	S486	4.933393241	-0.946684483	1.199125499
	S487	3.691544735	5.257681398	1.171723921
	S488	6.872254688	1.826287415	0.001368407
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pre-capture 2N2 associated 35, S=1/2			precapt2n2x1dte.car_4	
Fe(139) -2.391	C1	-7.585002415	-5.411784938	-1.926072816
Fe(140) -0.981	C2	-7.645401031	-6.309327111	-3.165938612
Fe(141) -2.566	C3	-8.800293620	-3.800016407	-0.530397341
Fe(142) 2.698	C4	-8.504437054	-4.349314519	0.860914836
Fe(143) 2.755	C5	-8.473129632	-6.289817320	2.348856879
Fe(144) 1.259	C6	-6.982395741	-6.376390733	2.688516305
Fe(145) 0.122	C7	-4.679286595	-6.391071255	1.880653513
	C8	-4.236267223	-4.994940154	2.333948745
	C9	-4.607000001	-2.583281401	2.057648312
	C10	-5.007912156	-2.309189632	3.515292398
	C11	-6.612659643	-2.611665413	5.297015959
	C12	-5.826709308	-3.384385135	6.366424131
	C13	-5.050502135	-5.587788570	7.121114384
	C14	-3.538038622	-5.854629205	7.123232227
	C15	-1.511239304	-6.194969461	5.764127420
	C16	-0.685666059	-4.934839755	5.498976034
	C17	-0.763944991	-2.539505201	4.938926295
	C18	-0.939934451	-1.573336607	6.127265484
	C19	-1.155796611	-1.955426012	3.555711867
	C20	-0.616161892	-0.538113956	3.335552375
	C21	-0.690564562	-2.891008770	2.433785029
	C22	-2.419454580	-0.100100940	7.414764690
	C23	-2.437425721	-0.734998482	8.818682275
	C24	-3.687257479	0.733696239	7.108550581
	C25	-4.039335726	1.663041809	8.275751396
	C26	-3.495663422	1.544281923	5.818960080
	C27	-3.295570411	-2.455982938	10.297385403
	C28	-1.939916605	-2.758867994	10.907405571
	C29	5.163163666	-12.244316458	2.635376877
	C30	5.858191315	-10.889328917	2.549710286
	C31	5.911899984	-8.636398927	3.609075276
	C32	6.853785125	-8.449848522	4.813998441
	C33	4.671559099	-7.733507105	3.724490112
	C34	5.034271058	-6.251375409	3.750617482
	C35	3.810509244	-5.349127257	3.603440016
	C36	3.849319269	-2.885776787	4.109525233
	C37	9.001942957	-7.529340047	5.556561746
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	C39	-4.638253877	-2.186078614	-3.456339744
	C40	-5.168312265	-0.875284906	-2.845660681
	C41	-3.164981482	-2.362148411	-3.017437925
	C42	-2.544529177	-3.750768799	-3.271998864
	C43	-1.894930496	-3.940158671	-4.642662237
	C44	-5.474144962	1.519286721	-3.354576367
	C45	-6.792535654	1.782248396	-2.613985202
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	C47	-9.127965398	1.109622600	-2.294491227
	C48	-9.125119516	0.802556567	-0.793751534
	C49	-7.889364743	-0.111374845	1.115908868
	C50	-6.841251629	0.748596958	1.824348789
	C51	-5.201680157	2.560080974	1.712205602
	C52	-5.853551464	3.695036576	2.538153790
	C53	-4.303025431	3.265064169	0.685624835
	C54	-3.459086314	2.395376120	-0.183148352
	C55	-3.091615527	1.073963967	-0.140738087
	C56	-2.144407692	1.981673294	-1.943621519
	C57	-7.686510110	5.343422431	2.544205405
	C58	-7.971762424	5.201838787	4.036246801
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	C60	-9.618392054	6.885430470	1.754404780
	C61	-9.796386024	7.802453117	2.772412053
	C62	-10.625868179	8.587565536	0.873559198
	C63	7.988100576	0.737426305	5.977329492
	C64	9.072646574	-0.311889603	5.826326294
	C65	6.718647117	0.162522344	5.296000261
	C66	5.522352636	1.077838198	5.399647806
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C71	3.296237165	2.798936035	5.582250861
C72	5.278741850	6.907860046	1.523523508
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C74	4.594769981	5.544272914	1.412270773
C75	3.662775130	9.943059879	-0.177613342
C76	2.289563255	9.638180600	-0.783247514
C77	0.785575763	7.807635937	-1.559938460
C78	-0.021934297	7.158637831	-0.407135108
C79	1.109600691	6.798760911	-2.687451547
C80	-0.024213448	5.979271769	-3.315114878
C81	-0.935235445	6.707108806	-4.316687860
C82	-2.599182309	8.507156060	-3.858190948
C83	-0.047423560	5.766095572	1.602920538
C84	-0.491657888	6.765680623	2.681271157
C85	0.777068576	4.664359636	2.298336347
C86	0.271721793	8.607850029	4.099449000
C87	-0.327611042	9.994697345	3.928240025
C88	-1.320978264	11.597308920	2.385160102
C89	-2.749124906	12.025305021	2.806745510
C90	-1.068326826	11.938914696	0.913877311
C91	-2.010357616	11.236575783	-0.056837662
C92	-4.975395221	11.285857469	3.527021105
C93	-5.212686421	12.139456020	4.766508523
C94	-5.703706032	9.920368631	3.672641829
C95	-5.628365061	9.097389760	2.405492979
C96	-6.579803509	9.271444259	1.389335887
C97	-4.583181720	8.184970314	2.184196532
C98	-6.476796467	8.585472107	0.177693248
C99	-4.444048644	7.514810435	0.964143829
C100	-5.395906883	7.726502652	-0.028009418
C101	6.443593110	-2.053077570	-8.222367613
C102	4.937428096	-1.891055809	-8.105127864
C103	3.128955284	-0.655429365	-6.933956969
C104	2.732806923	0.789345637	-7.263714979
C105	3.039276753	3.141408968	-6.625655174
C106	4.188367887	4.093332930	-6.306505512
C107	6.248256398	4.588167269	-5.117477516
C108	7.120055824	5.076958570	-6.258710019
C109	-0.130083791	-1.420868868	-10.082611714
C110	-1.244534397	-0.399839487	-9.826277319
C111	0.017921859	-2.363477051	-8.865650251
C112	0.841911684	-3.611645292	-9.231280291
C113	1.192062073	-4.408066482	-7.993838703
C114	-1.889792671	1.734674236	-8.824096892
C115	-1.292707517	3.111079763	-9.039473546
C116	-2.652644406	1.565734696	-7.486340910
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C118	-1.090267822	2.456786266	-5.708543252
C119	-1.260681063	0.063435050	-6.025032643
C120	-0.024560250	2.258257014	-4.824287899
C121	-0.194780389	-0.134055331	-5.144115173
C122	0.449165711	0.968261599	-4.572405895
C123	9.117813128	-5.226605731	-3.737497367
C124	10.013273336	-5.530096094	-2.523988549
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C126	6.640070162	-5.260370052	-4.455533888
C127	6.608874612	-5.572241795	-5.799448006
C128	4.692190874	-4.623454936	-5.225586623
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C131	0.894257311	-6.724204895	-1.432523979
C132	2.259317310	-6.866217561	-0.764936276
C133	3.467158742	-6.730182023	-1.737921369
C134	3.582771042	-8.007516426	-2.612577172
C135	4.876640875	-8.137497272	-3.420882835
C136	5.053777257	-9.513935667	-4.098935137
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C138	4.055110454	-0.271899655	-1.296029679
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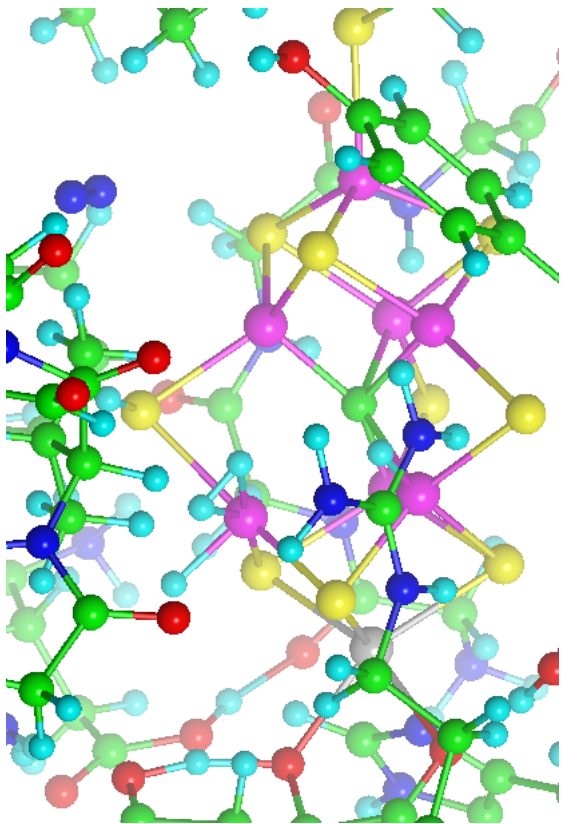
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O445	-5.272576278	4.214032654	3.494971472
O446	-7.981135541	6.132943754	4.823439481
O447	9.344505984	-1.149662981	6.674340026
O448	2.212155812	3.655437294	5.607522764
O449	3.331679056	8.280729923	2.056772407
O450	1.478473386	10.568428067	-0.957323116
O451	-1.247373402	7.344338154	-0.333220477
O452	-1.520372168	6.572682858	3.342360385
O453	1.734776001	5.218814463	3.202826642
O454	-0.260303025	10.831510125	4.836852823
O455	-3.091424233	13.213667101	2.731148079
O456	-3.227904568	11.145171811	0.158334558
O457	-6.264294008	12.721772145	4.977370137
O458	-5.221302003	7.086839338	-1.273550049
O459	4.159307557	-2.650401419	-8.731869790
O460	1.982524835	1.066339819	-8.221939437
O461	4.119205174	5.267561755	-6.705736238
O462	7.795432406	6.091041065	-6.197015318
O463	-2.400851443	-0.585227723	-10.240454711
O464	0.405022784	-5.162560259	-7.431045565
O465	2.424794299	-4.216799598	-7.481792458
O466	-1.706573961	4.133785188	-8.511171659
O467	10.767667849	-4.664365666	-2.039849374
O468	13.033781086	-6.578987801	-0.131939918
O469	0.855644803	-5.868256883	-2.460203459
O470	-0.111640200	-7.306055348	-1.027660229
O471	6.218386604	-10.044400807	-4.048825694
O472	4.046252723	-10.008809124	-4.678805955
O473	5.502014813	-5.541976591	-1.169389062
O474	5.097872157	-7.485827176	-0.120434916
O475	3.268256748	-5.551932374	-2.521605874
O476	8.617597166	-6.780591167	1.961078004
O477	6.819673085	-4.663903995	1.225952262

	O478	-3.769587781	5.251579394	-2.474069616
	O479	8.500588172	-9.794289135	-2.520051442
	O480	7.611375204	-8.545151501	0.081789557
	S481	3.831923948	5.249440714	-0.251949144
	S482	2.815132181	2.583414705	-2.322344972
	S483	2.945658717	-2.525723082	-3.338742330
	S484	3.535891657	1.614021050	1.133712627
	S485	0.935938181	-0.573472943	-1.769152033
	S486	5.397091312	0.308575291	-4.291222144
	S487	3.703727333	-3.532387693	0.059165443
	S488	6.213545381	2.289819518	-1.159877052
	S489	6.410278971	-2.475830063	-2.001292384
	S490	6.465491272	-0.844338385	1.043332584
	end			
pre-capture 2N2 dissociated 35, S=1/2			precapt2n2x1 dtg.car_3	
Fe(139) -2.580	C1	-7.556622263	-5.397754873	-1.924134747
Fe(140) -0.669	C2	-7.615532984	-6.298475917	-3.162587880
Fe(141) -2.360	C3	-8.791644655	-3.798686301	-0.528596197
Fe(142) 2.720	C4	-8.502854632	-4.351624322	0.863470478
Fe(143) 2.796	C5	-8.473336978	-6.296141213	2.346305718
Fe(144) 0.860	C6	-6.983236442	-6.382987898	2.688573653
Fe(145) 0.094	C7	-4.679184941	-6.394341041	1.881942688
	C8	-4.236664507	-4.997512785	2.332918761
	C9	-4.609471319	-2.587073173	2.063983794
	C10	-5.007228413	-2.318396186	3.523047183
	C11	-6.616427062	-2.619754888	5.301653188
	C12	-5.831414869	-3.394346879	6.370720268
	C13	-5.052058260	-5.597185024	7.123909049
	C14	-3.538196488	-5.853060218	7.123279127
	C15	-1.510243828	-6.170507637	5.760749396
	C16	-0.680264747	-4.914058923	5.486238447
	C17	-0.749387466	-2.519470977	4.909942402
	C18	-0.923734561	-1.555143444	6.100831528
	C19	-1.139888916	-1.933874384	3.532045490
	C20	-0.580904772	-0.525665291	3.315719078
	C21	-0.687215255	-2.873039484	2.410098422
	C22	-2.407775706	-0.093311007	7.398063868
	C23	-2.422036097	-0.737760620	8.797724428
	C24	-3.681632183	0.734946434	7.099438658
	C25	-4.035317638	1.657221027	8.271448695
	C26	-3.499117496	1.550903626	5.812687831
	C27	-3.275802504	-2.467904232	10.265678987
	C28	-1.924110371	-2.759375921	10.888694235
	C29	5.158260116	-12.240139729	2.624635331
	C30	5.858318761	-10.888119313	2.544785779
	C31	5.916059869	-8.638522470	3.608658620
	C32	6.858244456	-8.453520045	4.813356650
	C33	4.677524819	-7.732938828	3.726270718
	C34	5.043822717	-6.251500989	3.749803740
	C35	3.822854816	-5.345663489	3.603273116
	C36	3.864967779	-2.879613725	4.092612602
	C37	9.004242303	-7.527613045	5.556166561
	C38	9.142945157	-6.059656364	5.891093405
	C39	-4.611753068	-2.176134295	-3.451834991
	C40	-5.147904017	-0.866312490	-2.844016525
	C41	-3.139973219	-2.356059636	-3.014759703
	C42	-2.527761695	-3.748447723	-3.270053452
	C43	-1.880932187	-3.942080989	-4.641633757
	C44	-5.475351088	1.522883589	-3.361169428
	C45	-6.794032348	1.783043427	-2.620499465
	C46	-5.316261526	2.417861892	-4.598733864
	C47	-9.127471221	1.110097580	-2.297963718
	C48	-9.125125587	0.801585275	-0.797535607
	C49	-7.890779810	-0.119555774	1.110858019
	C50	-6.838025372	0.734159849	1.817470470
	C51	-5.195621370	2.541113274	1.699120943
	C52	-5.836430738	3.677888238	2.528600377
	C53	-4.309030356	3.243436241	0.660963181
	C54	-3.484815927	2.367402548	-0.222733876
	C55	-3.118487801	1.043636958	-0.184505390
	C56	-2.167121035	1.955461521	-1.981251246
	C57	-7.654031911	5.339264020	2.533865163
	C58	-7.934759069	5.204419825	4.028565244
	C59	-8.981067290	5.514228959	1.755208232
	C60	-9.595364750	6.883065850	1.756740026
	C61	-9.781089090	7.797940690	2.775741533
	C62	-10.610410975	8.581252175	0.876020155
	C63	7.991396222	0.739630655	5.974254313
	C64	9.078596905	-0.307069473	5.823018895
	C65	6.724016221	0.161247245	5.290979578
	C66	5.525962060	1.074569771	5.392364152



C67	4.648809251	1.011832776	6.490507000
C68	5.256991319	2.022236623	4.389201271
C69	3.535601339	1.854855185	6.581788259
C70	4.159146596	2.878833571	4.473328653
C71	3.297780559	2.792984701	5.570737775
C72	5.273770246	6.912492552	1.520440330
C73	4.270244687	8.050888187	1.276698804
C74	4.583582053	5.550939030	1.409681656
C75	3.660878907	9.945594554	-0.185406283
C76	2.288521807	9.637856556	-0.790728518
C77	0.787654458	7.800193444	-1.557990216
C78	-0.014849940	7.149679018	-0.400911549
C79	1.114072487	6.791934872	-2.687147622
C80	-0.016897817	5.969801405	-3.316777530
C81	-0.927698311	6.697742753	-4.317684505
C82	-2.591653529	8.497893276	-3.857788160
C83	-0.016125703	5.775944050	1.623596359
C84	-0.476241569	6.778703371	2.691124515
C85	0.834125823	4.700232296	2.333684564
C86	0.281169236	8.616499873	4.114395383
C87	-0.322320685	9.999369240	3.935895781
C88	-1.308990128	11.587961266	2.379033819
C89	-2.737506685	12.010860872	2.803341579
C90	-1.059271174	11.929279028	0.907860342
C91	-2.005294104	11.231984014	-0.061918630
C92	-4.962615438	11.268549775	3.520886831
C93	-5.202181013	12.126705310	4.756650577
C94	-5.694582186	9.905224251	3.666148119
C95	-5.619248827	9.083091341	2.399021047
C96	-6.570612537	9.256562982	1.382846877
C97	-4.573241621	8.171650504	2.178710427
C98	-6.465642878	8.572277463	0.170239327
C99	-4.431948842	7.502649681	0.958470290
C100	-5.384028867	7.713566158	-0.033560876
C101	6.448883140	-2.057196515	-8.249552418
C102	4.943601541	-1.893535425	-8.117315358
C103	3.146231036	-0.663967164	-6.924683948
C104	2.750315230	0.781276560	-7.251151433
C105	3.048452036	3.132910818	-6.614996361
C106	4.193934463	4.092529913	-6.306804870
C107	6.260976544	4.602585725	-5.136829078
C108	7.125193376	5.090483276	-6.283858865
C109	-0.126109009	-1.420716617	-10.087569992
C110	-1.238783108	-0.397161796	-9.831038490
C111	0.020548708	-2.363449298	-8.870000740
C112	0.843559454	-3.612291716	-9.233739086
C113	1.193769997	-4.408028456	-7.996541800
C114	-1.881107381	1.736737321	-8.824781782
C115	-1.281361184	3.112478679	-9.036810721
C116	-2.644207346	1.565494120	-7.487721370
C117	-1.688869053	1.351500064	-6.347544533
C118	-1.078741388	2.440140432	-5.702856969
C119	-1.269161147	0.049472100	-6.021791218
C120	-0.027560934	2.231375250	-4.803650157
C121	-0.215537928	-0.158628643	-5.127318913
C122	0.428258314	0.935250551	-4.540801511
C123	9.117160868	-5.231248793	-3.733023060
C124	10.013593313	-5.538753730	-2.520683802
C125	7.668740938	-5.652996949	-3.444137794
C126	6.634985462	-5.253262541	-4.450158832
C127	6.605610641	-5.567327807	-5.794282412
C128	4.687056760	-4.620291318	-5.223549343
C129	10.798763938	-7.117493690	-0.858713721
C130	12.256383497	-6.765523953	-1.061877180
C131	0.883003098	-6.725310744	-1.426673012
C132	2.252736334	-6.872692485	-0.765641257
C133	3.456691757	-6.734281257	-1.742989955
C134	3.577479354	-8.014037108	-2.613868127
C135	4.871891423	-8.142055700	-3.421026170
C136	5.053877956	-9.517310028	-4.101382789
C137	4.755720090	-6.589408163	-0.934672933
C138	4.088750302	-0.267179239	-1.315779249
Fe139	4.756405536	-1.247720488	-2.891014329
Fe140	2.618828066	0.807441967	-0.939310701
Fe141	5.016385759	0.698891954	0.131660386
Fe142	4.715318362	1.275370133	-2.414370041
Fe143	3.944516781	3.001540452	-0.453712075
Fe144	4.897971883	-1.783571890	-0.370021339
Fe145	2.390028544	-2.088355144	-1.115001152
H146	-5.854499910	-7.293430234	-2.890869608
H147	-5.741812810	-6.045193651	-3.936836534
H148	-9.518924931	-4.854529700	-2.236075066

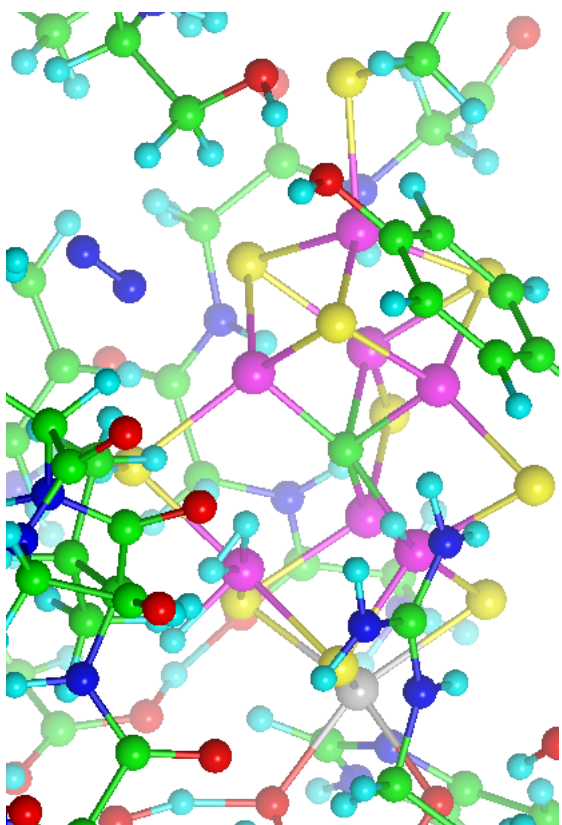
H149	-8.118427104	-5.744536207	-3.971607869
H150	-8.282323133	-7.142215029	-2.913074089
H151	-8.068412714	-2.987182860	-0.698363856
H152	-9.133613862	-6.215319206	0.299854517
H153	-9.796590513	-3.356848024	-0.521652346
H154	-8.896001367	-7.309057219	2.336799437
H155	-6.460839889	-6.377936134	0.692627145
H156	-8.950125351	-5.737646176	3.162650619
H157	-3.555485553	-2.302055510	1.956919774
H158	-5.457693514	-4.172239086	0.902057314
H159	-4.158777981	-6.665467968	0.953351526
H160	-6.517149567	-1.554095331	5.546264430
H161	-6.811803811	-3.285817276	3.259570478
H162	-4.381428490	-7.103061849	2.663644205
H163	-5.206864265	-1.954475517	1.394252092
H164	-5.955412226	-5.117638903	5.244675634
H165	-7.675785603	-2.901803457	5.376832659
H166	-1.084505999	-3.888421898	2.533151690
H167	-1.024866025	-2.502474726	1.429455737
H168	0.411234283	-2.938742101	2.378803351
H169	-2.235804312	-1.862114489	3.519975085
H170	-5.551379106	-6.572050927	7.018851929
H171	-3.306589364	0.912409754	4.940123580
H172	-3.782583050	-2.201167673	8.211490168
H173	-4.255101549	1.099457969	9.192489401
H174	0.513112125	-0.533630822	3.196636210
H175	-0.821919623	0.155007709	4.143575896
H176	7.777504938	0.847443416	7.054265306
H177	-4.403190105	2.138942546	5.598325284
H178	-4.921671478	2.255994792	8.016431398
H179	-2.657899104	2.254860034	5.925176359
H180	-3.207850734	2.352130294	8.485253653
H181	-4.516289489	0.025777977	6.952661013
H182	-1.540493320	0.585035834	7.420905751
H183	-2.939966366	-1.304835636	5.697358840
H184	-1.014370048	-0.085760153	2.404079346
H185	1.375713950	4.107792237	1.579079464
H186	0.133029909	4.037231027	2.860782618
H187	1.803091362	4.706842706	4.047324549
H188	1.651984013	3.450505992	6.366949451
H189	3.952418722	3.594855628	3.677949330
H190	5.901818105	2.071481637	3.508410227
H191	4.827694985	0.283505210	7.286504662
H192	-2.387553429	-3.894218041	5.001503606
H193	-1.321959623	-6.878883377	4.940599707
H194	-1.130184719	-6.618413752	6.687868516
H195	-3.477567842	-5.800536575	5.048169960
H196	-5.294946065	-5.187111323	8.111854672
H197	2.855629195	1.780817657	7.434761601
H198	0.327131897	-2.723172299	4.897742531
H199	-3.863865951	-1.849278940	10.965543950
H200	-3.788686668	-3.436313148	10.148987543
H201	-1.092694607	-2.930221675	10.164870027
H202	9.986838379	-7.933936762	5.270309712
H203	-0.379581936	-4.963301657	-5.583550888
H204	1.885710441	-5.568652272	-2.610779067
H205	0.246916841	-4.255541561	-9.895887078
H206	1.758702193	-3.319910701	-9.767633707
H207	-0.969279428	-2.680552741	-8.507135402
H208	-0.441222510	3.139936292	-9.769486550
H209	-0.510369434	-2.019935581	-10.927741202
H210	-2.526958919	-1.586727682	-3.513556026
H211	-3.303459848	-4.526307890	-3.162397169
H212	0.056293741	0.813757448	-8.745885641
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H214	1.606643411	-0.318103911	-9.781815321
H215	-0.415568462	-5.192619225	-3.837012982
H216	0.496267447	-1.808058342	-8.046518011
H217	1.728659253	-1.450789337	-10.971155221
H218	-5.604693218	-2.633411394	-5.203502430
H219	-3.103560365	-2.172273734	-1.930055493
H220	2.974108218	-3.579238920	-8.039757341
H221	-1.783491755	-3.961030487	-2.488759295
H222	-4.589055005	1.953257416	2.402111590
H223	-3.353504926	0.257635784	0.522142089
H224	-8.852715716	0.086348036	1.598797803
H225	-7.288386607	-0.159259631	-0.935085775
H226	-7.455202636	3.626480183	1.270289137
H227	-9.499124514	7.793725293	3.822979211
H228	-8.194447331	4.163463055	4.343827354
H229	-9.703183179	4.756884906	2.109615034
H230	-6.993450512	6.205535526	2.372372857

H231	-11.101985487	9.265358845	0.189259883
H232	-3.636978604	3.917800474	1.216701451
H233	-4.943596070	3.881524525	0.023440298
H234	-10.707467510	9.723077213	2.669915845
H235	-8.778398362	5.268957457	0.700543538
H236	-6.417924556	1.814841190	0.083619617
H237	-7.652587998	-1.174657963	1.308897188
H238	-9.526637302	2.128021306	-2.402230875
H239	-1.576445015	2.075392300	-2.885928580
H240	-9.830076668	0.424631716	-2.788618945
H241	9.123912652	2.445495480	5.890760485
H242	7.631283051	2.620215266	5.248617639
H243	1.661039260	6.119640873	0.313224404
H244	-0.933328904	5.301615789	1.246092957
H245	1.290016697	7.793975199	2.449887925
H246	-3.071320107	3.871904088	-1.723152380
H247	-4.351522332	4.760950420	-3.111935918
H248	-5.532776628	4.331046417	-4.987070586
H249	-4.336328503	5.772093732	-1.878025582
H250	-4.358871516	2.167245928	-5.084874067
H251	-6.136523024	2.228378273	-5.307964093
H252	-0.005180247	11.745929817	0.655488069
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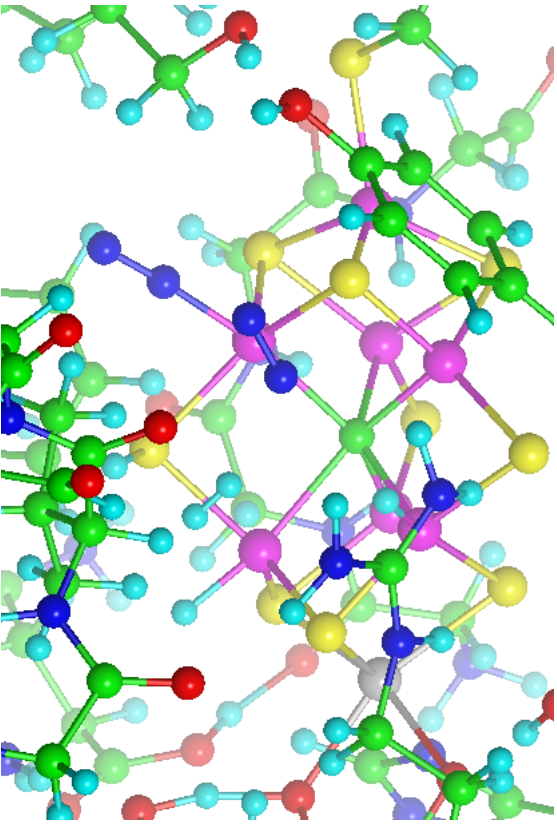
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C67	4.634827225	1.013965828	6.507523118
C68	5.250587727	2.031181246	4.411958175
C69	3.523206702	1.859400667	6.600028290
C70	4.156058767	2.892000047	4.498011453
C71	3.290249524	2.802060145	5.591869374
C72	5.275068694	6.908149029	1.529859213
C73	4.268192325	8.044032847	1.284875070
C74	4.590706517	5.546389725	1.398512265
C75	3.660966279	9.947270691	-0.167796409
C76	2.293431720	9.636594977	-0.781530341
C77	0.795281990	7.806213698	-1.561147468
C78	-0.015571916	7.162033791	-0.407018097
C79	1.115597944	6.788308434	-2.681248409
C80	-0.022600254	5.970384986	-3.302724298
C81	-0.931714441	6.696079712	-4.307849592
C82	-2.601155839	8.497051085	-3.853548604
C83	-0.038007682	5.775908847	1.608508542
C84	-0.483339122	6.778607070	2.682479768
C85	0.792527480	4.680866900	2.314643195
C86	0.289850534	8.615890527	4.097868227
C87	-0.311459722	10.000916152	3.924994390
C88	-1.315619421	11.593457124	2.378011405
C89	-2.742947041	12.016577855	2.801447158
C90	-1.069662717	11.926037264	0.904257461
C91	-2.009634914	11.210866141	-0.058070551
C92	-4.966925474	11.279503880	3.521823395
C93	-5.203281216	12.135698001	4.759942218
C94	-5.703425114	9.918750461	3.665766100
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C96	-6.578041115	9.271477858	1.382097711
C97	-4.588303142	8.176793111	2.181819360
C98	-6.479155129	8.580820950	0.172607683
C99	-4.452531172	7.501022906	0.964456597
C100	-5.401721229	7.716477480	-0.029730894
C101	6.440911776	-2.055223001	-8.235217745
C102	4.935562874	-1.887086950	-8.121029516
C103	3.129588588	-0.648030228	-6.950463522
C104	2.735100302	0.798567441	-7.271712716
C105	3.033261010	3.1466610895	-6.622532332
C106	4.176760466	4.105741101	-6.303359474
C107	6.235289062	4.611801586	-5.114013647
C108	7.135435139	5.072841390	-6.242684270
C109	-0.138569202	-1.422717026	-10.076205392
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C111	0.011812040	-2.370622064	-8.863508412
C112	0.840149705	-3.615519806	-9.230273387
C113	1.196299842	-4.407634437	-7.991610865
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C119	-1.261498716	0.058634125	-6.014269023
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C121	-0.184583188	-0.132041804	-5.145265058
C122	0.457633328	0.973603473	-4.578783235
C123	9.123498545	-5.225487543	-3.729095090
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C132	2.260849243	-6.872832873	-0.773181242
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C137	4.769020987	-6.606840961	-0.934951274
C138	4.073143840	-0.270126286	-1.302779160
Fe139	4.758298311	-1.243255112	-2.866833958
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Fe141	5.183137025	0.686936263	0.051632669
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Fe143	4.047480013	3.003545922	-0.495569316
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Fe145	2.473229360	-2.093211880	-1.127326149
H146	-5.903658684	-7.297932059	-2.914352614
H147	-5.807133684	-6.064262289	-3.978838396

H148	-9.540872226	-4.826308288	-2.224349429
H149	-8.183625739	-5.756540746	-3.971212376
H150	-8.328427279	-7.138682888	-2.888944485
H151	-8.042708528	-2.968237216	-0.717420300
H152	-9.120081592	-6.178929280	0.301433471
H153	-9.775079973	-3.307959920	-0.521182791
H154	-8.887025894	-7.263234757	2.344236987
H155	-6.449623195	-6.376096205	0.689379646
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H160	-6.478571378	-1.503777820	5.501810701
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H162	-4.363439601	-7.090281292	2.657143561
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H164	-5.891840799	-5.055353792	5.211705866
H165	-7.644434818	-2.847989337	5.362040175
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H173	-4.232309437	1.099622787	9.185224210
H174	0.222897867	-0.506354493	2.811207697
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H191	4.809238643	0.281146396	7.300384317
H192	-2.375835697	-3.955831628	5.024901719
H193	-1.284339030	-6.924657277	4.946726874
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H233	-4.922385068	3.886793419	0.044571563
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H236	-6.401658489	1.807914689	0.097614287
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H240	-9.823474051	0.400404722	-2.781784312
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H253	-1.259578246	13.003763156	0.784974396
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H261	1.844154678	6.071732718	-2.269334332
H262	2.821187423	7.672124048	-0.915432623
H263	-0.635774171	5.487803963	-2.524924766
H264	-7.680271894	0.256930762	-3.634291792
H265	4.210051277	10.581342605	-0.876410880
H266	-5.032271462	-0.173910800	-4.681149931
H267	1.641684010	7.336313699	-3.479773999
H268	-3.597589836	6.846017795	0.792333272
H269	3.464019088	10.544499658	0.733977687
H270	-1.411985063	9.041337704	-5.449272531
H271	-4.180076637	9.717993984	-3.398217058
H272	-3.949520885	-2.608322277	-5.334060279
H273	-5.214313061	-2.991619483	-2.956966912
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H278	0.462987045	5.154125418	-3.855079194
H279	-2.728069871	6.585428650	-3.170335063
H280	-0.319203389	8.081944113	4.842864719
H281	-0.838012768	9.526599601	2.006947777
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H306	3.208681800	-5.655320656	2.691864073
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H316	4.907348903	-3.810507322	2.675710901
H317	0.462492085	3.110819773	-4.348752402
H318	-1.745683031	-0.809569754	-6.466623730
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H320	7.671249201	-6.791664932	-3.407294376
H321	6.745468334	-8.087418961	-0.071186000
H322	7.656096402	-9.834389636	-3.067782440
H323	7.149339570	4.406490679	-7.138236032
H324	6.421008947	-5.014593781	0.384175234
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H326	5.218929088	-0.441401785	-6.698151051
H327	3.506763570	-8.875710500	-1.931795069
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H358	9.603371958	-0.307567669	4.878804871
H359	-4.350957567	12.174451113	5.478573379
H360	8.672466551	-8.051558445	6.476607560
H361	8.247444840	-5.443649489	5.713897789
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H366	4.319922905	-1.423853992	0.925086515
H367	-6.075050729	7.117213963	-1.759249603
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H369	2.193086971	-1.434730250	0.334781284
H370	1.681971043	-2.129252982	0.257048932
H371	-1.806272721	-0.037012449	-1.479582815
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N383	-3.164623531	-1.842819827	8.975221165
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N389	7.998067683	-7.781913767	4.537299804
N390	-4.770312751	-2.152082507	-4.894610488
N391	-0.837950538	-4.775029339	-4.683005364
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N410	-0.937583582	10.237286849	2.731417363
N411	-1.425940732	10.766167359	-1.203632736
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N419	9.656325460	-5.776537742	-4.987773840
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N422	9.992773513	-6.804409220	-2.022466599
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N424	0.450148348	2.108262224	-0.004164090
O425	-6.544068528	-5.245957981	-1.260912859
O426	-8.026101773	-3.567697500	1.739581549
O427	-6.589380507	-6.340627925	3.870613495
O428	-3.421493242	-4.806042504	3.256600779
O429	-4.289529710	-1.566933294	4.201354091
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O434	-1.751569474	-0.234768290	9.729846388
O435	-1.740758478	-2.893228603	12.098956321
O436	6.661799764	-10.657043171	1.633080652
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O438	10.171993361	-5.592433373	6.372158760
O439	-5.419704037	-0.744924629	-1.608214774
O440	-2.327073205	-3.361407644	-5.663084599
O441	-6.866762598	2.654502763	-1.719699547
O442	-5.346218476	3.795515199	-4.169611803
O443	-10.094202961	1.153082808	-0.099153125
O444	-6.657719866	0.619189777	3.052930286
O445	-5.275352712	4.203138640	3.500334053
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O447	9.304002174	-1.173049070	6.703609665
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O450	1.481198376	10.564770518	-0.962221361
O451	-1.240432934	7.351212734	-0.331308153
O452	-1.513390834	6.588920572	3.342561143
O453	1.722546380	5.241382892	3.241520838
O454	-0.239986630	10.842225211	4.828937730
O455	-3.089845845	13.203556269	2.723398714
O456	-3.223823161	11.101963536	0.166896992
O457	-6.254148353	12.718791649	4.971911064
O458	-5.229214231	7.070929227	-1.272513664
O459	4.154899088	-2.643452046	-8.748419801
O460	1.984698553	1.080368797	-8.228582904
O461	4.099213251	5.280172580	-6.700494411
O462	7.826697914	6.075924304	-6.177484020
O463	-2.414652215	-0.601373099	-10.210641037
O464	0.413237207	-5.163988427	-7.425704549
O465	2.429524874	-4.210553528	-7.483052173
O466	-1.726920378	4.124988874	-8.489882486
O467	10.779870241	-4.679261893	-2.033321833
O468	13.026414292	-6.561795470	-0.122380394
O469	0.860898046	-5.875551060	-2.469252984
O470	-0.103253610	-7.336484389	-1.056950933
O471	6.220176089	-10.054013176	-4.060567277
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O473	5.496910473	-5.543933908	-1.165715732
O474	5.100633764	-7.497962182	-0.130401526
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	O479	8.496193510	-9.803738849	-2.520672063
	O480	7.612854437	-8.549176020	0.082819770
	S481	3.817075064	5.277951320	-0.263961421
	S482	2.775731089	2.529379441	-2.350346589
	S483	2.938399334	-2.515242914	-3.336286909
	S484	3.379372319	1.584976983	1.112987883
	S485	0.897768194	-0.553034710	-1.700223802
	S486	5.415154970	0.313448487	-4.309310798
	S487	3.696334424	-3.537756256	0.049603439
	S488	6.164935253	2.314346948	-1.076946566
	S489	6.409814144	-2.482777390	-2.016629375
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Fe(139) -2.123				
Fe(140) -0.747				
Fe(141) -2.465				
Fe(142) 2.829				
Fe(143) 2.595				
Fe(144) 1.230				
Fe(145) 1.652				
				
