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The Mechanism of Nitrogenase: formation and release of the second NH_3 and completion of the cycle

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Supplementary Information

Contents

1. Protein model

2. Computational constraints

3. Density functional procedures

4. Validation

5. Determination of transition states

6. Movement of Val70 and the contiguous chain

7. Potential energy profile for Fe2-brNH2-Fe6-3b2 → Fe2NH3

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.

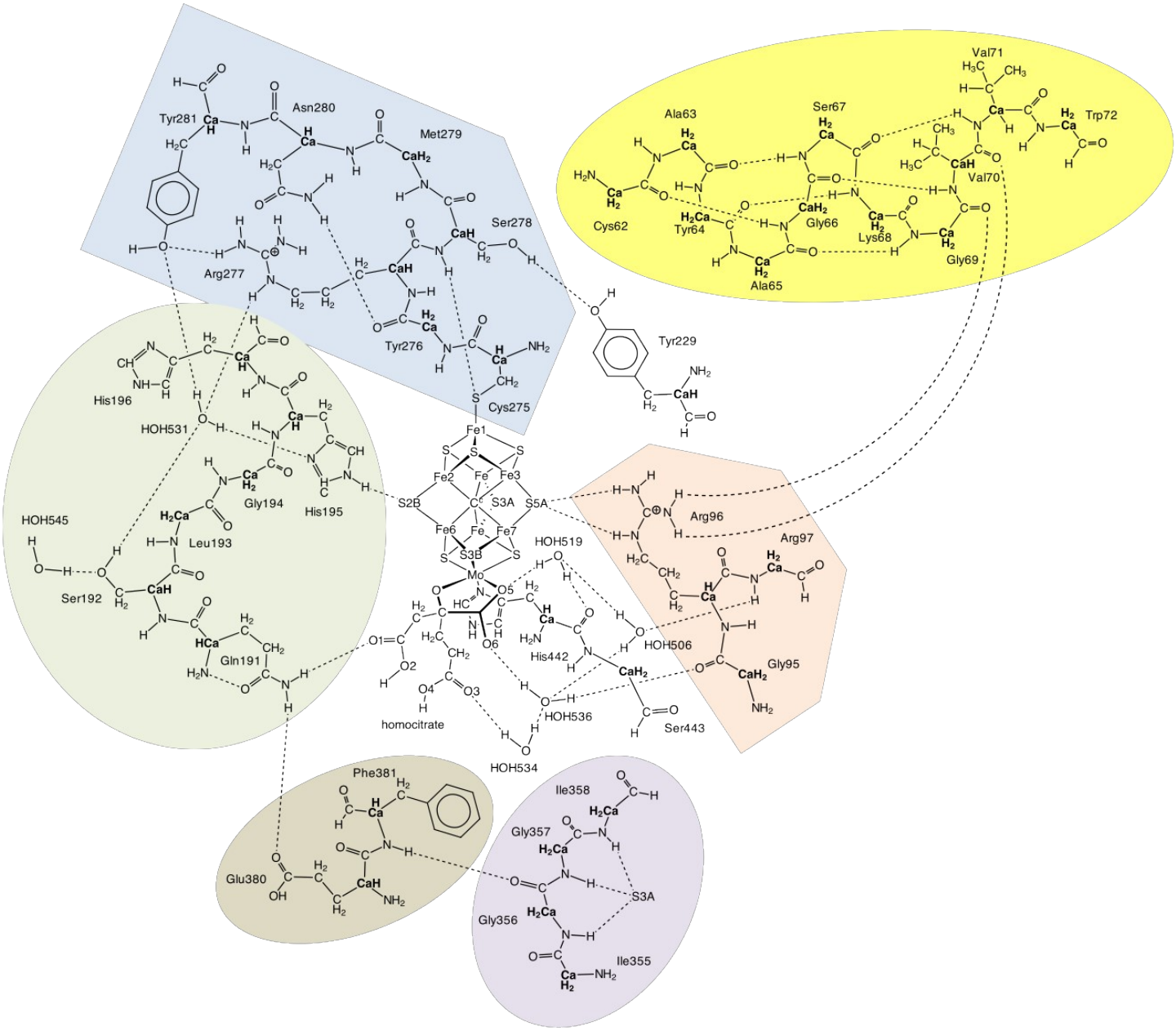


Chart S1. The quantum computed model, with residues and water molecules labelled according to *Azotobacter vinelandii* protein, crystal structure 3U7Q. Cα are labelled as Ca, and hydrogen bonds are broken lines. Non-influential sidechains are truncated to gly. In the 'front' chain (yellow highlight) that extends over the Fe2Fe3Fe6Fe7 face of FeMo-co the crucial residues Val70 and Val71 are complete, while 62, 63, 64, 65 6m7, 68 and 72 are modelled as Gly. In the 191 to 196 chain (highlight green) the significant sidechains of Gln191, Ser193, His195 and His196 are complete. In the 275-281 chain (blue highlight) Cys275, Arg277, Ser278, Asn280, Tyr281 near the N_2 pathway are complete: Tyr229 is included in full because it borders the reaction domain and has an important hydrogen bond with Ser278. In chain 95-97 (salmon highlight) the sidechain of Arg96 is included because it forms crucial hydrogen bonds with S5A, Gly69 and Val70: the sidechain of Arg97 is not nearby and is truncated to gly. In the rear chain (mauve highlight) with hydrogen bonds to S5A, Ile355 and Ile358 are truncated to gly. Glu380 and Phe381 (fawn highlight) are included in full. Ligand His442 is complete and Ser443 is truncated to gly. Homocitrate is complete. HOH531 has hydrogen bonds with two chains, Ser192, His195 and Arg277, Tyr281, and is part of the putative proton transfer from surface water (HOH545) to His195.[4] The four penultimate waters of the proton wire[5] (HOH519, HOH506, HOH536 and HOH534) are included. A proton on the coordinated alcoholate O atom of homocitrate is not shown in this Figure.

Experimental and computational studies are in general agreement that the redox level of the [CFe_7MoS_9] 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 N_2 and of H_2, and the diffusion of these molecules to and from FeMo-co. The constraints used here involved the Cα 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 Cα 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 explained[9] trial calculations on the modes of diffusion and coordination of N_2 / H_2 led to the conclusion that the front chain near Val70 should move away from FeMo-co. Details are provided in section 6 below. This is consistent with experimental data on mutation of amino acid 70 with smaller and larger side chains.[10-12]

In the present investigation of NH_3 formed in the reaction zone, and diffusing away between the side chains of Val70 and Arg96, it became apparent that a small separation of these sidechains should occur, by a libratory movement of the sidechain of Arg96, without changing the resting state hydrogen bond from NH2 of Arg96 to S5A. This is shown in Fig S1 Therefore the Cα(Val70) -- C^c and Cα(Val70) -- CZ(Arg96) distances were fixed, at 8.2 and 5.18 Å respectively.

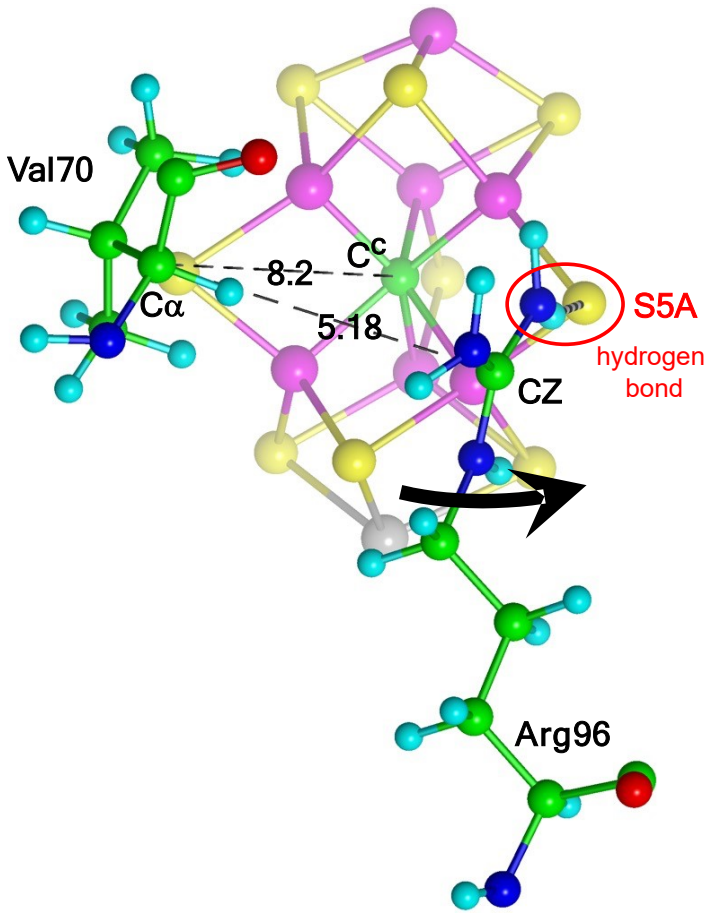


Fig S1. Expansion of the reaction zone by swinging the guanidine sidechain of Arg96 by about 1 Å around the unchanged hydrogen bond from NH2 to S5A

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.

3. Density functional procedures

Density functional (DF) calculations use the DMol methodology of Delley,[13-18] with accurate DNP (double numerical plus polarisation) basis sets.[16] 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 PBE[19] 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.[20] See section 4 Validation, below.

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.[16] These numerical basis sets avoid the need for basis set superposition corrections, and provide reliable energies at long intermolecular distances. This advantage of the DMol methodology obviates the need for empirical treatment[21] of the long-range dispersion energies that are involved when the computational model is comprised of separate molecular units. This ability of the DMol methodology to incorporate long-range dispersion has been well demonstrated. Zhang *et al* reported the excellent agreement between the experimental interatomic potential energy curves and the DMol/PBE calculated potential energy curves for the inert-gas pairs He_2, Ne_2, Ar_2, HeNe, HeAr and NeAr.[22] 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.[18] This set of molecular crystals ranged over amino acids, aliphatic and aromatic hydrocarbons, ice, H_2S, S_8, C_{60}, 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)[23-25] 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.[26]

4. Validation

Table S1 contains the results of calculations of the resting state of FeMo-co using the full protein model (482 atoms) and the computational methodology of this paper. The basis set is DNP, functional PBE, spin S=3/2, electronic state 235 (ie Fe2, Fe3 and Fe5 have negative spin densities). Results are for unprotonated and protonated His195. Calculated bonded and non-bonded distances are compared with the best crystallographic values, from PDB 3U7Q. The agreement between calculated and experimental lengths for C^c-Fe bonds and for Fe-S bonds is 0.01Å or better. The overall average deviation is 0.02Å. The longer distance between Nε of His195 and S2B, an interaction which may or may not be hydrogen bonded in the crystal structure, is calculated to be 0.12 Å longer with unprotonated His195 and 0.06Å shorter with His195 protonated at Nε.