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	C1	-7.740182194	-5.538245168	-0.374124809
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	C3	-8.788650067	-3.714431696	0.889858139
	C4	-8.359061109	-4.066130820	2.310635595
	C5	-8.181315515	-5.780125059	4.047847914
	C6	-6.664832896	-5.841424313	4.252638434
	C7	-4.446548695	-5.990333360	3.250610998
	C8	-3.977416056	-4.546469264	3.470128568
	C9	-4.400892804	-2.196161145	2.864992605
	C10	-4.667683179	-1.698068115	4.292887175
	C11	-6.051145366	-1.759194008	6.269535125
	C12	-5.128308758	-2.375141292	7.332650657
	C13	-4.250960487	-4.461139441	8.287682823
	C14	-2.737064527	-4.711704881	8.192207275
	C15	-0.847465768	-5.335017714	6.739725097
	C16	-0.057073274	-4.134540884	6.208574300
	C17	-0.262113944	-1.865553040	5.236569921
	C18	-0.294384470	-0.725670617	6.279370948
	C19	-0.965175621	-1.573646423	3.890577287
	C20	-0.698060967	-0.176825990	3.311635821
	C21	-0.624501168	-2.678131154	2.882386270
	C22	-1.613871329	0.942590261	7.507453008
	C23	-1.472236027	0.516712236	8.981872957
	C24	-2.909888713	1.747255042	7.236345877
	C25	-3.132197936	2.826209056	8.301797832
	C26	-2.868227081	2.380249606	5.838614491
	C27	-2.181598582	-0.930587389	10.793360441
	C28	-0.771798228	-1.184829137	11.287966139
	C29	5.431457105	-11.815770866	3.758267140
	C30	6.123905521	-10.499260703	3.425204937
	C31	6.254470917	-8.119582507	4.148335453
	C32	7.312914910	-7.763147663	5.209412651
	C33	5.008988959	-7.225820126	4.265067211
	C34	5.318443174	-5.750277613	4.036774603
	C35	4.050631443	-4.921828792	3.833238046
	C36	4.265760531	-2.440489425	4.115063585
	C37	9.524923706	-6.775896410	5.582671551
	C38	9.707217874	-5.279686703	5.719115089
	C39	-4.983376574	-2.591803736	-2.618382235
	C40	-5.449017239	-1.203469159	-2.140370324
	C41	-3.472276221	-2.716871024	-2.315610653
	C42	-2.870435824	-4.130347182	-2.449043124
	C43	-2.368831352	-4.509161664	-3.842426212
	C44	-5.799788213	1.103143011	-2.941911090
	C45	-7.039313041	1.483433634	-2.121898973
	C46	-5.752232482	1.812924472	-4.301914393
	C47	-9.329149639	0.886886831	-1.484695138
	C48	-9.176486451	0.788571563	0.037177995
	C49	-7.756541497	0.147139317	1.929520672
	C50	-6.645256574	1.087816486	2.397244139
	C51	-5.007765508	2.820968919	1.852266054
	C52	-5.575478918	4.071235734	2.565666599
	C53	-4.226654091	3.360926132	0.644630842
	C54	-3.451664108	2.377953000	-0.166433047
	C55	-3.019777223	1.093462755	0.044455025
	C56	-2.274502300	1.735640808	-1.955080257
	C57	-7.397836656	5.729699435	2.514989105
	C58	-7.518275826	5.795908928	4.036007403
	C59	-8.794895948	5.805916513	1.850386749
	C60	-9.411258486	7.169219833	1.728998979
	C61	-9.504238129	8.203812911	2.639445113
	C62	-10.499919287	8.756297822	0.738448058
	C63	8.556125671	1.475246538	4.905151391
	C64	9.613009872	0.390388530	4.804621827

C65	7.215416924	0.839262159	4.461348629
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C67	5.295051317	1.887262547	5.759752670
C68	5.694935203	2.625105773	3.500554696
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C71	3.892832024	3.596231530	4.781357206
C72	5.387598425	6.972753556	-0.042568303
C73	4.357951397	8.079011649	-0.326107655
C74	4.695907610	5.616587403	0.079976405
C75	3.586771371	9.781848189	-1.940450180
C76	2.167174122	9.405364341	-2.370908921
C77	0.599928871	7.499843459	-2.729876474
C78	-0.083376592	7.039519406	-1.416087374
C79	0.801719744	6.329762537	-3.721276360
C80	-0.401640794	5.458738306	-4.100188269
C81	-1.400326814	6.053785063	-5.106268030
C82	-3.022525120	7.912068253	-4.736523370
C83	0.115047950	5.935927731	0.762188371
C84	-0.227302823	7.080401862	1.726099567
C85	1.037667736	4.948019194	1.511043295
C86	0.679944511	9.085187205	2.796791276
C87	0.057930623	10.440795293	2.499416625
C88	-1.089847345	11.819339572	0.849208709
C89	-2.460757949	12.317090222	1.366280476
C90	-1.001661754	11.942707934	-0.674182583
C91	-2.039202899	11.123573158	-1.432366417
C92	-4.606898224	11.716451224	2.383947036
C93	-4.707022898	12.735289921	3.510190094
C94	-5.331906626	10.402926735	2.794220454
C95	-5.384362552	9.406821351	1.658086271
C96	-6.426948492	9.463595077	0.719508856
C97	-4.373933003	8.450900582	1.467564578
C98	-6.446567304	8.618588573	-0.391218155
C99	-4.364051067	7.612591118	0.347938617
C100	-5.403032447	7.709323734	-0.572819189
C101	5.551700885	-3.278350579	-8.517203524
C102	4.068085115	-3.070362684	-8.270457242
C103	2.391042901	-1.641449256	-7.125611783
C104	1.955885110	-0.253977176	-7.611782021
C105	2.302530797	2.162963715	-7.323276043
C106	3.475684195	3.138543071	-7.260124791
C107	5.643548499	3.770584950	-6.354595362
C108	6.409972595	4.101136291	-7.619290447
C109	-1.208701503	-2.824038390	-9.746458524
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C111	-0.928583929	-3.599109405	-8.438347153
C112	-0.116425960	-4.880680697	-8.701774728
C113	0.352251291	-5.483642502	-7.395146852
C114	-2.841876599	0.491268656	-8.754675718
C115	-2.303496813	1.823155804	-9.239215679
C116	-3.427312901	0.511363112	-7.320665170
C117	-2.338736657	0.466586058	-6.284003175
C118	-1.669455269	1.638126435	-5.891800483
C119	-1.877337252	-0.770749932	-5.802461748
C120	-0.522714736	1.563784690	-5.096129767
C121	-0.733646060	-0.843772933	-5.004184349
C122	-0.034400328	0.322435755	-4.678407261
C123	8.717641422	-5.823420541	-3.897824340
C124	9.725544427	-5.961734811	-2.747827984
C125	7.311904312	-6.224012741	-3.424711946
C126	6.198137130	-5.986917621	-4.391643313
C127	6.049470391	-6.532426238	-5.650363875
C128	4.194584963	-5.463502797	-5.091941625
C129	10.650215895	-7.283648697	-0.942660013
C130	12.082680062	-6.949576286	-1.295608130
C131	0.757984568	-6.820091094	-0.625122064
C132	2.180307065	-6.896159518	-0.078516791
C133	3.293138051	-6.937811953	-1.169472055
C134	3.334898242	-8.347420048	-1.818551969
C135	4.539590534	-8.612996671	-2.723310454
C136	4.646914001	-10.067975936	-3.230542462
C137	4.651555423	-6.675758628	-0.497771733
C138	3.889920199	-0.510198881	-1.703436486
Fe139	4.444091618	-1.649105797	-3.205605373
Fe140	2.334407393	0.920083715	-1.102774978
Fe141	5.189259663	0.609898713	-0.700803049
Fe142	4.291982908	0.875909333	-3.106585619
Fe143	4.111806647	2.904290845	-1.437451802
Fe144	4.814074798	-1.901170324	-0.687401696
Fe145	2.444174321	-2.222690009	-1.608577463
H146	-6.154480120	-7.566289868	-1.228062287

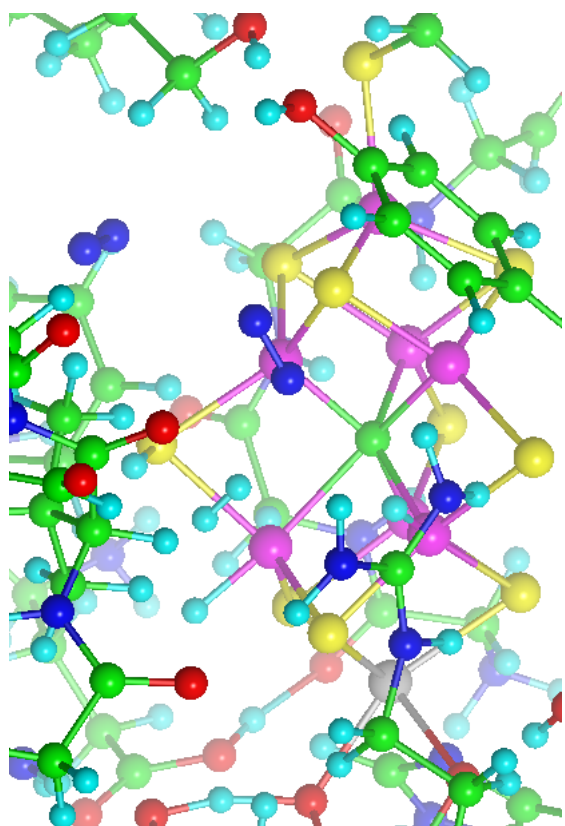
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H150	-8.571268529	-7.397007134	-1.002657812
H151	-8.073437393	-2.962196121	0.525162301
H152	-9.051551815	-5.978465252	2.091609925
H153	-9.779129604	-3.241662808	0.935070282
H154	-8.602141798	-6.779358251	4.221684894
H155	-6.331292278	-6.124843787	2.236029201
H156	-8.571042855	-5.107237154	4.823077598
H157	-3.368814761	-1.922688739	2.613810463
H158	-5.306112686	-3.938850821	2.028436267
H159	-4.009059449	-6.380637373	2.321256346
H160	-5.946874890	-0.668989664	6.346775384
H161	-6.461218161	-2.717296222	4.377437813
H162	-4.076194908	-6.593477639	4.088373534
H163	-5.065818435	-1.680317542	2.158782794
H164	-5.336482452	-4.229873386	6.460646130
H165	-7.087915791	-2.033310817	6.508398353
H166	-0.986862090	-3.657303819	3.218981815
H167	-1.082740313	-2.469989171	1.901885239
H168	0.461378599	-2.743306912	2.727978535
H169	-2.037679106	-1.620844033	4.111832882
H170	-4.748341890	-5.440948249	8.346791080
H171	-2.748140087	1.630632528	5.045303961
H172	-2.917112702	-0.972298279	8.789721794
H173	-3.268017988	2.401064403	9.306683543
H174	0.151491643	-0.179961613	2.621544553
H175	-0.507195140	0.581902048	4.082578912
H176	8.460314295	1.746602383	5.973536365
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H179	-2.036164284	3.100005820	5.767088173
H180	-2.277287171	3.519558245	8.339033384
H181	-3.758006235	1.040517850	7.276597994
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H188	2.345335633	4.378939635	5.648823781
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H207	-1.875927070	-3.873773697	-7.948970655
H208	-1.580025721	1.744103431	-10.084116938
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N2 / H2 exchange			bm52h2disn2dis2n2x3dtb.car 4	
2N2 dissociated	C1	-7.710685974	-5.522851799	-0.378340942
35, S=3/2	C2	-7.914353017	-6.600044446	-1.449113921
	C3	-8.780823948	-3.711895278	0.891161421
	C4	-8.357853310	-4.066793181	2.313162075
	C5	-8.183695926	-5.785699859	4.045390630
	C6	-6.667893487	-5.845396368	4.255687915
	C7	-4.44744501	-5.991146750	3.255808644
	C8	-3.980179697	-4.546639041	3.473638938
	C9	-4.407196237	-2.196866055	2.871709725
	C10	-4.671659107	-1.702072454	4.301436234
	C11	-6.055148627	-1.765557634	6.278617369
	C12	-5.130784831	-2.381965697	7.340233011
	C13	-4.250370890	-4.467666092	8.292264379
	C14	-2.734528768	-4.707740313	8.195451318
	C15	-0.840659467	-5.314710238	6.73907628
	C16	-0.047578863	-4.120336577	6.196621251
	C17	-0.252545653	-1.855721290	5.200730073
	C18	-0.282234836	-0.718527251	6.248250174
	C19	-0.967420373	-1.567867314	3.864752604
	C20	-0.700909914	-0.173249359	3.284336262
	C21	-0.637184164	-2.676887857	2.857549430
	C22	-1.601947122	0.943980121	7.487808868
	C23	-1.456120243	0.510646970	8.958703012
	C24	-2.902851478	1.744997722	7.227014514
	C25	-3.125089301	2.819100908	8.297893428
	C26	-2.870258707	2.384301726	5.831892105
	C27	-2.164875491	-0.943150377	10.762267656
	C28	-0.758539422	-1.192348306	11.268762618
	C29	5.423629353	-11.808918920	3.743881383
	C30	6.123129485	-10.495577296	3.419408330
	C31	6.256415612	-8.119576184	4.150577748
	C32	7.314932763	-7.762281703	5.210896650
	C33	5.010196164	-7.227188140	4.268142812
	C34	5.320609765	-5.752480637	4.037271097
	C35	4.054857585	-4.923579572	3.824559426
	C36	4.279549165	-2.445020081	4.103987638
	C37	9.524769330	-6.770096035	5.581248024
	C38	9.704652195	-5.273861595	5.718534248
	C39	-4.955954351	-2.581880284	-2.615749811
	C40	-5.430432575	-1.195991241	-2.138607033
	C41	-3.446301111	-2.710203198	-2.314075340
	C42	-2.854506823	-4.127505891	-2.448322273
	C43	-2.357340913	-4.510534043	-3.842710612
	C44	-5.799869747	1.105964544	-2.943524516
	C45	-7.039361862	1.484100276	-2.123297928
	C46	-5.750115781	1.816366300	-4.302959508
	C47	-9.328389062	0.887938542	-1.485547556
	C48	-9.177260918	0.787646256	0.036245066
	C49	-7.761620064	0.140507071	1.929678410
	C50	-6.647676953	1.077341524	2.397827826
	C51	-5.004037794	2.8043056406	1.847140014
	C52	-5.562801513	4.054741482	2.563458810
	C53	-4.235130958	3.343315327	0.632633450
	C54	-3.478651343	2.355818510	-0.189617192
	C55	-3.055049035	1.065264976	0.011465609
	C56	-2.297976354	1.720908187	-1.976827302
	C57	-7.369499115	5.725007097	2.503286901
	C58	-7.489843498	5.795742679	4.024078082
	C59	-8.771455470	5.804594189	1.846869057
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	C61	-9.491703365	8.198557484	2.642684236



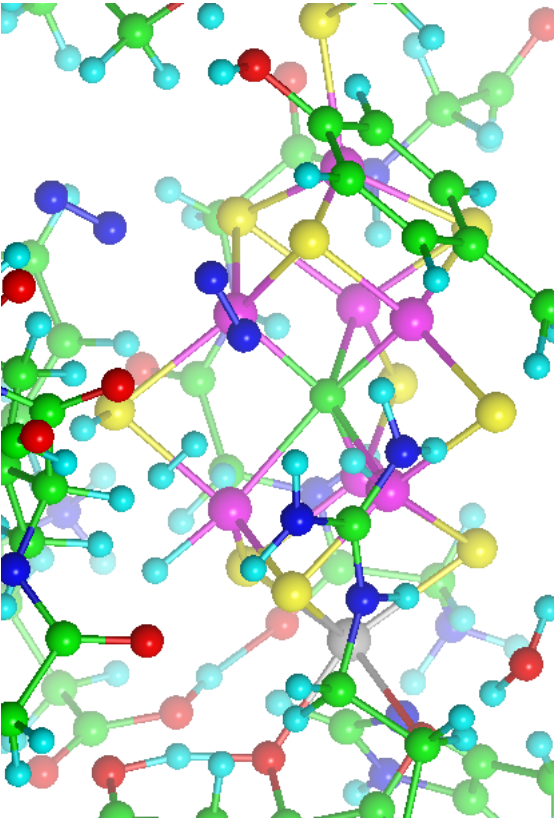
C62	-10.487362071	8.750802814	0.741662859
C63	8.559841193	1.478741733	4.901674014
C64	9.616686429	0.394381482	4.798840757
C65	7.220229254	0.842179357	4.456787572
C66	6.052749873	1.792842840	4.568885097
C67	5.300716366	1.892874394	5.754333634
C68	5.694638896	2.622073989	3.490972407
C69	4.225120678	2.781400074	5.862237612
C70	4.638894961	3.526954017	3.591045801
C71	3.896144148	3.597682655	4.773568490
C72	5.386336082	6.982113251	-0.045944139
C73	4.352020984	8.083944403	-0.331026141
C74	4.704433484	5.618307028	0.077651648
C75	3.582045226	9.785506240	-1.946981781
C76	2.163251745	9.407627086	-2.377623076
C77	0.599769087	7.497549466	-2.730943794
C78	-0.074082717	7.033187343	-1.413684951
C79	0.804903176	6.326803288	-3.721781718
C80	-0.396289804	5.453612064	-4.102058336
C81	-1.395449713	6.049299962	-5.106612431
C82	-3.017759978	7.907381676	-4.734950771
C83	0.144976450	5.940005049	0.767056485
C84	-0.212475737	7.084581084	1.725820524
C85	1.086986042	4.973709688	1.522878677
C86	0.685322708	9.087609834	2.803575608
C87	0.062456153	10.441609382	2.503964935
C88	-1.081887739	11.813040918	0.848051627
C89	-2.453154654	12.307879515	1.368097665
C90	-0.996438248	11.937906740	-0.675237730
C91	-2.037150574	11.122367995	-1.432878306
C92	-4.597528112	11.702259600	2.381010638
C93	-4.699090907	12.724517900	3.505310266
C94	-5.326651616	10.392795761	2.791577597
C95	-5.379901744	9.396228679	1.655864585
C96	-6.420839681	9.454452812	0.715493972
C97	-4.369703617	8.440056513	1.466152514
C98	-6.439619505	8.610073947	-0.395685689
C99	-4.358612818	7.602192011	0.346648831
C100	-5.396091948	7.700877448	-0.575057057
C101	5.554455208	-3.285416844	-8.541615097
C102	4.072877162	-3.073022446	-8.282688175
C103	2.406174368	-1.643350913	-7.125786010
C104	1.971072329	-0.255055888	-7.605631275
C105	2.312165557	2.159940862	-7.316024611
C106	3.481139279	3.140952769	-7.266654211
C107	5.651799380	3.787753036	-6.377761454
C108	6.410094699	4.115424845	-7.647022513
C109	-1.207889659	-2.824371472	-9.748814783
C110	-2.293623068	-1.772464613	-9.497777999
C111	-0.927871305	-3.599853380	-8.440490344
C112	-0.115882258	-4.881465684	-8.703823025
C113	0.353457161	-5.485361646	-7.397418890
C114	-2.837938686	0.491786068	-8.753710179
C115	-2.299939770	1.823481059	-9.240094911
C116	-3.414303602	0.510735286	-7.315819140
C117	-2.324965668	0.460838543	-6.279237468
C118	-1.653496682	1.629742615	-5.882097563
C119	-1.872154030	-0.777420802	-5.792980720
C120	-0.517983359	1.551689593	-5.069895426
C121	-0.739194153	-0.854354074	-4.978829890
C122	-0.042321043	0.309006617	-4.638263552
C123	8.714065364	-5.827763044	-3.888575911
C124	9.725052252	-5.967871424	-2.741170348
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C126	6.192549072	-5.985664240	-4.382079705
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C137	4.629034661	-6.655152068	-0.499356707
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Fe139	4.462840550	-1.685106614	-3.252695568
Fe140	2.547120366	0.663340572	-1.339736588
Fe141	5.049481973	0.634474825	-0.566125758
Fe142	4.448162618	0.873057502	-3.098127647
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	Fe144	4.765831862	-1.934176276	-0.674703538
	Fe145	2.395595230	-2.121347746	-1.677926245
	H146	-6.132414106	-7.567286797	-1.227250568
	H147	-6.143751199	-6.500262889	-2.462156102
	H148	-9.692224121	-4.983548938	-0.558532646
	H149	-8.511288614	-6.171381953	-2.270444537
	H150	-8.546180061	-7.384093115	-0.996563830
	H151	-8.069607174	-2.952551611	0.534575998
	H152	-9.045496696	-5.979929944	2.084395181
	H153	-9.775322191	-3.246979916	0.931712296
	H154	-8.604503657	-6.785489226	4.215537922
	H155	-6.330462590	-6.128597774	2.240456551
	H156	-8.577849975	-5.114349848	4.819718516
	H157	-3.375995741	-1.921677744	2.619274394
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	H159	-4.009046386	-6.382176944	2.327285424
	H160	-5.952854648	-0.675268318	6.357449519
	H161	-6.466032787	-2.719334132	4.384581261
	H162	-4.076758897	-6.592912004	4.094380249
	H163	-5.074721316	-1.680575937	2.168450582
	H164	-5.341430321	-4.236959084	6.468522902
	H165	-7.091397054	-2.041737795	6.517362175
	H166	-1.001841037	-3.653496081	3.199653627
	H167	-1.097668346	-2.471078569	1.877491753
	H168	0.447867340	-2.748713056	2.700530832
	H169	-2.038755824	-1.609995256	4.095221059
	H170	-4.742351452	-5.450354100	8.348716020
	H171	-2.751965925	1.638163808	5.034925971
	H172	-2.899160149	-0.979500798	8.761903590
	H173	-3.259648716	2.389671044	9.301302552
	H174	0.164401766	-0.171803624	2.614072108
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	H176	8.463623987	1.748516626	5.971253487
	H177	-3.807726480	2.926094169	5.640915749
	H178	-4.025138610	3.402731108	8.054692556
	H179	-2.039960787	3.106143634	5.759609793
	H180	-2.271285968	3.513900682	8.337760262
	H181	-3.748234163	1.034950722	7.268432864
	H182	-0.738947599	1.604385783	7.313843202
	H183	-2.329620154	-0.472662115	6.040331876
	H184	-1.570448770	0.158186416	2.697067960
	H185	1.566890459	4.302348548	0.791734832
	H186	0.459412637	4.369167474	2.194158892
	H187	2.192415570	5.228255476	3.132615848
	H188	2.353435539	4.386987740	5.645210328
	H189	4.357056643	4.148066119	2.740469470
	H190	6.235990851	2.540994426	2.545739687
	H191	5.552774813	1.260472709	6.610610027
	H192	-1.810169292	-3.207154383	5.739772468
	H193	-0.721715306	-6.142901102	6.024779689
	H194	-0.372370900	-5.617520904	7.684613388
	H195	-2.870086615	-5.059766416	6.153730696
	H196	-4.414790322	-3.939400202	9.238598053
	H197	3.633597516	2.823572382	6.780565472
	H198	0.814819592	-2.033359669	5.027325645
	H199	-2.651692511	-0.199594856	11.416225448
	H200	-2.716208435	-1.892135184	10.859126667
	H201	-0.027385346	-1.514301867	10.490863028
	H202	10.470061044	-7.218792328	5.238355435
	H203	-0.963057235	-5.666923819	-4.792750359
	H204	1.643753864	-5.904417497	-2.069170684
	H205	-0.755215543	-5.619699053	-9.209486773
	H206	0.743017502	-4.664301511	-9.354804210
	H207	-1.875483905	-3.873706540	-7.951300867
	H208	-1.579980881	1.744280966	-10.088634784
	H209	-1.679398527	-3.523416491	-10.455581557
	H210	-2.898056609	-2.011496181	-2.967434938
	H211	-3.608061799	-4.878271593	-2.153609412
	H212	-0.886396126	-0.403104459	-8.813230207
	H213	-3.686598198	0.282440582	-9.436423352
	H214	0.545165573	-1.707903552	-9.780984661
	H215	-0.804794400	-5.652030847	-3.038906302
	H216	-0.393140803	-2.938331138	-7.740450511
	H217	0.539873051	-2.989216254	-10.814283999
	H218	-6.119369565	-3.271332615	-4.179273109
	H219	-3.296988512	-2.382700773	-1.273982991
	H220	2.124907293	-4.704441293	-7.732313018
	H221	-2.027639706	-4.242147263	-1.731610152
	H222	-4.329713105	2.318902613	2.567774826
	H223	-3.218667547	0.384374440	0.837105440
	H224	-8.672746041	0.433567379	2.469323874
	H225	-7.358732574	-0.205452343	-0.137498845

H226	-7.293137587	3.847363179	1.480979107
H227	-9.121170810	8.318240995	3.654460597
H228	-7.684161959	4.806215725	4.504564140
H229	-9.448156211	5.105877882	2.369798796
H230	-6.739400598	6.561025079	2.160239289
H231	-11.039692744	9.350720545	0.022553429
H232	-3.530210555	4.102353023	1.011967217
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H234	-10.428316212	10.104429790	2.383855460
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H236	-6.377313660	1.858739804	0.484422689
H237	-7.510164892	-0.878847815	2.258339452
H238	-9.741134986	1.887039259	-1.683831263
H239	-1.793730675	1.712116647	-2.940578673
H240	-10.073365791	0.148932081	-1.807711947
H241	9.698478985	3.119013820	4.454544841
H242	8.146764899	3.248267048	3.961190964
H243	1.665239809	6.077071960	-0.755813608
H244	-0.801472407	5.419285284	0.561394567
H245	1.518774907	8.030414776	1.174825029
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H247	-4.673740044	4.330596836	-3.286805498
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H250	-4.823656109	1.509960087	-4.816105511
H251	-6.612642396	1.514698382	-4.916796755
H252	0.024309034	11.701575789	-1.006147726
H253	-1.181990626	12.994803720	-0.924120210
H254	-0.567472710	10.402601587	-2.706161843
H255	-2.223240872	9.869464415	-3.001195753
H256	-2.894617384	9.580882690	-5.912526347
H257	-1.778812959	5.256484845	-5.766659984
H258	-7.265200581	8.656240986	-1.110357936
H259	-3.563815798	8.327250697	2.196269157
H260	-4.293337579	7.950077479	-3.113609348
H261	1.565582374	5.661644754	-3.281750046
H262	2.685338659	7.439211283	-2.301155537
H263	-0.931214132	5.106829883	-3.203736664
H264	-8.030660705	-0.148603801	-2.848235725
H265	4.056532226	10.330278851	-2.773158142
H266	-5.501132481	-0.761077006	-4.082549185
H267	1.255482259	6.746088286	-4.636744766
H268	-3.528812459	6.912299285	0.186188308
H269	3.467076160	10.486306723	-1.106935320
H270	-2.060428654	8.201857388	-6.535799100
H271	-4.546769578	9.194861373	-4.290468688
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H273	-5.485405585	-3.314183190	-1.977606671
H274	-7.234314841	10.171348204	0.851827455
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H276	-0.053042899	8.267850958	-3.154517627
H277	-0.878180212	6.776849719	-5.745254456
H278	0.022175438	4.552617163	-4.571726888
H279	-3.069566099	6.108211662	-3.787323089
H280	0.160265610	8.662692493	3.671734094
H281	-0.629173016	9.710530039	0.724117770
H282	-0.375786207	12.545004545	1.270736669
H283	1.729840594	9.269404634	3.092975079
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H286	5.931041977	-3.848040154	-7.661789581
H287	8.718722867	-4.758312944	-4.146946610
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H289	5.176715677	-4.804165636	-9.841635188
H290	5.485843976	4.873756298	0.283224528
H291	5.449118838	7.417822777	1.949241029
H292	5.175866991	8.385844788	-2.191141255
H293	3.991041414	5.638935738	0.912697932
H294	6.659311007	8.117475761	1.099824064
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H297	4.547600868	-7.381809901	5.257064957
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H302	-0.387298407	-1.824706968	-4.622056895
H303	1.533840859	2.581650846	-6.656620079
H304	3.452354797	-4.878729169	4.739538150
H305	3.160088426	0.540927217	-6.150243025
H306	3.424238595	-5.379641147	3.045918791
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H308	5.949466668	-5.648736469	3.140437245
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H322	7.338618177	-10.260859754	-2.431829700
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H328	4.345208404	-6.480938266	-6.935176348
H329	3.173791165	-5.104660215	-5.163339278
H330	6.142549529	-12.618695228	3.532060052
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H335	2.786891508	-3.104643035	5.423903833
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O428	-7.822467252	-3.208415177	3.037296837
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O434	1.198396201	-4.158830754	6.158966344
O435	0.774003949	-0.331691439	6.771701425
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O456	0.207080088	11.393901808	3.280487209
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	O474	3.594915789	-10.618427378	-3.652681296
	O475	5.272282070	-5.591887978	-0.905590427
	O476	5.068893017	-7.418931419	0.381164926
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	O478	8.767656277	-6.548725050	1.979496930
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	O480	-4.013281705	4.886959717	-2.789545308
	O481	8.231517079	-10.161109712	-1.983853067
	O482	7.580476981	-8.546731902	0.484189012
	S483	3.780463460	5.145370902	-1.460560110
	S484	2.564213607	2.124474854	-2.959809627
	S485	2.714789635	-3.014812940	-3.660933662
	S486	3.337274431	1.761985891	0.397121881
	S487	0.691144508	-0.585238271	-1.413328189
	S488	5.031538021	-0.280392795	-4.889420240
	S489	3.253666548	-3.413525045	-0.107512644
	S490	6.039193499	2.049615043	-1.984639425
	S491	6.134919374	-2.804559334	-2.266879656
	S492	6.334997751	-0.781431090	0.543437194
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N2 / H2 exchange 2N2 TS 35, S=3/2				
Fe(139) -2.278				
Fe(140) 0.750				
Fe(141) -2.450				
Fe(142) 2.571				
Fe(143) 2.123				
Fe(144) 1.222				
Fe(145) 1.208				
				
	bm52h2disn2dis2n2x3dtd 1 53373.49			
	C1	-7.731302269	-5.521351012	-0.381872383
	C2	-7.948168583	-6.593222062	-1.454346910
	C3	-8.772912291	-3.695698404	0.888340404
	C4	-8.340631975	-4.047637787	2.307960571
	C5	-8.160902344	-5.757558342	4.047723721
	C6	-6.643523969	-5.828023585	4.244143499
	C7	-4.431892564	-5.989536115	3.230533320
	C8	-3.959977881	-4.545709514	3.443932542
	C9	-4.375849797	-2.197638403	2.824845261
	C10	-4.644193940	-1.684472915	4.247421959
	C11	-6.022118620	-1.731919505	6.228225382
	C12	-5.106318024	-2.346013248	7.298525924
	C13	-4.235920462	-4.430049858	8.265864677
	C14	-2.724168296	-4.691727342	8.168748246
	C15	-0.844919344	-5.343856685	6.714926268
	C16	-0.049662952	-4.139394389	6.198726366
	C17	-0.252965161	-1.865699219	5.231699394
	C18	-0.290055327	-0.730535355	6.279151337
	C19	-0.950645468	-1.574190709	3.885087217
	C20	-0.697988908	-0.167518432	3.317107541
	C21	-0.595314273	-2.673755207	2.876765657
	C22	-1.609447400	0.941591296	7.502832066
	C23	-1.466076934	0.519430975	8.977806832
	C24	-2.906581875	1.743961638	7.230459482
	C25	-3.131329535	2.826130528	8.292351756
	C26	-2.865386310	2.373284379	5.830983847
	C27	-2.170696962	-0.926135102	10.791205773
	C28	-0.761139674	-1.178767263	11.287897251
	C29	5.432665077	-11.802069848	3.775072735
	C30	6.122740685	-10.488233907	3.431079401
	C31	6.251091273	-8.104876561	4.141433595
	C32	7.309250408	-7.751308978	5.203291073
	C33	5.009364582	-7.206702842	4.255141083
	C34	5.327131851	-5.732954799	4.030454833
	C35	4.063466073	-4.896660858	3.837485834
	C36	4.282818191	-2.418628783	4.131272674
	C37	9.527201192	-6.782690435	5.579225980
	C38	9.720578953	-5.288653521	5.717084788
	C39	-4.969228394	-2.590573129	-2.607518841
	C40	-5.434441892	-1.201637287	-2.131429207
	C41	-3.456821581	-2.718933349	-2.312790429
	C42	-2.863842745	-4.136465921	-2.442835105
	C43	-2.364579284	-4.519205366	-3.836303480
	C44	-5.801970542	1.100440520	-2.937253253
	C45	-7.040898586	1.475403484	-2.114412156
	C46	-5.760910596	1.810590814	-4.296979116
	C47	-9.329249829	0.870976076	-1.477480788
	C48	-9.175235354	0.784583511	0.044858394
	C49	-7.757129593	0.151164777	1.941450368
	C50	-6.647366113	1.094057577	2.407353128
	C51	-5.002644986	2.817646065	1.855846919
	C52	-5.571290116	4.068749648	2.566395721
	C53	-4.225431199	3.354411150	0.645015586
	C54	-3.466000342	2.363617039	-0.171072233
	C55	-3.043877566	1.074851118	0.037780429
	C56	-2.300396305	1.711136803	-1.964191857
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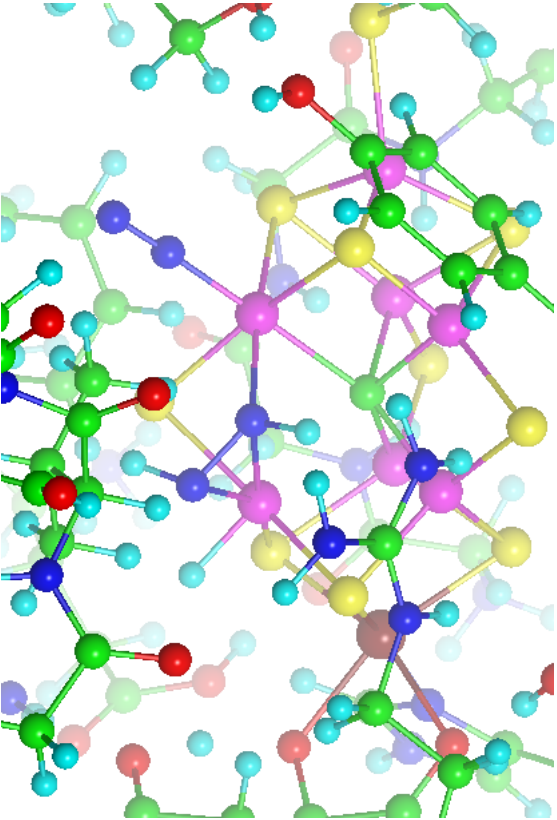
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C62	-10.514242837	8.743835625	0.730611389
C63	8.545558111	1.465633225	4.926782483
C64	9.604786267	0.381162943	4.837995286
C65	7.209020441	0.826409526	4.482233990
C66	6.039544128	1.774910984	4.589837611
C67	5.279664000	1.871903294	5.770389610
C68	5.685698371	2.603313942	3.510184491
C69	4.198502742	2.754672048	5.870283997
C70	4.625707125	3.503854163	3.603016796
C71	3.872930775	3.569385912	4.779255150
C72	5.384679008	6.980086198	-0.029487274
C73	4.356711838	8.085082538	-0.318124206
C74	4.691667238	5.619345173	0.080259984
C75	3.591334500	9.780894672	-1.941119760
C76	2.170627055	9.403493259	-2.366634076
C77	0.601648886	7.501913266	-2.729749831
C78	-0.084721437	7.041246044	-1.418195583
C79	0.801946524	6.328733925	-3.718897941
C80	-0.401456280	5.456072030	-4.093713819
C81	-1.402451435	6.045376727	-5.100713256
C82	-3.022299746	7.909476793	-4.732433490
C83	0.109762225	5.947207051	0.764216317
C84	-0.228309698	7.094895309	1.726947310
C85	1.025699565	4.958238678	1.520354276
C86	0.686154087	9.098315438	2.791581201
C87	0.064665125	10.452991366	2.489583317
C88	-1.093550349	11.821211792	0.838937222
C89	-2.465320675	12.316245364	1.356393495
C90	-1.010447751	11.941500387	-0.684709019
C91	-2.043063622	11.110148542	-1.435716993
C92	-4.607366786	11.714092419	2.381381335
C93	-4.709044353	12.734613011	3.506271790
C94	-5.330790557	10.400154128	2.791067595
C95	-5.383742344	9.403425382	1.654930479
C96	-6.429876240	9.455396759	0.719582073
C97	-4.371859794	8.449310420	1.461985991
C98	-6.451538890	8.608667677	-0.389956423
C99	-4.363650092	7.609540387	0.343681637
C100	-5.406011454	7.702720789	-0.573317617
C101	5.548628402	-3.274697082	-8.520549397
C102	4.064470545	-3.067444814	-8.274233140
C103	2.390216128	-1.642406797	-7.118662229
C104	1.955964786	-0.253226716	-7.599049287
C105	2.303572683	2.161383235	-7.311773756
C106	3.470658509	3.144176963	-7.248190577
C107	5.635933225	3.792956288	-6.349101209
C108	6.430149075	4.086304430	-7.605962796
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C124	9.720035124	-5.961255356	-2.750435341
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C138	3.903881505	-0.503180942	-1.704017563
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	H188	2.314054154	4.344982924	5.635132662
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	H192	-1.812161019	-3.226372767	5.736159741
	H193	-0.731690622	-6.157087381	5.983088167
	H194	-0.377082701	-5.667837612	7.653342478
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N419	9.123559418	-6.543412966	-5.108721953
N420	5.017095964	-5.309628884	-4.054468526
N421	4.775849346	-6.168400322	-6.072765585
N422	9.750811188	-7.148223197	-2.086699705
N423	-0.231161278	2.470637242	0.266572942
N424	2.161913814	1.263451191	3.562495621
N425	0.643691586	2.011593140	-0.246077796
N426	2.652548836	0.400175379	3.065978727
O427	-6.634153033	-5.313724287	0.165952877
O428	-7.793762665	-3.188973551	3.023314984
O429	-6.159633568	-5.664401436	5.376570161
O430	-3.083291528	-4.245077477	4.274200794
O431	-3.881456239	-0.867859329	4.785347606
O432	-4.678637807	-1.649215526	8.235175657
O433	-2.009683965	-4.593066058	9.173900690
O434	1.196386784	-4.172629337	6.167557814
O435	0.763806799	-0.343853012	6.808101554
O436	-0.717714297	1.136846498	9.754627778
O437	-0.444721165	-1.108120822	12.466414099
O438	6.837816545	-10.401009715	2.412512984
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O440	10.777527447	-4.777341174	6.053058474
O441	-5.568713070	-0.897913155	-0.929663988
O442	-2.916732618	-4.092712371	-4.877288774
O443	-7.026021851	2.460818285	-1.355444519
O444	-5.778985382	3.237629823	-4.095333780
O445	-10.060331156	1.261094324	0.767554081
O446	-6.336903789	1.138967956	3.601159094
O447	-4.907044191	4.708728924	3.386261868
O448	-7.479019701	6.815575252	4.680062293
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O451	3.497486238	8.426803847	0.512764475
O452	1.340307409	10.306319835	-2.586599588
O453	-1.294974482	7.251885844	-1.240956079
O454	-1.189975027	7.012850780	2.501862574
O455	2.041976872	5.636405134	2.260260935
O456	0.217614571	11.408001788	3.261037378
O457	-2.813343299	13.490817548	1.170296460
O458	-3.226160564	11.041947197	-1.074245630
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O461	3.224118414	-3.903683001	-8.686449928
O462	1.123399558	-0.103649127	-8.517128591
O463	3.346170907	4.251220160	-7.797269422
O464	7.160612977	5.057404509	-7.719259775
O465	-3.494459862	-2.017155778	-9.693637235
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	O469	10.515634754	-5.047237778	-2.456956367
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	O471	0.627325065	-6.138162849	-1.752339110
	O472	-0.214353711	-7.330893257	-0.040108288
	O473	5.806567762	-10.603650435	-3.242825710
	O474	3.584880478	-10.627198899	-3.660130993
	O475	5.308690705	-5.644122686	-0.899800271
	O476	5.067202563	-7.467273489	0.388820582
	O477	3.015075679	-5.924823178	-2.120413034
	O478	8.773804734	-6.549218162	1.972581702
	O479	6.877461928	-4.519777269	1.180020349
	O480	-4.025437149	4.888621996	-2.788852461
	O481	8.212337198	-10.161947705	-1.990085273
	O482	7.580008947	-8.546369368	0.483516922
	S483	3.786153652	5.136214726	-1.465765179
	S484	2.547004643	2.179804123	-2.887228217
	S485	2.687196452	-3.058198681	-3.575066170
	S486	3.628811136	1.839603807	0.428817447
	S487	0.718984272	-0.718849414	-1.586706033
	S488	4.949078489	-0.317755958	-4.894516137
	S489	3.369519691	-3.435509911	-0.033942206
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	C4	-4.844927548	-6.982360655	-4.642048448
	C5	-4.367850961	-9.258076657	-3.871616424
	C6	-3.242087947	-8.994463080	-2.869963139
	C7	-1.107436490	-7.892710725	-2.430423367
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	C9	-2.979587085	-4.794328162	-1.208340663
	C10	-3.929456725	-5.349575121	-0.137753965
	C11	-5.665000346	-6.913658176	0.465356156
	C12	-4.980756099	-7.725398740	1.574682898
	C13	-3.461234344	-9.578279500	2.087507502
	C14	-2.190459656	-9.196441747	2.859703907
	C15	0.004484239	-8.081454853	2.780654274
	C16	0.115708442	-6.629603255	3.248516871
	C17	-1.024712684	-4.429864494	3.266146942
	C18	-2.072264029	-4.155831679	4.356917337
	C19	-1.172644300	-3.571913207	1.988773346
	C20	-1.219099305	-2.082781191	2.345930059
	C21	-0.042385477	-3.884029981	1.003432213
	C22	-4.452608260	-4.115841598	4.964641145
	C23	-4.595543598	-5.288850059	5.955444608
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	C25	-6.929745661	-3.643454380	5.226382874
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	C27	-4.854546146	-7.674740385	6.314327940
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	C31	7.919784528	-6.666759158	4.047721946
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	C40	-2.645927534	-1.273327326	-5.188307532
	C41	-0.253040293	-1.726239101	-4.636620162
	C42	1.033828415	-2.549633155	-4.842446821
	C43	2.118659272	-1.885943697	-5.690562381
	C44	-3.933433776	0.828305588	-5.226055946
	C45	-5.358100976	0.259382077	-5.220132257
	C46	-3.843854909	2.163316376	-5.977457783
	C47	-6.958861878	-1.256061112	-6.290952372
	C48	-7.308235474	-2.161658666	-5.105018005
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	C50	-6.338227642	-2.584162664	-1.799843791
	C51	-5.948112036	-0.442504027	-0.676149700
	C52	-7.317916272	-0.042218170	-0.066670079
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C72	0.131154420	6.964769467	5.471845096
C73	-1.171636254	7.649903318	5.022777298
C74	0.324780603	5.638382213	4.735601154
C75	-2.161486261	9.630742315	3.925242359
C76	-2.870279095	9.165463314	2.651027621
C77	-2.848464868	7.436008919	0.850920490
C78	-3.545373241	6.117543534	1.274723998
C79	-1.698767249	7.203895721	-0.154361333
C80	-1.966537388	6.395342098	-1.428638265
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C82	-5.105388356	7.801269094	-2.627399680
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C93	-11.940875985	6.148394826	4.071706200
C94	-10.829445950	4.610784019	2.404887690
C95	-9.912032791	4.507344488	1.206625666
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C101	8.930954880	4.139360612	-4.065878817
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C104	4.241681909	4.854917809	-4.544969626
C105	3.038926650	6.638144105	-3.352645121
C106	3.342033497	7.664865540	-2.264801935
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C108	5.103794867	9.480237176	-0.548684999
C109	4.080888971	3.154317771	-8.781124929
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C113	5.920921288	0.224664277	-7.034277366
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C117	0.120992953	3.382601480	-5.834820413
C118	-0.207547957	4.255585428	-4.785232350
C119	1.029097036	2.335606677	-5.594814005
C120	0.427307879	4.132481299	-3.545258019
C121	1.650679692	2.208870491	-4.353498198
C122	1.384337732	3.137533023	-3.341337280
C123	11.164239644	0.470847625	0.269154738
C124	11.610868185	0.019920632	1.670368457
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C126	9.442617207	-0.105190509	-1.563836528
C127	10.031725008	0.218574037	-2.768529851
C128	7.843012986	0.041978939	-3.055872334
C129	12.445412172	-1.729860101	3.129136787
C130	13.482508009	-0.831323685	3.766587901
C131	4.597422132	-4.654870374	-2.176504242
C132	5.522242475	-4.559605038	-0.966383822
C133	6.735431452	-3.602330402	-1.162180168
C134	7.771166323	-4.252811063	-2.120319537
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Fe140	1.602473022	1.718346344	0.886742344
Fe141	3.678567510	2.343799977	2.827304709
Fe142	3.722906328	3.681074552	0.599158848
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Fe144	5.138859754	0.563429507	1.785248255
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H147	-0.063126800	-5.318301985	-7.407097625
H148	-4.243188595	-6.339441893	-7.830406152
H149	-2.030816513	-5.824727102	-8.676502358
H150	-1.852032641	-7.515160080	-8.220025556
H151	-4.679139729	-5.005968745	-5.393035169
H152	-4.235514556	-8.500860555	-5.880532501
H153	-5.870884920	-6.004984528	-6.252909951
H154	-4.203872316	-10.238371004	-4.338452230
H155	-2.174018346	-7.932837782	-4.276114970
H156	-5.296354204	-9.306080157	-3.290004324
H157	-2.222398733	-4.196635205	-0.686395488
H158	-2.514143836	-5.822482788	-3.032104664
H159	-0.262381238	-7.512615108	-3.021394664
H160	-6.222877829	-6.106716751	0.958372509
H161	-4.815286285	-6.628277866	-1.498915450
H162	-0.754531844	-8.729569187	-1.815759123
H163	-3.536463150	-4.126798249	-1.879857100
H164	-3.815173097	-8.688866329	0.172126551
H165	-6.379387443	-7.564258121	-0.057663589
H166	-0.020948673	-4.949092819	0.737537833
H167	-0.183997366	-3.316278074	0.070160745
H168	0.934297372	-3.584408589	1.408161009
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H170	-3.235687951	-10.488919268	1.513761351
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H173	-7.108510501	-4.576991777	5.778931571
H174	-0.275087106	-1.750902938	2.804154328
H175	-2.040327403	-1.850032600	3.040714764
H176	3.302609883	0.349453646	10.003435034
H177	-6.560673494	-2.224665350	2.920405869
H178	-7.853690701	-3.380546319	4.691629601
H179	-5.329464433	-1.643781364	4.066133412
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H181	-5.996442290	-4.603669508	3.538511490
H182	-4.160525487	-3.261498429	5.593700197
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H187	-2.356283583	2.818485989	5.335986669
H188	-2.639441590	0.704344084	6.941329619
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H191	1.183416000	-1.249617077	8.548333495
H192	-1.712430107	-6.279760756	2.440688658
H193	0.818213359	-8.253717711	2.060940545
H194	0.182766929	-8.725474653	3.651308145
H195	-1.435593644	-8.169072500	1.213788772
H196	-4.214805314	-9.823814234	2.844834078
H197	-1.191122431	-0.761736815	8.018746468
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H200	-4.764708987	-8.590283168	5.709932127
H201	-2.822616471	-7.280241730	7.144437825
H202	10.144963344	-5.380450779	7.683391209
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H204	5.148989891	-2.826628222	-2.420646660
H205	5.758002452	0.836257081	-9.067714232
H206	6.440272196	2.084756874	-7.990708321
H207	3.521183697	1.135558417	-8.160918975
H208	1.420566046	6.723523969	-7.670680322
H209	4.351066923	2.877539629	-9.812100475
H210	-0.002779308	-0.655884081	-4.556764231
H211	0.794653488	-3.516235961	-5.319031258
H212	2.649701815	4.558456483	-7.095863330
H213	0.407173701	4.656182555	-8.998079215
H214	4.789821068	4.568272100	-7.433306994
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H218	-1.266499359	-1.849431120	-7.782275189
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H221	1.458987663	-2.802207692	-3.859825093
H222	-5.440868523	-1.039503957	0.094577032
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H224	-7.547951016	-3.705090265	-3.139352454
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H231	-13.621389412	3.712747873	-3.265706673
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H233	-5.765890084	1.452639858	-1.687845204
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H236	-5.999124532	-0.786395285	-2.796486281
H237	-5.865845581	-4.240957609	-3.075561434
H238	-7.765750296	-0.513186291	-6.358485570
H239	-1.182654047	2.482667923	-2.528341196
H240	-6.985156503	-1.863479357	-7.204997792
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H245	-3.823748028	5.839479304	4.432999782
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H258	-9.960372192	4.936525076	-2.196384763
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H260	-6.640708658	6.504473523	-2.164210881
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H266	-2.256999364	0.172218417	-6.502620342
H267	-1.300733658	8.193851626	-0.431303359
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H273	-1.553055329	-2.984201399	-5.808459474
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H276	-3.635374861	8.062788993	0.417814558
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H287	10.698291102	1.455796952	0.423243915
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H290	1.258938621	5.190293677	5.101645814
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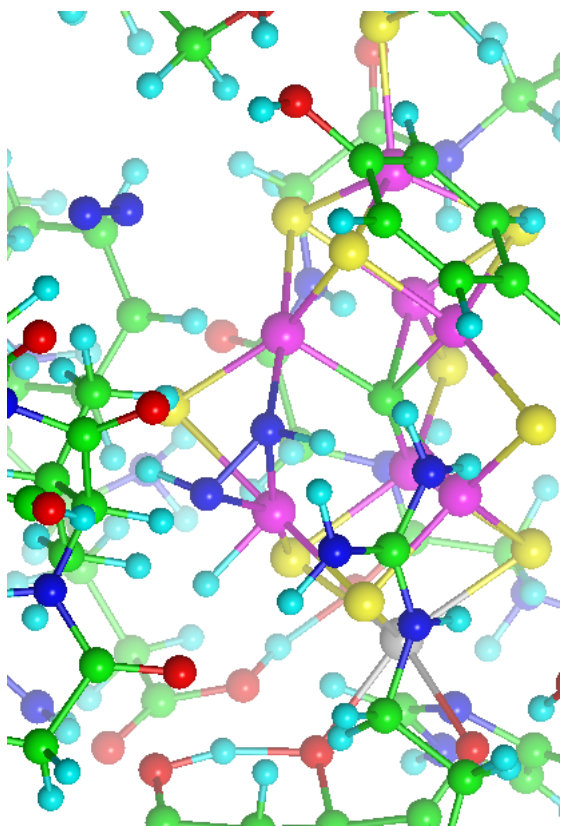
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H315	8.331049080	-11.180527924	1.944017274
H316	4.972675023	-2.622633128	3.919273468
H317	0.196988688	4.826431929	-2.734617740
H318	1.256611158	1.622115256	-6.390842300
H319	11.873654954	-4.267248781	0.630794919
H320	10.592446437	-1.482555450	-0.455821923
H321	9.479137830	-4.286882540	1.548074149
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H323	5.707811079	9.371616526	-1.481326048
H324	7.475370452	-2.045581194	2.455356480
H325	5.856106537	-5.566765480	-0.691570445
H326	6.616016340	4.456632254	-3.075129987
H327	7.906282202	-5.292469548	-1.782665418
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H329	6.885790204	0.016799952	-3.562000291
H330	10.542787283	-9.743923006	1.982312701
H331	3.755177743	-0.878675831	4.783756087
H332	8.851976667	-2.873889062	4.193686332
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H334	9.091706457	-4.849704709	5.444737335
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H340	-0.923461482	5.061786677	-4.963346335
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O429	-3.943500802	-4.889445733	1.015384557
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O432	1.152193584	-6.237202108	3.818560560
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O435	-3.971531513	-8.334717926	8.461121836
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O437	7.768961299	-7.678358455	6.247166947
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O439	-3.341968801	-1.790521201	-4.293301498
O440	1.843548056	-1.106403143	-6.631370327
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O443	-8.490820954	-2.475365494	-4.914514279
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O445	-7.423808446	0.264312212	1.124332997
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O449	-2.289978546	7.167662562	5.267562416
O450	-3.917558148	9.736245290	2.290748793
O451	-4.642188378	5.809553770	0.782778115
O452	-5.686596341	3.454833638	3.470174905
O453	-2.375311570	3.615090109	4.767074018
O454	-7.408510190	6.775887046	6.334074174
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O458	-7.304606815	4.570456869	-2.102534247
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O462	5.093760725	10.519098037	0.091551871
O463	1.894001926	3.072466882	-9.820243092
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O466	-0.523518298	6.589144295	-7.079750844
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O470	3.990465113	-5.680622998	-2.476665221
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O472	9.862602147	-4.898344103	-4.040269671
O473	7.561385239	-2.118111242	0.562685758
O474	7.859473679	-4.325172436	0.854319928
O475	6.235698438	-2.361791600	-1.665253632
O476	9.614043241	-3.442147485	4.463766835
O477	7.347043324	-1.999143946	3.436474092
O478	-4.813564435	4.090884166	-2.796521199
O479	12.581234398	-4.030104700	-0.009266925
O480	10.355298042	-4.442012731	1.990054305
S481	0.422802161	5.840223055	2.896881102
S482	1.516350153	3.958313815	0.234389480
S483	4.709804369	0.360204350	-1.879617606
S484	1.508139122	2.112055334	3.246023646
S485	1.635021149	0.787572144	-1.247660515
S486	5.380822182	4.084748722	-0.807020444
S487	4.696359546	-1.546219600	1.165221224
S488	4.059301566	4.540155058	2.653509601
S489	7.046889852	1.199993980	0.842804043
S490	4.983324830	0.962765603	3.936787545
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Fe2-brNH-NH-Fe6
2N2 dissociated
35, S=3/2

Fe(139) -2.056
Fe(140) 1.127
Fe(141) -2.301
Fe(142) 2.124
Fe(143) 1.372
Fe(144) 2.472
Fe(145) 0.162



bm526hx26n2h22n2xdtc.car_4

C1	-7.726926474	-5.334931881	-1.185212515
C2	-7.809604727	-6.356279643	-2.325913102
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C4	-8.641349169	-4.038022602	1.500044750
C5	-8.661876402	-5.848665509	3.146843375
C6	-7.164664034	-5.978105465	3.446697326
C7	-4.906059460	-6.171064223	2.534961758
C8	-4.397499929	-4.768444829	2.878397708
C9	-4.619492758	-2.363221282	2.447017808
C10	-4.967955411	-1.944036641	3.883128054
C11	-6.517431838	-2.011522199	5.731360033
C12	-5.687826383	-2.696815072	6.826349176
C13	-4.902526889	-4.832438880	7.739151264
C14	-3.380633442	-5.035280251	7.745339208
C15	-1.357567473	-5.484423024	6.415016657
C16	-0.503982735	-4.282186483	6.005441982
C17	-0.594001831	-1.939259863	5.196710704
C18	-0.707998866	-0.820580025	6.245659282
C19	-1.109757889	-1.568348151	3.790527798
C20	-0.477576945	-0.261183460	3.306190174
C21	-0.862276263	-2.717796907	2.810154139
C22	-2.179972967	0.725345090	7.463304621
C23	-2.169273057	0.193487260	8.910101487
C24	-3.457720456	1.526554627	7.118776524
C25	-3.761511067	2.568741111	8.201019279
C26	-3.316038900	2.198141553	5.746586821
C27	-3.010579422	-1.398864238	10.535776245
C28	-1.642475572	-1.710342833	11.108946869
C29	4.972046231	-12.073715211	3.574788982
C30	5.717928710	-10.760554232	3.363366556
C31	5.872903514	-8.429161707	4.219110660
C32	6.858276117	-8.166157894	5.372358839
C33	4.665786062	-7.479673946	4.295924900
C34	5.072049085	-6.012517169	4.187997069
C35	3.870236709	-5.089523989	4.003919549
C36	3.969496235	-2.599489470	4.286444702
C37	9.019814372	-7.183012148	5.978656603
C38	9.196966701	-5.691809375	6.160460154
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C42	-2.697071209	-3.968443733	-2.822037323
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C49	-7.850591238	0.151766754	1.343852427
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C51	-5.073228490	2.782382957	1.571406134
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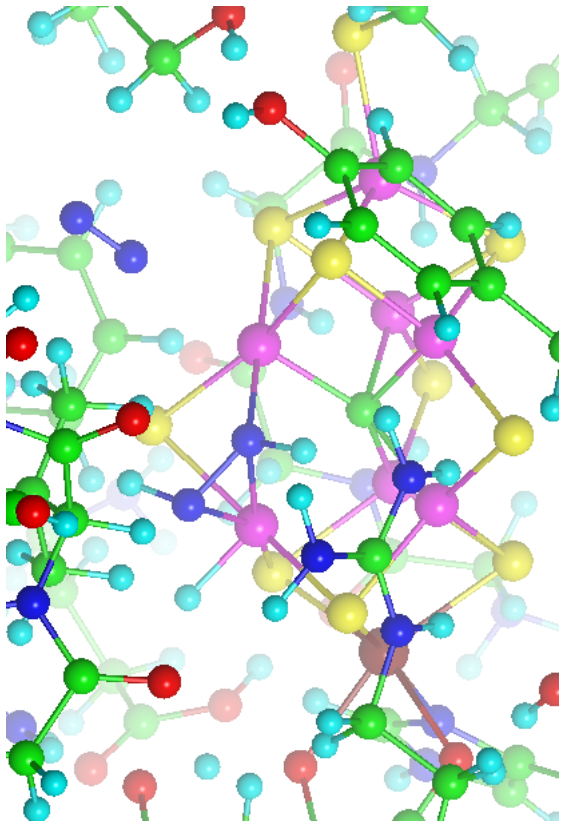
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C65	6.891085038	0.506940930	5.060789960
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C67	4.866675663	1.514214110	6.225925436
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C72	5.495073559	6.910978192	0.665003927
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C74	4.784451278	5.557251025	0.678343533
C75	3.854716523	9.812194213	-1.241853587
C76	2.467452885	9.473798124	-1.793849658
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C79	1.172125054	6.487359819	-3.370344707
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H321	6.573597441	-8.205495011	0.498528305
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	O470	4.007480543	-5.697657889	-2.514253708
	O471	11.404678275	-4.354183836	-2.476696020
	O472	9.889928254	-4.833993615	-4.086690761
	O473	7.537389923	-2.129768802	0.561415299
	O474	7.868595438	-4.334413099	0.828325799
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	O476	9.615135345	-3.451061497	4.462005963
	O477	7.345487684	-2.007165696	3.435041599
	O478	-4.802400441	4.089209376	-2.787114769
	O479	12.585015597	-4.042727910	0.001149607
	O480	10.353478394	-4.451487421	1.992166608
	S481	0.412758460	5.898738812	2.889103170
	S482	1.563336973	3.951402773	0.305168295
	S483	4.685593795	0.344377724	-1.886668855
	S484	1.422583088	2.219194141	3.062423506
	S485	1.648422645	0.788565496	-1.227310891
	S486	5.427471644	4.099150603	-0.805866554
	S487	4.705388487	-1.549851482	1.179838424
	S488	4.105714347	4.530499467	2.708625235
	S489	7.045398175	1.187792115	0.831801389
	S490	4.903846807	0.961024400	3.912887447
	end			
Fe2-brNH-NH2-Fe6 2N2 associated 35, S=1 Fe (139) -2.346 Fe (140) 0.124 Fe (141) -2.556 Fe (142) 2.597 Fe (143) 2.484 Fe (144) 2.337 Fe (145) -0.027			bm626x2nh6nh22n2xdt1f.car_4	
	C1	-2.350289601	-6.684021260	-6.504010976
	C2	-1.585004261	-6.916131982	-7.813110735
	C3	-4.577857881	-6.443496634	-5.490897320
	C4	-4.486966470	-7.385059712	-4.294198781
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	C6	-2.715008193	-9.166622878	-2.477101572
	C7	-0.683807279	-7.857238305	-2.147044479
	C8	-1.267261286	-6.743020447	-1.276402833
	C9	-2.878166706	-4.886689195	-1.154598942
	C10	-3.680749875	-5.412430116	0.045151311
	C11	-5.292764053	-7.006861138	0.889853436
	C12	-4.509831454	-7.725902684	1.995465761
	C13	-2.910416589	-9.495713126	2.528881629
	C14	-1.670531059	-8.896173899	3.197913848
	C15	0.320061102	-7.491712091	2.894587173
	C16	0.397510521	-6.018675905	3.277136866
	C17	-0.727383623	-3.807078022	3.208032467
	C18	-1.606749066	-3.471599899	4.423358150
	C19	-1.126988178	-3.030044632	1.937755288
	C20	-1.109061545	-1.525437258	2.225198434
	C21	-0.232188517	-3.462130542	0.773710837
	C22	-3.919655679	-3.364456691	5.283875083
	C23	-3.962746748	-4.548723844	6.263604930
	C24	-5.307651553	-3.028952219	4.683995938
	C25	-6.376212216	-2.901782292	5.774479016
	C26	-5.241117465	-1.745787675	3.846934637
	C27	-4.054814707	-6.955980627	6.566981309
	C28	-3.004954121	-6.976883172	7.658944787
	C29	10.139060485	-8.930468799	2.143116274
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	C31	8.330884382	-6.046146283	3.890511445
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	C34	6.293850234	-4.505704246	4.154376946
	C35	4.846684035	-4.260753086	3.713477483
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	C40	-2.697241732	-1.725275365	-5.108677580
	C41	-0.263972694	-1.992869837	-4.611853092
	C42	1.079444908	-2.722137596	-4.827658750
	C43	2.091174185	-2.009888365	-5.725746707
	C44	-4.100142982	0.306015849	-5.121743962
	C45	-5.494005263	-0.337001341	-5.090389981
	C46	-4.093064153	1.639622213	-5.881416246
	C47	-7.023101046	-1.955572655	-6.116472758
	C48	-7.317606981	-2.843078371	-4.901554888
	C49	-6.444670576	-3.918344859	-2.878819144
	C50	-6.301291110	-3.109351985	-1.589533852
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	C52	-7.336244489	-0.629930720	0.106545127

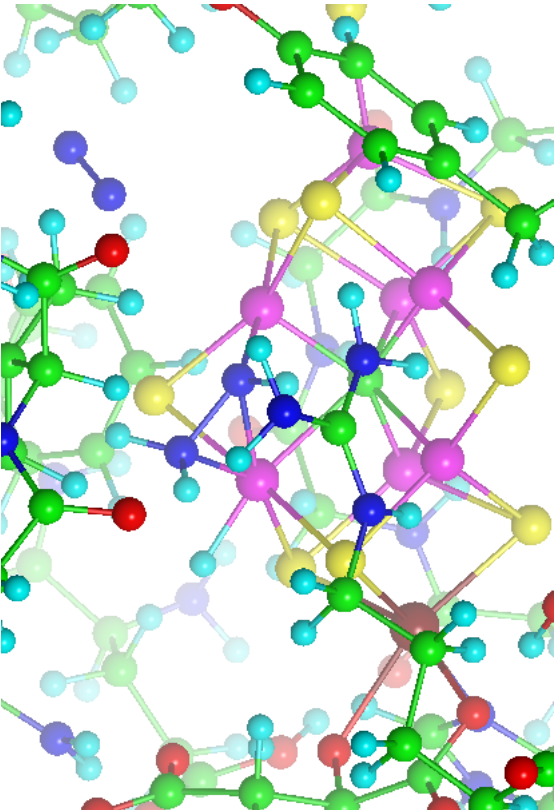
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C56	-2.089868291	1.499486785	-2.092730812
C57	-9.694639785	-0.120825321	-0.393900259
C58	-10.269283171	-1.058551384	0.667297931
C59	-10.580985051	-0.134893947	-1.660756666
C60	-11.827496396	0.700015309	-1.617970873
C61	-12.776309036	0.865400329	-0.627601220
C62	-13.313242556	2.056103879	-2.417619710
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C64	5.574284638	0.579955725	9.182302467
C65	3.614434793	0.296416870	7.706703188
C66	2.140311469	0.521363985	7.462511061
C67	1.173853571	-0.386493553	7.933194035
C68	1.690578499	1.657781410	6.765533862
C69	-0.190787431	-0.180253691	7.704675812
C70	0.332033719	1.884194095	6.543742947
C71	-0.607244406	0.958090370	7.004148014
C72	-0.149318523	6.875627559	5.375211029
C73	-1.491983757	7.492084591	4.941587507
C74	0.068719539	5.541337974	4.666879262
C75	-2.607297295	9.403819918	3.852170252
C76	-3.334638224	8.864709950	2.617952491
C77	-3.268391043	7.128527819	0.831682407
C78	-3.892869557	5.787923170	1.302794802
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C80	-2.416021029	6.068802459	-1.448956713
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C89	-9.631411215	7.173451530	3.755130538
C90	-7.725863219	8.606864146	2.907376969
C91	-7.780053768	8.063682197	1.485922509
C92	-11.170418207	5.359618060	3.146088849
C93	-12.178087624	5.403104244	4.286836876
C94	-11.028274841	3.903394446	2.618636300
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C99	-7.916362169	3.651001894	0.387176144
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C103	4.752565683	3.798970297	-4.582333651
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C107	3.642981876	8.329888223	-0.304797874
C108	4.455746258	9.553270451	-0.680001991
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C113	5.733888548	0.419720892	-7.198400574
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Fe139	5.143640448	2.119026648	-0.540372420
Fe140	1.372249823	1.806310130	0.875807312
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Fe143	1.692646100	4.220772030	2.348246764
Fe144	5.188680998	0.807126129	1.603041307
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H154	-3.596599161	-10.562799469	-3.865110509
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H240	-7.019256446	-2.589981739	-7.012413203
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H267	-1.781572022	7.910790119	-0.510666195
H268	-6.835815182	3.563766382	0.503624338
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H301	2.519357380	7.189090426	-4.525321256
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O455	-7.678688929	6.354649571	6.408301608
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O462	2.139307712	8.817761349	-2.555751204

	O463	4.435176801	10.594275216	-0.043575768
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	O465	5.409632061	-0.761242873	-7.236150014
	O466	6.420728716	0.898317425	-6.137815014
	O467	-1.173182832	6.252898718	-7.104896906
	O468	11.647826395	1.520634907	2.265902771
	O469	13.879872650	0.081034562	4.539788255
	O470	4.767579015	-3.130074827	-3.021735455
	O471	4.205319779	-5.273444702	-2.583708594
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	O473	10.226293103	-4.382889829	-4.329101372
	O474	7.800001162	-1.754974315	0.373404217
	O475	8.231488691	-3.945527910	0.642790308
	O476	6.616656830	-2.034732260	-1.911659679
	O477	10.019839657	-2.807028093	4.210377923
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	O479	-5.133036037	3.603070750	-2.751257322
	O480	12.862363397	-3.278961629	-0.324340523
	O481	10.720124154	-3.839780957	1.742838221
	S482	0.106828661	5.740041009	2.825406820
	S483	1.304718688	3.999065581	0.148813638
	S484	4.688562063	0.448646572	-1.945193308
	S485	1.459279785	2.200304268	3.210966124
	S486	1.379855798	0.869588380	-1.254325856
	S487	5.045932549	4.269094141	-1.061517449
	S488	4.841198638	-1.269746157	0.892773225
	S489	3.882364815	4.708989771	2.448106363
	S490	7.012191449	1.676786530	0.639464542
	S491	5.109207711	1.289098388	3.754305418
	end			
Fe2-brNH-NH2-Fe6 2N2 dissociated 35, S=1 Fe(139) -1.875 Fe(140) 1.120 Fe(141) -2.327 Fe(142) 2.091 Fe(143) 1.184 Fe(144) 2.512 Fe(145) 0.170			bm626x2nh6nh22n2xdt1b.car 4	
	C1	-2.343019338	-6.668544132	-6.496106681
	C2	-1.579806454	-6.907569059	-7.804882030
	C3	-4.572994182	-6.435987093	-5.484423185
	C4	-4.484121999	-7.380349959	-4.289711622
	C5	-3.830394076	-9.576007779	-3.437101431
	C6	-2.710926435	-9.164613149	-2.474654913
	C7	-0.680547644	-7.853677217	-2.144336278
	C8	-1.267151280	-6.739976214	-1.274916235
	C9	-2.880518286	-4.884965790	-1.157428108
	C10	-3.682708528	-5.409847767	0.042915441
	C11	-5.291632906	-7.006193625	0.890154922
	C12	-4.509192541	-7.725425277	1.996242932
	C13	-2.911070779	-9.495825170	2.529311151
	C14	-1.669553965	-8.896903840	3.196961917
	C15	0.319054924	-7.492404707	2.891862503
	C16	0.397449724	-6.019700829	3.274352723
	C17	-0.725273785	-3.806674729	3.205838366
	C18	-1.604048712	-3.467572519	4.421483462
	C19	-1.127948929	-3.033113975	1.934958808
	C20	-1.108051519	-1.528051892	2.209699734
	C21	-0.235732820	-3.463899295	0.769175153
	C22	-3.917705571	-3.358876640	5.282414707
	C23	-3.958471005	-4.542788149	6.262587041
	C24	-5.306181663	-3.025562691	4.683708480
	C25	-6.375417927	-2.900282957	5.774218346
	C26	-5.242050472	-1.742448055	3.845879911
	C27	-4.048738965	-6.950744467	6.562859398
	C28	-3.001654729	-6.972464239	7.656948850
	C29	10.132183487	-8.923676015	2.135008269
	C30	9.897199473	-7.480860871	2.584199423
	C31	8.329077466	-6.042738548	3.890845754
	C32	8.635918518	-6.067569792	5.401900162
C33	6.828518253	-5.834434928	3.621483853	
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C40	-2.691760307	-1.718092049	-5.099214941	
C41	-0.254845308	-1.985990484	-4.601578359	
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C44	-4.103295065	0.306101847	-5.125512567	
C45	-5.495026242	-0.339112798	-5.093993599	
C46	-4.095962926	1.640562654	-5.883774531	
C47	-7.022911600	-1.960239012	-6.116857369	
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C51	-5.950627368	-0.938572155	-0.526958250
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C67	1.174837582	-0.380172089	7.935028013
C68	1.696938876	1.652342323	6.749354691
C69	-0.188845121	-0.174739861	7.701552710
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C71	-0.602244671	0.958226015	6.990565067
C72	-0.137556209	6.898054788	5.383928003
C73	-1.484012223	7.506145333	4.948158487
C74	0.100625822	5.578953327	4.659627136
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C76	-3.336096244	8.872449998	2.620797478
C77	-3.270802696	7.135367588	0.834997590
C78	-3.888237232	5.795337534	1.313357481
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C82	-5.651308968	7.286223768	-2.606650412
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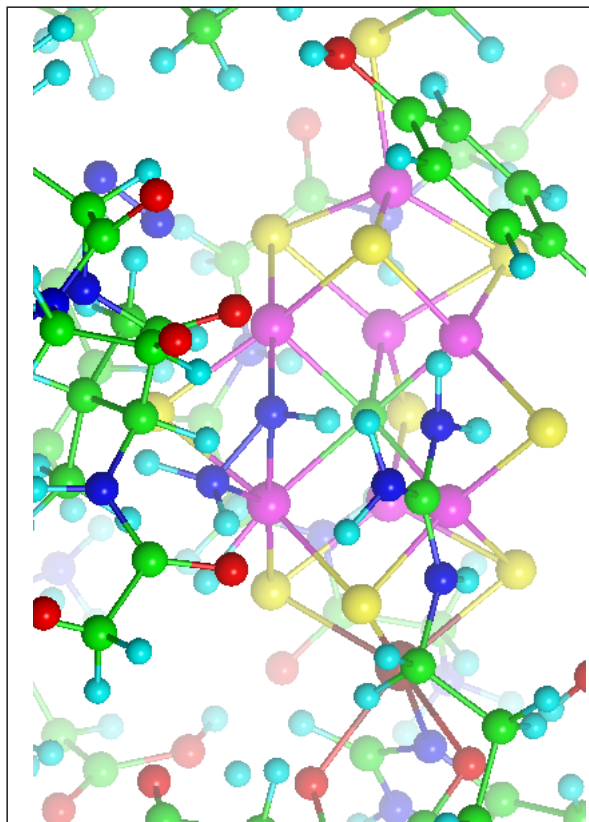
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N399	-8.362065688	-0.583465834	-0.776284894
N400	-12.172378154	1.448362951	-2.732466858
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N411	-7.220328596	6.518771079	4.174560268
N412	-6.726650036	8.418636778	0.699924141
N413	-9.868771756	5.851387343	3.577555193
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N419	1.540716427	4.109182049	-7.994157232
N420	12.235722279	1.608555710	-0.965058424
N421	8.160338702	0.335174657	-2.054591364
N422	8.954959276	0.861848769	-4.039595907
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N424	-1.931159722	2.133167239	0.674017611
N425	-1.103339769	1.507551691	1.073772373
O426	-1.787512847	-6.449668025	-5.406136045
O427	-4.808931536	-6.982764717	-3.155804916
O428	-2.768400884	-9.473318851	-1.273567995
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O430	-3.632884085	-4.855088917	1.153092221
O431	-4.727418436	-7.503260417	3.198367412
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O433	1.452531564	-5.596511172	3.782167732
O434	-1.107135748	-3.106966348	5.497832741
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O436	-3.155298080	-7.564250333	8.714989171
O437	10.703327573	-6.586587253	2.255236386
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O441	1.738554708	-1.350486834	-6.729682882
O442	-6.304710650	-0.054218106	-4.192407778
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O444	-8.478614433	-3.220218738	-4.692659867
O445	-6.427485451	-3.673163384	-0.495153353
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O447	-10.995482386	-0.705148740	1.577610120
O448	6.007879734	-0.314629479	9.901603902
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O452	-4.976935752	5.417991840	0.855231313
O453	-5.819679358	3.088001520	3.657184713
O454	-2.577824344	3.389163749	4.887560823
O455	-7.690207537	6.362423058	6.411933800
O456	-10.540000348	8.020284343	3.799477907
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O458	-13.384547278	5.364795271	4.107942611
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O460	7.198254998	3.440128924	-6.044968327