Table S1. Calculated distances, bonded and non-bonded, for the resting state of FeMo-co, for unprotonated and protonated forms of His195, in comparison with the crystallographic distances (PDB

3U7Q). Basis set DNP, functional PBE, S=3/2, electronic state 235. Cc is the C atom at the centre of FeMo-co.

distance	xtl 3U7Q	calculated with His195 unprotonated	calc - xtl	calculated with Hs195 protonated	calc - xtl
Cc-Fe2	1.997	1.945	**-0.052**	1.962	**-0.036**
Cc-Fe3	1.984	1.982	**-0.001**	1.982	**-0.002**
Cc-Fe4	1.990	2.005	**0.015**	1.995	**0.004**
Cc-Fe5	2.008	2.045	**0.036**	2.023	**0.015**
Cc-Fe6	2.018	1.969	**-0.049**	2.009	**-0.009**
Cc-Fe7	1.997	2.011	**0.014**	1.998	**0.000**
Fe1-Fe2	2.668	2.673	**0.005**	2.671	**0.003**
Fe1-Fe3	2.668	2.653	**-0.015**	2.652	**-0.015**
Fe1-Fe4	2.655	2.681	**0.027**	2.687	**0.032**
Fe2-Fe6	2.576	2.630	**0.054**	2.643	**0.067**
Fe3-Fe7	2.583	2.603	**0.021**	2.606	**0.024**
Fe4-Fe5	2.612	2.573	**-0.039**	2.555	**-0.057**
Mo-Fe5	2.727	2.733	**0.006**	2.731	**0.004**
Mo-Fe6	2.674	2.717	**0.044**	2.730	**0.056**
Mo-Fe7	2.681	2.679	**-0.002**	2.687	**0.006**
Fe2-S1A	2.261	2.257	**-0.004**	2.252	**-0.009**
Fe2-S2A	2.254	2.291	**0.037**	2.296	**0.042**
Fe3-S2A	2.275	2.285	**0.010**	2.288	**0.013**
Fe3-S4A	2.254	2.233	**-0.021**	2.228	**-0.026**
Fe2-S2B	2.206	2.178	**-0.028**	2.219	**0.013**
Fe3-S5A	2.221	2.236	**0.015**	2.226	**0.005**
Fe6-S2B	2.173	2.160	**-0.013**	2.219	**0.047**
Fe7-S5A	2.210	2.209	**0.000**	2.199	**-0.011**
Fe6-S1B	2.235	2.226	**-0.008**	2.234	**0.000**
Fe6-S3B	2.218	2.238	**0.020**	2.250	**0.032**
Fe7-S3B	2.245	2.254	**0.009**	2.252	**0.007**
Fe7-S4B	2.220	2.228	**0.009**	2.222	**0.002**
average deviation			**0.020**		**0.020**
HisN-S2B	3.216	3.341	**0.125**	3.153	**-0.063**
mean Fe--Fe	2.627	2.636	**0.009**	2.636	**0.009**
mean Fe-S	2.231	2.233	**0.002**	2.240	**0.010**
mean Fe--Mo	2.694	2.710	**0.016**	2.716	**0.022**
mean Cc-Fe	1.999	1.993	**-0.006**	1.995	**-0.004**

Thorhallsson et al consider that agreement with the dimensions of the crystal structure is essential for gauging the quality of the computational protocols.[27] Raugei et al[28] also present (their Figure S8) comparative results on the accuracy of the PBE functional to reproduce nearest neighbour Fe-Fe distances in resting FeMo-co.

The PBE/DMol method reproduces experimental enthalpy data on the binding of N_2. Relevant ΔH_{exp} / ΔH_{calc} comparisons from ref [20] are (kcal mol^{-1}) (a) exp 17.6, calc 20.0, 18.8 (b) exp ~10, calc 10.2 (c) exp 22.8, calc 25.9. Other assessments of DMol accuracy vs experiment have examined the electron affinities of atoms and molecules,[29] the enthalpies of formation for small (<100 electrons) molecular and atomic species,[30] the structures of metal-sulfide clusters,[31] photo-induced conversion of $[Os(NH_3)_5(\eta^1{-}N_2]^{2+}$ to $[Os(NH_3)_5(\eta^2{-}N_2]^{2+}$ (i.e. end-on to side-on bonding of N_2),[32] the geometry and vibrational frequencies of $[(NH_3)_5Ru(pyrazine)Ru(NH_3)_5]^{4+,5+,6+}$,[33] and protonation reactions involving hydrogen bonding.[4]

See ref [20] for further validation results relevant to the present work, including Fe_xH_y clusters, and hydrogen bonding by water.

5. Determination of transition states

The following pragmatic procedure is used to map reaction energy surfaces and locate transition states. [5, 8, 34, 35] A chemically reasonable geometry between energy minima is evaluated by observing the directions and extent of geometry change during an energy minimisation calculation that is restricted to small (ca 0.03 Å) atom displacements at each cycle. This reveals significant geometrical variables (i.e. which atoms are moving, which bond distances and angles are changing) and also the energy gradients involved. This calculation also indicates the direction of the energy saddle relative the 'reactant' and 'product' minima. Then, as illustrated in Figure S3, a point **Δ1** that is a short distance along this first optimization path is selected, and from this structure an atomic arrangement (**2** on Figure S2) on the other side of the saddle is found (by trial and error and chemical experience) and similarly evaluated with small-displacement energy minimisation steps. A point **Δ2** along the second optimisation path is selected, and from this the key moving atoms are adjusted to be just back across the suspected saddle-point towards the 'reactant' state. Repetition of this cycle, with subsequent short small-step energy minimisations, always starting from a point just on the other side of the barrier, allows the barrier to be straddled from opposing trial positions that progressively approach each other in geometry and energy, and converge at the transition state (TS). Confirmation of the TS is obtained by following the complete trajectory of geometries from positions nudged just away from the TS, linking the TS with the connected reactant and product energy minima on the same potential energy surface. The protocol uses human participation, which is itself insightful, and with chemical experience the procedure works efficiently.

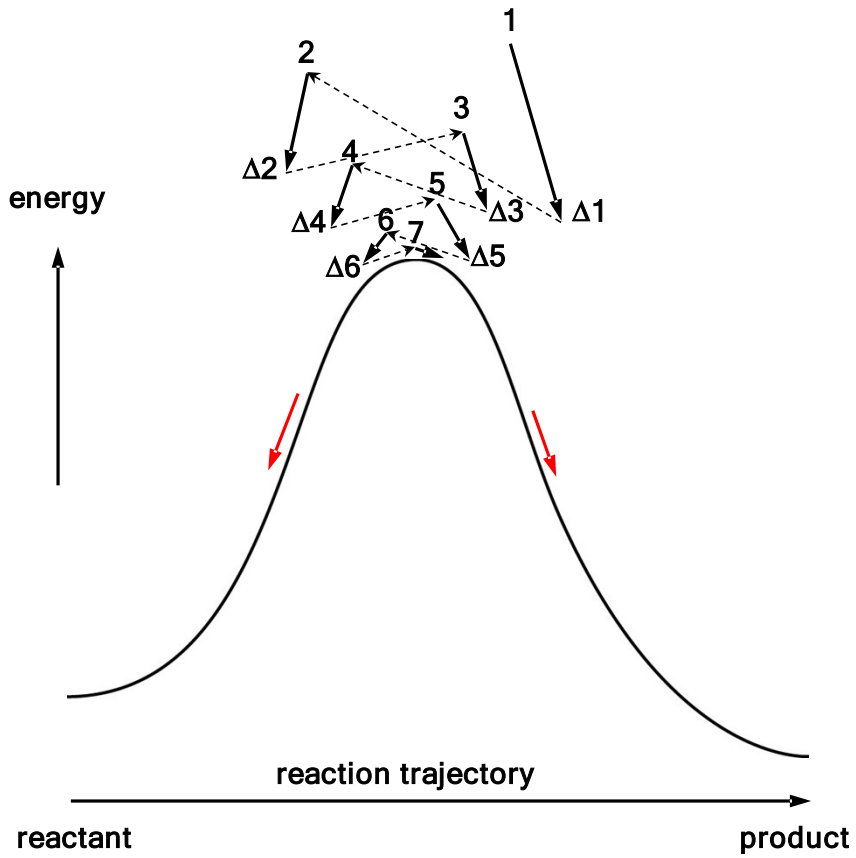
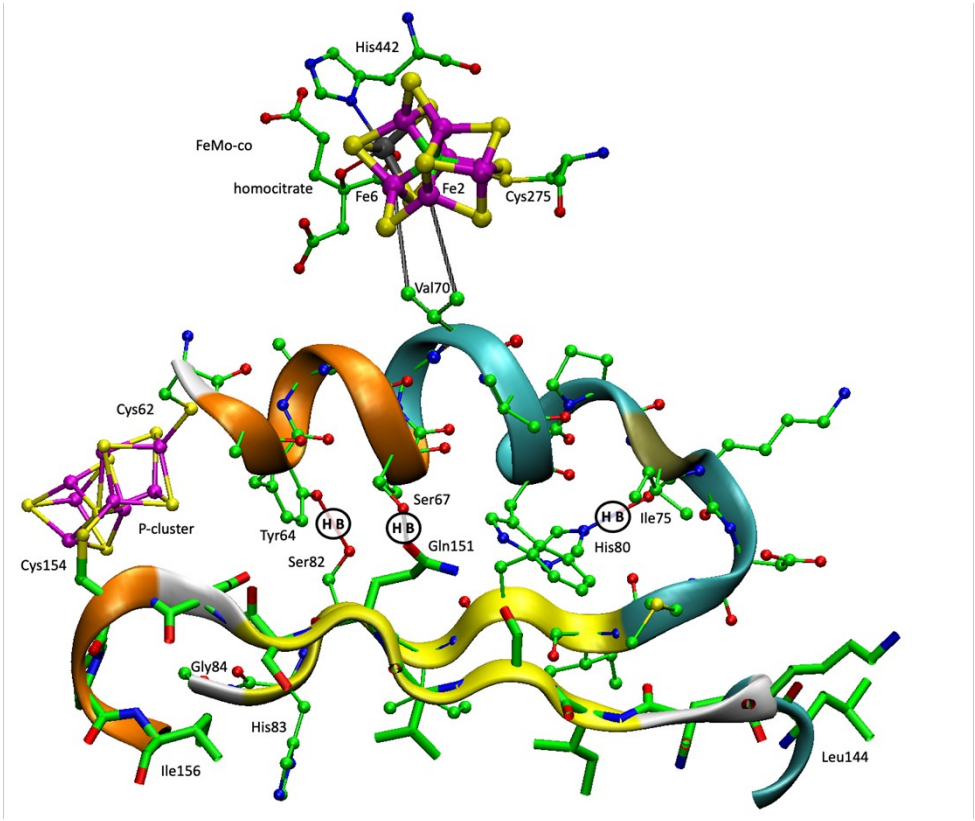


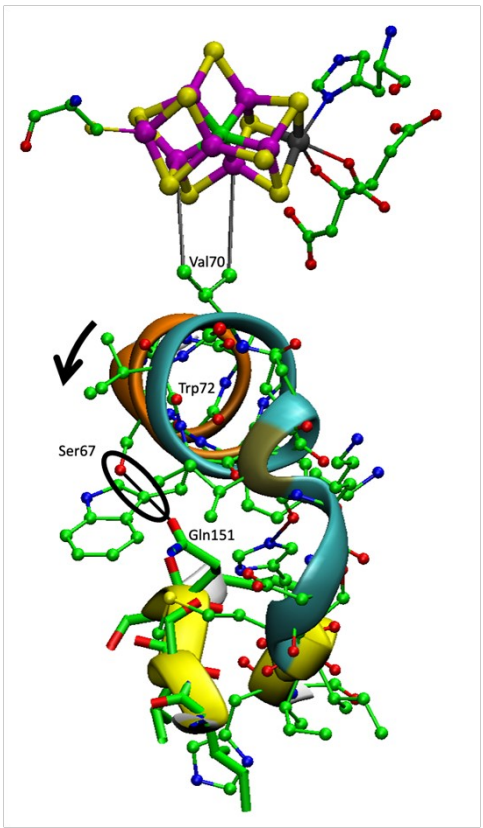
Fig. S2. Generalised diagram of the procedure for locating a reaction transition state. The solid arrows represent the course of limited small-step energy reductions from the numbered positions, which are generated (broken arrows) from Δ positions partway along the previous energy reduction, chosen according 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).