	O461	3.326408423	5.292909789	-5.869475348
	O462	2.126786831	8.819424448	-2.558044250
	O463	4.440830459	10.603582799	-0.043674019
	O464	1.406981391	2.906337484	-9.926471857
	O465	5.415553716	-0.762405301	-7.235506941
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	O467	-1.174104836	6.250039547	-7.098502260
	O468	11.650416672	1.521821287	2.267602947
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	O471	4.206188214	-5.278432616	-2.577281966
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	O473	10.229945359	-4.378610237	-4.334952558
	O474	7.818633743	-1.731444371	0.345943164
	O475	8.226650979	-3.923112612	0.642639690
	O476	6.616510143	-2.031751988	-1.933711234
	O477	10.019465642	-2.805419102	4.209755840
	O478	7.724483860	-1.466867523	3.191080987
	O479	-5.127257674	3.602418477	-2.752848310
	O480	12.857899380	-3.276826058	-0.324782241
	O481	10.716840939	-3.835531688	1.740577206
	S482	0.165478550	5.789139644	2.822277519
	S483	1.343854645	3.873742622	0.195661982
	S484	4.651697195	0.435579072	-1.993028418
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	S487	4.980344407	4.217287288	-1.059343317
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	S491	5.062685047	1.249190163	3.758493432
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Fe2-brNH-NH2-Fe6 2N2 TS 35, S=1 Fe(139) -2.509 Fe(140) 0.726 Fe(141) -2.576 Fe(142) 2.554 Fe(143) 2.338 Fe(144) 2.140 Fe(145) 0.097		bm626x2nh6nh22n2xdt1f_1_53327.67		
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	C3	-4.539997741	-6.406994305	-5.459534899
	C4	-4.454031934	-7.350923986	-4.264820553
	C5	-3.795447698	-9.539681487	-3.399915550
	C6	-2.667660195	-9.128139546	-2.447211981
	C7	-0.648356872	-7.806536508	-2.114698865
	C8	-1.249142281	-6.688654981	-1.261082698
	C9	-2.888476899	-4.854089809	-1.173952234
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	C13	-2.906794011	-9.494177720	2.533619859
	C14	-1.653240025	-8.903200796	3.185825896
	C15	0.295296959	-7.443273823	2.883428458
	C16	0.349415192	-5.973269627	3.281911584
	C17	-0.739175051	-3.746539316	3.154517636
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	C20	-1.172540749	-1.458719300	2.191082499
	C21	-0.291547018	-3.372055806	0.711742353
	C22	-3.910698934	-3.346560767	5.272440535
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	C28	-3.056664582	-6.970774361	7.669180785
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	C30	9.897173467	-7.497720231	2.560953877
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	C33	6.853996736	-5.830049791	3.604976380
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	C35	4.892877619	-4.229001925	3.665211838
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	C42	1.081724714	-2.727259565	-4.840770584
	C43	2.092782393	-2.012918531	-5.737242189
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	C46	-4.100597860	1.630165705	-5.855981380
	C47	-7.016017225	-1.986081193	-6.107013322
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C49	-6.444087364	-3.934065795	-2.859597936
C50	-6.297659740	-3.123015152	-1.572816537
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C52	-7.341264161	-0.647081298	0.114407838
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C54	-3.899647095	0.438091463	-1.276205247
C55	-2.833372157	-0.424545740	-1.187330716
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C61	-12.755407852	0.884843033	-0.634208895
C62	-13.321546655	2.035190301	-2.441541906
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C68	1.686541789	1.646708650	6.770658124
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C72	-0.147867961	6.869161362	5.382886731
C73	-1.487565511	7.489332379	4.951017184
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C75	-2.600045124	9.400602467	3.859643343
C76	-3.326016069	8.854767758	2.627953243
C77	-3.256561438	7.133376652	0.832931635
C78	-3.886296653	5.794228110	1.301302909
C79	-2.123503643	6.914023760	-0.195837536
C80	-2.401527230	6.066956076	-1.444809355
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C82	-5.648057853	7.277421427	-2.597881492
C83	-3.729921844	3.787129022	2.696235302
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C86	-5.772456513	5.141313443	5.583834436
C87	-6.967351502	6.065355919	5.423024806
C88	-8.154473406	7.606967438	3.965148174
C89	-9.627269375	7.171897315	3.760758468
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C91	-7.779453877	8.049113972	1.470344787
C92	-11.168271860	5.361048119	3.144716765
C93	-12.157232110	5.396758144	4.299616721
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C95	-10.139490781	3.819637865	1.389580546
C96	-10.679078275	4.000161519	0.106512929
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C98	-9.865803960	4.001060040	-1.027680727
C99	-7.919664598	3.636936694	0.378035430
C100	-8.487939504	3.837681679	-0.875867140
C101	8.476455676	4.588645741	-4.349962084
C102	7.187668945	4.070925194	-4.962943427
C103	4.749726064	3.785486576	-4.580512324
C104	3.740587370	4.929487893	-4.744703577
C105	2.461382689	6.649951143	-3.542528409
C106	2.704449935	7.704215621	-2.466376733
C107	3.620879819	8.321027760	-0.294497416
C108	4.483033586	9.518528630	-0.642940144
C109	3.606451630	3.145649138	-8.929848112
C110	2.093321876	3.381342459	-9.004848044
C111	3.911262181	1.916381241	-8.044929738
C112	5.356574164	1.428532545	-8.254931655
C113	5.740828552	0.424955051	-7.191324374
C114	0.113872526	4.384744966	-7.985035636
C115	-0.138298475	5.819458601	-7.565986066
C116	-0.778689475	3.336129325	-7.274536806
C117	-0.254204447	3.079378035	-5.891272894
C118	-0.588941928	3.932578915	-4.827060784
C119	0.741183432	2.105826132	-5.698868960
C120	0.134411245	3.879401039	-3.631643269
C121	1.456263349	2.049740756	-4.503137857
C122	1.184851554	2.969563065	-3.484527448
C123	11.145038322	1.160061007	-0.062326691
C124	11.667781937	0.735182302	1.318696532
C125	10.317234798	0.043098197	-0.714445998
C126	9.551267592	0.423768889	-1.940557977
C127	10.049592520	0.761858222	-3.180561449
C128	7.844911705	0.594091929	-3.306855662
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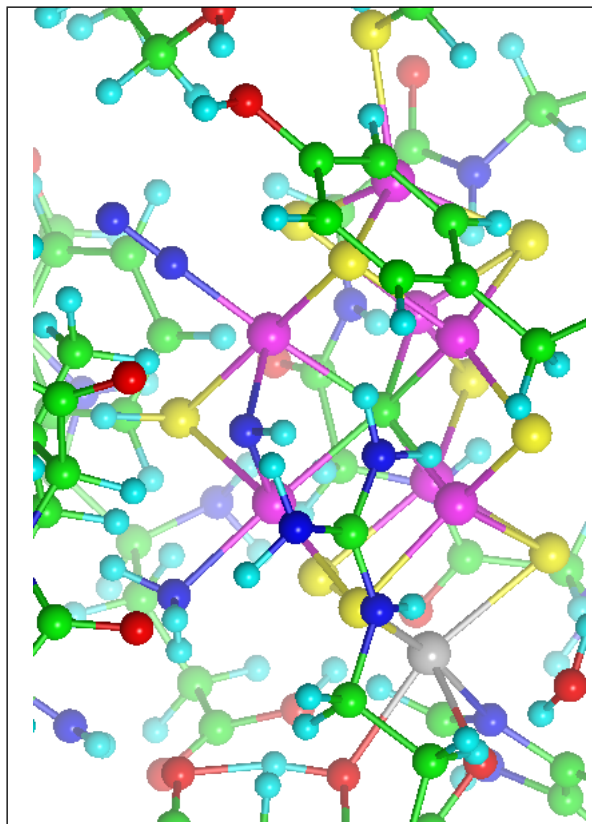
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C136	10.562498965	-3.823960156	-3.286371523
C137	7.766150892	-3.003685442	-0.039217201
C138	3.680857630	1.850554090	0.783914938
Fe139	5.149550007	2.130027860	-0.560555972
Fe140	1.582874719	1.833326517	0.846622508
Fe141	3.626035162	2.508436926	2.684724850
Fe142	3.465752304	3.768337221	0.406213714
Fe143	1.707237157	4.236699372	2.308090219
Fe144	5.155429274	0.780279471	1.575097726
Fe145	3.212045748	-0.046674777	-0.117638363
H146	0.298755331	-7.088939265	-7.111260878
H147	-0.054841403	-5.604348817	-7.693371535
H148	-4.133691496	-6.827266781	-7.507572574
H149	-2.120592571	-6.374706832	-8.637397321
H150	-1.733978205	-7.998613563	-8.080902389
H151	-4.285034977	-5.405673528	-5.082269593
H152	-3.760193773	-8.870346616	-5.445984618
H153	-5.585273894	-6.381618724	-5.795258434
H154	-3.572205515	-10.527802400	-3.821248618
H155	-1.689309379	-8.110488128	-3.955188650
H156	-4.702222972	-9.624207760	-2.787677857
H157	-2.225143711	-4.064908108	-0.807983632
H158	-2.318421229	-6.015206777	-2.876447667
H159	0.167307460	-7.405417475	-2.731145985
H160	-5.798062829	-6.146204389	1.377755380
H161	-4.537336328	-6.847116960	-1.128831843
H162	-0.224984565	-8.546854369	-1.425029666
H163	-3.583150871	-4.401262242	-1.892788615
H164	-3.465109421	-8.810421463	0.579979192
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H166	-0.512482815	-4.396906780	0.396783179
H167	-0.450547934	-2.709016076	-0.154156380
H168	0.774652324	-3.362852151	0.968802376
H169	-2.195999011	-3.255633229	1.643238091
H170	-2.606342888	-10.418834093	2.020051910
H171	-4.516770509	-1.789170860	3.036578604
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H173	-6.473265302	-3.834767689	6.358014508
H174	-1.507148044	-0.905815351	1.304166575
H175	-0.184584017	-1.067168069	2.471465339
H176	3.547188564	0.417026203	9.877641225
H177	-6.232154583	-1.527003835	3.395789213
H178	-7.343987977	-2.675847282	5.328724730
H179	-4.986011890	-0.870077842	4.486974955
H180	-6.122045031	-2.095059870	6.486725548
H181	-5.590912372	-3.855140078	4.020094596
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H184	-1.870788990	-1.210196355	3.004963945
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H191	1.478831114	-1.283764219	8.494869754
H192	-1.454665413	-5.614062862	2.386492529
H193	1.034322081	-7.570856917	2.076885354
H194	0.634686356	-8.026251151	3.748678688
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H196	-3.587983361	-9.763046048	3.351250164
H197	-0.935778885	-0.909764442	8.068540924
H198	0.283228190	-3.453826867	3.430641904
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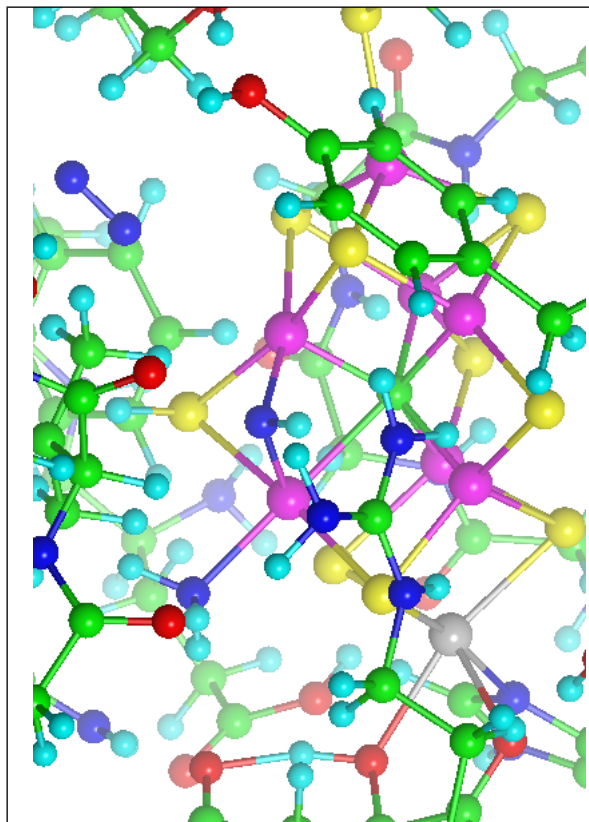
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	O460	-6.340646750	-7.742639403	-0.142722653
	O461	-3.637549317	-7.025443439	-3.408797832
	O462	1.039674084	-8.725248415	-3.490536973
	O463	2.769430002	-11.090479344	-1.013350908
	O464	-6.959104708	-4.471008967	-6.304813450
	O465	-8.371188398	-3.494260572	-0.509859102
	O466	-7.225234662	-5.259734449	0.232901958
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	O472	-9.131335305	-4.055040609	7.704738166
	O473	-9.903417336	-2.961737228	5.882392529
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	O480	-7.515141691	-4.765373471	9.804519062
	O481	-5.201906248	-2.827833675	9.855518544
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	S483	1.288658375	-3.958135169	-0.686083578
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	C5	-5.210884058	9.386033432	-1.039525312
	C6	-4.761760349	8.536890466	0.154628386
	C7	-4.772404127	6.350012511	1.239235864
	C8	-3.338777161	5.891107503	0.954464119
	C9	-1.677030992	5.354487313	-0.762243986
	C10	-0.644192989	6.432527624	-0.401493067
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	C12	0.113760300	9.078020354	1.125529966
	C13	-1.011960683	9.657709820	3.217529698
	C14	-0.812932828	8.548963733	4.257344957
	C15	-1.305601056	6.209291745	4.839338127
	C16	-0.361203523	5.037256893	4.576773720
	C17	0.988279614	3.778146709	2.909446972
	C18	2.461129374	4.232844464	2.977902103
	C19	0.605852999	3.192340669	1.536381420
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	C21	-0.810597963	2.613622642	1.574978191
	C22	4.217236881	5.634518877	1.947171525
	C23	4.483653112	6.743671480	2.977004125
	C24	4.550257562	6.082818859	0.500490882
	C25	5.922399716	6.763534837	0.416832291
	C26	4.486898070	4.895619358	-0.467977518
	C27	3.778829126	8.851137226	3.954940548
	C28	4.116118923	8.449891739	5.376499706
	C29	-6.938855075	1.656930280	11.652085640
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	C33	-2.934082253	1.258005411	9.097496969
	C34	-1.668878718	0.582545425	8.560426110
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	C37	-1.011353232	-0.633534946	13.015526791
	C38	0.408674557	-0.947908609	12.595942484
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	C40	-3.523617139	2.294460697	-4.357924045
	C41	-4.329408507	1.100541172	-2.295477130
	C42	-5.429796601	0.908117936	-1.230167653
	C43	-6.275076805	-0.360614707	-1.355404845
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C46	-1.899974396	0.244236819	-7.009961569
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C56	-0.317047415	0.055557236	-3.224344908
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C75	8.426466044	-5.560537711	-2.962304638
C76	7.550770457	-4.884921442	-4.021917591
C77	5.369674216	-3.760732111	-4.435018684
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C80	2.748625059	-3.709523107	-4.869796330
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C98	5.487487657	2.323660482	-8.910717204
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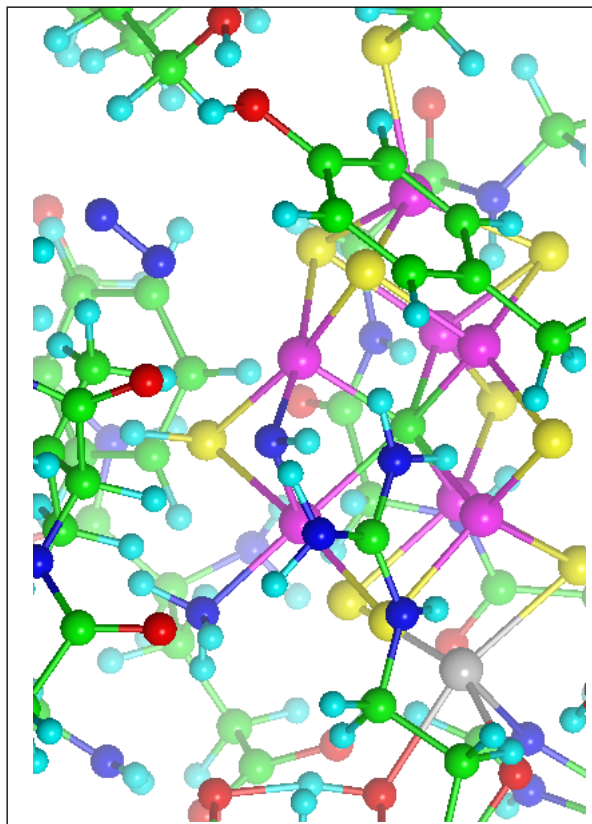
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C133	-5.744824720	-1.594916578	5.238820739
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Fe142	0.509725149	-4.929461240	1.159477362
Fe143	2.956985164	-3.976866852	0.907726642
Fe144	-0.704051930	-3.379941756	4.207932000
Fe145	-1.586626746	-1.720386434	2.139461902
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O441	-6.620706950	-0.818300168	-2.469821334
O442	-0.404128833	3.124571486	-6.935969759
O443	-0.619393018	0.151101742	-7.664729542
O444	-1.312529468	6.877474291	-7.465808290
O445	0.903168955	6.657228224	-3.331146205
O446	4.232621136	4.931393730	-4.105328561
O447	5.859142421	7.167689111	-6.308442719
O448	4.746044167	-1.791760850	10.390965355
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O450	8.425619660	-3.433054979	-1.131457223
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	O455	11.318893259	0.073323861	-3.659100371
	O456	11.289635980	0.119029573	-7.924793680
	O457	8.101908500	-0.797006693	-8.121217859
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	O459	3.696462762	0.972148805	-7.955841985
	O460	-6.337396725	-7.742415587	-0.151891614
	O461	-3.633212938	-7.002619544	-3.407090004
	O462	1.041493967	-8.718161423	-3.494657337
	O463	2.757421617	-11.107322692	-1.009119291
	O464	-6.952849241	-4.478664412	-6.304727480
	O465	-8.378777312	-3.499373503	-0.503740862
	O466	-7.229967629	-5.264454663	0.236411782
	O467	-2.139082758	-5.290848048	-7.670735073
	O468	-2.832253249	-7.670594217	8.791658761
	O469	-2.708807921	-7.462777651	12.257367536
	O470	-5.748702686	-0.502859189	2.547478381
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	O472	-9.147748815	-4.061137801	7.701242397
	O473	-9.925108918	-2.973112734	5.877555963
	O474	-4.015854477	-2.989302758	6.229387350
	O475	-5.030245218	-1.459393497	7.528501921
	O476	-5.357532583	-2.392916771	4.095959635
	O477	-2.527661642	-2.929981099	10.527146823
	O478	-1.672670384	-2.861115651	7.820584005
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	O480	-7.523117862	-4.765615568	9.797720583
	O481	-5.209661549	-2.833998438	9.851714198
	S482	4.799650091	-4.296688890	-0.410247919
	S483	1.243805981	-3.805865707	-0.641948471
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	S485	2.703210599	-2.099865555	2.108718304
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	S488	-1.997490591	-1.602854060	4.422790085
	S489	2.345901178	-5.663933005	2.327857143
	S490	-1.870404064	-5.272979893	4.543597498
	S491	1.192668341	-3.469046493	5.324361307
	end			
Fe2-brNH-Fe6NH3-S2BH 2N2 TS 35, S=1/2 Fe(139) -2.547 Fe(140) -0.477 Fe(141) -2.633 Fe(142) 2.561 Fe(143) 3.163 Fe(144) 2.251 Fe(145) -0.638		fe2brbhf6nh3s2bhdt2_2_53458.71		
	C1	-6.978986367	5.841784720	-3.098257332
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	C3	-5.025842533	7.010860854	-4.031829904
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	C5	-5.200778086	9.371702705	-1.032303559
	C6	-4.759406426	8.525668293	0.166887131
	C7	-4.770895779	6.341661758	1.256824193
	C8	-3.337996931	5.886241917	0.958370016
	C9	-1.703937034	5.356751251	-0.796027981
	C10	-0.668851500	6.425174510	-0.413794480
	C11	-0.056029619	8.763479761	-0.360558871
	C12	0.109301384	9.067046572	1.134154991
	C13	-1.017207594	9.668228369	3.220360989
	C14	-0.818320552	8.558392559	4.258583834
	C15	-1.289728531	6.209586469	4.818518242
	C16	-0.326075290	5.054048451	4.553867629
	C17	1.013277393	3.780245699	2.886947326
	C18	2.488850146	4.228524638	2.963623989
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	C21	-0.797216416	2.688641961	1.518370933
	C22	4.251129640	5.632268979	1.933859678
	C23	4.508866843	6.739626288	2.966270846
	C24	4.581542866	6.097173967	0.491347226
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	C26	4.512493155	4.924716975	-0.493859935
	C27	3.802124861	8.850728606	3.927972535
	C28	4.137133535	8.452664397	5.350917268
	C29	-6.950749961	1.669745321	11.650212677
	C30	-5.855161897	0.696576039	11.208354222
	C31	-3.492937351	0.601320476	10.394406603
	C32	-2.475013310	0.665475025	11.550523867
	C33	-2.945878142	1.244502822	9.105073463
	C34	-1.674326203	0.578442710	8.567664843
	C35	-1.290769244	1.124872152	7.186396193
	C36	0.931533657	0.720244136	6.047598067
	C37	-1.015116813	-0.636030411	13.023781811
	C38	0.401335611	-0.955503347	12.596957327
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	C40	-3.514244597	2.295359726	-4.356611851
	C41	-4.327133490	1.107098224	-2.297465721
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C43	-6.276251423	-0.354632964	-1.365735748
C44	-1.908976164	1.462129945	-6.064931365
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C47	-2.440527164	4.810043259	-7.828938909
C48	-1.786679989	5.863404155	-6.926212830
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C50	0.257879326	5.946946427	-4.103927819
C51	1.925492463	4.156467931	-4.012067420
C52	3.145143749	4.813449168	-4.683866059
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C54	0.976349945	1.819079356	-3.618037367
C55	0.078506701	2.052931424	-2.596880450
C56	-0.243870953	0.010436962	-3.194940902
C57	4.034241491	5.624813286	-6.826657029
C58	4.662593516	6.868914634	-6.202966151
C59	3.431740265	5.947166130	-8.214155521
C60	4.392730652	6.020764299	-9.362336476
C61	5.667954809	6.544894219	-9.446200844
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C64	4.837756037	-2.378160675	9.329296714
C65	4.460680920	-1.236010528	7.175057611
C66	5.038745887	-0.614083090	5.925923430
C67	5.442951829	0.733055251	5.900127856
C68	5.191638086	-1.369823478	4.749359609
C69	5.963149547	1.313334235	4.738302428
C70	5.721853265	-0.808607480	3.587153983
C71	6.096196758	0.536834271	3.580111264
C72	7.345401513	-4.713240621	0.638982072
C73	7.919850358	-4.508920625	-0.776479129
C74	6.103681468	-3.853148625	0.811465428
C75	8.410650940	-5.557347014	-2.960550778
C76	7.537436133	-4.875822666	-4.017759382
C77	5.353892654	-3.759301883	-4.436123361
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C80	2.734793780	-3.706894831	-4.865166818
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C82	3.847771628	-2.979040416	-8.262780166
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C84	6.798710019	0.152745375	-2.649706988
C85	5.197643592	-0.336190757	-0.821898931
C86	9.220236539	-0.084581516	-2.432513576
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C88	10.182800783	-0.889489430	-6.013114738
C89	10.481163211	0.274407485	-6.989874944
C90	9.619362742	-2.093832354	-6.774734730
C91	8.288320731	-1.817126823	-7.459796591
C92	9.900472659	2.549770946	-7.711173017
C93	11.246401284	3.256690634	-7.681861038
C94	8.762982989	3.562242245	-7.387501597
C95	7.385284407	2.949375662	-7.516205174
C96	6.719142396	2.950519414	-8.752417735
C97	6.751649827	2.321905938	-6.429984389
C98	5.477266573	2.330896338	-8.910082638
C99	5.521157592	1.674334611	-6.573866586
C100	4.896860450	1.680854931	-7.819499751
C101	-5.076800289	-9.158519505	1.329264211
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C104	-3.110713771	-6.783220370	-2.284279893
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C107	1.911491294	-8.835659914	-0.890500709
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C111	-7.076294653	-4.894438175	-3.063897739
C112	-8.124348921	-5.359831647	-2.035226476
C113	-7.951097608	-4.626614195	-0.723932694
C114	-4.208410105	-4.675919807	-6.571526427
C115	-3.110728789	-5.618930958	-7.022834900
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C117	-3.020206791	-3.137971200	-5.027941686
C118	-1.663444666	-3.488331574	-4.948909571
C119	-3.749415195	-2.945632527	-3.840418391
C120	-1.080073002	-3.744617925	-3.705753534
C121	-3.164178662	-3.205915637	-2.601572347
C122	-1.842100799	-3.657320206	-2.540591731
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C124	-3.912123167	-7.136443228	8.499913328

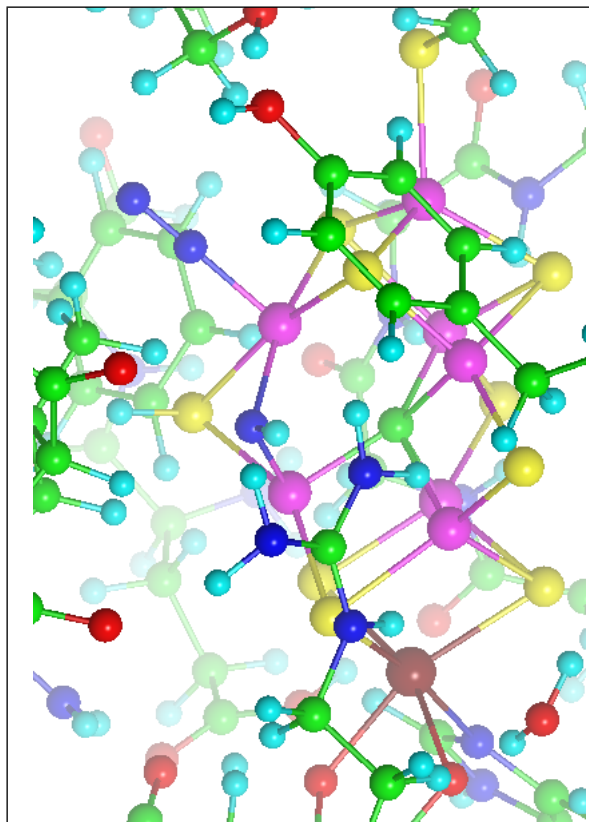
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C128	-5.765991833	-5.428315457	3.062533848
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C130	-3.572913619	-7.408781088	11.396942575
C131	-5.922297115	0.341343838	3.495362432
C132	-5.488971082	-0.120655176	4.900606286
C133	-5.750805318	-1.615731156	5.226616166
C134	-7.236829002	-1.858784492	5.578315886
C135	-7.560473901	-3.272432106	6.070982276
C136	-9.007789543	-3.438736189	6.585872183
C137	-4.882508708	-2.040366285	6.422454254
C138	-0.190751269	-3.496614319	2.288928240
Fe139	-1.754483716	-4.759410191	2.352850060
Fe140	0.641544097	-2.252764049	1.024480230
Fe141	1.597158667	-3.783590372	3.192507021
Fe142	0.498330615	-4.961044353	1.195059004
Fe143	2.967680046	-4.087640074	0.951038847
Fe144	-0.698113540	-3.398475486	4.220710447
Fe145	-1.496817818	-1.741852680	2.137102351
H146	-8.805474020	4.564725099	-1.542305213
H147	-8.424334240	3.497076181	-2.715342209
H148	-6.966883912	6.842376369	-4.894177009
H149	-8.561239475	5.187022965	-4.413211288
H150	-9.049914714	6.341493808	-3.176613554
H151	-4.403968177	6.103077863	-4.006741608
H152	-6.487585585	8.544618292	-2.547158082
H153	-4.791073795	7.549651847	-4.959155188
H154	-6.082442283	9.959924917	-0.746624215
H155	-5.863569437	6.908579449	-0.494278475
H156	-4.377972378	10.069369003	-1.239118870
H157	-1.363352754	4.407782901	-0.369164964
H158	-3.784012799	5.790303589	-1.040038321
H159	-5.433247674	5.465772537	1.288920951
H160	0.929926414	8.473141811	-0.743934772
H161	-1.878990884	7.921999761	-1.156625923
H162	-4.765078378	6.807653246	2.249273124
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H165	-0.381859155	9.678614434	-0.873515301
H166	-1.523301922	3.487371327	1.721855765
H167	-1.036241414	2.229636103	0.545923443
H168	-0.898386266	1.913303698	2.289697396
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H170	-1.969393519	10.167319073	3.450756895
H171	3.536222889	4.419730213	-0.474726781
H172	2.746551527	7.735356587	2.458584772
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H175	1.517186250	1.219612315	1.680613724
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H179	5.288228036	4.177611966	-0.260896372
H180	6.751684949	6.089172864	0.736540146
H181	3.817978354	6.842942209	0.201318474
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H191	5.333547737	1.348775723	6.796561428
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H193	-2.299535784	5.770558082	4.836233349
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H196	-0.204806870	10.390440524	3.374540091
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H198	0.906210064	2.993310844	3.643735722
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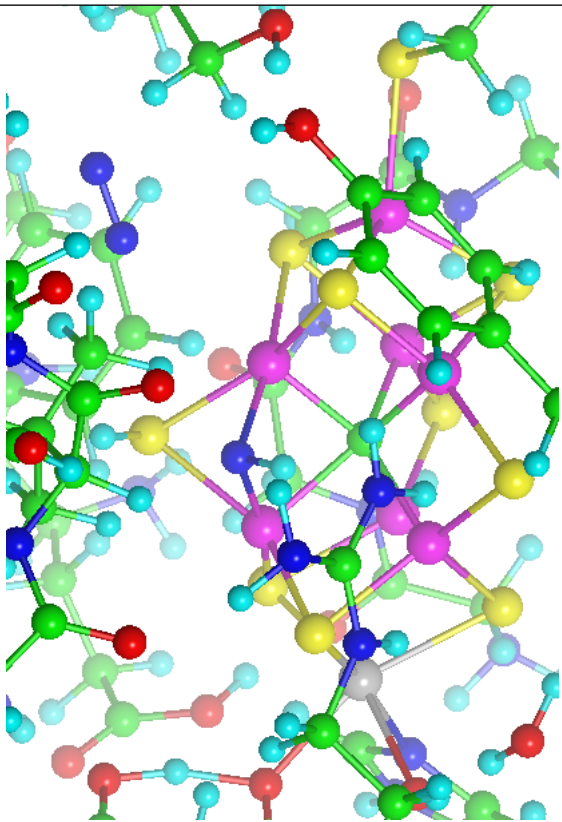
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C127	10.212790382	0.793761404	-2.491856120
C128	8.022386168	0.660562079	-2.789660422
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C130	13.411532922	-0.503802098	4.161916663
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C132	5.880485366	-4.277995165	-1.104379030
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C137	7.662509546	-3.148208955	0.265863425
C138	3.656001411	1.710695660	1.115884437
Fe139	5.225646621	2.049021654	-0.102772323
Fe140	1.291977178	1.626562839	1.072124555
Fe141	3.436434405	2.173147429	3.040881908
Fe142	3.485294956	3.646533941	0.894380782
Fe143	1.550816785	3.955879635	2.697432498
Fe144	5.040326875	0.521241691	1.926438942
Fe145	3.149748314	0.083563282	0.267285052
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H149	-1.637616178	-5.713431983	-9.169193810
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H151	-4.012139233	-4.978861113	-5.706483072
H152	-3.549670137	-8.416137252	-6.314195147
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H154	-3.423769084	-10.181736573	-4.812177196
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H164	-3.580795879	-8.719293475	-0.271538069
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H166	0.137250177	-4.169803064	0.226306554
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	O476	12.815851844	-3.509237450	0.229409086
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	S478	-0.010158196	5.502777482	3.221913011
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Fe2-brNH-Fe6-S2BH 2N2 dissociated 35, S=1/2 Fe(139) -2.334 Fe(140) 1.418 Fe(141) -2.530 Fe(142) 1.893 Fe(143) 3.069 Fe(144) 2.407 Fe(145) -1.455	bm602b26nh2n2x3dtb 5 53153.47			
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	C3	-8.965224887	-3.383678017	0.132128800
	C4	-8.685643531	-3.814512499	1.569038936
	C5	-8.718225203	-5.604923609	3.231907265
	C6	-7.212646107	-5.717643875	3.493224764
	C7	-4.979837866	-5.943316504	2.533286211
	C8	-4.419810458	-4.545153860	2.808756765
	C9	-4.620957615	-2.141842039	2.410286024
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	C11	-6.408337941	-1.622467322	5.736407472
	C12	-5.603640703	-2.336439962	6.830778357
	C13	-4.890506131	-4.483693273	7.756904061
	C14	-3.370353240	-4.649455875	7.648215361
	C15	-1.469119921	-4.968241905	6.128400813
	C16	-0.550202150	-3.849581875	5.644365247
	C17	-0.392781524	-1.573745924	4.642011754
	C18	-0.307196856	-0.472615289	5.718075093
	C19	-0.965232798	-1.069763074	3.301073813
	C20	-0.275006522	0.223604993	2.857158053
	C21	-0.850360687	-2.146225682	2.216962658
	C22	-1.548685640	1.232811893	7.007364313
	C23	-1.583395809	0.670600508	8.436719111
	C24	-2.738086150	2.183110859	6.716617293
	C25	-2.907774655	3.225703734	7.827894404
	C26	-2.559735721	2.877848875	5.360587059
	C27	-2.565750865	-0.884022132	10.015311214
	C28	-1.231168730	-1.246805665	10.633631976
	C29	4.737934729	-12.301895097	3.695567722
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	C38	9.115423050	-6.247397189	6.119664244
	C39	-4.923833675	-2.357022957	-3.060862838
	C40	-5.439682443	-1.012197638	-2.513910315
	C41	-3.442361057	-2.535315855	-2.666965116
	C42	-2.885909850	-3.966027093	-2.825069602



C43	-2.305309102	-4.313978515	-4.195681982
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C47	-9.216066908	1.252898616	-2.039413288
C48	-9.169104330	1.105729728	-0.513456844
C49	-7.922774712	0.336426100	1.448383181
C50	-6.825306467	1.212352682	2.056026115
C51	-5.065695180	2.885169256	1.722671975
C52	-5.630998464	4.121061476	2.443351109
C53	-4.157608769	3.394694845	0.591257055
C54	-3.453602113	2.314623675	-0.161816238
C55	-3.196775820	0.984234566	0.095926987
C56	-2.297340016	1.382788355	-1.816168242
C57	-7.354474972	5.865657315	2.333031867
C58	-7.609141150	5.808496739	3.837842513
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C61	-9.313984272	8.434996589	2.465598955
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C76	2.742163810	9.289103435	-1.606558264
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C79	1.322570645	6.345608895	-3.159490960
C80	0.109643455	5.569421747	-3.685351593
C81	-0.758958841	6.277678838	-4.739263199
C82	-2.364431466	8.160404966	-4.406725215
C83	0.283774170	5.832874755	1.246015757
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C86	0.895475230	8.868161212	3.427153614
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C88	-0.640712859	11.712528226	1.449049953
C89	-2.024832104	12.251794321	1.890071211
C90	-0.443583759	11.891719515	-0.058369013
C91	-1.462052550	11.149304898	-0.912667329
C92	-4.253847994	11.711768086	2.761094113
C93	-4.377276632	12.672825940	3.933205772
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C95	-5.080639217	9.475214503	1.865615466
C96	-6.064396754	9.610265611	0.875083750
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C98	-6.055166219	8.809205657	-0.267989396
C99	-4.053620615	7.698483109	0.537419033
C100	-5.035533960	7.870495449	-0.433733165
C101	5.971237126	-3.087874713	-8.201680113
C102	4.480776210	-2.831468501	-8.059176428
C103	2.776514892	-1.410372482	-6.940603644
C104	2.454435458	0.008510102	-7.430079099
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C106	4.071662955	3.308873611	-6.757763761
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C108	7.045736594	4.101424942	-6.746407420
C109	-0.618397408	-2.353050570	-9.869968845
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C111	-0.467649175	-3.205358265	-8.587975297
C112	0.268315662	-4.525340295	-8.882276401
C113	0.664819611	-5.215504502	-7.597907815
C114	-2.158442917	0.990439296	-8.829922320
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C116	-2.900792697	0.965423177	-7.470487463
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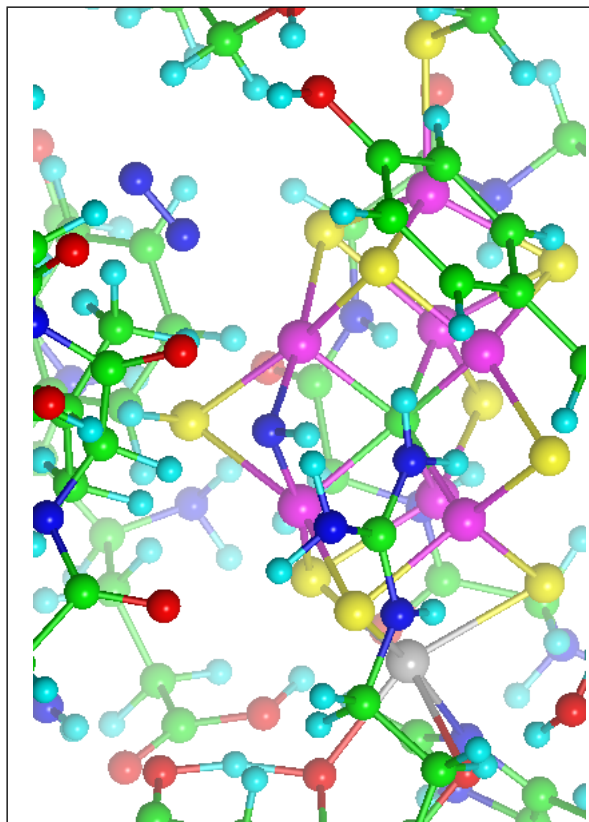
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C132	1.876419914	-7.092495271	-0.245745191
C133	3.050951829	-7.113161653	-1.268887929
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C136	4.406109118	-10.175096990	-3.440273084
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C138	3.923995359	-0.725955068	-1.340066832
Fe139	4.511107963	-1.804315524	-2.943798491
Fe140	2.401815184	0.294946678	-0.720111266
Fe141	4.959439030	0.353618592	-0.017078178
Fe142	4.370083707	0.718874459	-2.518762546
Fe143	3.984738943	2.697369960	-0.728441370
Fe144	5.006243349	-2.200174486	-0.447691649
Fe145	2.524128787	-2.170011170	-1.117766702
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H147	-6.407631897	-6.150804901	-3.250582926
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H151	-8.154408125	-2.694206121	-0.147491635
H152	-9.484258605	-5.667759962	1.219209894
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H154	-9.171107730	-6.601221102	3.325343615
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H174	-0.756512522	0.587980707	1.941307741
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H176	7.957197982	0.756618317	6.801462466
H177	-3.436387266	3.498196879	5.125086453
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Fe2-brNH-Fe6-S2BH 2N2 TS 35, S=1/2 Fe(139) -2.473 Fe(140) -0.317 Fe(141) -2.616 Fe(142) 2.624 Fe(143) 3.160 Fe(144) 1.866 Fe(145) 0.569			bm602b26nh2n2x3dte 1 53144.96	
	C1	-2.005358503	-5.935013350	-7.319312542
	C2	-1.192244808	-6.046408758	-8.614305264
	C3	-4.263867086	-5.715543284	-6.370823466
	C4	-4.269930445	-6.788874889	-5.286682765
	C5	-3.683618693	-9.067883108	-4.632144692
	C6	-2.629569450	-8.761573045	-3.561465652
	C7	-0.608961624	-7.525137898	-2.974013667
	C8	-1.204894411	-6.489444002	-2.017842451
	C9	-2.753886644	-4.618378707	-1.734161980
	C10	-3.675247775	-5.261124802	-0.686189317
	C11	-5.383159286	-6.900982651	-0.181903511
	C12	-4.711906504	-7.773601943	0.887527477
	C13	-3.172522083	-9.621360002	1.329695233
	C14	-1.955713093	-9.124838137	2.119531076
	C15	0.053740896	-7.713087573	2.061959193
	C16	0.128771494	-6.297629322	2.629127445
	C17	-0.850864263	-4.008498951	2.661273163
	C18	-1.828213962	-3.842644151	3.842939879
	C19	-1.155264757	-3.048133498	1.491575746
	C20	-1.351029808	-1.613779104	1.989089529
	C21	-0.063284743	-3.113531730	0.417141601
	C22	-4.185014353	-3.851810571	4.575721832
	C23	-4.312883473	-5.119198167	5.437700114
	C24	-5.539107340	-3.425895475	3.951900235
	C25	-6.660205758	-3.414194609	4.999033627
	C26	-5.421802348	-2.051484027	3.283008186
	C27	-4.574046728	-7.528355533	5.528376321
	C28	-3.599607168	-7.683050512	6.678229298
	C29	9.871914237	-9.334432396	1.779207968
	C30	9.634602513	-7.936699189	2.353167662
	C31	8.010383153	-6.597654408	3.704566100
	C32	8.206590716	-6.789865755	5.220518361
	C33	6.536223445	-6.321305323	3.351262522
	C34	5.977451714	-5.052322291	4.002820272
	C35	4.579699789	-4.711032568	3.475431218
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	C37	9.194767932	-5.857400023	7.259287101
	C38	8.393869400	-4.870888584	8.080747163
	C39	-1.028356945	-1.632309723	-5.953585009
	C40	-2.404714368	-1.167574778	-5.433551643
	C41	0.011097259	-1.474082261	-4.823353215
	C42	1.351552717	-2.204904485	-5.047252253
	C43	2.423838962	-1.424453375	-5.807171365
	C44	-3.783489701	0.890777825	-5.246541076