6. Movement of Val70 and the contiguous chain

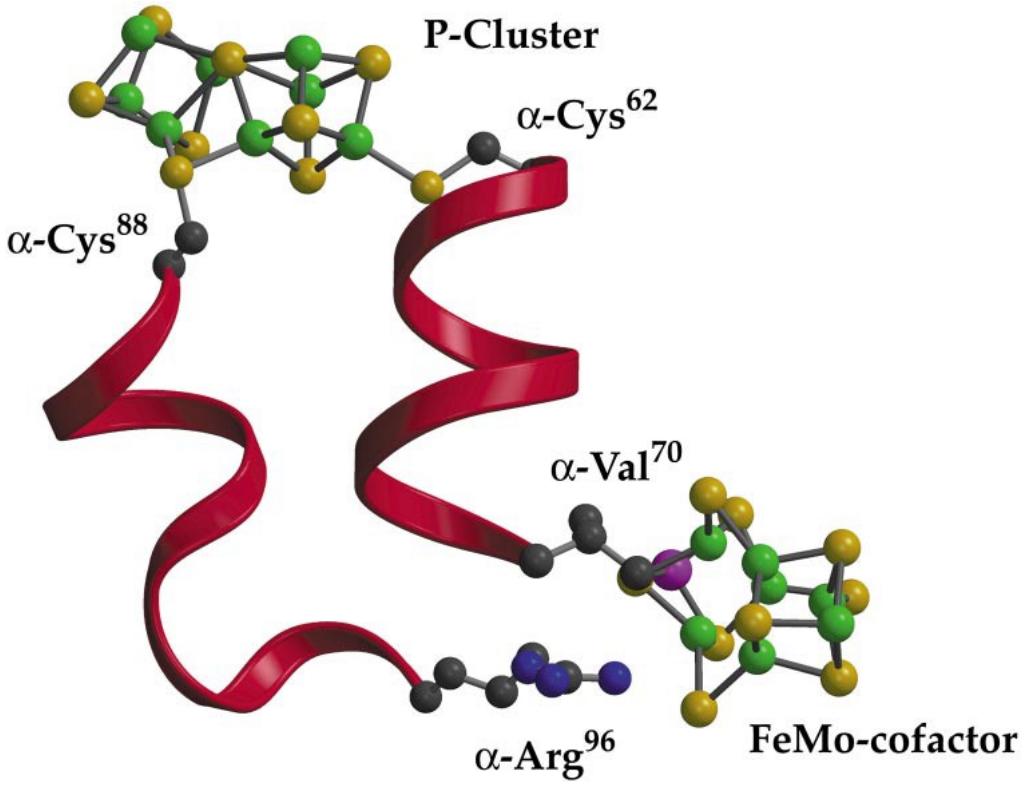
Previous calculations have revealed some steric interference between diffusing N_2 in the Fe2--Fe6 reaction zone and the immediately contiguous protein (mainly the side chain of Val70) in its resting position.[9, 36] This is consistent with experimental data on mutation of residue 70 to larger side chains.[11, 12] Therefore I postulated that the protein dynamics can accommodate and incorporate movement of Val70 and adjacent residues away from FeMo-co.[9] Figure S4 shows the relevant protein structure. The side chain of Val70 that protrudes towards Fe2 and Fe6 at Fe--C distances of 4.4Å extends from an α- and π-helical chain. This chain loops back along the opposite side of the helix, where it forms β-sheet with a later section of the chain. The helical section engages three hydrogen bonds (Fig. S4 (a)), of which Ser67 → Gln151 is most relevant because it is almost opposite Val70. Fig. S4 (b) shows how the helical section of the chain can rotate and slide slightly to increase the Val70 - Fe separations without disrupting this hydrogen bond. Qualitative manipulation of this protein assemblage confirmed that the Cα(Val70)-C^c and Cα(Trp72)-C^c distances in the constrained expanded model could be attained. Obviously analysis of the dynamics of the complete protein is required to explore and quantitate the protein dynamics that would increase the space between Fe2, Fe6 and Val70. The sidechain of Arg96 with possible hydrogen bonds to the mainchain at Gly69 and Val70 is also significant in this domain.


His442
FeMo-co
homocitrate
Fe6
Fe2
Cys275
Val70
Cys62
P-cluster
Cys154
Tyr64
Ser82
Ser67
Gln151
Ile75
His80
Gly84
His83
Ile156
Leu144

(a)


Val70
Trp72
Ser67
Gln151

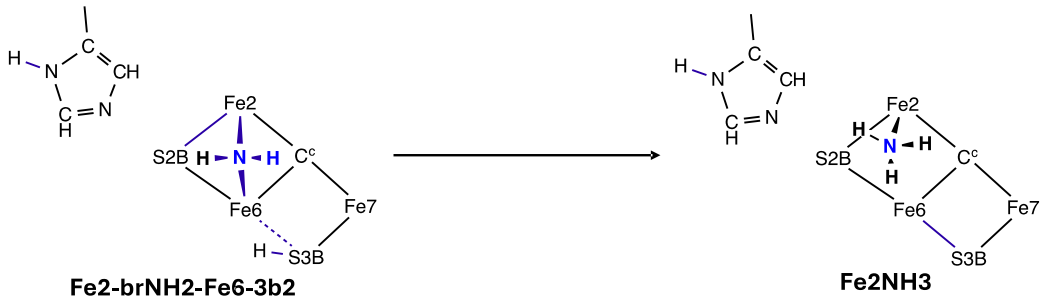
(b)



(c)

Fig. S3. (a) Structure of the protein containing Val70, adjacent to the Fe2,3,6,7 face of FeMo-co (from crystal PDB 3U7Q, all residues are in the a chain). The grey lines identify the approaches (C--Fe 4.37, 4.44Å) of the side chain methyl groups of Val70 to Fe2 and Fe6 of FeMo-co. Two relevant sections of the protein chain are drawn, with secondary structure superimposed as ribbons. The closest section of the chain, containing Val70, is drawn with thin bonds and spherical atoms and extends from Cys62 (a ligand of the P-cluster) to Gly84. A more distant part of the chain, drawn with thick bonds, is from Leu144 to Cys154 (P-cluster ligand). Both sections are part of a b-sheet (yellow ribbons). The a-helical section of the closest chain (residues 63-68, orange ribbon) changes to p-turn (cyan ribbon) through Val70, before looping back to the b-sheet. There are three hydrogen bonds (labelled HB) involving the closest section of chain, and only one of these (Ser67 → Gln151) connects the two sections of chain. (b) End view of (a), showing how the closest section of chain containing Val70 is located between FeMo-co and the distant section of chain containing Gln151. The large black arrow depicts the slight rotation and displacement of the section containing Val70 and Trp72 that can move them away from FeMo-co, without disrupting the Ser67 → Gln151 hydrogen bond. (c) Peptide chain connections between Val70 and Arg96 around FeMo-co and two Cys ligands of the P-cluster. From Ref [37].

7. Potential energy profile for Fe2-brNH2-Fe6-3b2 → Fe2NH3



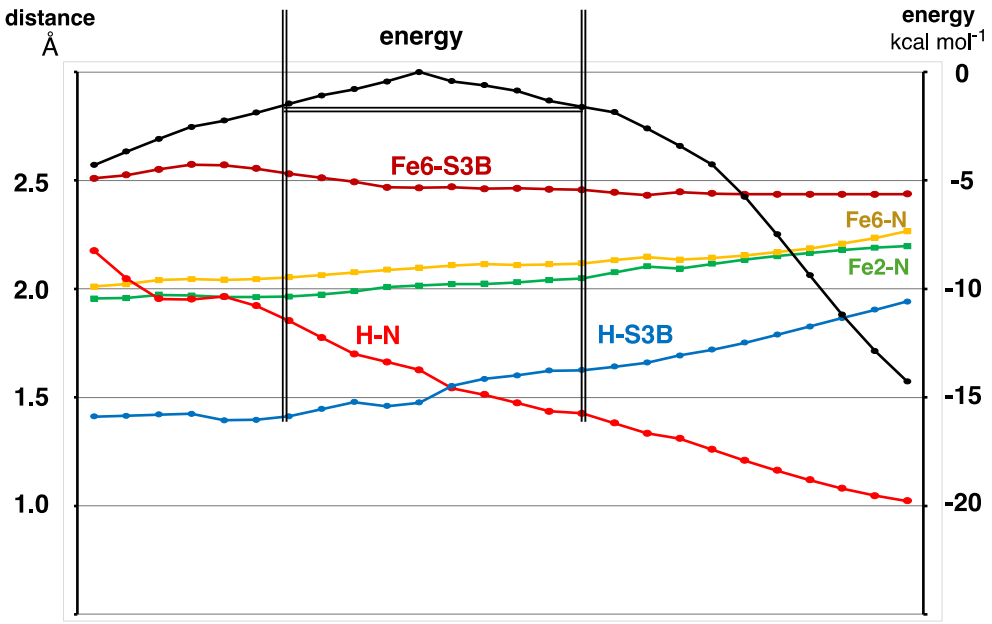


Fig S4. Potential energy profile near the transition state for the **Fe2-brNH2-Fe6-3b2** → **Fe2NH3** reaction step in the S=1, 35 electronic state.

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Coordinates

Translation of Fe numbering

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

structure, S **Fe spin densities**	**filename** **coordinates**
N2x-Fe2-brNH-Fe6-S2BH to N2x-Fe2-brNH2-Fe6 **reactant** **S=1/2, 35** Fe(139) -2.411 Fe(140) -0.235 Fe(141) -2.675 Fe(142) 2.396 Fe(143) 3.042 Fe(144) 2.229 Fe(145) -1.695	bm602n2x2b226nhtf.car_2 C1 -3.831191839 7.196884028 5.086084330 C2 -4.882123683 7.021120982 6.188156869 C3 -3.212276665 8.483624308 3.081283848 C4 -1.755357395 8.834141683 3.367475311 C5 -0.098734761 9.634724894 4.970860047 C6 0.762264162 8.372392360 5.094200879 C7 0.815284578 5.958129449 5.463310524 C8 1.155834571 5.483352552 4.049644351 C9 0.469251294 5.367725082 1.706809128 C10 1.648879659 6.143780908 1.100662139 C11 2.766435030 8.271494323 0.793405656 C12 4.146628969 8.015352373 1.413666734 C13 5.461667152 7.905500153 3.470299006 C14 5.994849714 6.487187660 3.699034590 C15 5.402581047 4.156290323 4.202202379 C16 5.252055030 3.061112409 3.148853377 C17 4.191708768 2.355379124 1.008295234 C18 5.112408801 2.639764630 -0.196798413

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	C23	6.970870362	4.791536629	-1.668603090
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	C25	5.675694842	5.582172864	-4.187256193
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	C27	8.143898216	6.418629480	-0.306472586
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	C37	9.563090662	-5.162387165	7.287061136
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	H220	-5.699233934	-5.037682645	5.324115275
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	H238	-6.113755604	7.690721644	-2.288307627
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H282	0.717325605	-0.155129256	-12.525445872
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H284	0.248865163	2.623247447	-10.660236062
H285	-4.561779763	-9.054265008	3.178158644
H286	-3.797160636	-8.388792561	4.636294561
H287	0.551949150	-9.041040430	5.613980678
H288	-5.321012226	-10.080485795	5.317892999
H289	-6.074786531	-8.672742725	5.674821221
H290	2.866923610	-4.939128671	-4.397699618
H291	4.265225392	-4.531438393	-7.066315142
H292	0.420062935	-6.247466600	-7.708681176
H293	2.707737957	-3.445351266	-5.376620724
H294	4.020162142	-6.066448625	-7.575891840
H295	-1.904748413	-8.288743000	-2.555821852
H296	2.060614805	-6.303805422	-6.277919479
H297	6.838356139	-0.919605182	7.255539992
H298	6.027479617	-3.697206446	8.275695799
H299	-3.116371174	-6.925181572	-1.206922418
H300	5.411959853	-2.028193256	0.288301951
H301	-6.490782175	-5.766135869	-1.516804680
H302	-4.212223916	-1.756661590	2.092753732
H303	-5.260220959	-4.605769103	-2.029624033
H304	6.128982627	-0.518849596	4.652816379
H305	-3.929882364	-5.581952473	0.052430093
H306	4.535457129	-1.062018106	5.209870577
H307	5.180781309	-1.520985353	7.517975073
H308	5.600319890	-3.324268689	5.780056420
H309	7.180092783	-2.604879904	5.433641129
H310	-8.234632241	0.291981906	0.591967962
H311	7.137582815	-1.334440904	9.749576540
H312	5.324272180	-1.583623016	12.189264641
H313	-3.189134270	-2.736742389	0.032132234
H314	8.197796019	-1.092756191	12.070678800
H315	6.974890801	-0.062054021	12.436416529
H316	4.668874182	-2.890883803	3.556484757
H317	-4.239987366	-2.393359980	-2.151210921
H318	-6.400981616	-0.580568800	1.941557307
H319	2.953506374	-6.668104709	10.412595182
H320	0.637709610	-7.291994288	8.129509826
H321	3.650666100	-4.986621328	8.617947767
H322	1.499212750	-6.650047928	10.964306846
H323	-4.313726922	-9.685953121	-2.275858210
H324	3.464951151	-5.088382955	5.485767714
H325	1.747085582	-0.989218415	7.976846367
H326	-4.074016032	-7.074022257	2.154684614
H327	0.880429405	-2.582613603	9.418357143
H328	-4.002687802	-6.402561111	6.978278350
H329	-2.902947908	-4.691008190	5.477515873
H330	6.597595662	-2.655347005	12.791399235
H331	4.677683787	-3.233199263	1.317430979
H332	5.484919562	-5.986768294	6.354666048
H333	4.114906033	-5.775397361	4.253637242
H334	7.417047310	-5.173978821	7.436168984
H335	6.179340134	0.316640925	2.742915652
H336	-0.902192657	-4.909113570	8.530465721
H337	0.810990801	-5.087311755	8.929694353
H338	-0.793886963	-2.458245837	8.854753358

H339	-4.124137359	-4.640762347	2.213020369
H340	-6.458837682	-1.225609881	-2.322571252
H341	-8.273977159	0.098237032	-1.182273183
H342	1.734022368	-1.220011842	6.219460208
H343	5.366613961	-6.124503456	7.897161947
H344	4.713045035	-5.077052686	9.739567634
H345	6.356492584	-0.151417940	1.126700050
H346	-2.314730559	-8.111210416	7.898490411
H347	1.247772149	-6.787637028	6.560379263
H348	-5.741062107	-4.748640327	2.966604463
H349	-2.781681436	-7.660831023	-3.969522517
H350	7.894394606	-3.614944284	0.447783287
H351	6.581677029	-4.736871617	0.011989494
H352	0.069630630	-10.764597980	7.134370549
H353	0.128424202	-9.772476312	8.434622876
H354	4.546792667	-8.872893381	9.213619114
H355	2.394397797	-8.307927629	8.735341390
H356	3.746090813	-11.303937588	8.216688323
H357	4.904089553	-8.538486966	7.505350864
H358	8.196827092	-6.849262976	0.496342034
H359	1.679428917	4.160622722	-13.189824487
H360	10.332346426	-4.443361489	7.619727697
H361	9.214758035	-4.811672515	5.109231074
H362	-1.269804223	4.166242962	-12.480153256
H363	0.819231243	5.105133981	-10.412951510
H364	-0.398321205	6.130862998	-11.194179795
H365	-4.864075686	3.965892877	-7.034459576
H366	2.344973602	-1.969330553	1.079490638
H367	-0.670613377	-0.069503470	1.100539659
Mo368	0.284428547	-4.297271564	4.608542039
N369	1.368314907	-1.631557022	1.097873105
N370	-4.856098258	5.763196790	6.911624729
N371	-4.035527626	8.267250367	4.262154429
N372	-1.472749250	9.374827981	4.575561079
N373	0.122612547	7.238515597	5.476824232
N374	0.210297455	5.689698399	3.101544146
N375	1.704729313	7.466982635	1.378701106
N376	4.191971766	8.013557180	2.772991431
N377	5.055475120	5.507532440	3.810593364
N378	4.461433733	3.318013590	2.081771157
N379	4.843392109	3.775683086	-0.902268829
N380	6.933889976	5.705692986	-0.665833782
N381	7.246178936	-0.823615229	11.812186707
N382	6.665052467	-2.229499029	9.588022940
N383	5.252846225	-2.053510811	3.513616438
N384	6.273551589	-0.477437525	2.090453947
N385	5.118690041	-2.299999108	1.222011512
N386	8.265276406	-4.575609285	7.554172362
N387	-5.959974915	3.018603248	2.716910892
N388	-3.879402424	-0.155377810	5.550140474
N389	-5.345367559	3.613290736	0.239054419
N390	-5.781427643	6.090264440	-0.963763327
N391	-3.302987968	7.386361447	-0.672537676
N392	-1.538067983	5.914256090	-2.306266581
N393	-2.578749898	1.830306536	-2.531218348
N394	-1.891392234	1.850264595	-0.413402360
N395	-1.425834454	6.630815972	-4.963568040
N396	-4.387905632	8.532588536	-8.152636553
N397	-3.182733298	9.138638117	-9.913743248
N398	7.900379457	-6.032544330	-1.956717384
N399	3.902366217	-5.443596456	-6.771655373
N400	0.656867262	-5.356541840	-8.138107218
N401	-1.342916418	-3.498100335	-7.669113730
N402	-5.189704292	-0.392760013	-6.483014302
N403	-6.395000104	-1.130806971	-8.353955581
N404	-5.398243420	0.957469577	-8.357599833
N405	-0.150797156	-1.312520702	-6.207047596
N406	1.716372607	-0.420100096	-8.077187958
N407	0.702760234	0.317182983	-10.527854161
N408	-3.140783940	-0.678564136	-10.290218268
N409	0.110758211	2.809580962	-11.650369686
N410	-5.768189972	-9.263768134	4.896509225
N411	-4.795494361	-6.571750766	2.679589927
N412	-4.940545495	-5.523602423	-0.158355755
N413	-3.598773107	-7.196494403	-2.068328649
N414	-9.086722759	-4.608926596	2.934956924
N415	-8.721730043	-2.473095051	1.047146772
N416	-0.114906125	-9.804371467	7.439096626
N417	-1.082405394	-5.773750040	5.896504579
N418	-3.015999947	-6.423191383	6.735147628

	N419	2.859648717	-8.861520718	8.011297230
	N420	-0.076772731	-0.160891112	-2.252563200
	N421	0.059669961	-0.949801694	-1.464874147
	O422	-2.832653606	6.466475073	4.966554937
	O423	-0.883360811	8.612240918	2.508740548
	O424	1.983308471	8.420756938	4.871635862
	O425	2.245234855	4.948700291	3.786627818
	O426	2.498966606	5.579114815	0.391706730
	O427	5.156636058	7.861275977	0.707954859
	O428	7.213295152	6.296082431	3.813340552
	O429	5.838003366	1.980339235	3.356349704
	O430	6.036137423	1.865019521	-0.493218156
	O431	8.033692706	4.496994436	-2.240703979
	O432	10.469307943	5.803687018	-0.111566284
	O433	5.661233191	-3.941444627	10.772968485
	O434	9.096065140	-2.504131490	8.105238226
	O435	10.617936304	-6.259867578	5.419661335
	O436	-3.461514596	4.806954342	0.807872981
	O437	-5.580472090	0.733345179	4.335064824
	O438	-4.566127002	5.430808201	-2.775834775
	O439	-6.309231786	2.954324288	-3.258349166
	O440	-4.082149753	9.164188001	-1.904315419
	O441	0.194761667	7.299355264	-1.763713797
	O442	0.621889413	5.656492534	-5.168846482
	O443	0.478339525	8.284093381	-7.448004763
	O444	9.949720824	-5.871802760	0.873727021
	O445	5.518286862	-0.519355704	-4.341591252
	O446	2.044967180	-3.548422487	-8.113386739
	O447	-1.785057792	-3.277193627	-9.915424886
	O448	-1.733039812	-0.023232132	-7.239521727
	O449	1.592451010	1.682832156	-7.166251762
	O450	2.900436865	-1.117996067	-5.475564391
	O451	2.786922747	0.321888246	-11.479815459
	O452	-0.496589173	1.851924737	-13.627276961
	O453	-2.636858691	1.401423864	-11.096066884
	O454	0.404413903	5.597431023	-13.888795343
	O455	-4.091709927	3.367836069	-7.017960840
	O456	-6.027801993	-6.521668560	4.617985072
	O457	-6.959099584	-4.907551781	0.735137651
	O458	-5.328428433	-6.912521877	-3.516518909
	O459	-3.393183411	-10.223169555	-4.016663260
	O460	-10.123458567	-1.289597500	2.402547480
	O461	-5.848264002	-2.255024773	6.626626016
	O462	-5.293522498	-4.258327340	5.813376603
	O463	-9.021668295	-2.000178439	-2.487506629
	O464	2.860807808	-9.903923718	5.998970063
	O465	5.699611984	-11.031627467	7.697008300
	O466	-1.096409171	-0.807272292	6.323480685
	O467	0.042489615	0.848077925	7.332850510
	O468	0.096081726	-5.653458475	11.243278350
	O469	-1.332133053	-3.905530875	11.112049960
	O470	1.805484279	-4.620373016	6.165905556
	O471	2.903091371	-3.601524114	7.841465781
	O472	-0.284422658	-3.083131766	6.285694175
	O473	6.012089960	-6.251568596	7.149092586
	O474	4.340400864	-5.279321017	5.062532502
	O475	-4.401467148	1.854922699	-4.889100676
	O476	2.314672762	-7.233224892	10.901889853
	O477	4.175088212	-5.652302003	9.139134075
	S478	0.527047052	-4.300292289	-4.724497010
	S479	-1.308720797	-3.556670164	-1.687398073
	S480	-1.584203211	-3.548994955	3.421211749
	S481	2.186051322	-2.930314105	-1.482239415
	S482	-1.303405988	-1.258905341	1.226454656
	S483	-1.941838411	-6.411142778	0.902325726
	S484	1.907248117	-2.775348584	3.740987013
	S485	1.006768287	-6.302392588	-1.388231861
	S486	0.869654767	-6.300612396	3.460802424
	S487	3.604419751	-5.201149808	1.273367452
	end			
N2x-Fe2-brNH-Fe6-S2BH to N2x-Fe2-brNH2-Fe6 **TS** **S=1/2, 35** Fe(139) -2.306 Fe(140) -0.203	bm602n2x2b226nhte_1_53148.76			
	C1	-3.841462336	7.369867265	4.830261183
	C2	-4.894292392	7.251768867	5.939477332
	C3	-3.204970770	8.573074377	2.781517378
	C4	-1.749059866	8.941180659	3.051215305
	C5	-0.090007583	9.785895171	4.630488080
	C6	0.771473468	8.527595851	4.793400480
	C7	0.823359050	6.128306577	5.248152106
	C8	1.151982913	5.611102580	3.846848923
	C9	0.450234391	5.434869638	1.510809037