C45	-5.184572224	0.292808072	-5.408013196
C46	-3.688110478	2.303356452	-5.840414982
C47	-6.634995375	-1.198768894	-6.693791823
C48	-7.010272096	-2.205737531	-5.599563956
C49	-6.293391255	-3.476692529	-3.632948737
C50	-6.257062565	-2.813001174	-2.254710597
C51	-5.950979774	-0.782891079	-0.918020026
C52	-7.367199889	-0.537962152	-0.366759312
C53	-5.271762775	0.591256208	-1.030054545
C54	-3.839669314	0.550205652	-1.451897869
C55	-2.893778046	-0.452149880	-1.525799765
C56	-1.900415354	1.329371902	-2.208521913
C57	-9.650372081	0.131787673	-0.982046678
C58	-10.293709027	-0.896882888	-0.055063254
C59	-10.448158016	0.252480611	-2.300872419
C60	-11.691479392	1.090531992	-2.253416575
C61	-12.666057063	1.209374730	-1.282229238
C62	-13.128550381	2.524484796	-3.004827207
C63	3.555891021	-0.135545244	9.325103152
C64	4.998949188	-0.551602493	9.536702106
C65	3.141558863	-0.616551075	7.911228480
C66	1.692791946	-0.327295015	7.599105541
C67	0.684524443	-1.265749428	7.889839432
C68	1.305390826	0.891311105	7.011843456
C69	-0.657951101	-1.009191335	7.593116298
C70	-0.031789971	1.168830116	6.727504442
C71	-1.012006922	0.212393395	7.006980049
C72	-0.374016648	6.243216577	6.073522783
C73	-1.683201014	6.938909264	5.651838766
C74	-0.155306674	5.000881996	5.221740361
C75	-2.699187473	8.971664713	4.682135327
C76	-3.347742879	8.584729562	3.348875957
C77	-3.204962965	7.045700260	1.396223675
C78	-3.887342225	5.681651153	1.680649578
C79	-2.005198636	6.912724806	0.429007408
C80	-2.207838182	6.234021692	-0.930354906
C81	-2.931770449	7.052655040	-2.012071870
C82	-5.359080498	7.631732020	-2.134531478
C83	-3.835457367	3.523925374	2.838262026
C84	-5.096738480	3.619572515	3.705716931
C85	-2.849006329	2.575613911	3.556446221
C86	-6.007193047	4.623018163	5.741974707
C87	-7.168291367	5.597647844	5.631957028
C88	-8.269601360	7.291676805	4.272526778
C89	-9.732668069	6.916051956	3.927382406
C90	-7.762441537	8.396300453	3.340888756
C91	-7.730663200	7.994932602	1.871843088
C92	-11.258732831	5.208869116	3.038905712
C93	-12.323694284	5.133011473	4.122892001
C94	-11.098933229	3.817236470	2.360225559
C95	-10.142707210	3.850883878	1.187943204
C96	-10.604966716	4.170723574	-0.098798428
C97	-8.767273355	3.613733398	1.353293227
C98	-9.726447991	4.275633767	-1.179812180
C99	-7.868852185	3.744755103	0.290452775
C100	-8.360663268	4.080780802	-0.968600650
C101	8.809884582	4.834581568	-3.307523085
C102	7.553705573	4.398273424	-4.040037100
C103	5.092340706	4.134728409	-3.836579699
C104	4.122202604	5.317629420	-3.946891907
C105	2.802257747	6.940907991	-2.659555617
C106	2.976570012	7.855976484	-1.450672938
C107	3.779541894	8.215555874	0.819699914
C108	4.655190701	9.440699573	0.645352369
C109	4.219459636	3.991643216	-8.310522412
C110	2.718822685	4.265336022	-8.454647148
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C112	5.896938109	2.171918080	-7.727482238
C113	6.196846255	1.043732729	-6.768573835
C114	0.691119604	5.192080646	-7.457083305
C115	0.433422590	6.574778550	-6.889809622
C116	-0.255909266	4.090694576	-6.920048487
C117	0.172353958	3.698957017	-5.537273442
C118	-0.229378931	4.456653354	-4.427222510
C119	1.151143369	2.705454510	-5.368618729
C120	0.400814714	4.282016651	-3.192965099
C121	1.778542476	2.533622997	-4.134740250
C122	1.430199122	3.350934944	-3.055642671
C123	11.117045514	0.909340841	0.736317798
C124	11.556871202	0.329799200	2.089074245
C125	10.291527701	-0.113503485	-0.061136255
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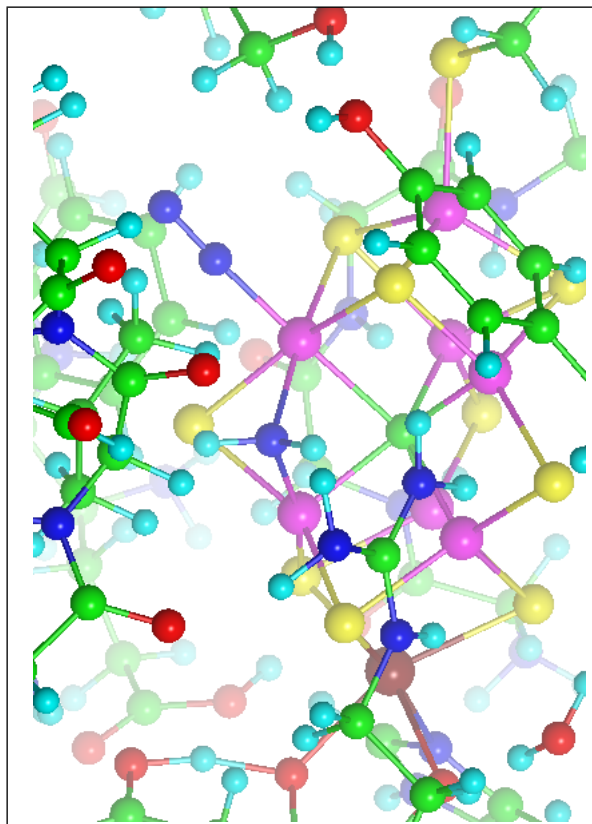
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C130	13.420025627	-0.647691508	4.144729936
C131	4.993394507	-4.179458555	-2.516173375
C132	5.886929298	-4.246194361	-1.273913045
C133	7.082838026	-3.250420160	-1.288198600
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C136	10.663975995	-3.649890371	-3.007927485
C137	7.660055364	-3.116272134	0.126565259
C138	3.655843162	1.667363526	1.193164295
Fe139	5.244161040	2.072029303	0.002794403
Fe140	1.675015963	1.515477833	1.000258453
Fe141	3.439532083	2.089244721	3.160467300
Fe142	3.448268619	3.603886273	1.047205318
Fe143	1.505373466	3.851206325	2.800717801
Fe144	5.035674859	0.471154773	1.982725549
Fe145	3.391802711	0.007607472	0.079443733
H146	0.653467688	-6.299406921	-7.782380933
H147	0.346974816	-4.759962817	-8.228296747
H148	-3.739663236	-5.923359363	-8.427719142
H149	-1.658915179	-5.406426842	-9.380418041
H150	-1.309819335	-7.083240430	-8.973281925
H151	-4.004789200	-4.769734205	-5.871380072
H152	-3.515872457	-8.178787225	-6.585812153
H153	-5.284065166	-5.618551949	-6.764565450
H154	-3.407934997	-9.999915824	-5.143036302
H155	-1.568315717	-7.578685647	-4.881043047
H156	-4.631954384	-9.232163552	-4.104273129
H157	-2.037344745	-3.991385300	-1.192240891
H158	-2.226325741	-5.599309039	-3.567017436
H159	0.244959032	-7.084119735	-3.505067694
H160	-5.953578981	-6.124183650	0.343692524
H161	-4.473317234	-6.531350278	-2.104182479
H162	-0.242735289	-8.356145469	-2.358477193
H163	-3.342489089	-3.971157079	-2.397530055
H164	-3.587548193	-8.725832522	-0.571687410
H165	-6.083847914	-7.522178733	-0.756435367
H166	0.070878909	-4.134404836	0.031667156
H167	-0.330915544	-2.456579367	-0.425412953
H168	0.897285286	-2.745623891	0.807811427
H169	-2.104053916	-3.380890638	1.040059820
H170	-2.847918811	-10.490991147	0.739911297
H171	-4.627274651	-2.024299256	2.524078158
H172	-4.365718968	-6.361386301	3.761917756
H173	-6.824476063	-4.402541449	5.452283762
H174	-1.654226963	-0.985887685	1.142644657
H175	-0.418806509	-1.192282429	2.393623086
H176	2.938999864	-0.681394667	10.064156341
H177	-6.364203034	-1.780109033	2.786175581
H178	-7.602607833	-3.095226407	4.529424839
H179	-5.202404910	-1.275538330	4.034206822
H180	-6.429299800	-2.705628881	5.810564761
H181	-5.801186750	-4.172493114	3.179233006
H182	-3.851161737	-3.068777139	5.272383099
H183	-3.431872693	-4.208110094	2.591832208
H184	-2.134131187	-1.535780894	2.757539916
H185	-1.847007297	2.696570295	3.116946264
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H191	0.954198178	-2.224114633	8.343359144
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H194	0.334528727	-8.392194145	2.876455366
H195	-1.440573218	-7.851784472	0.568313458
H196	-3.908755570	-9.962678570	2.068969179
H197	-1.421053497	-1.765119556	7.794950198
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H199	-5.602513169	-7.602448150	5.919055183
H200	-4.410324495	-8.373590883	4.841577161
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H206	6.603830484	2.999333693	-7.570767224
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H208	1.322732292	7.247976851	-6.882763658

H209	4.548487345	3.829130067	-9.348644680
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H214	4.776877212	5.320581483	-6.812269177
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H325	6.234963003	-5.277171308	-1.136600082
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H335	1.976060260	-4.813789357	4.416604620
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O436	-3.136310635	-1.873997102	-4.714264948
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O438	-6.071309897	0.511840663	-4.564689389
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O451	-7.895479434	5.828867795	6.606019221
O452	-10.628448635	7.767990572	4.012074118
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	O455	-7.439615824	4.255644054	-2.018288277
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	O457	3.788603397	5.795845319	-5.050754251
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	O459	4.633404548	10.394643031	1.406325159
	O460	2.099018833	3.929165805	-9.477546156
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	O463	-0.661580391	6.972241096	-6.517858492
	O464	11.487008581	1.000944805	3.137653939
	O465	13.586549515	-0.721399399	5.354634125
	O466	4.888787799	-2.975446256	-3.068331757
	O467	4.375148772	-5.162175535	-2.932855600
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	O469	10.380515955	-4.038444991	-4.175863130
	O470	7.639967194	-1.917235549	0.654870662
	O471	8.132234644	-4.111485089	0.707669959
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	O477	10.549935843	-4.239545637	1.949478521
	S478	-0.039170084	5.420136853	3.426753700
	S479	1.291757883	3.850466251	0.484936742
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	S483	5.159991204	4.256448194	-0.247257921
	S484	4.628687435	-1.550194584	1.084498904
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Fe2-brNH2-Fe6 2N2 associated 35, S=1/2			bm6026nh22n2x1dtd.car_4	
Fe(139) -2.351	C1	-2.478964365	-5.726699413	-7.309602796
Fe(140) -0.217	C2	-1.692939551	-5.825407949	-8.621068510
Fe(141) -2.629	C3	-4.709507021	-5.487700468	-6.306197535
Fe(142) 2.567	C4	-4.695151840	-6.579142240	-5.238088898
Fe(143) 2.718	C5	-4.147830048	-8.888004532	-4.654960795
Fe(144) 2.195	C6	-3.046506527	-8.628626152	-3.621732219
Fe(145) -1.549	C7	-0.958558883	-7.467554346	-3.109038848
	C8	-1.470462770	-6.436173832	-2.101838843
	C9	-2.927842611	-4.515943805	-1.696126450
	C10	-3.824997844	-5.148227670	-0.622037076
	C11	-5.570471932	-6.737619689	-0.082272685
	C12	-4.881071900	-7.656547588	0.936354076
	C13	-3.381195993	-9.556032802	1.275979197
	C14	-2.122052422	-9.110440405	2.028505248
	C15	-0.043898952	-7.804819852	1.897536403
	C16	0.116997094	-6.407583483	2.485913326
	C17	-0.824209449	-4.106981691	2.647269273
	C18	-1.752413940	-3.924702272	3.864737784
	C19	-1.109334531	-3.113101303	1.500272989
	C20	-1.214736332	-1.681908422	2.033794743
	C21	-0.041229397	-3.247490601	0.408941802
	C22	-4.080042053	-3.848007824	4.676439401
	C23	-4.204997397	-5.132821813	5.512887247
	C24	-5.435601098	-3.366448303	4.106158852
	C25	-6.522339722	-3.335674880	5.190036981
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	C27	-4.457458049	-7.544126090	5.553361611
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	C29	9.670288222	-9.599885828	1.172114621
	C30	9.486900190	-8.209332939	1.781637911
	C31	7.950876256	-6.864234274	3.223937559
	C32	8.215649533	-7.091067104	4.725434135
	C33	6.468224493	-6.553490001	2.947941709
	C34	5.979075603	-5.277544759	3.639407358
	C35	4.545254596	-4.919295214	3.235969957
	C36	3.064660714	-3.188278271	4.328666782
	C37	9.320121804	-6.222930991	6.731458676
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	C39	-1.317602614	-1.472563597	-5.931006173
	C40	-2.670176947	-1.001364420	-5.363268348
	C41	-0.231673664	-1.340034096	-4.844163809
	C42	1.073488152	-2.110952078	-5.129736997
	C43	2.134667716	-1.356444733	-5.930195896
	C44	-3.982944653	1.090965636	-5.066308819
	C45	-5.411313773	0.549675013	-5.176316240
	C46	-3.855172020	2.515986439	-5.624613298



C47	-6.969649722	-0.869404641	-6.417258542
C48	-7.319740235	-1.886217955	-5.323823490
C49	-6.546978192	-3.228237875	-3.427485356
C50	-6.438243662	-2.597138224	-2.037294476
C51	-6.015727123	-0.610375473	-0.667218167
C52	-7.394972414	-0.334119084	-0.046192068
C53	-5.300137592	0.743949874	-0.780120088
C54	-3.899440974	0.652156590	-1.286283970
C55	-3.018638756	-0.397375367	-1.458365940
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C59	-10.541139092	0.582069430	-1.802243140
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C61	-12.699898722	1.571798409	-0.685889358
C62	-13.181783378	2.940384088	-2.360913664
C63	3.963178669	-0.384514835	9.145246418
C64	5.400519382	-0.847241215	9.284332591
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C69	-0.340699368	-1.139833985	7.549140345
C70	0.298960755	1.046433387	6.712771151
C71	-0.690679345	0.102520195	7.003887164
C72	0.039729919	6.150893696	6.181935211
C73	-1.268721816	6.884706758	5.839149489
C74	0.196769928	4.908566073	5.305236570
C75	-2.272152689	8.960489211	4.955430915
C76	-2.988026296	8.620751466	3.643863081
C77	-2.962801237	7.104138161	1.663304314
C78	-3.666978393	5.752120333	1.947108275
C79	-1.805872252	6.968818021	0.647265235
C80	-2.073089695	6.332866039	-0.720145869
C81	-2.830561731	7.192666343	-1.745384729
C82	-5.244826276	7.821821022	-1.760761088
C83	-3.619251204	3.562780146	3.042044375
C84	-4.836029187	3.658479533	3.973061853
C85	-2.619917481	2.570227214	3.670120491
C86	-5.640642366	4.636708170	6.070156950
C87	-6.774841532	5.650172734	6.038578330
C88	-7.877106727	7.418308456	4.778501746
C89	-9.361295231	7.087915381	4.488899108
C90	-7.380353831	8.529695585	3.849892387
C91	-7.431063407	8.168131213	2.370509968
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C94	-10.887074991	4.063279096	2.916151166
C95	-9.982570747	4.089060440	1.704880173
C96	-10.483358174	4.469146042	0.450059757
C97	-8.612510362	3.794961308	1.807695727
C98	-9.645097934	4.574955326	-0.662176627
C99	-7.752800260	3.921852118	0.712984246
C100	-8.279913844	4.323534436	-0.512583624
C101	8.792558449	4.687244722	-3.624999347
C102	7.491448543	4.278800011	-4.295749262
C103	5.035339682	4.067491270	-3.972999863
C104	4.097665823	5.281536985	-4.019698425
C105	2.869195310	6.907074602	-2.640924673
C106	3.146222308	7.810991826	-1.444025902
C107	4.065561489	8.131052212	0.784197072
C108	4.909167006	9.372223119	0.571711299
C109	3.981307528	4.055028700	-8.427017977
C110	2.485028238	4.379230636	-8.500685427
C111	4.197702222	2.708943387	-7.698480430
C112	5.621017817	2.169842666	-7.942925254
C113	5.923579550	1.014544100	-7.017927485
C114	0.531986175	5.346934919	-7.399739121
C115	0.339197148	6.725420951	-6.801406577
C116	-0.418857191	4.262008186	-6.836955512
C117	0.045301984	3.826045796	-5.478318814
C118	-0.307268608	4.560057399	-4.335731594
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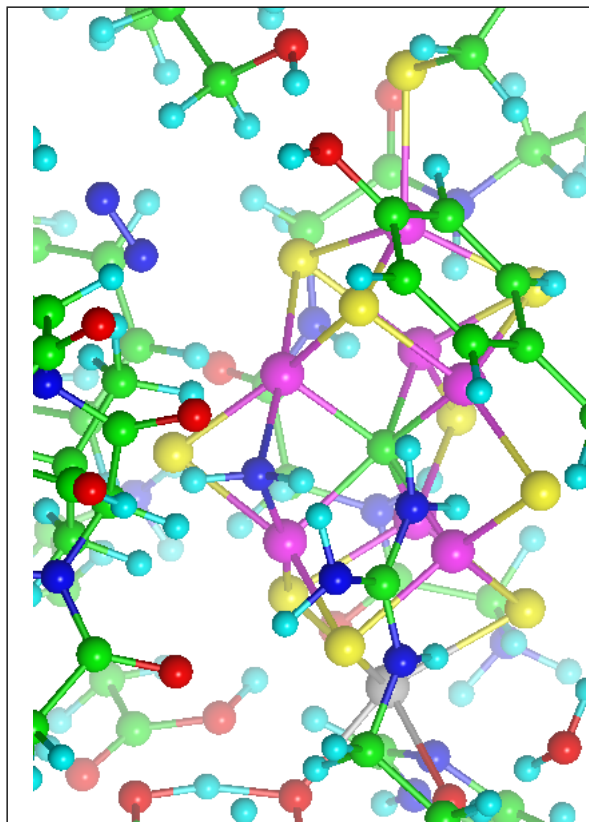
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O425	-1.143359803	-6.482654059	-0.905321878
O426	-3.790468069	-4.763313639	0.558893627
O427	-5.140908353	-7.591256800	2.148963524
O428	-1.826604151	-9.637933962	3.109537054
O429	1.140123248	-6.175314964	3.158247072
O430	-1.285585353	-3.716767681	4.995683930
O431	-4.243441510	-5.104891052	6.754402622
O432	-3.667255315	-8.400705386	7.661584838
O433	10.339500829	-7.323213853	1.567325986
O434	7.784087684	-8.107343717	5.299620294
O435	9.043903246	-4.860235460	8.700150079
O436	-3.395659341	-1.716552351	-4.647049193
O437	1.839352888	-0.563613727	-6.854650280
O438	-6.250396496	0.782707078	-4.289186085
O439	-4.786224750	3.394397279	-4.962497453
O440	-8.501160880	-2.240580789	-5.192006229
O441	-6.641081574	-3.294853014	-1.034808815
O442	-7.583126403	-0.286739582	1.175302229
O443	-11.055041906	-0.290476914	1.335788398
O444	5.742894142	-1.859099934	9.879241500
O445	-1.998868367	0.445089235	6.716962255
O446	-2.384993871	6.385677467	6.059475623
O447	-4.046006362	9.212067675	3.348852784
O448	-4.780759309	5.517858135	1.453769274
O449	-5.770044332	2.850963181	3.892282779
O450	-2.440035345	2.824408159	5.068100246
O451	-7.457852388	5.868283163	7.046997123
O452	-10.233849781	7.955851758	4.635249423
O453	-8.407340914	7.594058475	1.867991143
O454	-13.195726378	5.460298225	4.550386451
O455	-7.394372891	4.504000326	-1.592037614
O456	7.493580805	3.777559662	-5.446827048

	O457	3.740254048	5.797526568	-5.099414610
	O458	2.629049648	8.940344615	-1.410720072
	O459	4.899280967	10.326452050	1.333318646
	O460	1.809132144	4.079848571	-9.499421329
	O461	5.571019288	-0.139206633	-7.235113832
	O462	6.576110182	1.318829329	-5.876159403
	O463	-0.714570515	7.135324586	-6.336710327
	O464	11.621376858	0.628316995	2.640614366
	O465	13.752784899	-1.143634805	4.726959983
	O466	4.593046009	-3.098125084	-3.322727804
	O467	4.095306555	-5.286095799	-3.172778051
	O468	11.549115702	-3.917053897	-3.017197824
	O469	10.019767834	-4.275337060	-4.643863016
	O470	7.585935796	-2.091318238	0.280607510
	O471	7.996929888	-4.296930726	0.291299743
	O472	6.362195404	-2.095659807	-2.019180995
	O473	9.791814069	-3.790120027	3.973142534
	O474	7.587478222	-2.214049419	3.107401820
	O475	-4.893902874	4.177500542	-2.338996722
	O476	12.700614454	-3.848453731	-0.523536461
	O477	10.490452485	-4.545577001	1.400798075
	S478	0.259103897	5.314863720	3.499406278
	S479	1.510566213	3.867968640	0.546714917
	S480	4.804914423	0.679076034	-1.911166125
	S481	1.431324178	1.596168476	3.286514166
	S482	1.776806321	0.747530089	-1.304814829
	S483	5.329046704	4.156195377	-0.373576041
	S484	4.622703914	-1.670972813	0.810723683
	S485	3.954420822	4.151720851	3.139945670
	S486	7.049219832	1.078773587	0.992952071
	S487	5.014640085	0.504809480	3.986671655
	end			
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	C1	-2.475784955	-5.722992627	-7.305756327
	C2	-1.687005373	-5.821786050	-8.616064728
	C3	-4.707622968	-5.486352810	-6.304151224
	C4	-4.693309937	-6.577861618	-5.236986890
	C5	-4.146284966	-8.887236855	-4.655856429
	C6	-3.044782090	-8.628813787	-3.622082969
	C7	-0.956353614	-7.468897495	-3.109915532
	C8	-1.467817993	-6.437251325	-2.102768737
	C9	-2.923688925	-4.516174117	-1.697113375
	C10	-3.821420184	-5.147103924	-0.622428195
	C11	-5.568127759	-6.736710277	-0.082048739
	C12	-4.879068037	-7.656025473	0.935977511
	C13	-3.379502125	-9.555955719	1.275855065
	C14	-2.121115130	-9.110635274	2.028848789
	C15	-0.040736552	-7.809125705	1.897383528
	C16	0.120516060	-6.411828916	2.486639688
	C17	-0.817503994	-4.112616056	2.648693638
	C18	-1.746864061	-3.925515597	3.864844597
	C19	-1.095954900	-3.119532833	1.501465053
	C20	-1.190417510	-1.685970795	2.031431221
	C21	-0.029823698	-3.254802916	0.408975553
	C22	-4.075837672	-3.846915900	4.675314725
	C23	-4.200168798	-5.131883848	5.511488118
	C24	-5.432448477	-3.366053755	4.105272482
	C25	-6.518543602	-3.335515858	5.188773213
	C26	-5.284551128	-1.982389906	3.46056817
	C27	-4.451758792	-7.545237539	5.551724388
	C28	-3.445428299	-7.715484832	6.670303379
	C29	9.670914228	-9.597872609	1.171559536
	C30	9.487473151	-8.207909519	1.781989959
	C31	7.951087962	-6.863268001	3.224648865
	C32	8.216596732	-7.090813692	4.726130277
	C33	6.468772446	-6.553158331	2.949376511
	C34	5.981168394	-5.276821998	3.639602591
	C35	4.546047044	-4.919942905	3.240269851
	C36	3.066210056	-3.187413472	4.330526774
	C37	9.322220657	-6.223053369	6.731496418
	C38	8.607028234	-5.233585191	7.623955617
	C39	-1.313234532	-1.470880733	-5.927078562
	C40	-2.666849625	-0.997787025	-5.361622989
	C41	-0.225904558	-1.338197098	-4.841340762
	C42	1.078564800	-2.110296043	-5.126939224
	C43	2.141241689	-1.357096807	-5.928036867
	C44	-3.984467397	1.091975526	-5.077813450
	C45	-5.411801157	0.549178917	-5.185888284
	C46	-3.855121282	2.518036686	-5.631948440
	C47	-6.970436373	-0.872805918	-6.420815938
	C48	-7.320066247	-1.888965180	-5.326331231
Fe2-brNH2-Fe6 2N2 dissociated 35, S=1/2				
Fe(139) -2.425				
Fe(140) -1.073				
Fe(141) -2.562				
Fe(142) 2.768				
Fe(143) 3.011				
Fe(144) 2.143				
Fe(145) -1.397				



C49	-6.547442995	-3.235194946	-3.432962635
C50	-6.438806118	-2.603785119	-2.043303100
C51	-6.010456943	-0.610096494	-0.681193805
C52	-7.385975882	-0.331155677	-0.051426596
C53	-5.295029999	0.744017047	-0.810991203
C54	-3.901177448	0.648545628	-1.335467836
C55	-3.014942516	-0.400105720	-1.484539454
C56	-1.972083515	1.337241668	-2.200705965
C57	-9.665162062	0.443296359	-0.528921954
C58	-10.281768020	-0.568086184	0.434308762
C59	-10.536156395	0.584331354	-1.799984620
C60	-11.753181886	1.456014120	-1.687563559
C61	-12.695902991	1.573573823	-0.684554664
C62	-13.177761745	2.941509423	-2.359867630
C63	3.965255942	-0.383526004	9.148418664
C64	5.401896881	-0.847656664	9.286732065
C65	3.479283924	-0.827135287	7.744320447
C66	2.026227456	-0.500609148	7.492027019
C67	1.008960432	-1.425061394	7.797399963
C68	1.644416803	0.736312728	6.940783569
C69	-0.336510197	-1.137775786	7.547064715
C70	0.304600082	1.044504658	6.702148587
C71	-0.685632291	0.102348390	6.997473406
C72	0.046699295	6.153782069	6.188834150
C73	-1.262497742	6.887591235	5.846375429
C74	0.203503802	4.915119776	5.308787081
C75	-2.269527968	8.961296022	4.959584398
C76	-2.981930185	8.622286578	3.646712060
C77	-2.957897076	7.109435264	1.667181586
C78	-3.661290876	5.758582435	1.958964503
C79	-1.803300098	6.968953294	0.648617970
C80	-2.071090598	6.331630125	-0.718685418
C81	-2.827853394	7.191356166	-1.744635804
C82	-5.242550029	7.821581361	-1.761604852
C83	-3.619993703	3.584415759	3.086198939
C84	-4.838140936	3.681709124	4.009029635
C85	-2.621367884	2.601030778	3.735833957
C86	-5.649116974	4.650893133	6.102477483
C87	-6.784595191	5.660827705	6.057919015
C88	-7.875150064	7.420674400	4.779417055
C89	-9.359304636	7.088511940	4.488009372
C90	-7.375684055	8.529167467	3.848460062
C91	-7.426023600	8.167673472	2.369700482
C92	-10.964743073	5.448670262	3.621111667
C93	-11.989341479	5.396944498	4.744104978
C94	-10.883645982	4.064018298	2.915787027
C95	-9.978163497	4.088787350	1.705397659
C96	-10.477416293	4.469199375	0.449862123
C97	-8.607922695	3.793865463	1.807273660
C98	-9.638371657	4.575483399	-0.662476505
C99	-7.747660402	3.921146293	0.712126397
C100	-8.273275823	4.322783194	-0.513898620
C101	8.795080970	4.686886564	-3.624845473
C102	7.494201778	4.278823016	-4.295612225
C103	5.037273599	4.068767656	-3.971964990
C104	4.101360534	5.282964511	-4.018500870
C105	2.871800542	6.906848288	-2.641582557
C106	3.148008721	7.813251333	-1.445091586
C107	4.070547632	8.134276897	0.781658254
C108	4.911343638	9.377137478	0.568493683
C109	3.985396854	4.054398456	-8.424331368
C110	2.489079046	4.380102426	-8.497280327
C111	4.201561097	2.708034980	-7.696627282
C112	5.624208134	2.169479940	-7.941922844
C113	5.927024903	1.014043289	-7.017020783
C114	0.536402438	5.346914851	-7.397931280
C115	0.343015312	6.725220322	-6.798658715
C116	-0.416124558	4.261882327	-6.840288641
C117	0.044827201	3.821554473	-5.481314995
C118	-0.306204869	4.554573453	-4.337291172
C119	0.989280694	2.786455539	-5.365874385
C120	0.330545368	4.305200227	-3.119366428
C121	1.620624608	2.538925215	-4.146801618
C122	1.316397239	3.321521103	-3.029890746
C123	11.134586401	0.596914307	0.258339700
C124	11.624919497	-0.022126144	1.575770780
C125	10.216617775	-0.373273604	-0.500964984
C126	9.502765713	0.184110011	-1.690800478
C127	10.064299729	0.664378053	-2.856366181
C128	7.867832519	0.554875006	-3.098860632
C129	12.534667228	-1.909912310	2.786635861
C130	13.556510052	-1.070989997	3.521019658

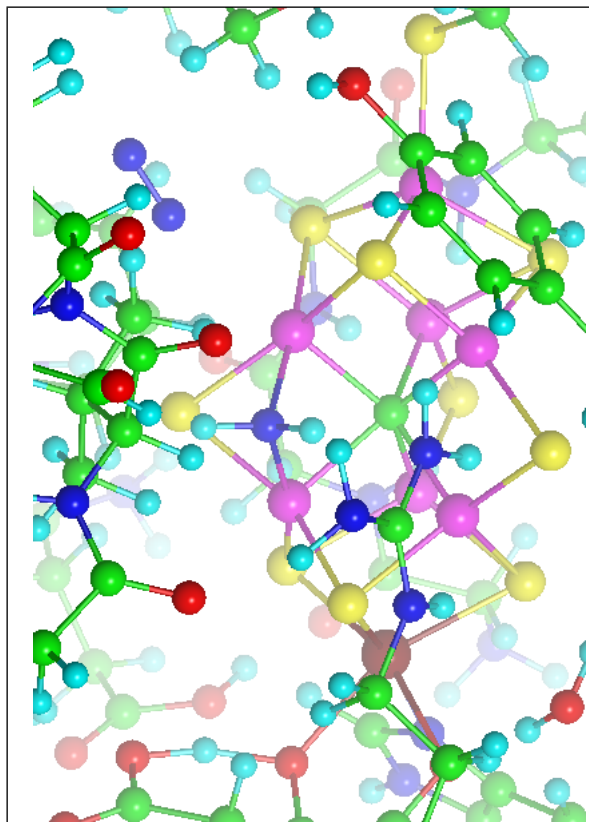
C131	4.728906525	-4.302933497	-2.769668329
C132	5.664625942	-4.367532095	-1.563516723
C133	6.875246466	-3.388019665	-1.638026222
C134	7.930757334	-3.927438407	-2.641676322
C135	9.280785715	-3.206795236	-2.623554496
C136	10.368177369	-3.866160895	-3.501884057
C137	7.542021308	-3.287843177	-0.257782282
C138	3.763152808	1.587288645	1.057439468
Fe139	5.319269303	1.967280319	-0.153230487
Fe140	1.795926976	1.497292196	0.870524252
Fe141	3.572037806	1.905378606	3.013238514
Fe142	3.645973129	3.554607028	0.975255057
Fe143	1.661581393	3.704605114	2.750978547
Fe144	5.166941802	0.328280150	1.790588070
Fe145	3.524247673	-0.041995423	-0.166838825
H146	0.164112209	-6.140866161	-7.821178929
H147	-0.108471156	-4.583565543	-8.227320654
H148	-4.232035314	-5.656562778	-8.376910571
H149	-2.149414688	-5.154861996	-9.361729108
H150	-1.834976221	-6.846805568	-8.997413425
H151	-4.428249924	-4.550292477	-5.797674165
H152	-4.037467763	-7.961812627	-6.596687817
H153	-5.736529905	-5.376606091	-6.671318228
H154	-3.913004654	-9.812239824	-5.198841047
H155	-2.010997684	-7.451032817	-4.965221149
H156	-5.078850161	-9.041953246	-4.097454504
H157	-2.159055419	-3.928458337	-1.176650676
H158	-2.515948170	-5.460127617	-3.579611876
H159	-0.118734951	-7.043067094	-3.679016263
H160	-6.086720930	-5.956523820	0.489762213
H161	-4.726536501	-6.352717423	-2.031605053
H162	-0.583815089	-8.322100387	-2.529577977
H163	-3.516081537	-3.828235495	-2.315093468
H164	-3.847441681	-8.610575100	-0.590195233
H165	-6.312264229	-7.323172272	-0.638508535
H166	-0.040277654	-4.253479135	-0.049786410
H167	-0.197528084	-2.510926521	-0.386188389
H168	0.980586150	-3.093491663	0.817161534
H169	-2.070715339	-3.384878501	1.061479070
H170	-3.099290476	-10.420885023	0.657199116
H171	-4.536583192	-1.975529513	2.654640880
H172	-4.330321950	-6.331949504	3.809491152
H173	-6.696127890	-4.325839238	5.632536078
H174	-1.377875632	-1.003917583	1.193525556
H175	-0.259678271	-1.363891140	2.522894939
H176	3.361466904	-0.925779636	9.901806933
H177	-6.238112868	-1.651144888	3.024989686
H178	-7.464962423	-2.984027235	4.751937811
H179	-4.976733790	-1.239092951	4.214816295
H180	-6.240514711	-2.645708182	6.001697057
H181	-5.748742132	-4.086642339	3.328154967
H182	-3.698417618	-3.090184844	5.378795575
H183	-3.404756281	-4.162668849	2.656239908
H184	-2.012214365	-1.559493919	2.752045392
H185	-1.643906404	2.693170762	3.235440208
H186	-3.017567092	1.589701691	3.559590941
H187	-2.365526771	1.980449341	5.583531483
H188	-2.584140904	-0.298861400	6.933529296
H189	0.024318821	1.997334012	6.252386509
H190	2.410341802	1.460063778	6.654602561
H191	1.272304961	-2.397138410	8.222679812
H192	-1.606743005	-5.798988917	1.594438674
H193	0.694481698	-7.893190681	1.081126373
H194	0.244857947	-8.518331556	2.684531604
H195	-1.594653336	-7.860507811	0.460423927
H196	-4.094558711	-9.893274443	2.036506250
H197	-1.108118108	-1.882511468	7.757524928
H198	0.193585058	-3.929700876	3.031308302
H199	-5.468587708	-7.643163789	5.965926786
H200	-4.294617419	-8.372688223	4.841719324
H201	-2.458474769	-7.227491336	6.499637956
H202	10.409328954	-6.113926020	6.861881976
H203	4.167799633	-1.170292838	-6.138709394
H204	5.347362366	-2.461982624	-2.782509339
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H206	6.360584608	2.973304978	-7.795885519
H207	3.471531866	1.960423074	-8.045772288
H208	1.241076602	7.384957273	-6.857325510
H209	4.266244112	3.903892974	-9.479171372
H210	-0.005809811	-0.271022918	-4.685242775
H211	0.857190970	-3.036461547	-5.686728060
H212	2.516266181	5.193768007	-6.585252876

H213	0.266743459	5.492059407	-8.465436638
H214	4.643452888	5.327737252	-6.919815759
H215	3.684084065	-2.234021640	-4.822883436
H216	4.012728257	2.847213686	-6.620952623
H217	5.752933499	5.049174971	-8.104362625
H218	-1.306977195	-1.147804756	-7.968589177
H219	-0.648012484	-1.694322272	-3.892196354
H220	6.830369114	2.291072846	-5.825646960
H221	1.519907941	-2.436275388	-4.173669001
H222	-5.475982029	-1.266880805	0.019529122
H223	-3.181787720	-1.447371756	-1.245387349
H224	-7.571318480	-3.620600347	-3.530693004
H225	-5.332144049	-2.032795185	-4.720136065
H226	-8.163059387	-0.137217437	-1.940713029
H227	-12.793700323	1.097868218	0.284966050
H228	-10.012449265	-1.627584806	0.202351350
H229	-10.799414232	-0.422660583	-2.169827145
H230	-9.581265465	1.415589293	-0.017214470
H231	-13.712474436	3.690619143	-2.938483613
H232	-5.300381254	1.207157298	0.189281513
H233	-5.893857724	1.398426633	-1.465320466
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	O466	4.599277585	-3.092893451	-3.314001790
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	O476	12.701517875	-3.848275581	-0.522646569
	O477	10.491845095	-4.544519017	1.400564755
	S478	0.245704017	5.334459403	3.507332456
	S479	1.439209839	3.755543453	0.450557318
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Fe(139) -2.417	C1	-2.476513833	-5.718727865	-7.314041582
Fe(140) -0.993	C2	-1.702771500	-5.824356728	-8.634258597
Fe(141) -2.582	C3	-4.703301324	-5.484262853	-6.296691755
Fe(142) 2.788	C4	-4.686819731	-6.575882533	-5.230207932
Fe(143) 2.976	C5	-4.133137403	-8.883102745	-4.647364022
Fe(144) 2.160	C6	-3.032431146	-8.622260360	-3.612153192
Fe(145) -1.449	C7	-0.948744609	-7.456731965	-3.096240351
	C8	-1.468776871	-6.424405258	-2.094448010
	C9	-2.941402501	-4.511556498	-1.700985237
	C10	-3.833446085	-5.145981634	-0.624996579
	C11	-5.572354170	-6.742349065	-0.078333313
	C12	-4.881356502	-7.657468574	0.940776985
	C13	-3.378991719	-9.555910101	1.282321900
	C14	-2.114951651	-9.114120014	2.025942799
	C15	-0.050736943	-7.787812050	1.894905316
	C16	0.104149439	-6.389741171	2.488217628
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	C19	-1.133531200	-3.097891162	1.499023166
	C20	-1.248860360	-1.665539131	2.030379045
	C21	-0.073914361	-3.214527448	0.396941416
	C22	-4.088932397	-3.838466718	4.682491162
	C23	-4.210186748	-5.120698298	5.518407273
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	C46	-3.859720054	2.513417069	-5.623588612
	C47	-6.963514441	-0.878137668	-6.415589145
	C48	-7.312830476	-1.896155528	-5.323099212
	C49	-6.541004123	-3.233683258	-3.425338913
	C50	-6.430243845	-2.601080504	-2.035484609



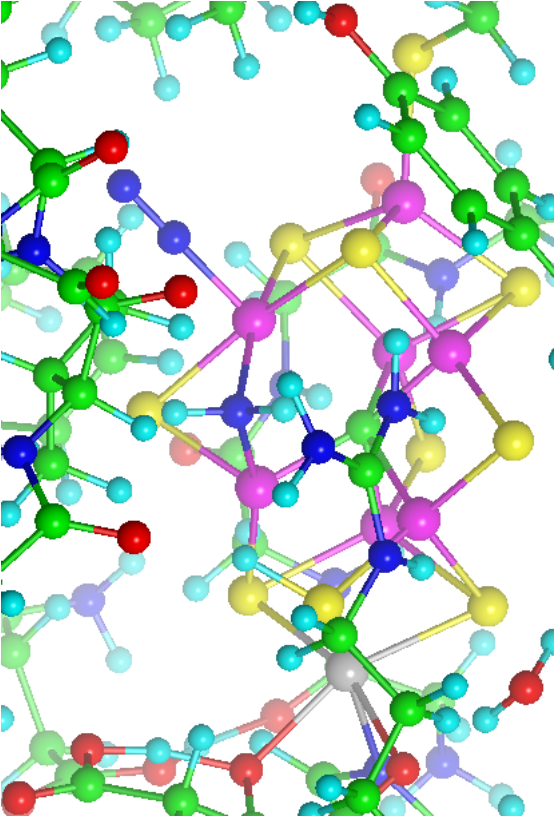
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C54	-3.899099011	0.658073551	-1.318436070
C55	-3.009425013	-0.385567113	-1.474394262
C56	-1.971020184	1.361328111	-2.172101451
C57	-9.663744543	0.430342107	-0.542172965
C58	-10.285006994	-0.589103450	0.409715529
C59	-10.530281492	0.580701556	-1.816391322
C60	-11.747762493	1.451037873	-1.700970218
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C62	-13.173490762	2.940302684	-2.362431720
C63	3.959473973	-0.393700927	9.148893636
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C65	3.472818646	-0.838517891	7.746441892
C66	2.019236630	-0.509589775	7.497584422
C67	0.999685954	-1.430822041	7.806439574
C68	1.638212670	0.729036665	6.949480212
C69	-0.346254488	-1.139174446	7.561687253
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C71	-0.693905497	0.102365656	7.015136290
C72	0.044283219	6.145367138	6.190605350
C73	-1.261082329	6.880814364	5.843254666
C74	0.202237592	4.908397993	5.309158149
C75	-2.263155101	8.957528910	4.955898861
C76	-2.978493031	8.613673701	3.646472515
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C78	-3.661311288	5.757228886	1.950561119
C79	-1.800659768	6.961090683	0.645152652
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C81	-2.824372317	7.189105917	-1.747800947
C82	-5.238417678	7.821616732	-1.761724819
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C89	-9.360013392	7.089214129	4.486343027
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C95	-9.977037300	4.088617047	1.702627118
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C138	3.762302682	1.580746749	1.058678543
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Fe140	1.779446901	1.518511682	0.888792701
Fe141	3.593654186	1.913523172	3.019234013
Fe142	3.665289316	3.559810684	0.974594449
Fe143	1.698722401	3.724217997	2.758849557
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Fe145	3.504627409	-0.043466657	-0.158474576
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H148	-4.242211770	-5.660440292	-8.371843825
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H164	-3.849671877	-8.613300893	-0.584170904
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H167	-0.250025304	-2.462968314	-0.388909207
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H176	3.359500395	-0.936893676	9.903074574
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H204	5.381037767	-2.448726137	-2.790581044
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H218	-1.314566588	-1.145254697	-7.963393243
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H230	-9.586632023	1.399359971	-0.022669178
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H235	-9.892204663	1.047884752	-2.582178922
H236	-5.952208641	-0.735337184	-2.816293815
H237	-5.871707120	-4.106649363	-3.446611677
H238	-7.782604385	-0.145127679	-6.419859503
H239	-1.211396890	2.047588124	-2.537973506
H240	-6.972132352	-1.391184453	-7.386905996
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H248	-4.839207163	4.203569891	-5.496399678
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H256	-5.717936659	9.817739337	-1.650568317
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H258	-10.055377644	4.839906099	-1.640222902
H259	-8.178623085	3.462391799	2.753921523
H260	-6.730778312	6.425590865	-1.490799849
H261	-1.015088941	6.359229037	1.129392044
H262	-1.504439905	7.272460526	3.215226028
H263	-2.571371354	5.346476025	-0.617834472
H264	-4.925882826	-0.411559395	-6.911334415
H265	-1.934647735	10.003468936	4.895521540
H266	-2.266248098	0.662436089	-6.358418335
H267	-1.366691967	7.963604386	0.493040814
H268	-6.676525907	3.752758134	0.827181022
H269	-3.019666339	8.887032948	5.750256227
H270	-4.070569105	9.491359046	-2.088760587
H271	-7.270426085	8.018644783	-1.907130216
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H275	-3.777723811	1.113469629	-3.983787184
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H279	-4.531767776	5.919311714	-1.923444836
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H289	9.815463703	4.385511171	-5.352213864
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H299	4.287952740	6.391345441	-0.430848663
H300	2.127774697	-1.588651116	5.165637278
H301	2.949325112	7.527114627	-3.547086798
H302	2.364809808	1.732692325	-4.053497939
H303	1.812945791	6.589388630	-2.575430252
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H306	4.496266252	-4.902180373	2.109076378
H307	6.387847840	-6.443082235	1.848236344
H308	6.663350171	-4.441023701	3.399959968
H309	6.009777497	-5.407655579	4.732514485
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H312	9.459287442	-9.486047059	0.091945515
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H316	4.831323082	-2.817775118	3.395140757
H317	0.096915678	4.883543827	-2.224789864
H318	1.230527009	2.171696189	-6.236258956
H319	12.004589607	-4.182786012	0.076210660
H320	10.835844043	-1.228875583	-0.859041323
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H323	5.600303764	9.311105689	-0.300946860
H324	7.659544966	-2.183045170	2.114599261
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H326	6.470143574	4.750977862	-2.585306802
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H332	9.048847627	-3.178798394	3.764150193
H333	7.422302159	-1.297214121	3.370392658
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H348	5.099341923	3.657216771	-4.988777754
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H351	4.106958145	-0.353004536	6.986738148
H352	12.809611243	1.749360610	-0.040840493
H353	12.887748441	0.294506288	-0.786476144
H354	13.018525504	-2.868370343	2.532122273
H355	12.134449083	-1.864975032	0.694968424
H356	14.182321523	-0.414636737	2.878263890
H357	11.686582349	-2.133136951	3.454502325
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H360	9.051036617	-7.235399182	7.079440612
H361	7.623122322	-4.879520935	7.226970809
H362	-11.302654293	6.204197546	2.885449397
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H366	2.257990476	-0.766578365	2.017799612
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Mo368	6.270903566	-0.555410602	-0.534333774
N369	2.016389385	-0.429594857	1.081399832
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N371	-3.837955948	-5.729357392	-7.440860531
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N375	-4.658561059	-6.138143061	-1.034783623
N376	-4.008147979	-8.564932105	0.425670689
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N420	-1.985017768	1.732653866	0.929030411
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O423	-5.021532552	-6.314119526	-4.061622824
O424	-3.123679556	-9.079798750	-2.461026882
O425	-1.145740224	-6.464985290	-0.896695458
O426	-3.800651257	-4.755650511	0.554107240
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O451	-7.458007844	5.882912650	7.050811415
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O457	3.730650633	5.796242200	-5.102163997
O458	2.609128742	8.935229639	-1.408189952
O459	4.924605804	10.304433605	1.349600902
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	O461	5.572442423	-0.138310893	-7.227894880
	O462	6.584423285	1.321182353	-5.875570347
	O463	-0.725384716	7.124706255	-6.334803254
	O464	11.628752745	0.623801416	2.644648462
	O465	13.751142610	-1.148248101	4.732581748
	O466	4.622067472	-3.071710449	-3.330241565
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	O469	10.044123313	-4.260129920	-4.663292746
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	O472	6.400517818	-2.100285578	-2.032914564
	O473	9.798233676	-3.792068098	3.972181696
	O474	7.591104167	-2.220869515	3.103401979
	O475	-4.888112236	4.175805271	-2.341100176
	O476	12.703249046	-3.848198732	-0.529537449
	O477	10.493823344	-4.548084007	1.399505810
	S478	0.257862624	5.333825098	3.508320079
	S479	1.451514138	3.763343615	0.463959235
	S480	4.800278199	0.657855702	-1.918923305
	S481	1.367958419	1.571447501	3.192789708
	S482	1.734884380	0.740280536	-1.241576528
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	S484	4.664743563	-1.663626732	0.816844023
	S485	3.915248024	4.103009770	3.180801829
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	S487	5.006718673	0.503117638	3.982106960
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Fe (139) -2.158				
Fe (140) -0.018				
Fe (141) -2.512				
Fe (142) 2.538				
Fe (143) 2.616				
Fe (144) 2.153				
Fe (145) -0.821				
				