Fe(141) -2.676 Fe(142) 2.575 Fe(143) 2.584 Fe(144) 2.197 Fe(145) -1.701	C10	1.636150856	6.182711348	0.881721230
	C11	2.775168843	8.286760447	0.507275873
	C12	4.154873388	8.051526596	1.135518105
	C13	5.474010480	8.023487782	3.193161723
	C14	5.994518655	6.609789985	3.473360675
	C15	5.384187854	4.300297473	4.035988795
	C16	5.247958534	3.177847986	3.009528972
	C17	4.174042739	2.400860575	0.901410444
	C18	5.097787574	2.638141478	-0.310376364
	C19	2.678884357	2.344877263	0.522403767
	C20	2.452318730	1.406046979	-0.666599655
	C21	1.826183887	1.943829581	1.730139742
	C22	5.628422717	4.082623868	-2.234688812
	C23	6.967458436	4.725650284	-1.845816882
	C24	4.821503550	4.958730770	-3.226853941
	C25	5.695061285	5.432052506	-4.396031038
	C26	3.598995342	4.196110814	-3.750624880
	C27	8.138543417	6.408029953	-0.558363001
	C28	9.294610813	5.489039608	-0.223619050
	C29	6.336115359	-1.535916690	12.037394449
	C30	6.195500768	-2.437405487	10.808692345
	C31	6.702325928	-2.548191713	8.362693207
	C32	8.143777312	-3.011778859	8.076211455
	C33	6.187871215	-1.577014712	7.284287228
	C34	6.157954321	-2.186132754	5.878503924
	C35	5.459876052	-1.262726360	4.873946547
	C36	5.546374308	-1.525590718	2.361936280
	C37	9.563343740	-4.912817817	7.469997286
	C38	9.808553792	-5.227068981	6.010325423
	C39	-4.556642085	3.525392987	2.399402963
	C40	-4.377732980	4.064816829	0.966725879
	C41	-3.584566146	2.348546579	2.625982861
	C42	-3.382963885	1.938063963	4.100016177
	C43	-4.368607936	0.909469688	4.651180718
	C44	-5.224866433	3.668345611	-1.339804403
	C45	-5.164244418	5.090883877	-1.904577238
	C46	-6.399409618	2.867671002	-1.923197946
	C47	-5.687685609	7.453581770	-1.550903670
	C48	-4.270658099	8.038747032	-1.586643139
	C49	-1.909166106	7.756677772	-1.000745322
	C50	-0.993314378	6.897982381	-1.875227828
	C51	-0.721275091	4.986472637	-3.378071203
	C52	-0.420353731	5.678709481	-4.716062957
	C53	-1.421183712	3.660180851	-3.714951600
	C54	-1.726715915	2.809361565	-2.528029423
	C55	-1.319419144	2.840190712	-1.209628242
	C56	-2.666264908	1.173728358	-1.356484035
	C57	-1.392689762	7.024695761	-6.514950577
	C58	-0.125471941	7.865485246	-6.665293494
	C59	-2.652222681	7.908415513	-6.682701602
	C60	-3.050944128	8.239529855	-8.090928141
	C61	-2.288168475	8.582782646	-9.189440704
	C62	-4.440114429	8.565839479	-9.718982536
	C63	8.484726798	-5.189797521	-0.746938253
	C64	8.923222156	-6.012632482	0.449661209
	C65	7.437064458	-4.168024521	-0.239183501
	C66	6.958535593	-3.233493617	-1.324739166
	C67	7.601973033	-2.005783878	-1.566274107
	C68	5.855025781	-3.566032741	-2.130218920
	C69	7.154147828	-1.131086840	-2.561690602
	C70	5.408291865	-2.711622481	-3.139105678
	C71	6.051338628	-1.487725925	-3.345326743
	C72	2.471650847	-5.515333178	-6.273954396
	C73	1.709538344	-4.906738091	-7.463344507
	C74	2.314855599	-4.629526872	-5.037209824
	C75	-0.130787407	-5.216652474	-9.080118828
	C76	-1.160876705	-4.112763955	-8.824185977
	C77	-2.174144493	-2.656732418	-7.076474655
	C78	-1.326489092	-1.381224816	-6.828312028
	C79	-2.905858113	-3.134065345	-5.800622945
	C80	-3.808414193	-2.152010222	-5.046022695
	C81	-5.182354658	-1.857272629	-5.673186821
	C82	-5.668078920	-0.463420048	-7.691389844
	C83	0.687319222	-0.366287292	-5.874138490
	C84	1.361677957	0.206556114	-7.128965957
	C85	1.794300802	-0.659070912	-4.839513241
	C86	2.669250067	-0.388596046	-9.110850711
	C87	2.063658373	-0.166826152	-10.487356553
	C88	0.027459555	-0.079181179	-11.817404892
	C89	-0.167223103	1.301839805	-12.490465463

C90	-1.287186669	-0.865584084	-11.808138751
C91	-2.400770648	-0.192461528	-11.016929408
C92	-0.256245657	3.735395940	-12.197514703
C93	0.677309740	4.212054119	-13.298448913
C94	-0.204120893	4.724398277	-10.997480881
C95	-1.207315435	4.376756854	-9.919915106
C96	-2.517197768	4.877084377	-9.980554291
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C118	-5.973283643	-1.386181824	-1.310985356
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C121	-4.724439383	-1.632103219	1.180384973
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C126	-0.874377172	-6.677271154	6.956533888
C127	-2.088020091	-7.062278734	7.491345313
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	H173	6.545294115	6.045448713	-4.064762749
	H174	1.389087045	1.411544634	-0.936221341
	H175	2.723220684	0.368672278	-0.421277099
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	H177	2.991599801	4.838215860	-4.403806595
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	H189	4.539263119	-2.973600078	-3.742785250
	H190	5.313382274	-4.497112746	-1.948299746
	H191	8.461618405	-1.715870634	-0.955439321
	H192	3.944406507	4.282555207	1.891326440
	H193	4.755129685	4.015395565	4.894339598
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	H196	6.253488600	8.533969303	2.612545873
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	H203	-4.503799281	-0.646648835	5.969284644
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	H205	-8.296322825	-2.828239403	6.260763596
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	H208	-9.398569921	-3.538067579	-1.057725065
	H209	-9.838758241	-2.903307773	4.195810337
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	N399	3.905466117	-5.664795609	-6.571004524
	N400	0.653284033	-5.634482706	-7.932134284
	N401	-1.350034609	-3.770865048	-7.534285982
	N402	-5.186473425	-0.621634897	-6.461297717
	N403	-6.376746528	-1.422106656	-8.315303071
	N404	-5.397888587	0.674583098	-8.373304305
	N405	-0.151417209	-1.534418261	-6.155022234
	N406	1.718204120	-0.717523579	-8.066002084
	N407	0.700619757	-0.056043498	-10.531961515
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	N409	0.112768565	2.399080015	-11.742907454

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Fe2-brNH2-Fe6
product
S=1/2, 35

Fe(139) -2.364
Fe(140) -0.318
Fe(141) -2.632
Fe(142) 2.596
Fe(143) 2.737
Fe(144) 2.209
Fe(145) -1.510

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C2	-4.872063147	7.219877004	5.938678345
C3	-3.218324381	8.593586296	2.783728519
C4	-1.760396335	8.952082358	3.053589524
C5	-0.103429990	9.813337990	4.627820588
C6	0.758159412	8.555598101	4.791984174
C7	0.814683301	6.158734281	5.255203233
C8	1.153669223	5.623805287	3.862881194
C9	0.471735899	5.414916343	1.525010865
C10	1.648873442	6.170408894	0.889423833
C11	2.760106468	8.289357574	0.505010922
C12	4.138914281	8.056917343	1.134740907
C13	5.458659190	8.023101055	3.190645055
C14	5.994531017	6.612775712	3.462598811
C15	5.408152996	4.304920797	4.066210605
C16	5.254005072	3.168866755	3.059206022
C17	4.209152614	2.394914365	0.936354634
C18	5.123469040	2.632398143	-0.280968581
C19	2.711767228	2.322054607	0.569448911
C20	2.484043580	1.374602279	-0.613997917
C21	1.880378954	1.928023841	1.794724924
C22	5.633186892	4.080788196	-2.211522024
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C26	3.585485545	4.174534982	-3.703632458
C27	8.142547924	6.393651557	-0.508207792
C28	9.294031769	5.467708688	-0.176507065
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C31	6.696421085	-2.539177075	8.344581327
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C33	6.203183616	-1.558582945	7.264151369
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C35	5.517095838	-1.227402296	4.841185288
C36	5.537570744	-1.501423765	2.328888316
C37	9.555362507	-4.910439870	7.456125675
C38	9.820819528	-5.215779536	5.998306710
C39	-4.568573700	3.517182549	2.401904760
C40	-4.389566668	4.066786595	0.971840101
C41	-3.597966670	2.338423057	2.615422280
C42	-3.384922153	1.916172889	4.083409482
C43	-4.376205661	0.896938902	4.642147022
C44	-5.230712030	3.666043573	-1.336312792
C45	-5.168585303	5.086289320	-1.905990547
C46	-6.402980168	2.862560560	-1.919367233
C47	-5.694080836	7.449467408	-1.554033509
C48	-4.278567504	8.038019627	-1.601109852
C49	-1.914819815	7.771020497	-1.015772229
C50	-0.996146867	6.920074745	-1.894912614
C51	-0.710979376	4.997593409	-3.382689559
C52	-0.414709206	5.677222577	-4.728303378
C53	-1.398234532	3.660828371	-3.706056552
C54	-1.708844095	2.819868758	-2.512765491
C55	-1.302494858	2.857794970	-1.193889228
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C59	-2.641147700	7.898175739	-6.708653572
C60	-3.040195388	8.236240701	-8.115202285
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C65	7.418807999	-4.183259066	-0.239202506
C66	6.941017925	-3.245550260	-1.322444335
C67	7.573809691	-2.010000997	-1.550727044
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C69	7.119323102	-1.130516236	-2.539153016
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C73	1.699407972	-4.899921927	-7.469218388
C74	2.299752263	-4.639760961	-5.037783784
C75	-0.138905588	-5.212545602	-9.093077983
C76	-1.170026950	-4.110706882	-8.835120664
C77	-2.170855483	-2.646432550	-7.084219107
C78	-1.326552038	-1.370501167	-6.828979907
C79	-2.911004157	-3.131814639	-5.817245259
C80	-3.810764395	-2.150852219	-5.057480569

C81	-5.186975452	-1.855041373	-5.678552001
C82	-5.678511184	-0.467311361	-7.697716064
C83	0.675048717	-0.350064506	-5.858153814
C84	1.357637660	0.215156769	-7.111250953
C85	1.770159746	-0.637067487	-4.812405387
C86	2.664922846	-0.371967336	-9.094714263
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C90	-1.270714504	-0.870676451	-11.814752279
C91	-2.394588381	-0.201620716	-11.033725048
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C94	-0.197213285	4.729512718	-11.000441810
C95	-1.203410966	4.381619336	-9.926916520
C96	-2.517269208	4.869142291	-9.996571290
C97	-0.873459579	3.520263195	-8.866238732
C98	-3.481591353	4.486555126	-9.059957674
C99	-1.831279728	3.102345385	-7.937627940
C100	-3.131418192	3.589388896	-8.048834426
C101	-4.778894216	-8.376082900	4.426109795
C102	-5.269643119	-6.982706029	4.071515543
C103	-5.062564050	-5.131367415	2.426167936
C104	-5.745934161	-5.164343684	1.053966891
C105	-5.401026012	-5.633117753	-1.332129528
C106	-4.771281694	-6.718282471	-2.199376888
C107	-2.915444055	-8.214671027	-2.682583517
C108	-3.623684938	-9.548667069	-2.790424758
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C116	-8.050768547	-0.407809845	-0.225564437
C117	-6.620474007	-0.861419385	-0.185897427
C118	-5.998217254	-1.381258740	-1.332395273
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H147	-5.008847140	5.186667416	6.076382750
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H150	-4.727939230	8.068871602	6.629189662
H151	-3.205580983	7.674020898	2.179488461
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H155	-0.901224836	7.429215447	5.285872051
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H230	-1.381380314	6.206233599	-7.298214453
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H232	-0.735846607	3.123851901	-4.406049543
H233	-2.331346216	3.870685258	-4.256233796
H234	-2.947563531	9.055668570	-11.189148226
H235	-3.492727558	7.358098190	-6.265801390
H236	-2.526644732	5.610015535	-2.404373254
H237	-1.466067080	7.821557872	-0.012166853
H238	-6.122427115	7.608119529	-2.553918112
H239	-3.270627651	0.327894265	-1.104318859
H240	-6.289213997	8.035678195	-0.841240314

	H241	8.643239896	-6.608887075	-2.221837721
	H242	7.425655209	-5.546988200	-2.471130067
	H243	0.072145495	-2.413301210	-5.670175202
	H244	0.041672489	0.462283347	-5.472453538
	H245	1.640948446	-1.696167859	-7.801966397
	H246	-3.110837962	1.484909134	-3.422714231
	H247	-5.077558909	2.113826580	-4.376469378
	H248	-7.164288982	2.495340659	-3.684939769
	H249	-4.113084821	2.358161239	-5.611047637
	H250	-6.360457439	1.844283753	-1.498134409
	H251	-7.354599355	3.332070666	-1.622249144
	H252	-1.080201160	-1.892359541	-11.457814745
	H253	-1.605328447	-0.943050197	-12.861282477
	H254	-2.782223507	-1.974528255	-10.041577273
	H255	-3.776836768	-0.583230690	-9.622088081
	H256	-6.568074558	-1.377552828	-9.311699012
	H257	-5.941295961	-1.750619210	-4.883641973
	H258	-4.496524102	4.886778755	-9.119206163
	H259	0.150514013	3.157713313	-8.742381642
	H260	-4.870114014	1.413945538	-7.941105988
	H261	-2.147144903	-3.487586761	-5.107294529
	H262	-0.782978914	-4.243325109	-6.837706451
	H263	-3.285840743	-1.205288089	-4.851346037
	H264	-6.181014747	5.790092300	-0.279271930
	H265	-0.673646242	-6.085014768	-9.490386364
	H266	-6.037978180	3.025079221	0.598338213
	H267	-3.501709081	-4.017791945	-6.103151044
	H268	-1.568566993	2.386619229	-7.158237642
	H269	0.525181045	-4.837442226	-9.884456185
	H270	-6.693210540	-2.260756435	-7.822586816
	H271	-6.041850124	0.948406258	-9.127617918
	H272	-5.988716962	2.299960934	3.258821866
	H273	-4.251960878	4.341997861	3.069968031
	H274	-2.798309526	5.563166881	-10.792423311
	H275	-4.288226512	3.194290728	-1.650307768
	H276	-2.874327989	-2.390438561	-7.882799775
	H277	-5.498712754	-2.700739606	-6.305762741
	H278	-3.994509995	-2.610989037	-4.077918464
	H279	-4.861062215	0.233207885	-5.972224533
	H280	3.204073074	0.544550574	-8.812097706
	H281	0.184693167	-0.245369408	-9.672507210
	H282	0.727368164	-0.589768723	-12.506385716
	H283	3.398672828	-1.183718609	-9.194619893
	H284	0.262132060	2.250633295	-10.747205854
	H285	-4.566760553	-8.942484974	3.506960600
	H286	-3.805498676	-8.226623115	4.938206020
	H287	0.551610723	-8.853339165	5.926785513
	H288	-5.331286185	-9.887971335	5.675524968
	H289	-6.083530800	-8.466286583	5.983493253
	H290	2.862377817	-5.112523187	-4.222468494
	H291	4.250196611	-4.762108238	-6.905602144
	H292	0.416040010	-6.507077521	-7.488756833
	H293	2.705789370	-3.636631987	-5.229013153
	H294	4.013373005	-6.318027747	-7.356599028
	H295	-1.915730406	-8.400850130	-2.257872473
	H296	2.051103007	-6.516327992	-6.066343715
	H297	6.849869459	-0.665184055	7.276245653
	H298	6.019817049	-3.402021498	8.386076920
	H299	-3.114355097	-6.982374830	-0.952907845
	H300	5.420718144	-2.010468557	0.351740611
	H301	-6.483497581	-5.810711538	-1.310393241
	H302	-4.235837428	-1.712056670	2.117957999
	H303	-5.246217934	-4.678289086	-1.863585437
	H304	6.156662162	-0.356508058	4.659517600
	H305	-3.923152822	-5.578692335	0.252225217
	H306	4.554604853	-0.854049611	5.229268620
	H307	5.189152077	-1.243414563	7.557948692
	H308	5.587280219	-3.109849964	5.884378818
	H309	7.179019714	-2.424391418	5.517037448
	H310	-8.263658009	0.305765931	0.583961776
	H311	7.138877131	-0.997709752	9.785981998
	H312	5.322984594	-1.167895942	12.241592445
	H313	-3.232952507	-2.763329262	0.110007262
	H314	8.193474827	-0.669320559	12.096470899
	H315	6.969021041	0.369119116	12.421895445
	H316	4.686899902	-2.763187577	3.645694800
	H317	-4.300127547	-2.482404768	-2.105617284
	H318	-6.413334341	-0.513050838	1.942069132
	H319	2.959087324	-6.299745058	10.637851157
	H320	0.649411136	-6.981240035	8.354962409

H321	3.646966961	-4.686209183	8.782237635
H322	1.505224308	-6.256691420	11.185282675
H323	-4.339888101	-9.769426236	-1.962174835
H324	3.459244202	-4.887872996	5.655475414
H325	1.764378495	-0.710907619	7.994197566
H326	-4.071158348	-7.000666964	2.412173162
H327	0.870308193	-2.234999694	9.498855611
H328	-4.000999767	-6.156734397	7.213242759
H329	-2.908551454	-4.478056325	5.668250242
H330	6.607791499	-2.211630112	12.864502571
H331	4.653485266	-3.158387688	1.417310550
H332	5.480668628	-5.761440157	6.553903042
H333	4.108086271	-5.613282435	4.445140888
H334	7.409112857	-4.909592245	7.598995176
H335	6.186135510	0.422086224	2.726000596
H336	-0.892037640	-4.605602567	8.682158620
H337	0.820546380	-4.753333871	9.096553015
H338	-0.800657802	-2.139814750	8.915685714
H339	-4.118041192	-4.567905202	2.373233746
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H344	4.710448570	-4.730540232	9.904758764
H345	6.334868913	-0.087657339	1.118647616
H346	-2.309915117	-7.845101142	8.160073557
H347	1.247364503	-6.559205571	6.757908182
H348	-5.735005078	-4.640471593	3.132630247
H349	-2.776549436	-7.797270433	-3.691478455
H350	7.876102260	-3.607412700	0.579214317
H351	6.565897125	-4.743678309	0.176061412
H352	0.064644489	-10.504743771	7.525243059
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H354	4.544833022	-8.547164417	9.518789737
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H357	4.906620068	-8.267763391	7.801539742
H358	8.168113318	-6.812847587	0.756265911
H359	1.674903682	3.694296002	-13.342366698
H360	10.325763252	-4.188286988	7.780911338
H361	9.220673850	-4.616644572	5.270052108
H362	-1.266799089	3.726378804	-12.614064437
H363	0.821569899	4.735326054	-10.581543173
H364	-0.393723908	5.733885907	-11.402215580
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H366	2.258311228	-1.753513155	1.125380782
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Mo368	0.281235361	-4.118903767	4.754037117
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N375	1.698727641	7.503314277	1.115027773
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N379	4.848373779	3.740359307	-1.025339981
N380	6.933966495	5.672238052	-0.849834499
N381	7.242339700	-0.412535880	11.824699087
N382	6.663035840	-1.896237401	9.653364293
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N386	8.259174311	-4.309657042	7.696295647
N387	-5.965086888	3.107439022	2.610148553
N388	-3.886284766	0.052822760	5.571142816
N389	-5.346552681	3.619673952	0.112637225
N390	-5.782728604	6.050820225	-1.178760725
N391	-3.303827404	7.359187178	-0.935646595
N392	-1.535724057	5.835298170	-2.517251969
N393	-2.586130915	1.753919321	-2.580845663
N394	-1.902029850	1.857691177	-0.462546864
N395	-1.425342138	6.448330387	-5.200726734
N396	-4.384341739	8.238160739	-8.456229390
N397	-3.181765153	8.792384570	-10.235905914
N398	7.893573207	-6.099688567	-1.747409004
N399	3.892051487	-5.664784373	-6.577266497
N400	0.648452304	-5.629708172	-7.946977246