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	C1	-7.910980374	-5.031903361	1.570313873
	C2	-8.339946491	-6.176837442	0.645822890
	C3	-8.625299489	-2.992761976	2.740364150
	C4	-8.034734590	-3.234015398	4.126633464
	C5	-7.721757996	-4.775292173	5.997314038
	C6	-6.199063056	-4.944155196	5.944221939
	C7	-4.235794865	-5.395383186	4.559261426
	C8	-3.623490935	-3.993191235	4.500383915
	C9	-3.892145589	-1.687430624	3.716124895
	C10	-3.800461058	-1.025639787	5.100057820
	C11	-4.788238971	-0.696031701	7.288328737
	C12	-3.764770781	-1.311521941	8.254582610
	C13	-3.007289579	-3.353857443	9.378520656
	C14	-1.576099576	-3.754446938	8.996820055
	C15	-0.102308511	-4.574100577	7.204334743
	C16	0.695331880	-3.494894275	6.466721501
	C17	0.627271784	-1.424135794	5.166750900
	C18	0.988265091	-0.182721266	5.995282675
	C19	-0.105057992	-1.096084758	3.845448155
	C20	0.546596993	0.093542079	3.131271393
	C21	-0.131095425	-2.330577782	2.937043044
	C22	0.191279795	1.741427202	7.3036067800
	C23	0.544521040	1.407721613	8.764842358
	C24	-0.982024104	2.740471203	7.161503739
	C25	-0.759146499	3.975991448	8.042872256
	C26	-1.156511534	3.155129339	5.693882277
	C27	0.078999420	0.132710896	10.772163352
	C28	1.516394850	-0.328725650	10.916378330
	C29	5.455362808	-11.693447297	4.067163295
	C30	6.097786817	-10.459529068	3.436118965
	C31	6.463101203	-8.020140966	3.788897225
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	C39	-5.454495203	-2.570450089	-1.449620814
	C40	-5.853330487	-1.150324892	-0.998977687
	C41	-3.917764904	-2.697186385	-1.432976675
	C42	-3.370692527	-4.138647167	-1.487408522
	C43	-3.172838598	-4.732872807	-2.881529303
	C44	-6.131067341	1.134488749	-1.949086268
	C45	-7.226979503	1.687668877	-1.032215998
	C46	-6.238063304	1.691041781	-3.375889181
	C47	-9.412702491	1.306797269	0.001479007
	C48	-9.026462729	1.347634255	1.484632073
	C49	-7.365854072	0.814004235	3.201693794
	C50	-6.170158530	1.742170805	3.431525238
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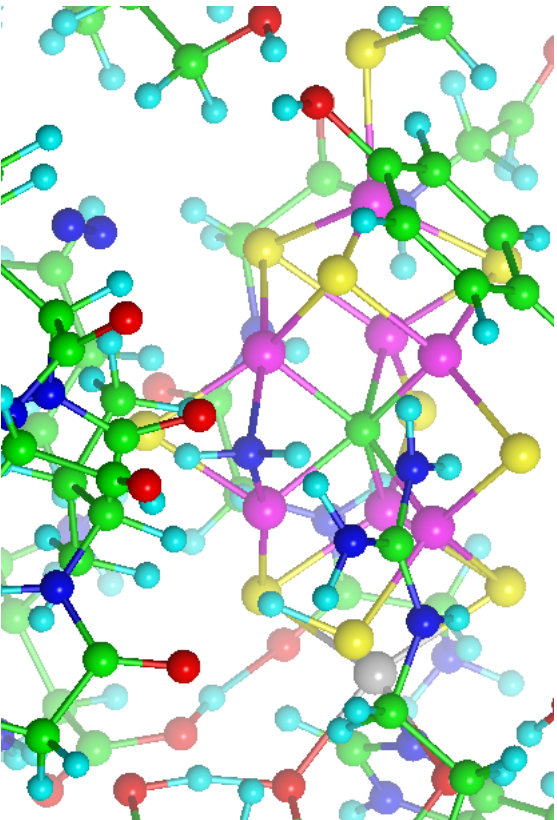
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C54	-3.377430706	2.398246121	0.385306281
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C56	-2.636856010	1.206492843	-1.339097644
C57	-6.528197656	6.440766708	3.111062710
C58	-6.363843952	6.671786023	4.611241752
C59	-8.017117015	6.552937130	2.703809050
C60	-8.592886097	7.932320403	2.577530823
C61	-8.434822827	9.057877340	3.364083106
C62	-9.826925737	9.474719755	1.690785723
C63	9.208369862	1.252728667	3.405775931
C64	10.172629380	0.088136027	3.280613952
C65	7.780231965	0.687229880	3.202739443
C66	6.706432291	1.732373528	3.392235756
C67	6.117354473	1.952658236	4.650300314
C68	6.262895298	2.515996197	2.311184208
C69	5.114148217	2.911065286	4.826572075
C70	5.276092470	3.486958699	2.475686271
C71	4.695945035	3.677458734	3.732350625
C72	5.571562947	6.580718121	-1.571692161
C73	4.573387220	7.735154497	-1.767958676
C74	4.829049894	5.306318772	-1.166619433
C75	3.578190800	9.314945118	-3.387135882
C76	2.093376317	8.979321922	-3.545989290
C77	0.411775662	7.139859308	-3.461292163
C78	-0.075914463	6.852314664	-2.017823931
C79	0.408407653	5.882179317	-4.356621099
C80	-0.870614575	5.044173914	-4.464407540
C81	-1.999346884	5.615657775	-5.336270124
C82	-3.462053884	7.587568657	-4.882069062
C83	0.392708001	5.898353104	0.188414296
C84	0.292312595	7.140800062	1.083218065
C85	1.359452993	4.908560406	0.869586126
C86	1.486052150	9.161711330	1.780793616
C87	0.957380339	10.541705761	1.428854093
C88	-0.348083165	11.876877962	-0.133815461
C89	-1.564958390	12.510776095	0.582095688
C90	-0.549295191	11.883787003	-1.653598283
C91	-1.773136627	11.102905259	-2.118429175
C92	-3.563966504	12.137585979	1.931556473
C93	-3.418031466	13.274045382	2.931605806
C94	-4.293641913	10.939057762	2.598352795
C95	-4.593755759	9.840982870	1.605146265
C96	-5.769211075	9.875674492	0.839982394
C97	-3.681230305	8.798923581	1.370778984
C98	-6.017934161	8.918551266	-0.144975307
C99	-3.900573742	7.847272318	0.371520660
C100	-5.069212327	7.923393846	-0.382288791
C101	3.776133844	-4.331294732	-8.995771980
C102	2.377440717	-4.015214078	-8.494896208
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C104	0.558980189	-1.057580251	-7.746717462
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C106	2.216760067	2.262800907	-7.996876432
C107	4.537595043	2.828660885	-7.560719505
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C109	-2.1963132554	-3.665964945	-9.095182238
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C112	-1.868064977	-5.688285179	-8.003215313
C113	-1.188858462	-6.187402131	-6.747901954
C114	-4.220308451	-0.156279834	-8.240247323
C115	-3.620247220	1.076692871	-8.886704846
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C122	-0.920388437	-0.017978517	-4.722552403
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C135	3.652504481	-9.096252784	-2.503743161
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C138	3.517900454	-0.921468223	-2.275801835
Fe139	3.675378821	-2.254763111	-3.728183195
Fe140	1.866769038	0.450751952	-1.312505141
Fe141	4.862748134	0.268518904	-1.431240772
Fe142	3.577605877	0.371097069	-3.725469447
Fe143	3.763649950	2.501342639	-2.165533212
Fe144	4.693656812	-2.288977963	-1.365333775
Fe145	2.109411886	-2.012488097	-1.746321271
H146	-6.593566057	-7.230300477	0.679079225
H147	-6.751424504	-6.277816328	-0.635393947
H148	-9.831470287	-4.293580576	1.553417500
H149	-9.035896643	-5.780370049	-0.110513738
H150	-8.928451653	-6.879095755	1.261553347
H151	-7.906265450	-2.356974313	2.202405363
H152	-8.909147389	-5.083991355	4.228801868
H153	-9.559412468	-2.427159918	2.856531242
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H157	-2.906023084	-1.591693336	3.245634268
H158	-5.132670025	-3.372783010	3.250558933
H159	-4.033440684	-5.921957505	3.616930090
H160	-4.551762986	0.372277231	7.204594750
H161	-5.629072694	-1.810283610	5.643719422
H162	-3.743219729	-5.938598368	5.373839949
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H164	-4.459422420	-3.209659201	7.810500918
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H175	1.599979250	-0.108651011	2.878871569
H176	9.280228067	1.630939049	4.443324857
H177	-1.988369389	3.867411300	5.589628315
H178	-1.590354098	4.683658395	7.907354394
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H182	1.103512001	2.210367065	6.905997325
H183	-1.003127911	0.243329392	6.312220337
H184	0.518649318	1.010657016	3.736963830
H185	1.611713905	4.107959247	0.157945945
H186	0.819963928	4.462784258	1.717012905
H187	2.792365734	5.205706522	2.192448070
H188	3.341143038	4.635611148	4.738373086
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	S479	3.602884760	4.749973713	-2.437599021
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	S481	1.832772127	-3.504781677	-3.369453286
	S482	3.594358140	1.578242262	-0.157978405
	S483	0.248810357	-1.017607440	-2.023603544
	S484	3.862699077	-0.930405780	-5.515772998
	S485	3.674262196	-3.819813198	0.055308491
	S486	5.483865844	1.477647141	-3.207646174
	S487	5.537541263	-3.350340642	-3.127614635
	S488	6.205200682	-1.072245151	-0.309346942
	end			
Fe2-brNH2-Fe6-3b2 2N2 dissociated 35, S=1				
Fe(139) -2.199				
Fe(140) -0.915				
Fe(141) -2.351				
Fe(142) 2.796				
Fe(143) 2.817				
Fe(144) 2.302				
Fe(145) -0.801				
				
	fe2brnh2Fe63b22n2xdtdb.car_3			
	C1	-7.903842839	-5.030651174	1.566443656
	C2	-8.334280096	-6.176189270	0.643914190
	C3	-8.621772462	-2.993715581	2.738733497
	C4	-8.032215686	-3.235570945	4.125543674
	C5	-7.719985507	-4.777158132	5.995829548
	C6	-6.197386370	-4.946055204	5.942906769
	C7	-4.234114654	-5.397365426	4.557844915
	C8	-3.622210433	-3.995121522	4.499268346
	C9	-3.890651838	-1.689563648	3.715186408
	C10	-3.798613872	-1.027414743	5.098983743
	C11	-4.786469687	-0.697704292	7.287327791
	C12	-3.763013121	-1.313098497	8.253692503
	C13	-3.004940726	-3.355605715	9.377175460
	C14	-1.573681059	-3.755712929	8.995068471
	C15	-0.100019152	-4.574224420	7.201965339
	C16	0.696736004	-3.495064862	6.463982074
	C17	0.628936470	-1.425863801	5.162945485
	C18	0.989266838	-0.183145066	5.990172913
	C19	-0.100939773	-1.100681944	3.840889741
	C20	0.557387156	0.083085005	3.124528953
	C21	-0.128041581	-2.335037696	2.932464101
	C22	0.192984468	1.739385886	7.301441967
	C23	0.546129488	1.405550651	8.762663180
	C24	-0.980098776	2.738869667	7.159783524
	C25	-0.757228342	3.974227119	8.041632057
	C26	-1.154540508	3.153999676	5.692271133
	C27	0.080977171	0.130999586	10.770413660
	C28	1.518438017	-0.330328208	10.914924960
	C29	5.455789228	-11.692923274	4.064763577
	C30	6.099478962	-10.459855129	3.434299521
	C31	6.465349655	-8.021059833	3.787749717
	C32	7.713063266	-7.688884219	4.626882413
	C33	5.369300205	-6.961433526	3.988631971
	C34	5.823980170	-5.561315145	3.580467846
	C35	4.678184436	-4.555816292	3.618197983
	C36	4.779589993	-2.047941541	3.539647579
	C37	10.011465152	-6.851640371	4.566586643
	C38	10.326018884	-5.374052599	4.523091075
	C39	-5.446666633	-2.569998970	-1.452234441
	C40	-5.849331891	-1.151075960	-1.002245448
	C41	-3.909842922	-2.697760616	-1.435391011
	C42	-3.366481770	-4.140402564	-1.489191313
	C43	-3.169960267	-4.734946540	-2.883437112
	C44	-6.136320536	1.131523706	-1.952984548
	C45	-7.231827163	1.683650154	-1.034988501
	C46	-6.240868855	1.689225060	-3.379573712
	C47	-9.415534124	1.303322308	0.002196698
	C48	-9.030269666	1.344001007	1.485698390
	C49	-7.373785466	0.805728571	3.205465572
	C50	-6.180105886	1.735692868	3.435312964
	C51	-4.521036759	3.270203930	2.482625213
	C52	-4.873369149	4.620218855	3.125046955
	C53	-3.905142242	3.584901920	1.109909464

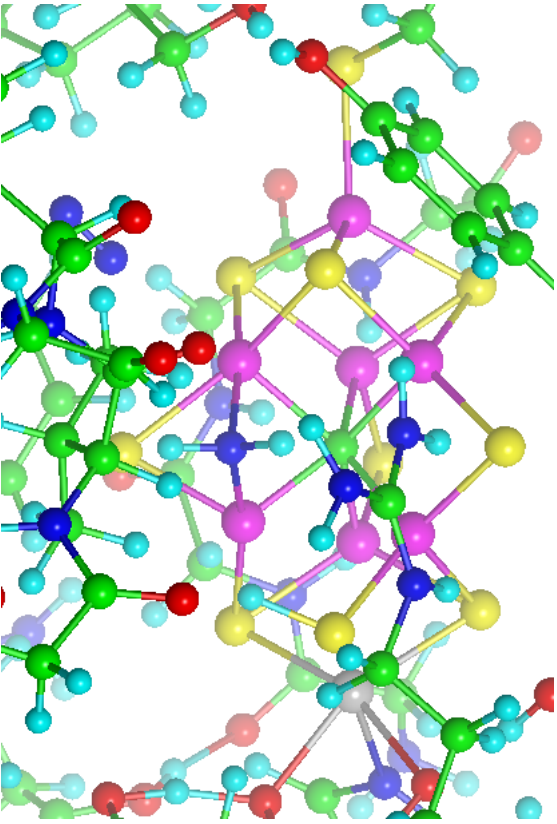
C54	-3.424408666	2.385165934	0.368211887
C55	-3.168125826	1.078447447	0.737597030
C56	-2.646486442	1.197340711	-1.342278419
C57	-6.523579402	6.440409687	3.108229679
C58	-6.359562195	6.671840059	4.607959751
C59	-8.012415385	6.553165843	2.701675588
C60	-8.588905142	7.932190578	2.575676490
C61	-8.432598483	9.057430004	3.363059535
C62	-9.824840109	9.473694133	1.689696349
C63	9.212253832	1.253064093	3.409085172
C64	10.175651683	0.087769561	3.282449475
C65	7.784726845	0.686462563	3.203277142
C66	6.708605462	1.729952058	3.389474879
C67	6.119247297	1.952060658	4.647136426
C68	6.262511432	2.509796910	2.306485212
C69	5.115015409	2.909753052	4.822303441
C70	5.274393492	3.479809539	2.469694835
C71	4.695574565	3.673450629	3.726725572
C72	5.578673742	6.583556966	-1.575118956
C73	4.579860934	7.738166109	-1.770290549
C74	4.831280911	5.308132175	-1.183625846
C75	3.580957458	9.315608386	-3.389130505
C76	2.096227506	8.978757732	-3.548844553
C77	0.414112737	7.140219909	-3.463333321
C78	-0.066496390	6.850474385	-2.017788113
C79	0.409720795	5.880783026	-4.357705392
C80	-0.868334582	5.041174161	-4.465107020
C81	-1.997924921	5.613023613	-5.336167331
C82	-3.460417467	7.585555055	-4.882107976
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C84	0.307844614	7.149177677	1.079917839
C85	1.403546824	4.934197200	0.872996527
C86	1.494088890	9.170595288	1.782298683
C87	0.961670726	10.548806217	1.429920528
C88	-0.346672294	11.877506674	-0.134974578
C89	-1.563821501	12.509958933	0.581121516
C90	-0.547940640	11.881482770	-1.654549551
C91	-1.771558508	11.100104366	-2.118971372
C92	-3.563167448	12.136290103	1.930711043
C93	-3.416420567	13.272379264	2.930651527
C94	-4.292084556	10.936612868	2.596898466
C95	-4.591433682	9.838259808	1.603503026
C96	-5.766812197	9.872137063	0.838073709
C97	-3.678798054	8.796053645	1.369808232
C98	-6.015213180	8.914576801	-0.146600897
C99	-3.897928435	7.843953921	0.370835626
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C101	3.777557004	-4.331818001	-8.995687439
C102	2.378571288	-4.015937448	-8.496447421
C103	1.022282405	-2.404031400	-7.178757995
C104	0.559347370	-1.057816729	-7.747984091
C105	1.010690850	1.358409814	-7.761030240
C106	2.216885731	2.262224699	-7.997965757
C107	4.538035125	2.829075734	-7.564791625
C108	4.997969077	3.070837530	-8.987845242
C109	-2.958329768	-3.665783407	-9.092825233
C110	-3.931828803	-2.513469584	-8.818509587
C111	-2.505015951	-4.309086691	-7.762751362
C112	-1.865861757	-5.689491077	-8.003814538
C113	-1.186530953	-6.189471069	-6.749202082
C114	-4.215320694	-0.157028565	-8.238518270
C115	-3.616780717	1.075880170	-8.885475368
C116	-4.670976179	0.040352958	-6.770706217
C117	-3.469603408	0.057179519	-5.872602949
C118	-2.741567873	1.242542063	-5.677266599
C119	-2.951837533	-1.153338380	-5.384194326
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C121	-1.684314011	-1.197885285	-4.801750782
C122	-0.924025402	-0.028586041	-4.704117086
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C138	3.525479958	-0.918964618	-2.277020198
Fe139	3.666883029	-2.277450060	-3.729267124
Fe140	2.141646447	0.309071960	-1.528254748
Fe141	4.818385950	0.289092926	-1.385098223
Fe142	3.702103721	0.349385466	-3.775800424
Fe143	3.714857550	2.519523217	-2.188406601
Fe144	4.686293798	-2.300491970	-1.366179984
Fe145	2.093422240	-2.059871147	-1.769168130
H146	-6.589807462	-7.232744112	0.676505406
H147	-6.747517949	-6.281001428	-0.638835867
H148	-9.825570205	-4.296292168	1.551878433
H149	-9.031138965	-5.779909435	-0.111732452
H150	-8.922734064	-6.876621638	1.261467820
H151	-7.903303085	-2.356208295	2.202245883
H152	-8.906719664	-5.085802001	4.226810693
H153	-9.556762207	-2.429451714	2.854379861
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H155	-6.273687904	-5.420562426	3.936140199
H156	-7.924663392	-4.006351608	6.750340672
H157	-2.904471104	-1.593923835	3.244671086
H158	-5.130632866	-3.375020914	3.248225513
H159	-4.031886288	-5.923723036	3.615390055
H160	-4.550060480	0.370570437	7.203672046
H161	-5.626605513	-1.812911514	5.643125811
H162	-3.741453388	-5.940691482	5.372266110
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H164	-4.457475446	-3.211359696	7.809417613
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H166	-0.599034947	-3.200297027	3.419795941
H167	-0.687688589	-2.121673623	2.008467973
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H171	-1.366421628	2.296125947	5.039375574
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H174	0.033519223	0.278636964	2.179868321
H175	1.613648888	-0.119530935	2.885676833
H176	9.283730810	1.631283005	4.446828352
H177	-1.986463524	3.866207573	5.587990710
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H201	1.972522648	-0.753994503	9.988222415
H202	10.857287926	-7.418701433	4.147743446
H203	-1.983328283	-6.036962272	-3.925658059
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H205	-2.651324623	-6.407635242	-8.279396021
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H207	-3.362800166	-4.429025973	-7.082450240
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H211	-4.040741220	-4.822425813	-0.941435792
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H219	-3.538816997	-2.219412369	-0.519103326
H220	0.505453328	-5.501408942	-7.470137030
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H222	-3.781195241	2.793447757	3.140971415
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H224	-8.191914221	1.170895664	3.841579297
H225	-7.301557840	0.233245070	1.143962143
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H238	-9.799579307	2.304984878	-0.235273000
H239	-2.305317478	0.968107893	-2.348799006
H240	-10.242807031	0.591598396	-0.121156434
H241	10.369216414	2.767800099	2.657185853
H242	8.778644928	2.933645889	2.323185193
H243	1.681282960	5.793706635	-1.556861470
H244	-0.577417665	5.442101504	0.180002374
H245	1.961963465	7.916987361	0.149652944
H246	-3.207589361	3.272541880	-1.566205656
H247	-4.954303351	4.213843086	-2.777783715
H248	-6.448423681	3.436558681	-4.239566316
H249	-4.608298947	5.469368953	-1.873954741
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H251	-7.183679350	1.352653518	-3.840615856
H252	0.371636758	11.535656743	-2.146887645
H253	-0.708998356	12.930382802	-1.949364148
H254	-0.613789555	10.070747980	-3.491789165
H255	-2.330512948	9.662709967	-3.422722017
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H258	-6.940564546	8.946254103	-0.727529093
H259	-2.776006010	8.701196686	1.978861178
H260	-4.436843733	7.817889574	-3.087430702
H261	1.206205793	5.213761875	-3.991397615
H262	2.536441860	6.999870379	-3.331734724
H263	-1.261210633	4.773997750	-3.471920293
H264	-8.379026958	0.030556420	-1.384335387
H265	3.926639302	9.767586362	-4.328419624
H266	-6.044218877	-0.815480246	-2.951038299
H267	0.719169240	6.196144822	-5.368404612
H268	-3.152346675	7.074474192	0.168746626
H269	3.638174630	10.083772729	-2.604572096
H270	-2.694240515	7.691863186	-6.794747519
H271	-4.863693688	8.957421778	-4.316292963
H272	-5.347956787	-3.480940103	-3.294132490
H273	-5.851324146	-3.245181478	-0.673905815
H274	-6.505956470	10.657744603	1.013176189
H275	-5.196208036	1.483527226	-1.505624403
H276	-0.258416922	7.908748054	-3.856318113
H277	-1.564098828	6.240116941	-6.126308984
H278	-0.561416770	4.094997060	-4.931629455
H279	-3.407807568	5.886738943	-3.759194461
H280	1.054026743	8.880500181	2.748443607
H281	-0.072171346	9.735201786	-0.137964916
H282	0.472141121	12.581317939	0.082789473
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H289	3.072311382	-5.931845322	-10.033173279
H290	5.572537637	4.509999314	-1.047496358
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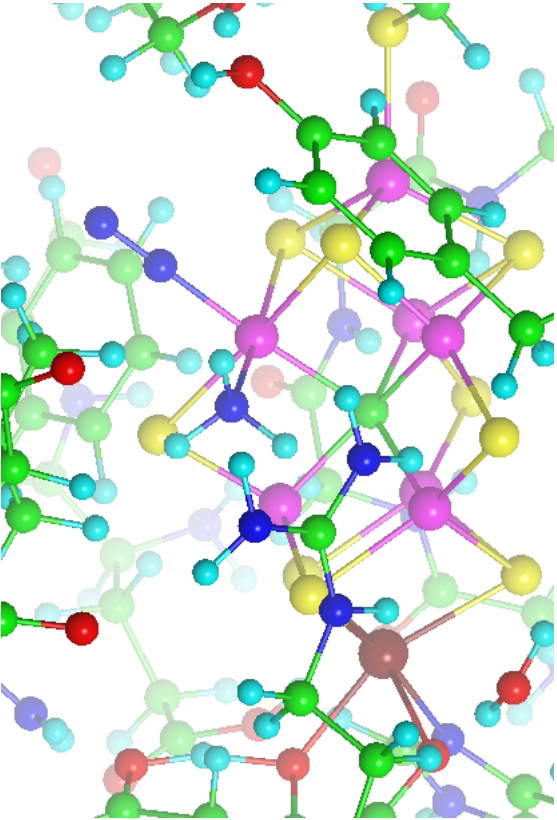
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C110	-3.938282410	-2.509454797	-8.808422685
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C119	-2.958323408	-1.157621066	-5.370286139
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C121	-1.691203496	-1.204698371	-4.787272025
C122	-0.929131925	-0.036727613	-4.689369656
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C124	8.772305411	-6.830565353	-3.729616415
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C132	1.884367142	-6.980855092	0.302786828
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C134	2.623913682	-8.650209580	-1.468504768
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N417	-1.903863011	-3.245442314	-10.013769762
N418	-3.383921702	-1.312032943	-8.469591415
N419	7.735965875	-7.582605430	-5.880680845
N420	3.973707705	-5.861629903	-4.271804475
N421	3.300527594	-6.855198638	-6.121371716
N422	8.852487572	-7.953639384	-2.964792965
O423	-6.737164698	-4.887056493	1.953956574
O424	-7.313452736	-2.366064122	4.656935348
O425	-5.493019114	-4.719018297	6.938357692
O426	-2.566242867	-3.703488086	5.092582000
O427	-2.854192438	-0.261828580	5.380373932
O428	-2.988091040	-0.588401276	8.916412748
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O430	1.933183710	-3.621647533	6.328585670
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O433	2.151383166	-0.302485039	11.960382625
O434	6.654183198	-10.547162560	2.335038726
O435	7.704625316	-7.839923299	5.871178287
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O438	-3.936596513	-4.454621495	-3.839964551
O439	-7.066638029	2.758351435	-0.412646919
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O448	1.286001370	9.893471100	-3.727638584
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O452	1.309894826	11.532570064	2.063051271
O453	-1.844746702	13.698877586	0.408119939
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O455	-4.341194115	14.004416895	3.237762202
O456	-5.262248881	6.989692159	-1.421318536
O457	1.434018863	-4.820169737	-8.676817165
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O460	5.671892977	4.040885791	-9.306768542
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O462	-1.780724838	-6.729017767	-5.825279522
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	O465	9.659133085	-5.956761135	-3.669895765
	O466	12.301423299	-7.587540665	-2.039765206
	O467	0.106930338	-6.218425218	-1.141889512
	O468	-0.477822155	-7.215223158	0.789351815
	O469	4.680150415	-11.206837191	-3.051152608
	O470	2.421100897	-11.087857015	-3.044287604
	O471	4.899485774	-6.057504258	-1.248991916
	O472	4.775793659	-7.669099723	0.317859051
	O473	2.391012439	-6.242226611	-1.945522189
	O474	8.704098799	-6.878369222	1.120056227
	O475	6.911076932	-4.804782761	0.328516736
	O476	-4.216828248	4.831696343	-2.501619309
	O477	7.279641499	-10.815926335	-2.256268235
	O478	7.159015556	-8.933053008	0.103378389
	S479	3.598501301	4.795279368	-2.486595079
	S480	1.873501048	1.702876865	-3.321773214
	S481	1.819575083	-3.530763203	-3.367931868
	S482	3.506746958	1.635534051	-0.188798034
	S483	0.268697120	-0.986148174	-1.961502735
	S484	3.857734124	-0.998147732	-5.557372443
	S485	3.634987537	-3.824630236	0.035610697
	S486	5.498064774	1.509078744	-3.167025421
	S487	5.532157547	-3.345709230	-3.135348789
	S488	6.183031272	-1.047468517	-0.306950420
	end			
Fe2-NH3 2N2 associated 35, S=1 Fe (139) -2.269 Fe (140) 0.009 Fe (141) -2.749 Fe (142) 2.766 Fe (143) 3.199 Fe (144) 2.326 Fe (145) -1.822		bmexpprot2nh32n2xdtd.car_3		
	C1	-3.092612840	-4.747867519	-7.617806296
	C2	-2.243743789	-4.786416586	-8.893216973
	C3	-5.333399693	-4.370813106	-6.685025176
	C4	-5.429240816	-5.540167147	-5.711115548
	C5	-5.148603882	-7.939656454	-5.335912845
	C6	-4.035921946	-7.948046425	-4.282060460
	C7	-1.852113601	-7.113230485	-3.582004107
	C8	-2.279494296	-6.137703121	-2.479212451
	C9	-3.518378043	-4.086381972	-1.969246753
	C10	-4.519700410	-4.746362614	-1.010637289
	C11	-6.388779399	-6.252972954	-0.708736948
	C12	-5.813535397	-7.328648696	0.224478463
	C13	-4.509345949	-9.399642999	0.381124758
	C14	-3.179530244	-9.316636617	1.142944081
	C15	-0.875338648	-8.444275250	1.146912062
	C16	-0.627515855	-7.112695181	1.859037905
	C17	-1.478223267	-4.839568972	2.282372125
	C18	-2.491159138	-4.724492533	3.438815411
	C19	-1.521483994	-3.677805110	1.265986591
	C20	-1.615298539	-2.325928760	1.978558109
	C21	-0.307509138	-3.750496633	0.332783965
	C22	-4.833994006	-4.494664541	4.136146156
	C23	-5.108139850	-5.788901595	4.922412410
	C24	-6.114234748	-3.876573576	3.522827321
	C25	-7.248139454	-3.807523476	4.552259874
	C26	-5.821454446	-2.478991323	2.960375982
	C27	-5.628835002	-8.156216938	4.885974621
	C28	-4.616424640	-8.494377837	5.963239580
	C29	8.401889445	-10.602940218	0.164875793
	C30	8.439506101	-9.345015627	1.025035147
	C31	7.108821792	-8.068984109	2.698035117
	C32	7.322961329	-8.403091585	4.185787805
	C33	5.668211491	-7.605778544	2.424490464
	C34	5.305034824	-6.330928571	3.182630954
	C35	4.015513476	-5.699862177	2.657258949
C36	2.793863460	-4.017864621	4.061157498	
C37	8.372375767	-7.665009869	6.275898618	
C38	7.738817813	-6.603086429	7.145638880	
C39	-1.471821377	-0.728848445	-5.950087616	
C40	-2.742493626	-0.125260275	-5.324999869	
C41	-0.371610481	-0.809261890	-4.871427439	
C42	0.825341109	-1.718494653	-5.218198463	
C43	1.965356388	-1.062058403	-5.996220242	
C44	-3.769088745	2.089604076	-4.851100897	
C45	-5.253688725	1.730224909	-4.984959371	
C46	-3.481584902	3.523790728	-5.320024745	
C47	-6.969336655	0.624846312	-6.335543970	
C48	-7.442660024	-0.447889748	-5.346285394	
C49	-6.837171934	-2.037578711	-3.582580653	
C50	-6.675932819	-1.553424212	-2.138809194	
C51	-6.040545161	0.244136148	-0.595652464	
C52	-7.375860989	0.626242953	0.061653586	
C53	-5.171292343	1.511944725	-0.597666219	
C54	-3.784058933	1.300551090	-1.101620582	
C55	-3.046316313	0.176243422	-1.408963925	

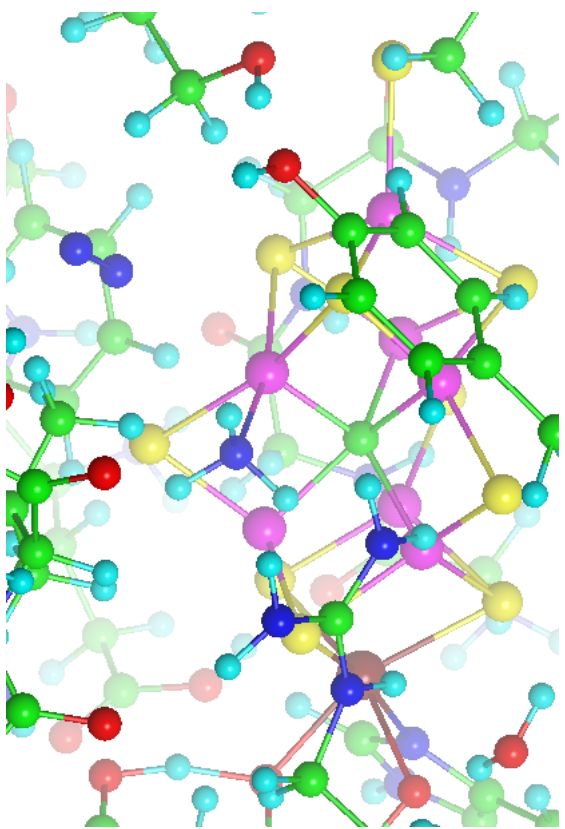
C56	-1.760158046	1.840251853	-1.847399279
C57	-9.516891530	1.759431242	-0.331255157
C58	-10.259556990	0.785542299	0.580343986
C59	-10.367906076	2.095902957	-1.578569310
C60	-11.472429932	3.095820697	-1.399718493
C61	-12.404658244	3.250016951	-0.392113304
C62	-12.716418915	4.773565625	-1.970674754
C63	3.883771029	-1.211351114	9.144602062
C64	5.274904807	-1.806479424	9.256518255
C65	3.360272705	-1.547019696	7.724870475
C66	1.954371737	-1.051685809	7.480323827
C67	0.830911034	-1.853794170	7.751697058
C68	1.732256168	0.239317210	6.970400104
C69	-0.468848003	-1.391871515	7.509204488
C70	0.443692003	0.721195284	6.743680149
C71	-0.657282294	-0.100305151	7.001284708
C72	0.779128218	5.828204945	6.597964222
C73	-0.450044954	6.708459095	6.304316740
C74	0.876106855	4.702668300	5.575664307
C75	-1.234597296	8.939859560	5.583391196
C76	-1.927958921	8.800181838	4.225574175
C77	-2.029610936	7.465164331	2.124639688
C78	-2.896156555	6.191816664	2.296352805
C79	-0.887283413	7.264043776	1.102596748
C80	-1.231184939	6.745140152	-0.298827968
C81	-1.893366936	7.745260153	-1.260987750
C82	-4.206281627	8.672345755	-1.151631938
C83	-3.105228167	3.925864342	3.200837279
C84	-4.307731023	4.066501734	4.145014668
C85	-2.217282021	2.781621214	3.731123091
C86	-5.004220308	4.903255588	6.339294961
C87	-6.011753702	6.036235916	6.450372129
C88	-6.943635052	8.028629515	5.393343889
C89	-8.455998826	7.896861610	5.090837120
C90	-6.319959217	9.161562009	4.571757299
C91	-6.431027855	8.964234619	3.063674224
C92	-10.232985123	6.526295165	4.106729582
C93	-11.268979509	6.527428091	5.220612327
C94	-10.313091952	5.201646817	3.297070799
C95	-9.413990483	5.228222878	2.082521152
C96	-9.872352657	5.760596263	0.869088021
C97	-8.081149537	4.788999636	2.150784691
C98	-9.024530892	5.876344253	-0.235253364
C99	-7.209274506	4.922961862	1.066251867
C100	-7.692240535	5.475133790	-0.117950135
C101	9.333798285	3.867132886	-3.392799204
C102	7.979250240	3.718354075	-4.064030508
C103	5.524626220	3.823722891	-3.717289088
C104	4.729283165	5.132235652	-3.661057725
C105	3.665542336	6.759649180	-2.155259782
C106	4.077540595	7.561566003	-0.924423259
C107	5.147298485	7.648712669	1.257454493
C108	6.015601074	8.876320749	1.061859535
C109	4.478074412	4.252671329	-8.126236943
C110	3.035926304	4.773280561	-8.164485087
C111	4.519119470	2.842112825	-7.493448985
C112	5.849960551	2.131793284	-7.807447362
C113	6.000265558	0.878874124	-6.974364543
C114	1.225854270	5.911655696	-6.974972163
C115	1.218475766	7.256856044	-6.277851501
C116	0.159848800	4.910177750	-6.470931065
C117	0.588850037	4.244704382	-5.193541377
C118	0.388666841	4.869957512	-3.952444679
C119	1.309670167	3.038865580	-5.238636960
C120	0.939604491	4.326098193	-2.789892700
C121	1.860713151	2.498870476	-4.075155021
C122	1.698159238	3.155061559	-2.851706191
C123	11.196270649	-0.744028819	0.261384322
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C125	10.080925399	-1.486387307	-0.489333785
C126	9.504728555	-0.794324727	-1.681952876
C127	10.168263591	-0.394272585	-2.823999636
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C130	13.271568626	-2.918571268	3.457735660
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C132	5.041904042	-4.726299765	-1.831181786
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C136	9.762956360	-4.791566929	-3.778190995
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C138	3.958008882	1.197998371	1.170994095
Fe139	5.620924512	1.490017887	-0.016230138
Fe140	1.819387143	1.096730039	1.190814841
Fe141	3.861776139	1.459754788	3.167752955
Fe142	4.071042714	3.155395350	1.204510434
Fe143	2.214461542	3.577754581	2.979744419
Fe144	5.171192838	-0.303659795	1.785948619
Fe145	3.705431921	-0.058458345	-0.323030403
H146	-0.527302620	-5.495935747	-8.052832535
H147	-0.524001154	-3.880250704	-8.267974285
H148	-4.774412049	-4.377013058	-8.746125778
H149	-2.547089415	-3.946985438	-9.539615126
H150	-2.525576699	-5.704232072	-9.436768944
H151	-5.018081635	-3.498296557	-6.093344031
H152	-4.895122435	-6.862325901	-7.179774869
H153	-6.338150485	-4.168748101	-7.080121027
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H157	-2.744153845	-3.606683349	-1.358366890
H158	-3.041453079	-4.867454157	-3.905677204
H159	-0.943259776	-6.738325345	-4.072698461
H160	-6.879870887	-5.506377799	-0.070368414
H161	-5.483078193	-5.679594691	-2.581464507
H162	-1.615457247	-8.070905852	-3.103447502
H163	-4.019893043	-3.303888316	-2.553807627
H164	-4.742175563	-8.147530375	-1.339835425
H165	-7.147030857	-6.721328962	-1.351403416
H166	-0.271743907	-4.708442051	-0.205241299
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H171	-5.049374836	-2.497738529	2.179495540
H172	-5.386505034	-6.900132369	3.180119963
H173	-7.540690154	-4.799731446	4.924771593
H174	-0.782012846	-2.188707272	2.685219835
H175	-2.547691112	-2.226498750	2.551640980
H176	3.239173645	-1.730347368	9.879215699
H177	-6.727226778	-2.045459075	2.512494286
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H179	-5.486658226	-1.804988501	3.765538503
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H187	-2.047158503	2.012941622	5.539499493
H188	-2.585094150	-0.273828474	6.869411152
H189	0.288373601	1.714568396	6.322231375
H190	2.585242074	0.868609453	6.706637130
H191	0.969714072	-2.865063998	8.145011996
H192	-2.264060946	-6.303281875	0.933197560
H193	-0.095484616	-8.560477911	0.379703792
H194	-0.734943142	-9.239004727	1.890830288
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H196	-5.273423007	-9.665434823	1.121099304
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H198	-0.505244411	-4.812725178	2.787665668
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H201	-3.590222115	-8.094412782	5.788547748
H202	9.458053648	-7.683067788	6.459504409
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H204	4.981042901	-2.730382730	-2.942059254
H205	5.862235871	1.841490376	-8.867607415
H206	6.695310585	2.810590514	-7.623462848
H207	3.687851201	2.229685830	-7.876356315
H208	2.184269281	7.811230910	-6.343916434
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H210	-0.020248375	0.210032568	-4.650986741
H211	0.484223760	-2.579476608	-5.820738944
H212	3.172640267	5.446344188	-6.205461317
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H214	5.292443129	5.329407034	-6.547476006
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H217	6.362443146	4.969072642	-7.743891212
H218	-1.449671668	-0.259944466	-7.962651389
H219	-0.828938501	-1.171078771	-3.940158515