N401	-1.342119710	-3.755867389	-7.546248964
N402	-5.191656089	-0.621194440	-6.470597413
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N404	-5.401752863	0.663448918	-8.391158805
N405	-0.162600830	-1.519078828	-6.136280935
N406	1.712397494	-0.706080678	-8.052003321
N407	0.702782450	-0.047791972	-10.528778967
N408	-3.154042200	-1.046960695	-10.282192576
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N410	-5.779124098	-9.085978429	5.227039522
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N412	-4.933257322	-5.527545275	0.038484293
N413	-3.599585078	-7.277842416	-1.806281054
N414	-9.096989711	-4.505257819	3.096316721
N415	-8.729145950	-2.440217288	1.132202832
N416	-0.115139249	-9.530304369	7.785053854
N417	-1.087040889	-5.553665653	6.097937478
N418	-3.015766347	-6.182868960	6.964209773
N419	2.859963209	-8.569250411	8.311476084
N420	-0.195922614	-0.218962656	-2.223746532
N421	-0.070275723	-1.015889371	-1.440946874
O422	-2.821130915	6.644101808	4.731040077
O423	-0.888316922	8.695172125	2.204757505
O424	1.979375060	8.596156915	4.567606292
O425	2.240426048	5.072303034	3.623983108
O426	2.502691299	5.582483822	0.203315989
O427	5.148718972	7.876781362	0.434961440
O428	7.213742500	6.422476532	3.567603544
O429	5.814608436	2.087027576	3.322203997
O430	6.043683321	1.845231380	-0.553396735
O431	8.032947392	4.426283993	-2.396586606
O432	10.467514767	5.790556713	-0.292184816
O433	5.643289893	-3.558873289	10.896251053
O434	9.096723054	-2.228743068	8.198860493
O435	10.638280940	-6.041150572	5.622341745
O436	-3.468598230	4.840729595	0.649416877
O437	-5.577583298	0.861732554	4.289160845
O438	-4.567713552	5.324594897	-2.967943218
O439	-6.308000347	2.821478892	-3.355979366
O440	-4.089730707	9.097849452	-2.216701287
O441	0.195011652	7.237472312	-2.016325191
O442	0.620404377	5.466007867	-5.371781156
O443	0.479475255	8.011092399	-7.744530241
O444	9.954231743	-5.870807046	1.054967518
O445	5.511242597	-0.664488456	-4.311249977
O446	2.028899836	-3.814280830	-7.977325792
O447	-1.789101148	-3.614394932	-9.797031624
O448	-1.715355090	-0.272727487	-7.257858429
O449	1.607154072	1.423870713	-7.205580848
O450	2.882553581	-1.316524185	-5.405991008
O451	2.790121961	-0.051745500	-11.472887663
O452	-0.506480263	1.376436531	-13.679539447
O453	-2.623998189	1.012822557	-11.120803703
O454	0.405572969	5.122913894	-14.064341412
O455	-4.096054716	3.121485674	-7.137632877
O456	-6.032502859	-6.354563731	4.845769193
O457	-6.958325331	-4.900563553	0.911110196
O458	-5.323230631	-7.028680728	-3.269351018
O459	-3.414856518	-10.348576992	-3.687895920
O460	-10.127057449	-1.206756280	2.446866610
O461	-5.856702665	-2.026483985	6.713647554
O462	-5.298928265	-4.048661668	5.954064179
O463	-9.045257859	-2.085002147	-2.418993299
O464	2.861761439	-9.692488492	6.343042245
O465	5.700639528	-10.752263601	8.089298132
O466	-1.078467497	-0.564385849	6.336037304
O467	0.068838322	1.115297624	7.297093391
O468	0.103729653	-5.241519892	11.425815543
O469	-1.339746643	-3.512139164	11.226044174
O470	1.807255763	-4.387316472	6.306143583
O471	2.898538661	-3.329948931	7.961056993
O472	-0.287158817	-2.847571641	6.387055032
O473	6.008178723	-5.996622531	7.357505084
O474	4.334848008	-5.095117084	5.239646629
O475	-4.400195287	1.681070781	-4.958274369
O476	2.318346163	-6.843117331	11.147287212
O477	4.175804016	-5.330126522	9.325341468
S478	0.525544329	-4.454045974	-4.539031532
S479	-1.316797949	-3.668643899	-1.602727026
S480	-1.640830218	-3.438924139	3.584017323

S481	2.156917428	-2.920593292	-1.373447326
S482	-1.358593016	-1.405120593	1.232605725
S483	-1.923794189	-6.414719158	1.147435952
S484	1.836492507	-2.592445876	3.807573843
S485	1.056548417	-6.319988426	-1.183681752
S486	0.873968172	-6.148880965	3.670025053
S487	3.610014939	-5.101673900	1.447117628
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N2x-Fe2-brNH2-Fe6-3b5 to 3b3
S=1, 35
reactant
Fe(139) -2.192
Fe(140) -0.056
Fe(141) -2.528
Fe(142) 2.514
Fe(143) 2.653
Fe(144) 2.068
Fe(145) -0.671

bm5expro2b2n2x3b5.car_3

C1	-7.916052984	-5.025655274	1.542412966
C2	-8.374212012	-6.176213622	0.638691139
C3	-8.602361485	-2.978880857	2.719126065
C4	-8.013859977	-3.221709390	4.105911707
C5	-7.692335725	-4.766523665	5.970951386
C6	-6.169365410	-4.931797148	5.907542466
C7	-4.216604256	-5.380731073	4.509912403
C8	-3.612242139	-3.974367752	4.465032063
C9	-3.891927264	-1.664818011	3.686476266
C10	-3.792167162	-0.994646686	5.065283795
C11	-4.743093900	-0.660998459	7.264758620
C12	-3.714174342	-1.281188508	8.222561895
C13	-2.950137150	-3.329934720	9.332281937
C14	-1.526505389	-3.743354959	8.936749451
C15	-0.076342231	-4.605007660	7.149448057
C16	0.715955436	-3.508228990	6.432676590
C17	0.626294141	-1.420717940	5.161395636
C18	0.995058475	-0.183653958	5.991963139
C19	-0.117797222	-1.085077775	3.849241133
C20	0.525996260	0.111937076	3.138760558
C21	-0.149824112	-2.310591118	2.928174682
C22	0.222726892	1.767784841	7.268487774
C23	0.586644927	1.437573630	8.727652486
C24	-0.945564266	2.773265242	7.129260856
C25	-0.722822876	4.005334229	8.015562484
C26	-1.114191024	3.195838276	5.662789128
C27	0.134931005	0.140757410	10.728518611
C28	1.574521228	-0.310435490	10.876926533
C29	5.444453338	-11.683300948	4.095225814
C30	6.074022754	-10.448626708	3.456041889
C31	6.437274153	-8.010248607	3.804086833
C32	7.682512043	-7.672549859	4.645099385
C33	5.338940890	-6.951137097	3.995892528
C34	5.802150643	-5.551289510	3.594407785
C35	4.661006762	-4.539983675	3.602157088
C36	4.778039898	-2.029283195	3.535770379
C37	9.991754149	-6.861284513	4.581450246
C38	10.307188762	-5.383826521	4.535925873
C39	-5.447455311	-2.561620686	-1.428805143
C40	-5.843090754	-1.141656434	-0.975725337
C41	-3.913072678	-2.699383535	-1.415899061
C42	-3.383878598	-4.147882671	-1.479955242
C43	-3.188334946	-4.733125494	-2.878229893
C44	-6.129750378	1.143874351	-1.921223890
C45	-7.235949525	1.688148229	-1.012083965
C46	-6.231813727	1.702525751	-3.348070390
C47	-9.427170679	1.287294329	0.004491935
C48	-9.043856624	1.344056077	1.488546475
C49	-7.385101604	0.827718944	3.212655983
C50	-6.175200625	1.738960477	3.433355690
C51	-4.508524169	3.267542323	2.488584268
C52	-4.885682263	4.614942038	3.124464982
C53	-3.871021857	3.589032054	1.127252906
C54	-3.366197445	2.397733232	0.386908957
C55	-3.103560656	1.092332867	0.749009224
C56	-2.615149985	1.215655302	-1.339642118
C57	-6.543116006	6.424230459	3.082905255
C58	-6.403528453	6.643445873	4.587511633
C59	-8.028064106	6.532531328	2.657449360
C60	-8.613084191	7.908612722	2.538738166
C61	-8.471019103	9.028671569	3.335834529
C62	-9.862904732	9.444461919	1.661985831
C63	9.189180879	1.240967756	3.432212718
C64	10.146622128	0.071594258	3.299165269
C65	7.758070439	0.679532000	3.239594337
C66	6.688728799	1.729426689	3.427045159
C67	6.123865923	1.979525528	4.691041056
C68	6.223404675	2.487297116	2.336772580
C69	5.121663297	2.939429853	4.863715249
C70	5.235905858	3.458559544	2.496696652
C71	4.678374087	3.677091378	3.759034580