H220	7.076066104	1.926164285	-5.706774630
H221	1.230140141	-2.148698471	-4.289742890
H222	-5.589499711	-0.533301507	0.036701972
H223	-3.360553088	-0.860436858	-1.336567488
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	H338	6.921375885	-4.398258802	-3.900544829
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	H366	-7.306249017	5.824272173	-1.992616562
	H367	2.514481933	-1.242757398	2.145404955
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O437	-3.551656339	-0.791340337	-4.652410352
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O457	7.894592245	3.306246532	-5.247014440
O458	4.438898863	5.769091189	-4.696243379
O459	3.654487265	8.722591934	-0.786175856
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	O470	9.354328005	-5.097860232	-4.933318719
	O471	7.245749583	-2.886744221	0.154684471
	O472	7.354776298	-5.124273680	0.004130441
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	O474	9.145359008	-5.182587546	3.654463922
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	O477	12.101108274	-5.249639522	-0.842534690
	O478	9.811447549	-5.781340778	1.036156897
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	S482	1.657846828	1.487815093	3.551530859
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Fe2-NH3 2N2 dissociated 35, S=1 Fe(139) -2.403 Fe(140) 0.055 Fe(141) -2.559 Fe(142) 2.780 Fe(143) 3.197 Fe(144) 2.436 Fe(145) -2.120			bmexpprot2nh32n2xdtg.car 1	
	C1	-3.089011829	-4.745734287	-7.612890061
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	C3	-5.333005298	-4.372906971	-6.684884045
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	C5	-5.146621636	-7.939856694	-5.337888066
	C6	-4.034315836	-7.950744272	-4.282910652
	C7	-1.852019781	-7.115316448	-3.580255319
	C8	-2.278817381	-6.140711576	-2.478599432
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	C10	-4.520470894	-4.749377018	-1.009976167
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	C15	-0.874648294	-8.446424545	1.144975511
	C16	-0.625411093	-7.117491050	1.858737761
	C17	-1.469899848	-4.843915158	2.284040954
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	C20	-1.606004199	-2.338666742	1.981025179
	C21	-0.301408847	-3.753823861	0.335073093
	C22	-4.830554401	-4.495115657	4.133565860
	C23	-5.105923317	-5.790297984	4.920694178
	C24	-6.111949447	-3.877034742	3.521077608
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	C30	8.441103508	-9.346166527	1.023744864
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	C32	7.325727864	-8.405466498	4.184730556
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	C34	5.309385404	-6.333343178	3.184837678
	C35	4.020818914	-5.699580489	2.661391039
	C36	2.800291617	-4.014678355	4.063882419
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C41	-0.364478660	-0.806626166	-4.868073240	
C42	0.831076007	-1.718062872	-5.217254386	
C43	1.970331608	-1.061700378	-5.995603720	
C44	-3.766769926	2.090305817	-4.851526222	
C45	-5.251825918	1.730033981	-4.985484622	
C46	-3.478720390	3.524297103	-5.318866969	
C47	-6.968467850	0.626201959	-6.335287531	
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C49	-6.837989006	-2.039553139	-3.585482990	
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C52	-7.369896267	0.629058146	0.060454992	
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C54	-3.782733599	1.299254211	-1.127813962	
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C56	-1.757152928	1.837927051	-1.873588847	

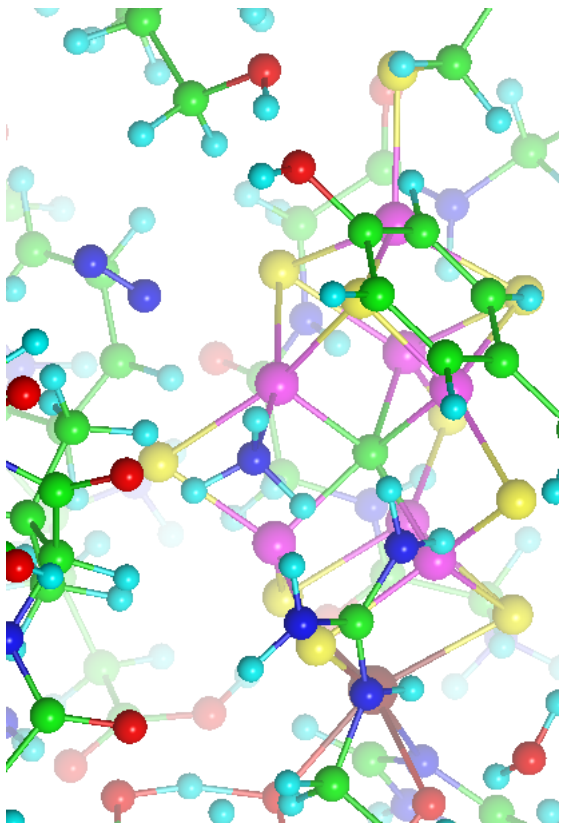
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C60	-11.469022061	3.096871821	-1.394578479
C61	-12.402738678	3.249856811	-0.388329998
C62	-12.713437592	4.774391353	-1.966392606
C63	3.882744073	-1.212326198	9.149965154
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C65	3.361652629	-1.547241258	7.729382255
C66	1.957600163	-1.049031086	7.482154771
C67	0.833583401	-1.850623929	7.752822277
C68	1.738850181	0.239246866	6.964603794
C69	-0.465376747	-1.387624205	7.508070905
C70	0.450642561	0.722266151	6.737447139
C71	-0.651941792	-0.096207269	6.997327675
C72	0.778996515	5.832294259	6.598643220
C73	-0.450378984	6.712253342	6.304077131
C74	0.876074480	4.705902827	5.578248946
C75	-1.233918282	8.942515381	5.581985642
C76	-1.926226969	8.802547789	4.223162262
C77	-2.023850303	7.469077183	2.121834166
C78	-2.887263124	6.192796993	2.294154530
C79	-0.882460212	7.267022015	1.099667462
C80	-1.227645261	6.744653429	-0.300312775
C81	-1.891536440	7.743519705	-1.263822523
C82	-4.203159991	8.670558657	-1.151485607
C83	-3.089482659	3.931115202	3.217844696
C84	-4.302914637	4.076641694	4.149880251
C85	-2.203745570	2.798249249	3.777959883
C86	-5.008312321	4.906330371	6.345424478
C87	-6.016121869	6.037786486	6.456703676
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C101	9.332789525	3.866295990	-3.393271261
C102	7.978598681	3.718369698	-4.065071448
C103	5.525713345	3.822922285	-3.716570857
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C112	5.851264415	2.129302468	-7.806227778
C113	6.002742714	0.877643711	-6.972918298
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Fe142	4.096443307	3.158403610	1.174184549
Fe143	2.218699718	3.589799481	2.979290742
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H148	-4.768778840	-4.378620382	-8.743041396
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H262	-0.603301575	7.335543036	3.706801624
H263	-1.832350875	5.825708095	-0.248307529
H264	-4.886635243	0.874271624	-6.802551303
H265	-0.818480610	9.956427936	5.648723215
H266	-2.122258839	1.552133170	-6.193395023
H267	-0.351087171	8.229124527	1.009579000
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H269	-2.029025641	8.856480737	6.336460975
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H271	-6.193358601	9.122461887	-1.244248079
H272	-0.001522562	0.043609558	-7.168173601
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H274	-10.907023559	6.089437742	0.775569815
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H286	9.516762180	2.897923264	-2.883082430
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H295	5.704460960	6.951656517	1.901663795
H296	1.688758337	6.449987906	6.544341976
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H298	7.804524114	-7.276251013	2.389417087
H299	5.159686968	5.988012999	-0.079856646
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H302	2.421562641	1.563152220	-4.115206605

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H305	4.570940725	4.862581081	-1.648016300
H306	4.080722895	-5.558413439	1.570361091
H307	5.596270445	-7.423162893	1.340778939
H308	6.117426306	-5.596194082	3.069014653
H309	5.200929966	-6.532302075	4.262669715
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H312	8.112820514	-10.269476531	-0.846024142
H313	2.127323254	2.732314177	-1.947484418
H314	7.887344688	-12.248306725	1.286461192
H315	7.108621786	-12.172504385	-0.151688108
H316	4.598492994	-3.734894919	3.171472520
H317	0.787882257	4.802181656	-1.819427691
H318	1.442424453	2.522055984	-6.193736558
H319	11.361385366	-5.518376893	-0.253905163
H320	10.475824981	-2.467951105	-0.827726080
H321	8.963383691	-5.444284420	0.645470840
H322	11.648780586	-5.125141238	-1.729118089
H323	6.590921735	8.903322120	0.103792650
H324	7.144605837	-3.214337749	1.982124314
H325	5.230574310	-5.806416489	-1.746882502
H326	7.053480493	4.208833392	-2.302350090
H327	7.349585101	-5.650377315	-2.711663726
H328	9.371532927	0.300905746	-4.680660607
H329	7.077498868	0.038266332	-3.645983198
H330	9.439123549	-10.970649712	0.084685860
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H332	8.445474538	-4.506192570	3.501881365
H333	7.024266819	-2.457453936	3.330293984
H334	8.474333302	-6.673841253	4.375111255
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H338	6.922094644	-4.410807545	-3.901942532
H339	5.052874798	3.053474004	-3.086111753
H340	-0.187026046	5.797569278	-3.910989700
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H343	9.476311978	-5.388020792	2.735227321
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H345	0.973863862	-4.479541859	4.850562368
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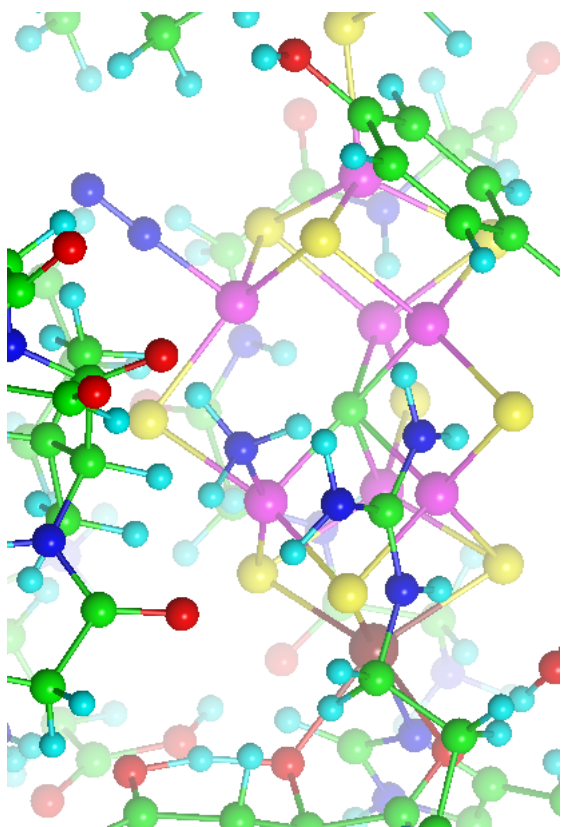
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O470	9.362494355	-5.085579323	-4.951137763
O471	7.234472929	-2.902147467	0.153859803
O472	7.371322906	-5.138149135	-0.018299552
O473	6.076688389	-2.567654149	-2.166401463
O474	9.153980037	-5.187487928	3.649628029
O475	7.028351668	-3.361817603	2.946744004
O476	-4.330465666	5.036815220	-1.913373199
O477	12.105142215	-5.256256897	-0.851487909
O478	9.818846592	-5.785453718	1.031692137
S479	1.014594103	5.378726894	3.830583325
S480	1.870729351	3.494874736	0.661754267
S481	5.072863238	0.501530517	-1.976752198
S482	1.638019935	1.574215852	3.558629635
S483	1.672664638	0.364426372	-0.871923982
S484	5.863641968	3.691380631	-0.108262968
S485	4.317639634	-2.009291709	0.595755325
S486	4.498843572	3.612729318	3.334777930
S487	7.199626459	0.285228867	1.052240110
S488	4.952839918	-0.249669322	3.992021327
end			

Fe6-NH3 2N2 associated 35, S=1	bmexpprot2n2x6nh31.car_2			
Fe (139) -2.415	C1	-7.522959862	-5.812281982	0.290854687
Fe (140) -0.918	C2	-7.631335450	-7.001099916	-0.669100925
Fe (141) -2.703	C3	-8.682938135	-3.875122023	1.255866354
Fe (142) 2.527	C4	-8.298481746	-4.021237464	2.724809047
Fe (143) 2.801	C5	-8.114432749	-5.488938994	4.672153035
Fe (144) 2.254	C6	-6.601078251	-5.467065986	4.909433325
Fe (145) 0.371	C7	-4.362365658	-5.659026135	3.958294305
	C8	-3.941274871	-4.185610200	3.980820012
	C9	-4.405199847	-1.943534516	3.099187432
	C10	-4.698595032	-1.295091779	4.459640767
	C11	-6.155278941	-1.131175958	6.385197996
	C12	-5.260049668	-1.575229876	7.550801533
	C13	-4.338944642	-3.482910201	8.790665331
	C14	-2.816008928	-3.672302957	8.730287089
	C15	-0.888371530	-4.330301021	7.345212712
	C16	-0.135223518	-3.191496944	6.656470145
	C17	-0.338771644	-1.061732770	5.434276014
	C18	-0.432614581	0.188516172	6.330506650
	C19	-0.871508162	-0.883838256	3.994232704
	C20	-0.344787556	0.404388620	3.3515804196
	C21	-0.525693822	-2.120324746	3.157711227
	C22	-1.844431682	1.945426228	7.303466694
	C23	-1.731335785	1.706319277	8.821095588
	C24	-3.159471541	2.654601067	6.897214627
	C25	-3.444837136	3.863364392	7.795202418
	C26	-3.105604627	3.081406519	5.424322086
	C27	-2.422002110	0.433538229	10.768840847
	C28	-1.013505098	0.309454934	11.312186679
	C29	5.692613539	-11.028643581	5.459180819
	C30	6.362214646	-9.748926500	4.967543154
	C31	6.419931418	-7.289471250	5.352074663
	C32	7.435206148	-6.759014532	6.380141568
	C33	5.160164446	-6.409645075	5.302317876
	C34	5.466273003	-4.969476885	4.899480638
	C35	4.199792222	-4.178817040	4.578573222
	C36	4.222962894	-1.668615291	4.479146730
	C37	9.594959513	-5.639267854	6.676482994
	C38	9.714156626	-4.133696829	6.586549680
	C39	-4.812965149	-3.098349822	-2.332066198
	C40	-5.394944022	-1.702726450	-2.032289263
	C41	-3.304100371	-3.096927331	-2.009837119
	C42	-2.647940780	-4.489593034	-1.903399828
	C43	-2.131945678	-5.094349646	-3.209089224
	C44	-5.723802301	0.506535216	-3.122262572
	C45	-7.018569269	0.961009101	-2.440700325
	C46	-5.622352337	1.010784991	-4.568743900
	C47	-9.297653416	0.354871271	-1.782957779
	C48	-9.180856274	0.478727851	-0.258751376
	C49	-7.802611868	0.154038413	1.738622052
	C50	-6.756119148	1.200750610	2.132308258
	C51	-5.129768657	2.897227847	1.438580411
	C52	-5.760519755	4.203173338	1.948414263
	C53	-4.299636304	3.270063146	0.199691834
	C54	-3.552797275	2.130451940	-0.410374301
	C55	-3.195986162	0.876362704	0.044515831
	C56	-2.446614527	0.994132259	-1.964806824
	C57	-7.579550848	5.802545056	1.541874667
	C58	-7.724856970	6.082770731	3.035219746



C59	-8.972782291	5.729229664	0.868368269
C60	-9.646061357	7.035420335	0.568540796
C61	-9.755520867	8.190260302	1.319249101
C62	-10.804412684	8.427339415	-0.618914731
C63	8.392014493	2.439951401	4.830636342
C64	9.507586679	1.414161667	4.905451762
C65	7.103014608	1.675369755	4.435328245
C66	5.883583654	2.565106180	4.382364084
C67	5.090412997	2.790844211	5.522785693
C68	5.512394661	3.206289017	3.185929886
C69	3.961902366	3.616411263	5.475728945
C70	4.398926723	4.044073703	3.126612783
C71	3.620611436	4.246592901	4.271606209
C72	5.160701542	7.066913295	-0.891033773
C73	4.117298449	8.106938385	-1.342103336
C74	4.479352002	5.735572946	-0.608857976
C75	3.322147145	9.533317647	-3.193250902
C76	1.933255967	9.036263228	-3.605773122
C77	0.449033619	7.039515946	-3.739463597
C78	-0.269643353	6.761678999	-2.393950720
C79	0.728396189	5.753189492	-4.548621786
C80	-0.428986642	4.795448909	-4.853484812
C81	-1.420961506	5.235744335	-5.942629975
C82	-3.105973297	7.070172882	-5.843789747
C83	-0.150959773	5.932105421	-0.095757154
C84	-0.529875848	7.185840468	0.703557042
C85	0.738677075	5.060113689	0.811786902
C86	0.321386025	9.330788590	1.518041967
C87	-0.287698369	10.631739764	1.022218791
C88	-1.448273932	11.761526752	-0.797791801
C89	-2.842556305	12.279049213	-0.367555529
C90	-1.335732018	11.697829475	-2.323983372
C91	-2.341962665	10.762977457	-2.984435391
C92	-4.995047639	11.750920829	0.671967334
C93	-5.144875780	12.916130723	1.638827996
C94	-5.702506711	10.491573829	1.246792558
C95	-5.704191679	9.348330925	0.259054392
C96	-6.727146092	9.227801848	-0.693654467
C97	-4.649307695	8.420105318	0.216050123
C98	-6.685763211	8.236536104	-1.678103455
C99	-4.574606783	7.441897961	-0.779061130
C100	-5.595204450	7.367172215	-1.724049747
C101	5.838053813	-4.207920323	-7.894847919
C102	4.343607627	-4.016342923	-7.697038591
C103	2.607664835	-2.509577345	-6.753603224
C104	2.141111986	-1.226325949	-7.452346261
C105	2.382879646	1.218079431	-7.503024034
C106	3.530906531	2.221721312	-7.562609717
C107	5.657850197	3.025972108	-6.710589189
C108	6.386220915	3.243951959	-8.021373904
C109	-0.849526729	-4.173748428	-9.288737114
C110	-1.967080644	-3.125851296	-9.219720603
C111	-0.592623913	-4.752233143	-7.877599381
C112	0.243681770	-6.043576753	-7.943088056
C113	0.709720134	-6.450692224	-6.563014481
C114	-2.593705161	-0.802368540	-8.803460611
C115	-2.063036289	0.474420409	-9.425195417
C116	-3.254240058	-0.619162344	-7.416037340
C117	-2.213041268	-0.494595801	-6.340008266
C118	-1.589416953	0.736854623	-6.079534528
C119	-1.740579471	-1.649663045	-5.691982788
C120	-0.467445507	0.792536863	-5.248651369
C121	-0.619776740	-1.590638276	-4.863161119
C122	0.040545312	-0.373667440	-4.671565821
C123	8.995767949	-6.045015365	-2.908479531
C124	9.976025111	-5.986862450	-1.726606923
C125	7.585124374	-6.406090039	-2.420454629
C126	6.475979941	-6.299602498	-3.419687048
C127	6.339890633	-6.993401036	-4.604920166
C128	4.467056124	-5.888524149	-4.186173369
C129	10.908210112	-7.014140416	0.262817340
C130	12.333175443	-6.692081281	-0.131599358
C131	1.032388776	-6.708986905	0.358169806
C132	2.448674370	-6.680236153	0.933531249
C133	3.568432912	-6.859551689	-0.131518977
C134	3.629095043	-8.342010445	-0.592761712
C135	4.860858399	-8.725237622	-1.417243238
C136	5.005650209	-10.241660889	-1.680253433
C137	4.929407140	-6.507803523	0.490033420
C138	3.970247963	-0.625446323	-1.528626008
Fe139	4.599747633	-1.931765226	-2.928864587
Fe140	2.189169461	0.902449929	-1.447336285

Fe141	4.999732884	0.780684078	-0.514549713
Fe142	4.434071128	0.571834767	-3.012290721
Fe143	3.965363481	2.860756016	-1.739835881
Fe144	5.275949111	-1.758751072	-0.474401282
Fe145	2.741542701	-2.018769546	-0.833421696
H146	-5.824412076	-7.850618022	-0.255329943
H147	-5.815646047	-6.931273503	-1.602196600
H148	-9.489296800	-5.330931337	-0.077867793
H149	-8.197037097	-6.684842684	-1.560054359
H150	-8.256578631	-7.760872075	-0.169179832
H151	-7.983289463	-3.146555764	0.820390781
H152	-8.908413303	-5.975394993	2.733289734
H153	-9.691115248	-3.442256930	1.207766344
H154	-8.505423362	-6.470769770	4.969087045
H155	-6.220643611	-5.968215565	2.942777283
H156	-8.547111965	-4.736610419	5.345220745
H157	-3.375066179	-1.685580695	2.827301952
H158	-5.270390616	-3.795108083	2.463571292
H159	-3.899190093	-6.157042195	3.095573472
H160	-6.085965288	-0.036899287	6.326628199
H161	-6.482661773	-2.320968116	4.616082979
H162	-3.984428383	-6.126660126	4.875412005
H163	-5.070182818	-1.518623384	2.335912225
H164	-5.406305583	-3.538687453	6.936649494
H165	-7.192884342	-1.405633161	6.621171463
H166	-0.999831003	-3.026587111	3.558337232
H167	-0.853734186	-1.993726772	2.114573661
H168	0.562712729	-2.296020944	3.157197868
H169	-1.965857902	-0.795504530	4.061878852
H170	-4.789551722	-4.469383011	8.977071294
H171	-2.952220924	2.229229033	4.747976291
H172	-3.108550273	0.142657086	8.769817368
H173	-3.577075188	3.578194940	8.849395109
H174	0.751082635	0.387155415	3.242617006
H175	-0.612020368	1.294732535	3.938871417
H176	8.246708144	2.850725707	5.847987597
H177	-4.045752262	3.569019179	5.128241320
H178	-4.367469106	4.360908727	7.461798655
H179	-2.285521143	3.800746262	5.263576290
H180	-2.622605547	4.594189590	7.741691936
H181	-3.984000138	1.929591993	7.024505578
H182	-0.997542167	2.609214761	7.071280564
H183	-2.477481453	0.316885094	6.045287146
H184	-0.783628311	0.527320048	2.349870994
H185	1.202880992	4.267344482	0.208341747
H186	0.078467273	4.591513948	1.556760992
H187	1.874030164	5.505269561	2.362300486
H188	2.021190864	5.080799190	4.987594000
H189	4.109506022	4.518913697	2.188392834
H190	6.089748886	3.026652925	2.276538350
H191	5.352737786	2.305598786	6.467267814
H192	-1.910785326	-2.381096761	6.043132579
H193	-0.730175657	-5.241365166	6.749192863
H194	-0.417210766	-4.483273286	8.324688370
H195	-2.916613115	-4.211784268	6.724969018
H196	-4.533860587	-2.840759789	9.657396043
H197	3.346421369	3.767066503	6.366072835
H198	0.740376100	-1.251862314	5.373398921
H199	-2.954011585	1.214944723	11.335986056
H200	-2.926598466	-0.527666231	10.953101825
H201	-0.252729389	-0.046184510	10.578533753
H202	10.570106302	-6.095824974	6.447334729
H203	-0.657471858	-6.300655898	-3.951856571
H204	1.974278574	-5.947966598	-1.168359991
H205	-0.375462712	-6.857283541	-8.347988819
H206	1.107316134	-5.901323888	-8.608703946
H207	-1.549420003	-4.968556088	-7.378047522
H208	-1.235296560	0.322371379	-10.157423150
H209	-1.286596535	-4.977910316	-9.900334218
H210	-2.781793190	-2.486201408	-2.762513030
H211	-3.363852951	-5.214697520	-1.477122103
H212	-0.623724782	-1.644991219	-8.653223461
H213	-3.399567247	-1.117944642	-9.497962726
H214	0.862243015	-3.005946552	-9.444597140
H215	-0.496941896	-5.955546417	-2.232242075
H216	-0.086908380	-3.989052785	-7.265119635
H217	0.946239669	-4.441326915	-10.247074315
H218	-5.938260621	-3.967159945	-3.832606815
H219	-3.160534681	-2.572274273	-1.055548929
H220	2.445858606	-5.627983978	-6.973735373
H221	-1.815867386	-4.438104124	-1.185488507
H222	-4.482584856	2.527814869	2.245713587

H223	-3.417241394	0.434835411	1.013599828
H224	-8.746673009	0.458930998	2.211639292
H225	-7.315546622	-0.449903710	-0.253780251
H226	-7.371652596	3.830206440	0.737394399
H227	-9.365519102	8.470821030	2.290519889
H228	-7.934323453	5.169540251	3.644434806
H229	-9.625791920	5.077754710	1.475833889
H230	-6.976874527	6.604299941	1.085741643
H231	-11.385882805	8.899676526	-1.407030916
H232	-3.607542411	4.070632423	0.511382083
H233	-4.971327465	3.713127044	-0.555060174
H234	-10.755702771	10.009799848	0.804883348
H235	-8.841330864	5.219872650	-0.099055047
H236	-6.355916693	1.686166273	0.152725231
H237	-7.507659759	-0.800342616	2.200680184
H238	-9.750388536	1.294530064	-2.129362450
H239	-1.948240875	0.786421772	-2.908209293
H240	-10.001880683	-0.457482209	-2.007262352
H241	9.447334008	4.076329121	4.190653850
H242	7.918166464	4.017852223	3.615458276
H243	1.435056579	5.881591833	-1.563273151
H244	-1.088689293	5.388914997	-0.280729873
H245	1.194072457	8.084056190	0.051971048
H246	-3.185227643	2.988315664	-2.337999991
H247	-4.678203900	3.655485133	-3.890506984
H248	-5.870896329	2.703613166	-5.524888008
H249	-4.616731494	4.969114368	-3.007681307
H250	-4.651668354	0.684843711	-4.978034163
H251	-6.430290040	0.567592778	-5.172704274
H252	-0.303571507	11.446092644	-2.605579357
H253	-1.543264794	12.709815007	-2.705082248
H254	-0.830975158	9.896229977	-4.104886636
H255	-2.466165423	9.288738749	-4.352916634
H256	-3.030279611	8.564168205	-7.246720434
H257	-1.777260253	4.355384892	-6.499703162
H258	-7.497670906	8.144511827	-2.404244284
H259	-3.859055924	8.438657616	0.971478095
H260	-4.397976279	7.281036391	-4.254828119
H261	1.489419566	5.174061875	-4.001255480
H262	2.511684330	7.118381828	-3.209246173
H263	-0.976630749	4.523158924	-3.937491430
H264	-7.897219521	-0.819182280	-2.912300099
H265	3.793758672	9.983109368	-4.077116215
H266	-5.272060144	-1.451731805	-3.999499856
H267	1.201605723	6.062349904	-5.495522830
H268	-3.716920688	6.769595505	-0.825981866
H269	3.154211526	10.334568260	-2.459109387
H270	-2.150317205	7.136480614	-7.666241907
H271	-4.695579898	8.332602454	-5.595851858
H272	-4.285819643	-4.048639434	-4.078609583
H273	-5.310681719	-3.777593353	-1.613557038
H274	-7.576080717	9.915442131	-0.670902376
H275	-4.920133333	0.968233173	-2.531548394
H276	-0.203049703	7.723551890	-4.292619808
H277	-0.908418373	5.885706615	-6.664458108
H278	0.035347898	3.864001119	-5.208708426
H279	-3.118785920	5.414351566	-4.659930507
H280	-0.239409787	9.020805009	2.412336397
H281	-0.974271968	9.663080319	-0.643440513
H282	-0.768212646	12.557414895	-0.456899236
H283	1.354503978	9.550107850	1.820124791
H284	-3.269011678	10.500210522	0.511841624
H285	6.323837725	-3.232904599	-8.047349919
H286	6.212636763	-4.603984402	-6.927626357
H287	8.984286100	-5.026902252	-3.323902956
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H289	5.507212445	-5.909770911	-8.957382582
H290	5.249648159	5.023776308	-0.283430469
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H292	4.940091185	8.139519538	-3.228505965
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H294	6.384394398	8.380021013	0.108282513
H295	6.401978122	2.691969701	-5.970293283
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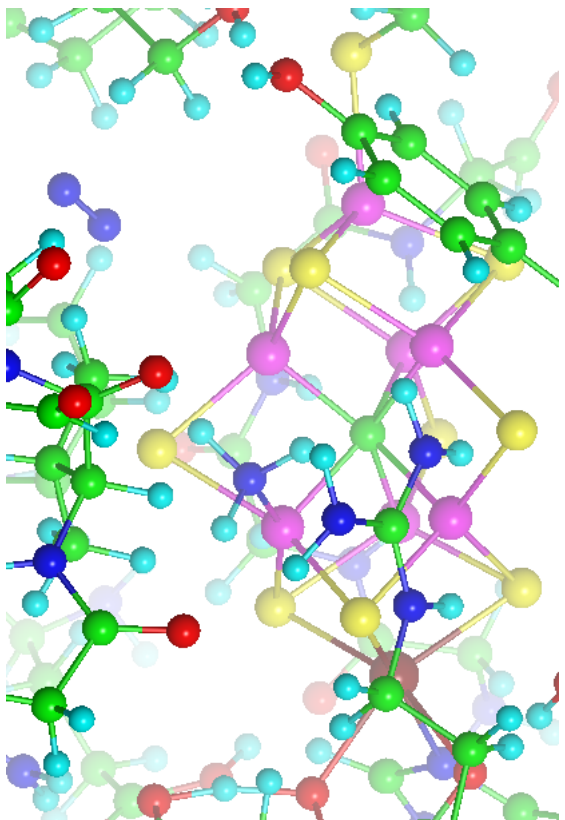
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H309	6.020876153	-4.449159819	5.696425864
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H312	4.899074468	-11.247825907	4.728270624
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H315	4.307492223	-11.545429251	6.889928039
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H318	-2.248729098	-2.603657712	-5.849429084
H319	8.318949927	-9.533598286	0.384348896
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H321	6.966643974	-7.745081539	1.599171942
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H323	6.341005445	2.383523444	-8.731767356
H324	6.597855086	-4.650692716	1.207297866
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H326	4.703493115	-2.222257927	-6.774902826
H327	3.610508986	-8.955507460	0.321457333
H328	4.634636762	-7.122542250	-5.890405619
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O451	1.748878340	5.845251129	1.453719339
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O476	-4.061880861	4.338756421	-3.519630243
O477	8.575355226	-10.082413864	-0.390578547
O478	7.843138029	-8.163627270	1.813327150
S479	3.627887041	5.080476884	-2.115048926
S480	2.664154039	1.898540829	-3.371812791
S481	2.786312360	-3.250407416	-2.753669195
S482	3.291566827	2.052891311	0.225841818
S483	0.954158089	-0.931740140	-1.583274907
S484	5.061136768	-0.700719825	-4.724382330
S485	3.947360518	-3.230249605	0.618655171
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end			

Fe6-NH3
2N2 dissociated
35, S=1

Fe(139) -2.376
Fe(140) -2.267
Fe(141) -2.351
Fe(142) 2.765
Fe(143) 2.962
Fe(144) 2.229
Fe(145) 1.084



bmexpprot6nh312n2xdta.car 2

C1	-1.803365135	-6.553186548	-6.604300517
C2	-1.075751098	-6.537006731	-7.953372881
C3	-3.989265574	-6.759560514	-5.492673753
C4	-3.656747139	-7.752792160	-4.383011266
C5	-2.595222808	-9.865996353	-3.756639327
C6	-1.485928143	-9.365132241	-2.827340220
C7	0.349019529	-7.795125011	-2.470665462
C8	-0.301284900	-6.842629283	-1.461059227
C9	-2.105425871	-5.229773482	-1.081349336
C10	-2.789898572	-6.010352439	0.048847939
C11	-4.051866658	-7.957212236	0.736288966
C12	-3.106140640	-8.651475186	1.726496990
C13	-1.195626100	-10.159418681	2.002358092
C14	0.075324255	-9.549191388	2.611224884
C15	1.966697096	-8.003691131	2.276540798
C16	1.808870813	-6.568577237	2.783621936
C17	0.292811030	-4.634102260	2.984639496
C18	-0.626104706	-4.674043885	4.222042214
C19	-0.177663099	-3.708337410	1.839678585
C20	-0.571240359	-2.327179614	2.372900092
C21	0.916227957	-3.627148243	0.768915629
C22	-2.870217716	-5.091818316	5.130809276
C23	-2.656142996	-6.274458747	6.092819762
C24	-4.315049209	-5.006976232	4.581413093
C25	-5.351092802	-5.149257563	5.702755898
C26	-4.521148153	-3.682552351	3.833496651
C27	-2.374116689	-8.663974709	6.394983741
C28	-1.264934822	-8.514297361	7.416030944
C29	11.399521304	-7.286169969	0.630968062
C30	11.078134534	-5.961442048	1.318650416
C31	9.494680751	-4.923169597	2.936774186
C32	9.889088951	-4.953084375	4.424496165
C33	7.968701537	-4.977257465	2.763840160
C34	7.260533704	-3.788971465	3.408405048
C35	5.792996724	-3.700023343	2.989078301
C36	4.156850518	-2.287861422	4.270856602
C37	10.752825675	-3.630410977	6.300189483
C38	9.841340025	-2.726989803	7.101313443
C39	-1.490948328	-2.022441787	-5.616228719
C40	-2.865089285	-1.770443553	-4.964417659
C41	-0.368040006	-1.581476861	-4.655982912
C42	1.034287883	-2.130791524	-5.002904356
C43	1.864796569	-1.287193826	-5.968306636
C44	-4.559265704	0.028806654	-4.718665848
C45	-5.848375353	-0.792462427	-4.651395761
C46	-4.767291221	1.399577749	-5.377164198
C47	-7.179327042	-2.593906247	-5.633110298
C48	-7.213549546	-3.572616432	-4.454096224
C49	-6.006750608	-4.601590395	-2.590665365
C50	-5.917756350	-3.880801085	-1.242696405
C51	-5.796310614	-1.768095737	-0.009964012
C52	-7.139841959	-1.717346484	0.733158311
C53	-5.384674888	-0.307347013	-0.261719971
C54	-4.061077208	-0.155435715	-0.934973069
C55	-2.972919584	-0.994173192	-1.079863676
C56	-2.438826242	0.824094310	-2.093883005
C57	-9.547405368	-1.362020665	0.421649217
C58	-9.875927004	-2.361209949	1.529548510
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C60	-11.898204490	-0.913090345	-0.590139406
C61	-12.756643492	-0.896671218	0.492035183
C62	-13.664196295	0.162760974	-1.230527568
C63	4.568437136	1.451196386	8.779687124
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C66	2.622128054	0.749822815	7.286512864
C67	1.848019849	-0.311322747	7.793648242
C68	1.953448442	1.787705056	6.613925898
C69	0.458084254	-0.337459925	7.637523517
C70	0.566003154	1.781835648	6.462067360
C71	-0.180611743	0.715507169	6.974303443
C72	-0.769895912	6.655756262	5.734572771
C73	-2.230343437	7.069308911	5.466610663
C74	-0.405656319	5.446051658	4.878879119
C75	-3.724469367	8.815507878	4.553399896
C76	-4.423027189	8.248315812	3.315542063
C77	-4.215638586	6.631951463	1.428197846
C78	-4.597216557	5.187971082	1.846466865
C79	-3.136463777	6.672441436	0.325030577
C80	-3.357457775	5.878836300	-0.968650167
C81	-4.364475807	6.467563395	-1.971860990
C82	-6.839944768	6.617425785	-1.764504948
C83	-4.018442319	3.149901102	3.068796330
C84	-5.167257048	3.070405488	4.078428126
C85	-2.802320011	2.431185804	3.689283022
C86	-5.966985333	3.961822760	6.206955097
C87	-7.265013915	4.745773752	6.259232218
C88	-8.826893147	6.159096496	5.037788090
C89	-10.226825274	5.509606587	4.913128858
C90	-8.659735559	7.284760005	4.012949340
C91	-8.777424540	6.828468699	2.563870696
C92	-11.517177815	3.529978587	4.281489977
C93	-12.420803556	3.380992527	5.496729841
C94	-11.232559265	2.138156450	3.652414772
C95	-10.449009662	2.251014806	2.364562942
C96	-11.111468374	2.434176049	1.140640654
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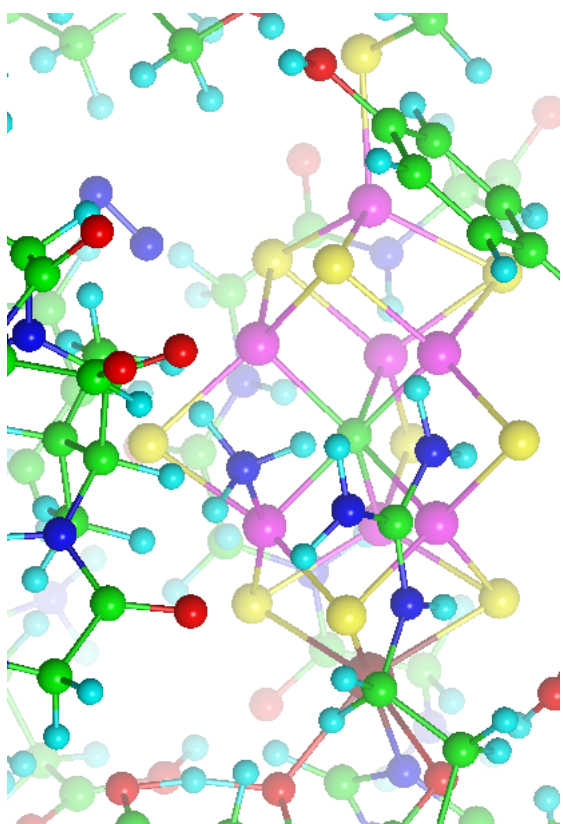
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N416	2.369482076	8.059097907	-1.312767397
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N422	12.230364894	1.316582398	0.554338552
O423	-1.224984850	-6.368799513	-5.519432809
O424	-3.966746739	-7.500937074	-3.205727707
O425	-1.387816940	-9.814341292	-1.672632455
O426	0.052393052	-6.797707923	-0.268462337
O427	-2.791849126	-5.584601490	1.214788781
O428	-3.361070839	-8.663375604	2.943429197
O429	0.465514107	-9.916232156	3.728208962
O430	2.757900651	-6.024887352	3.382224663
O431	-0.188697145	-4.326902525	5.331483174
O432	-2.633917708	-6.111502751	7.325134234
O433	-1.238716188	-9.135812543	8.468720895
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O436	10.189958664	-2.142495494	8.114813926
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O438	1.350895703	-0.668267416	-6.928256141
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O447	-3.189463343	6.350522659	5.797073048
O448	-5.593565625	8.600282359	3.066251792
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O450	-5.936763330	2.100754709	4.095561917
O451	-2.621994444	2.798599322	5.061838212
O452	-7.871379287	4.903512176	7.326742965
O453	-11.247532171	6.186067436	5.107586874
O454	-9.653513749	6.031701239	2.196781213
O455	-13.623979384	3.186370655	5.415248682
O456	-8.262356831	2.995821287	-1.156956691
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O458	2.068247014	6.045183838	-5.751377286
O459	0.617464324	9.188491668	-2.224165543
O460	2.648500017	11.376909368	0.056275563
O461	0.159486139	3.722517658	-9.868546096
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O463	5.660503249	2.170258052	-6.540762784
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O471	7.902276795	-0.416686603	-0.278827961
O472	8.673166851	-2.521232100	-0.139267481
O473	6.458161367	-0.850468231	-2.414561480
O474	10.547530397	-1.433698641	3.333371715
O475	7.941108641	-0.464477655	2.597436799
O476	-5.806489751	3.066797017	-2.095349198
O477	13.097080935	-1.279918157	-1.428079627
O478	11.228613651	-2.181332823	0.758762099
S479	-0.557850998	5.809230355	3.067639183
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S481	4.280926952	1.425992371	-2.291945172
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S483	1.278253447	0.996606966	-1.097720666
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S485	5.054372950	-0.447463667	0.607640266
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**Fe6-NH3
2N2 TS
35, S=1**

**Fe(139) -2.461
Fe(140) -1.625
Fe(141) -2.653
Fe(142) 2.623
Fe(143) 2.935
Fe(144) 1.965
Fe(145) 1.309**



bmexpprot6nh312n2xdtd.car_1

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C6	-1.483523926	-9.354770210	-2.823331878
C7	0.350348884	-7.784362118	-2.470583983
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C10	-2.793683390	-5.996126664	0.043796289
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C12	-3.107948294	-8.638152401	1.729184804
C13	-1.194921252	-10.144164091	2.012062870
C14	0.077053433	-9.535923528	2.620460774
C15	1.985598640	-8.017717052	2.276574486
C16	1.821864162	-6.584987872	2.788162901
C17	0.297740459	-4.655551920	2.988578005
C18	-0.620908153	-4.693453747	4.226696214
C19	-0.177139788	-3.742637375	1.840347690
C20	-0.596595876	-2.361804034	2.357748617
C21	0.919406684	-3.643072707	0.774124843
C22	-2.867587410	-5.098418866	5.135265009
C23	-2.661818420	-6.279815370	6.101433030
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C40	-2.871023331	-1.780725541	-4.970467405
C41	-0.379845203	-1.606545439	-4.664810481
C42	1.025109777	-2.141111829	-5.010662681
C43	1.851334573	-1.289645756	-5.974002877
C44	-4.551704703	0.030476349	-4.705867199
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C47	-7.172766935	-2.588966199	-5.628357418
C48	-7.207639274	-3.576602277	-4.455739070
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C81	-4.366609566	6.468375691	-1.973950334
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C91	-8.779097224	6.826542038	2.561088214
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C93	-12.430814478	3.376314186	5.496435677
C94	-11.239100288	2.137382297	3.652464066
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C96	-11.119177062	2.430318596	1.141639828
C97	-9.048928182	2.251992530	2.359130519
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C99	-8.323425042	2.491347026	1.188648186
C100	-9.015880463	2.694696584	-0.002706236
C101	7.369303504	6.077708881	-4.772707469
C102	6.116784193	5.378875565	-5.272919017
C103	3.794669756	4.725327815	-4.675526975
C104	2.616794269	5.707707375	-4.700396788
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C107	2.438933827	8.971072589	-0.188400160
C108	2.864804640	10.359813394	-0.612185605
C109	2.368255785	4.182029731	-9.010545861
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C111	2.902978706	2.963179577	-8.225198375
C112	4.381320968	2.690264719	-8.555767306
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C115	-1.607502190	6.207764359	-7.222913056
C116	-1.841068136	3.647160294	-7.025381908
C117	-1.172243773	3.381516947	-5.707034857
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C120	-0.739166692	4.036160023	-3.409768027
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C122	0.398160814	3.227465017	-3.386882494
C123	10.826106005	2.863723290	-0.792399235
C124	11.490883784	2.465849283	0.536075204
C125	9.987725363	1.697443505	-1.338198963
C126	9.107805922	1.993618610	-2.510962212
C127	9.490057728	2.431051770	-3.761953392
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C129	12.807742841	0.884656361	1.816400963
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C131	5.184188387	-3.350182788	-2.822857467
C132	6.222328582	-3.140269210	-1.719559074
C133	7.209990737	-1.969987303	-1.993316374
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C136	10.557933948	-1.991153044	-4.156407516
C137	7.982118182	-1.636069879	-0.709885394
C138	3.430077559	2.533419994	0.591257499
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H148	-3.598523747	-6.904094912	-7.589891979
H149	-1.701036394	-5.983308000	-8.693293435
H150	-1.070953569	-7.588704328	-8.335269135
H151	-3.940593273	-5.756334160	-5.057837888
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H154	-2.245456294	-10.758474135	-4.266050475
H155	-0.810442281	-8.023631862	-4.251701285
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H161	-3.472523432	-7.427051030	-1.279800466
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H164	-1.909587703	-9.296620671	0.182180611
H165	-4.658008277	-8.716299759	0.237083912
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H168	1.861589155	-3.283019878	1.219063413
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H174	0.242547348	-1.832126245	2.835842528
H175	-1.412688919	-2.428918786	3.092364450
H176	4.164024309	0.856998493	9.615455272
H177	-5.531754602	-3.618475956	3.428406678
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H181	-4.453958057	-5.841744063	3.873453437
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H195	0.397817534	-8.390355130	0.916555074
H196	-1.791090650	-10.517905155	2.853662835
H197	-0.132798317	-1.180043571	8.023472029
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H211	0.946724449	-3.146215986	-5.462516815
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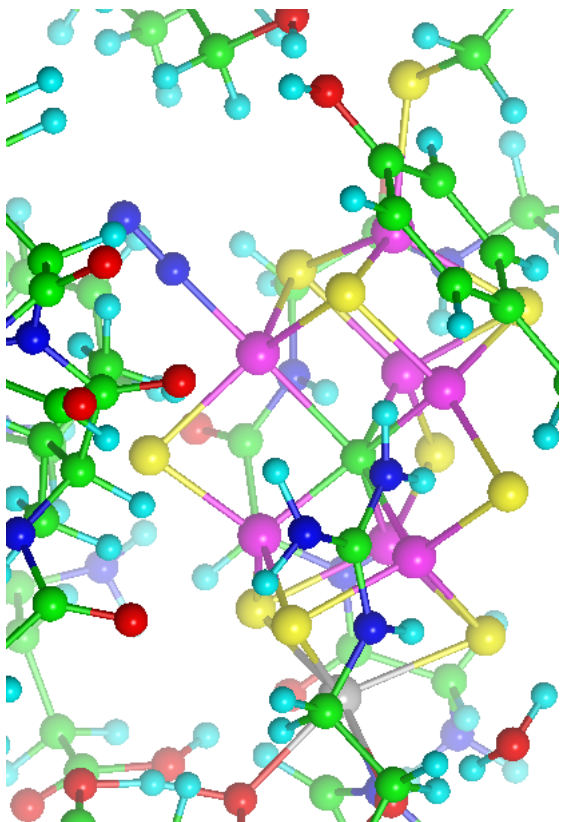
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O433	-1.226712851	-9.137297790	8.471825393
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O457	6.117845372	4.778139656	-6.375700952
O458	2.062708547	6.047362852	-5.767385490
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O464	-2.689520272	6.439154589	-6.701153363
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O477	13.092094177	-1.276663104	-1.424953511
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core 2N2 associated 35, S=1	bm522bz22n2xdta.car_4			
Fe (139) -2.312	C1	-8.407818188	-4.487151901	-0.716217807
Fe (140) -1.625	C2	-8.757243132	-5.514793970	-1.798998878
Fe (141) -2.771	C3	-9.152852656	-2.467319397	0.469617576
Fe (142) 2.409	C4	-8.888208087	-2.852250330	1.922896340
Fe (143) 2.874	C5	-9.083812799	-4.541967386	3.676924364
Fe (144) 2.062	C6	-7.596879256	-4.805874430	3.936569931
Fe (145) 1.170	C7	-5.409528438	-5.317034250	2.972856222
	C8	-4.719218111	-3.964149040	3.158271276
	C9	-4.662650071	-1.597974073	2.538830448
	C10	-4.817463558	-1.023176664	3.954221903
	C11	-6.213900123	-0.757794751	5.918647245
	C12	-5.462448538	-1.528792332	7.013074424
	C13	-5.072197756	-3.703672939	8.069160733
	C14	-3.603954434	-4.140580523	7.969624500
	C15	-1.813648650	-4.930033941	6.476411257
	C16	-0.806715970	-3.909376578	5.940718175
	C17	-0.449444348	-1.811154839	4.704988396
	C18	-0.169890875	-0.693886787	5.725522735
	C19	-0.933261596	-1.296761028	3.334416563
	C20	-0.070306658	-0.125233981	2.850757864
	C21	-0.927717542	-2.436765090	2.309322461
	C22	-1.107845344	1.155613197	7.060496846
	C23	-1.102209152	0.643015959	8.513855830
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	C25	-2.155121353	3.322035239	7.885046182
	C26	-2.018666724	2.850830018	5.413973451
	C27	-2.164320327	-0.730767904	10.214431901
	C28	-0.844020853	-1.225035172	10.765732896
	C29	3.615978343	-12.407667487	4.202532691
	C30	4.441928574	-11.184218473	3.813276677
	C31	4.882478645	-8.812390068	4.435386900
	C32	5.919383406	-8.637150389	5.560842787
	C33	3.840277336	-7.680830514	4.456573555
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	C35	3.410900131	-5.223428823	4.033658157
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	C37	8.236092503	-8.047808536	6.091642168
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C138	3.845664228	-1.067404445	-1.398197499
Fe139	4.376444791	-2.252664110	-2.977807250
Fe140	2.269406014	0.398218222	-1.011773223
Fe141	5.062157283	-0.057365540	-0.130097848
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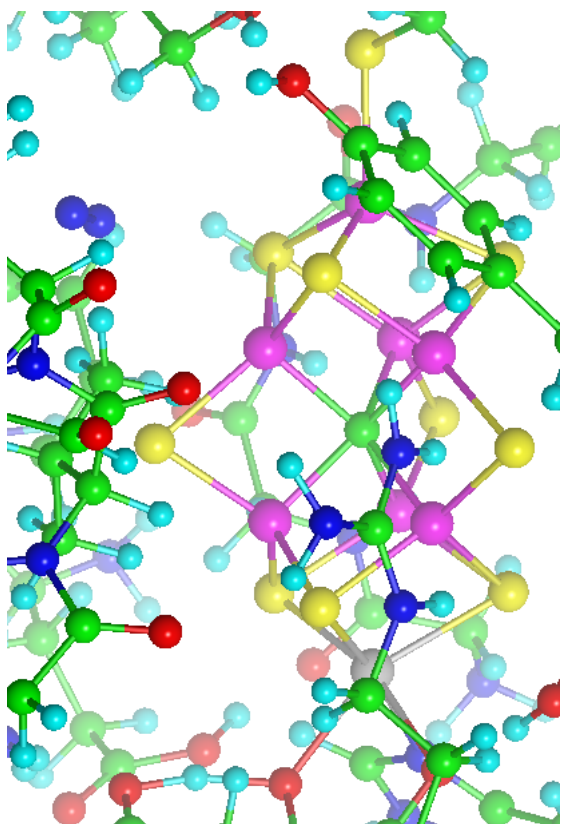
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H164	-6.156457929	-3.327865709	6.259466105
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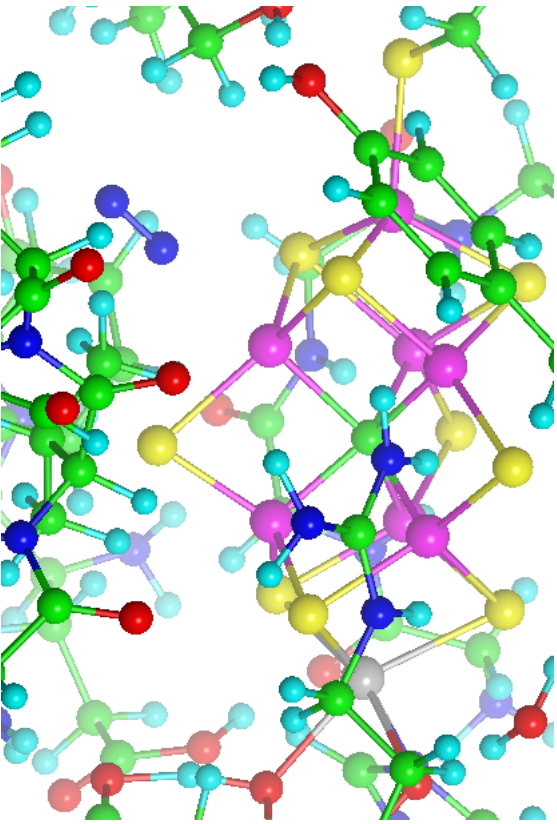
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H183	-2.144795020	-0.118252834	5.659312757
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O473	6.836231729	-11.220414607	-1.507788166
O474	6.294778627	-9.534462723	0.917386364
S475	4.355588973	4.596584562	-1.073682023
S476	2.795244924	1.733455905	-2.697177892

	S477	2.410437135	-3.331262161	-3.348094489
	S478	3.378309351	1.246487244	0.817360894
	S479	0.728463382	-1.039724840	-0.937179318
	S480	5.133940263	-0.857241798	-4.527669992
	S481	2.954488097	-3.720217098	0.199255886
	S482	6.186743593	1.270313337	-1.434477382
	S483	5.865728826	-3.638786606	-2.068609040
	S484	6.024210739	-1.607846011	1.031974588
	end			
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	C1	-8.408782440	-4.489001107	-0.722540719
	C2	-8.776663634	-5.510920423	-1.805228115
	C3	-9.130728391	-2.464084848	0.470205144
	C4	-8.879878173	-2.846530334	1.926215707
	C5	-9.072129622	-4.539491231	3.676908699
	C6	-7.583787356	-4.801437550	3.933415440
	C7	-5.397346517	-5.304038944	2.965719845
	C8	-4.709706412	-3.950867401	3.157210256
	C9	-4.655963572	-1.581966325	2.542358415
	C10	-4.812492466	-1.013970252	3.959878804
	C11	-6.208976507	-0.750155844	5.922402932
	C12	-5.451819831	-1.517760430	7.016101910
	C13	-5.052702661	-3.692747974	8.069436533
	C14	-3.588447314	-4.144082682	7.970178107
	C15	-1.799419473	-4.939632800	6.476703569
	C16	-0.793596695	-3.910427107	5.953552893
	C17	-0.444603106	-1.811591751	4.715302535
	C18	-0.163357109	-0.699930165	5.741397613
	C19	-0.935460497	-1.288527047	3.351908881
	C20	-0.081471353	-0.106157943	2.879850211
	C21	-0.922859113	-2.415678407	2.313683858
	C22	-1.098084354	1.154727029	7.069783248
	C23	-1.095483670	0.648221962	8.523291635
	C24	-2.179458271	2.231784104	6.809967315
	C25	-2.145394663	3.326960557	7.882675484
	C26	-2.003501481	2.841639827	5.413476282
	C27	-2.163108803	-0.720116482	10.221900222
	C28	-0.849830025	-1.211519415	10.792893974
	C29	3.617242262	-12.403809936	4.209777257
	C30	4.444540308	-11.182242905	3.817610166
	C31	4.876272603	-8.805550304	4.429516344
	C32	5.910046701	-8.630720153	5.558475783
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	C34	4.458520679	-6.294630197	4.256114395
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	C37	8.226421160	-8.050718690	6.096579892
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	C39	-5.153852994	-2.019685895	-2.817613588
	C40	-5.555089183	-0.611054161	-2.336187246
	C41	-3.677312903	-2.285877439	-2.459504736
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C49	-7.837552751	1.179926740	1.582367063	
C50	-6.664576417	1.996284108	2.130268176	
C51	-4.748991888	3.458314999	1.697502646	
C52	-5.194752703	4.776760724	2.348614634	
C53	-3.808345760	3.828692622	0.539936434	
C54	-3.220069467	2.654333417	-0.164871665	
C55	-3.134572899	1.311407425	0.141724503	
C56	-2.203446716	1.521682669	-1.782755686	
C57	-6.739242840	6.671389069	2.115776480	
C58	-6.997885865	6.721233220	3.620538915	
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C62	-9.395608041	10.053641413	0.217273073	
C63	8.247717375	0.205265663	5.563851027	
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C65	6.869681100	-0.216785083	4.996052630	
C66	5.854229720	0.901872807	5.025904699	
C67	5.040299767	1.120639870	6.153481494	
C68	5.691664338	1.759605162	3.921519707	
C69	4.089686263	2.147477652	6.178684163	
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C71	3.951504075	2.984687706	5.064736559	

C72	6.192130286	6.176046325	0.358222676
C73	5.362074093	7.426188089	0.017248777
C74	5.280160308	4.958793127	0.486833717
C75	4.896173442	9.169899757	-1.669853264
C76	3.466868332	8.976365451	-2.183764230
C77	1.678218781	7.294476274	-2.610064022
C78	0.853420925	6.965205606	-1.339796647
C79	1.784752239	6.090267210	-3.574306930
C80	0.503419081	5.385140701	-4.034739829
C81	-0.339265653	6.108190158	-5.098980646
C82	-1.749082122	8.151030028	-4.815069475
C83	0.735452066	5.858722209	0.840760557
C84	0.529611458	7.063507121	1.770335041
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C89	-0.911904970	12.527697071	1.238220659
C90	0.577186933	11.959404342	-0.730761836
C91	-0.526404134	11.265316524	-1.518822656
C92	-3.168147431	12.229278775	2.145260007
C93	-3.170249319	13.258568039	3.264437206
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C95	-4.221958278	10.034426435	1.403243136
C96	-5.216125036	10.197600445	0.427365179
C97	-3.327987699	8.958722369	1.262068108
C98	-5.302689861	9.337358913	-0.670161153
C99	-3.378140634	8.109167073	0.153855294
C100	-4.365579958	8.312065330	-0.806195649
C101	5.464613113	-3.958991382	-8.162871883
C102	4.008365103	-3.562616049	-7.980920624
C103	2.469846445	-1.968454441	-6.860783898
C104	2.243002702	-0.549009646	-7.392834655
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C106	4.136033993	2.640262482	-6.974572318
C107	6.302508158	2.994174970	-5.921942403
C108	7.207966152	3.142673788	-7.128274837
C109	-1.052495355	-2.740638066	-9.713940818
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C111	-0.957937738	-3.538069818	-8.392863440
C112	-0.352432737	-4.933865101	-8.632271991
C113	0.016746921	-5.594859943	-7.323900026
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C115	-1.522430670	2.017735613	-9.233550433
C116	-2.944175021	0.856199411	-7.422312508
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C121	-0.694011492	-0.880497274	-4.886368675
C122	0.106145699	0.177458504	-4.446999170
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C124	8.907254150	-7.235897957	-2.211932743
C125	6.514273934	-7.229608046	-3.050720319
C126	5.496466716	-6.789402724	-4.054707330
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C131	-0.145179465	-6.848613411	-0.599227847
C132	1.219546799	-7.133201396	0.044390931
C133	2.371051393	-7.347486627	-0.974162949
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C137	3.721542058	-7.239358936	-0.252957515
C138	3.843927581	-1.064024155	-1.392041498
Fe139	4.361563401	-2.241511667	-2.986767029
Fe140	2.365441881	0.299150315	-1.005016843
Fe141	5.002737744	-0.049904271	-0.142500262
Fe142	4.513924554	0.300222849	-2.691929510
Fe143	4.206364174	2.317026166	-0.978544142
Fe144	4.725437115	-2.587673071	-0.446902407
Fe145	2.384189658	-2.320639427	-1.362358495
H146	-7.155348622	-6.729984764	-1.593445581
H147	-7.018757703	-5.676039166	-2.832188968
H148	-10.213677983	-3.546666658	-1.015451018
H149	-9.299910135	-4.989527845	-2.622474278
H150	-9.519700979	-6.192148446	-1.354774141
H151	-8.246856741	-1.897207210	0.140707984
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H153	-9.996322543	-1.789053245	0.435780088

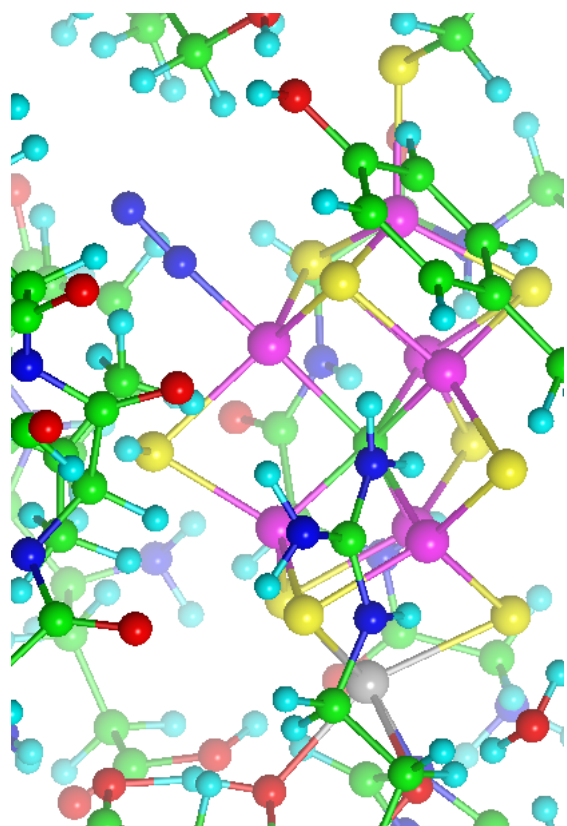
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H157	-3.587651526	-1.555793428	2.297085304
H158	-5.898020057	-3.115972606	1.704540142
H159	-5.018934403	-5.777188179	2.049301432
H160	-5.884438796	0.296460902	5.979611119
H161	-6.758823335	-1.690529669	4.060119984
H162	-5.122161010	-5.933070999	3.820978415
H163	-5.183451022	-0.942672881	1.821130074
H164	-6.127294223	-3.319468100	6.253830858
H165	-7.285715564	-0.796143718	6.137150939
H166	-1.543080800	-3.268430377	2.624782174
H167	-1.289602832	-2.045407491	1.345323963
H168	0.104585917	-2.774556316	2.144305247
H169	-1.965654365	-0.923371992	3.487575003
H170	-5.675533321	-4.596293522	8.137398612
H171	-2.062849398	2.084384361	4.619466707
H172	-2.803180593	-0.503941864	8.208878332
H173	-2.340975034	2.932107803	8.890000843
H174	-0.460870759	0.251154412	1.913688234
H175	0.968943245	-0.400555314	2.728192087
H176	8.107027028	0.485093550	6.626298150
H177	-2.786005666	3.590434703	5.222250956
H178	-2.908325667	4.087217440	7.661601532
H179	-1.025048902	3.344393753	5.336530925
H180	-1.162962860	3.825277854	7.898952126
H181	-3.165343794	1.733363041	6.853657344
H182	-0.103623140	1.602656524	6.927026323
H183	-2.137890834	-0.117930976	5.681254767
H184	-0.104658503	0.735426924	3.587909069
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H186	0.674157373	4.288460286	2.297872614
H187	2.542065669	4.789542151	3.285945570
H188	2.485800541	3.999781026	5.830127436
H189	4.622892089	3.438384847	3.066791256
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H197	3.449078520	2.287053641	7.052789856
H198	0.534472424	-2.283025376	4.556475675
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H202	9.101504963	-8.660879991	5.823660490
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H299	5.062428678	1.275212625	-5.691175138
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H303	2.085797141	2.330527441	-6.520572518
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H314	3.601237443	-12.626064270	6.257192003
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H325	1.138797036	-7.998702061	0.712189084
H326	4.585086037	-2.024380622	-6.751118327
H327	2.123415784	-9.463976838	-0.796971389
H328	3.727534075	-6.900448836	-6.708212119
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H355	7.974203247	-9.064078399	-1.764238965
H356	11.282937008	-8.804025160	-1.825148292
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N385	-1.801751210	-5.214871111	-3.839600959
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N388	-8.039520902	1.212702104	0.144823148
N389	-5.883463513	2.663811532	1.235342666
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N392	-6.279237211	5.342190993	1.760458593
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N395	8.855955006	1.251405192	4.737549844
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N403	1.549338229	7.968705634	1.770394534
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N408	3.790573507	-2.471674795	-7.217043279
N409	2.930438740	0.411729179	-6.736806235
N410	5.136452662	2.169546263	-6.188090204
N411	0.218784419	-2.331520113	-10.325911455
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N415	4.170554744	-6.706293764	-5.814038531
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N417	0.016842710	2.414482518	0.151512549
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O419	-7.326429052	-4.504468915	-0.110388642
O420	-8.250730432	-2.079333742	2.675384052
O421	-7.114041192	-4.682488755	5.077408890
O422	-3.784509309	-3.800436837	3.975141988
O423	-3.902783270	-0.359941215	4.494099279
O424	-4.819545906	-0.916336042	7.901041278
O425	-2.904737096	-4.265188614	8.997201897
O426	0.421803428	-4.098695664	6.142485373
O427	0.987514538	-0.509247048	6.179761607
O428	-0.263316851	1.050169938	9.353404052
O429	-0.610482715	-1.220643219	11.992204082
O430	5.228964482	-11.245243644	2.847831945
O431	5.600792510	-8.841541667	6.744302668
O432	9.763327843	-6.270790136	6.631228538
O433	-5.880000713	-0.360456985	-1.160620141
O434	-3.259580769	-3.871867020	-4.951030133
O435	-6.657635040	3.335664307	-1.714849671
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O439	-4.565092051	5.317098772	3.264562050
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O443	4.548286323	7.922672696	0.814699232
O444	2.784690160	9.976606239	-2.485133808
O445	-0.303146176	7.398880107	-1.220158485
O446	-0.468113046	7.152204522	2.496540431
O447	2.508161147	5.282259102	2.440762045
O448	1.539863701	11.293174229	3.259012560
O449	-1.082287017	13.741742249	1.055510459
O450	-1.724726401	11.417935085	-1.239827913
O451	-4.075845237	14.061625709	3.427536879
O452	-4.371055693	7.475152062	-1.937713721
O453	3.089196669	-4.253497984	-8.484500351
O454	1.495777976	-0.324002972	-8.367797150
O455	4.202133845	3.744433058	-7.540274590
O456	8.041297099	4.027054512	-7.235648192
O457	-3.201991599	-1.631599125	-9.853413051
O458	-0.785154328	-6.189156421	-6.611984954
O459	1.301870169	-5.461187380	-6.928718941
O460	-1.801136150	3.149860630	-8.863225468
O461	9.837612717	-6.464878785	-1.903139616
O462	11.926112302	-8.436001476	0.075258872
O463	-0.091057605	-6.168389416	-1.724299943
O464	-1.197892539	-7.194944787	-0.045920289
O465	4.453727552	-11.350922407	-2.880416511
O466	2.299253665	-11.023581990	-3.486526732
O467	4.530785909	-6.289564839	-0.641475831
O468	4.006313875	-8.051389587	0.648304012
O469	2.288358796	-6.291987461	-1.962486026
O470	7.734126748	-7.703579376	2.425124624
O471	6.276321280	-5.464335097	1.438796226
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O473	6.824178631	-11.215021892	-1.500431391
O474	6.288435008	-9.529346486	0.922003125
S475	4.365298207	4.603970835	-1.081466966
S476	2.797134421	1.771450721	-2.705599068
S477	2.428232623	-3.316952261	-3.354945540
S478	3.467732230	1.263496026	0.847433903
S479	0.677223984	-1.199225380	-0.860952576
S480	5.108727918	-0.831783368	-4.525451439
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	S482	6.197063141	1.263520636	-1.466749491
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2N2 associated	1	-8.338077991	-4.658608075	0.732112488 C
35, S=3/2	2	-8.768923583	-5.761269761	-0.242291423 C
	3	-9.036649919	-2.630001207	1.928683026 C
	4	-8.476184384	-2.918114484	3.318530556 C
	5	-8.289201703	-4.494276046	5.176350807 C
Fe (139) -2.317	6	-6.776182184	-4.731986262	5.172703805 C
Fe (140) -1.082	7	-4.784613135	-5.281721140	3.870349472 C
Fe (141) -2.479	8	-4.070141713	-3.928740433	3.855732281 C
Fe (142) 3.021	9	-4.134097797	-1.593504220	3.140477561 C
Fe (143) 2.778	10	-4.092639701	-0.964140866	4.541620880 C
Fe (144) 2.218	11	-5.261520009	-0.539573126	6.626701733 C
Fe (145) 0.451	12	-4.389536238	-1.226668792	7.685755543 C
	13	-3.795435880	-3.328927898	8.792449391 C
	14	-2.361274483	-3.793173240	8.500717352 C
	15	-0.801933123	-4.609757418	6.775989204 C
	16	0.163593444	-3.624790483	6.107111356 C
	17	0.425785691	-1.655545968	4.636484934 C
	18	0.766560654	-0.480843635	5.582839689 C
	19	-0.228590342	-1.199359322	3.318860249 C
	20	0.585396492	-0.074216611	2.669752707 C
	21	-0.400369894	-2.396399506	2.375509674 C
	22	-0.110339457	1.338809413	7.005695371 C
	23	0.077178494	0.932331424	8.483097376 C
	24	-1.254284623	2.365536679	6.813638935 C
	25	-1.135140316	3.520221469	7.815390391 C
	26	-1.264342442	2.901130565	5.376193143 C
	27	-0.807158913	-0.159886307	10.463950105 C
	28	0.527979749	-0.757783176	10.858698199 C
	29	4.472905156	-12.080297129	4.328187969 C
	30	5.200790391	-10.865319691	3.756545743 C
	31	5.641034931	-8.443248453	4.175958840 C
	32	6.810093611	-8.185141907	5.146277594 C
	33	4.571315037	-7.342572962	4.277117860 C
	34	5.112606073	-5.945702953	3.966708991 C
	35	3.981065326	-4.931071495	3.805323310 C
	36	4.239542497	-2.434479246	3.964902951 C
	37	9.170906954	-7.553488371	5.326385906 C
	38	9.559561309	-6.091101475	5.339285371 C
	39	-5.471648846	-2.212593737	-1.975912392 C
	40	-5.763710494	-0.759103770	-1.561169918 C
	41	-3.970053808	-2.501578390	-1.779109998 C
	42	-3.581916709	-3.994373545	-1.838381256 C
	43	-3.228262536	-4.534729483	-3.223469949 C
	44	-5.846702811	1.534129635	-2.500533376 C
	45	-6.977352053	2.126641389	-1.653027848 C
	46	-5.825866695	2.122868413	-3.918058485 C
	47	-9.254658109	1.838338557	-0.804149708 C
	48	-8.971508989	1.820254132	0.703270076 C
	49	-7.482276068	1.101570041	2.511171550 C
	50	-6.263071777	1.954756642	2.863801168 C
	51	-4.514419724	3.507461147	2.148111960 C
	52	-4.929151132	4.829780291	2.814133501 C
	53	-3.739641421	3.884800408	0.874475759 C
	54	-3.178350302	2.721989718	0.126084813 C
	55	-2.885724829	1.416421798	0.470078885 C
	56	-2.418605939	1.580211163	-1.619367269 C
	57	-6.583895013	6.642321335	2.759143285 C
	58	-6.637120798	6.774452496	4.280043506 C
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	61	-8.383191620	9.324979460	2.874356938 C
	62	-9.498317829	9.893456208	1.045059173 C
	63	8.941409231	0.674312778	4.351539432 C
	64	9.872113052	-0.519362149	4.255192609 C
	65	7.518133812	0.167945824	4.000458338 C
	66	6.466455574	1.247407214	4.107334869 C
	67	5.801830371	1.493935289	5.322350379 C
	68	6.114257629	2.029691335	2.993835919 C
	69	4.809308791	2.473786182	5.424879441 C
	70	5.135492528	3.020299962	3.084063580 C
	71	4.476254148	3.233615828	4.298319914 C
	72	5.968383946	6.319785616	-0.782043453 C
	73	5.053716649	7.522789063	-1.065688213 C
	74	5.126520214	5.084363823	-0.465615949 C
	75	4.320096650	9.176769535	-2.748610217 C
	76	2.848530595	8.916688387	-3.081510019 C



77	1.066035418	7.172980337	-3.174415481	C
78	0.422885335	6.870890647	-1.795344590	C
79	1.097846805	5.936119311	-4.103976126	C
80	-0.197480870	5.165492706	-4.385411730	C
81	-1.196051801	5.818739684	-5.353827334	C
82	-2.568059545	7.872033343	-4.978476635	C
83	0.627902901	5.891467431	0.438372388	C
84	0.508892076	7.135787328	1.329990696	C
85	1.453790347	4.842912109	1.213561883	C
86	1.758812851	9.058537133	2.183856806	C
87	1.318961577	10.470069598	1.832678232	C
88	0.203393870	11.893143486	0.199027766	C
89	-1.055584307	12.575377148	0.788660176	C
90	0.175255016	11.932440442	-1.332321548	C
91	-1.010796324	11.206802095	-1.957855704	C
92	-3.175575835	12.283450158	1.979782533	C
93	-3.058831019	13.366315768	3.043351297	C
94	-4.021636241	11.095647635	2.520619036	C
95	-4.261620285	10.038100389	1.467602964	C
96	-5.370777456	10.122346357	0.611786628	C
97	-3.357844722	8.978822743	1.276475059	C
98	-5.558592286	9.199487251	-0.420179622	C
99	-3.512698884	8.065092130	0.230588405	C
100	-4.611051492	8.194349901	-0.616558944	C
101	4.410261323	-4.322474806	-8.562119471	C
102	2.988472753	-3.926938322	-8.200995539	C
103	1.599461758	-2.272856916	-6.972770000	C
104	1.288305697	-0.887174531	-7.546292264	C
105	1.864082544	1.498218747	-7.444461727	C
106	3.129455539	2.346869305	-7.500405916	C
107	5.442666684	2.716273595	-6.860192256	C
108	6.056704415	3.000816748	-8.217043497	C
109	-2.226172692	-3.239855320	-9.374552477	C
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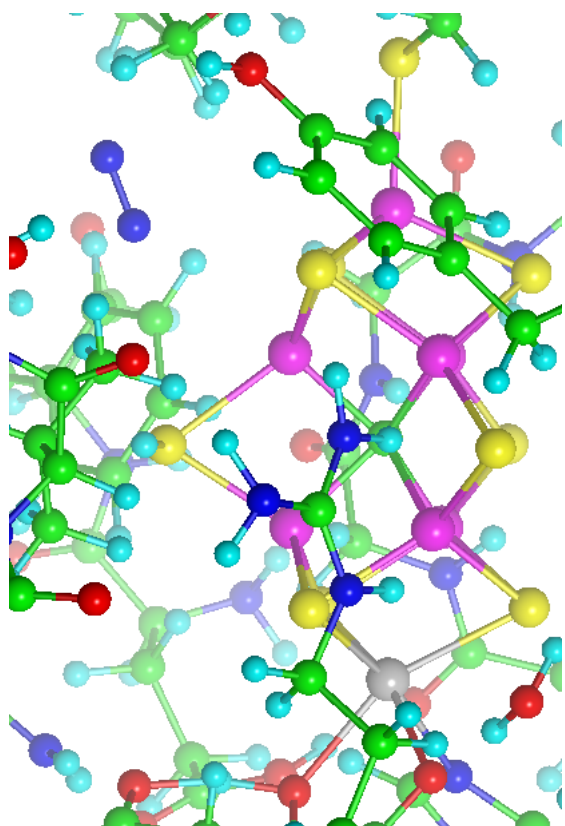
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408	-0.717143746	10.471625999	-3.064048527	N
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427	1.388479369	-3.765189087	6.270751079	O
428	1.950059022	-0.163736910	5.814155452	O
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451	-2.163434786	11.335822470	-1.519230200	O
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453	-4.723161200	7.308273550	-1.703709378	O
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478	2.041773479	-3.400140760	-3.460477372	S

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Fe(140) -2.213	C				
Fe(141) -2.454	4	-8.471770543	-2.915849849	3.322938551	
Fe(142) 2.810	C				
Fe(143) 2.933	5	-8.287880801	-4.496114617	5.177798123	
Fe(144) 2.218	C				
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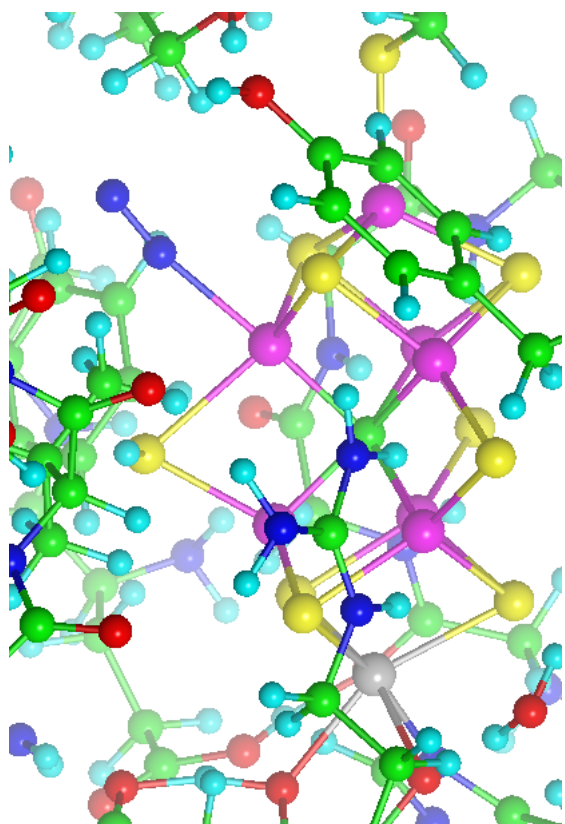
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35, S=3/2

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