C72	5.564285949	6.577546981	-1.549072261
C73	4.567491636	7.729332011	-1.754077802
C74	4.814383465	5.303681816	-1.148736553
C75	3.583687435	9.307597708	-3.381202440
C76	2.098745227	8.970420525	-3.535449914
C77	0.414551392	7.135290733	-3.450787612
C78	-0.085640469	6.854600219	-2.010247118
C79	0.413096031	5.876190843	-4.345097282
C80	-0.864455996	5.037302596	-4.452794993
C81	-1.996682412	5.607346480	-5.320949411
C82	-3.458103117	7.583058665	-4.874920159
C83	0.351866840	5.905829194	0.202749110
C84	0.278906829	7.154474360	1.090821006
C85	1.284639220	4.892180633	0.894297575
C86	1.495578467	9.167876991	1.769278280
C87	0.935904519	10.537666772	1.422251804
C88	-0.366973642	11.865436969	-0.143950077
C89	-1.583919795	12.494279694	0.573882062
C90	-0.566606574	11.879747291	-1.664375171
C91	-1.784936084	11.095412782	-2.137009349
C92	-3.584938657	12.120476704	1.919519422
C93	-3.428798899	13.262926235	2.911293988
C94	-4.312054380	10.927448759	2.598562255
C95	-4.617970610	9.827776997	1.610084271
C96	-5.796348676	9.862400330	0.849276808
C97	-3.704784717	8.787585679	1.370221402
C98	-6.046168012	8.908570947	-0.138789775
C99	-3.925360156	7.839466159	0.367847815
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C101	3.771495220	-4.315228052	-9.009407318
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C103	1.029933193	-2.389167506	-7.167516519
C104	0.562259607	-1.044406653	-7.739156397
C105	1.019793686	1.372624538	-7.768170319
C106	2.220598841	2.287538678	-7.987929266
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C113	-1.186101018	-6.175088403	-6.751581535
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C116	-4.686487220	0.038688341	-6.713369731
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Fe140	1.870759457	0.421191753	-1.324452378
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	H247	-4.937525680	4.216499786	-2.757234770
	H248	-6.454367137	3.451037403	-4.201934292
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	H254	-0.612673422	10.063693674	-3.494819391
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	H267	0.723565137	6.193176731	-5.354802900
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	H273	-5.856485499	-3.235581215	-0.651391917
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	H321	6.290840559	-8.429373878	0.082678600
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	H323	4.798605505	2.230993956	-9.644317282
	H324	6.302999044	-5.324718824	-0.323764500
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	H327	2.666228719	-9.302403925	-0.603669618
	H328	2.660667296	-7.138277498	-6.848642858
	H329	1.970316493	-5.522510245	-5.028715402
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N2x-Fe2-brNH2-Fe6-3b5 to 3b3 **S=1, 35** **TS** Fe(139) -2.458 Fe(140) -0.153 Fe(141) -2.598 Fe(142) 2.480 Fe(143) 2.697 Fe(144) 1.954 Fe(145) -0.852	bm5expro2b2n2x3b4c.car_1 C1 -7.916992291 -5.032058910 1.552174689 C2 -8.364671816 -6.178212319 0.639437564 C3 -8.606845451 -2.984631726 2.723463697 C4 -8.015316497 -3.226636460 4.109359473 C5 -7.695649383 -4.770257790 5.976873391 C6 -6.173029192 -4.936666332 5.915190691 C7 -4.217351308 -5.384814506 4.520288372 C8 -3.609999315 -3.980167960 4.471992935 C9 -3.887099920 -1.671032722 3.692792679 C10 -3.790116697 -1.005620346 5.074132557 C11 -4.752782726 -0.673850386 7.269878981 C12 -3.723746612 -1.291992176 8.228680273 C13 -2.962425910 -3.338632517 9.343893371 C14 -1.537464922 -3.752655105 8.953737989 C15 -0.080396761 -4.602903949 7.165249156 C16 0.712436964 -3.512006515 6.440871413 C17 0.630031309 -1.423524586 5.173293600 C18 0.996342320 -0.184837709 6.000716039 C19 -0.111557111 -1.087373462 3.857286512 C20 0.530793881 0.113628508 3.153067387 C21 -0.136210569 -2.311919209 2.934973261 C22 0.217431627 1.761607373 7.281249922 C23 0.578548870 1.431130967 8.740963734 C24 -0.951449941 2.765727411 7.139066673 C25 -0.726783777 3.999144464 8.022730949 C26 -1.120350619 3.184206723 5.671669529 C27 0.126410674 0.139235807 10.742669948 C28 1.566777361 -0.314035744 10.883878007 C29 5.451291277 -11.685979628 4.089285670 C30 6.089949022 -10.453665530 3.453262216 C31 6.452199832 -8.013267701 3.796460069 C32 7.698703651 -7.680347012 4.636507930 C33 5.357274419 -6.951628652 3.991259602 C34 5.812972072 -5.552515413 3.578543460 C35 4.658691792 -4.556077796 3.587447130 C36 4.762731827 -2.047105764 3.505380704 C37 10.002421451 -6.858203410 4.574843972 C38 10.317991910 -5.380743498 4.532227871 C39 -5.452109335 -2.567303198 -1.435634899 C40 -5.846912748 -1.147514168 -0.981799591 C41 -3.915044419 -2.700263997 -1.421827836 C42 -3.377845348 -4.144861446 -1.483415288 C43 -3.183412623 -4.733630828 -2.880511324 C44 -6.125237465 1.139083766 -1.928785894 C45 -7.228464648 1.687042926 -1.017700644 C46 -6.228858266 1.696340121 -3.355595977 C47 -9.418383458 1.291401563 0.003079761 C48 -9.034786082 1.343365303 1.486789964 C49 -7.375585211 0.824574129 3.209785929 C50 -6.172380505 1.743653516 3.434962611 C51 -4.507304843 3.275918433 2.491833868 C52 -4.881962045 4.622582925 3.129444913 C53 -3.871612639 3.595719352 1.128391619 C54 -3.373128467 2.400830996 0.390058205 C55 -3.112956472 1.096928444 0.758913453 C56 -2.626292622 1.207705992 -1.330396195 C57 -6.543797621 6.431082395 3.096033747 C58 -6.396184957 6.653909744 4.599240289 C59 -8.027492681 6.537555122 2.671775531 C60 -8.610348813 7.914354066 2.549516043 C61 -8.461736455 9.036510960 3.342631915

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H148	-9.831802335	-4.281307522	1.551455273
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H166	-0.603485122	-3.182698896	3.416080357
H167	-0.699712864	-2.092519636	2.014611197
H168	0.887631046	-2.594553898	2.637954534
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H174	-0.013511242	0.339172400	2.225289619
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H177	-1.950367153	3.898492221	5.566340667
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H181	-1.877759877	2.263121664	7.472277136
H182	1.129078858	2.224251091	6.874399591
H183	-0.992250103	0.274266697	6.291152555
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H188	3.348059739	4.652541738	4.764289680
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N2x-Fe2-brNH2-Fe6-3b5 to 3b3 **S=1, 35** **product** Fe(139) -2.383 Fe(140) 0.055 Fe(141) -2.612 Fe(142) 2.696 Fe(143) 3.138 Fe(144) 1.275 Fe(145) -0.430	bm5expro2b2n2x3b3.car_2 C1 -7.912921835 -5.028200451 1.545689061 C2 -8.371154145 -6.177179027 0.640843677 C3 -8.598214729 -2.980560935 2.721125428 C4 -8.007813800 -3.222661774 4.107285168 C5 -7.686037731 -4.766960781 5.973355821 C6 -6.163244687 -4.932334633 5.908907368 C7 -4.210497445 -5.380307355 4.511231640 C8 -3.605034427 -3.974612016 4.466587126 C9 -3.885993541 -1.664677536 3.688268677 C10 -3.785225735 -0.996016885 5.067424975 C11 -4.736920958 -0.661318880 7.266316827 C12 -3.707462617 -1.281423782 8.223493327 C13 -2.944400255 -3.330163801 9.334010401 C14 -1.520889289 -3.744365176 8.939005464 C15 -0.070513758 -4.606503696 7.152088273 C16 0.722178010 -3.511439205 6.432976671 C17 0.634863741 -1.421042172 5.166615911 C18 1.002274272 -0.183956286 5.997432303 C19 -0.111363367 -1.084410944 3.855190339 C20 0.530780422 0.114677027 3.147988453 C21 -0.142486048 -2.309646900 2.934153868 C22 0.229003937 1.768321131 7.271872725 C23 0.592512140 1.437925063 8.731021382 C24 -0.939440554 2.773499401 7.132017655 C25 -0.716799929 4.006227084 8.017270344 C26 -1.107970103 3.195710949 5.665699208 C27 0.140825204 0.140629105 10.730940366 C28 1.581082962 -0.309744642 10.878131306 C29 5.456153329 -11.687270791 4.103684406 C30 6.081123232 -10.451484317 3.461293593 C31 6.445704745 -8.012753168 3.805739497 C32 7.690124792 -7.675407554 4.647482241 C33 5.346469367 -6.954546423 3.994445912 C34 5.801468050 -5.554845224 3.584418668 C35 4.645619104 -4.559688882 3.577818253 C36 4.766040633 -2.050553872 3.497155747 C37 9.999294864 -6.865129543 4.586318688 C38 10.314566068 -5.387838355 4.540349991 C39 -5.443820213 -2.563000147 -1.428661707 C40 -5.839975564 -1.143373009 -0.974950139 C41 -3.908179568 -2.700482855 -1.414917976 C42 -3.378313934 -4.148165409 -1.475501158 C43 -3.179744814 -4.734918852 -2.872546666 C44 -6.123709776 1.143373050 -1.919400316 C45 -7.229310194 1.688518394 -1.010208294 C46 -6.225447151 1.702571161 -3.345864870 C47 -9.420623532 1.288486758 0.005289177 C48 -9.037330845 1.344656877 1.489117507 C49 -7.379086609 0.827943370 3.213812041 C50 -6.168591522 1.738170576 3.434936194 C51 -4.500588539 3.264656147 2.489089354

C52	-4.877460147	4.612741105	3.123818690
C53	-3.862622528	3.583249529	1.126669331
C54	-3.356532310	2.392186207	0.385805797
C55	-3.090079006	1.087053791	0.746170770
C56	-2.602321655	1.214693495	-1.342567442
C57	-6.534834986	6.422789050	3.082926379
C58	-6.395460499	6.642366405	4.587332183
C59	-8.019781949	6.532266891	2.659077573
C60	-8.605647971	7.908668333	2.540866478
C61	-8.463624365	9.029185595	3.337606998
C62	-9.856303881	9.444246347	1.664270448
C63	9.193925083	1.240126467	3.433240950
C64	10.152457643	0.071296012	3.300267684
C65	7.763746045	0.677743627	3.239594867
C66	6.692747633	1.726347164	3.427707201
C67	6.128469139	1.975349568	4.692312333
C68	6.229424039	2.487793267	2.338890184
C69	5.127307173	2.935955849	4.866116586
C70	5.243446269	3.460153565	2.500210079
C71	4.685127607	3.676094447	3.762602841
C72	5.580350918	6.566631365	-1.547747121
C73	4.588771307	7.728226497	-1.751048273
C74	4.811445584	5.310171733	-1.163743549
C75	3.596156118	9.306126746	-3.373652328
C76	2.111604925	8.963538997	-3.529335262
C77	0.427357054	7.129860609	-3.448951986
C78	-0.076106787	6.851253350	-2.009348480
C79	0.423678646	5.870570472	-4.342980541
C80	-0.855228947	5.032905312	-4.450321056
C81	-1.986951199	5.603455709	-5.318674334
C82	-3.447583198	7.579130250	-4.872088816
C83	0.358637008	5.904010722	0.204256594
C84	0.285521649	7.152742063	1.091728579
C85	1.291011940	4.891701738	0.898630190
C86	1.504593920	9.164280167	1.770612761
C87	0.944381223	10.533264693	1.423006768
C88	-0.357363759	11.859246552	-0.144208469
C89	-1.574597701	12.488047507	0.573688844
C90	-0.557224492	11.875112601	-1.664032012
C91	-1.776044112	11.091883485	-2.137009971
C92	-3.574976169	12.116010393	1.919570950
C93	-3.419220531	13.259371839	2.910296045
C94	-4.304065802	10.924936721	2.599302953
C95	-4.611215090	9.824828591	1.611732404
C96	-5.789563425	9.859996013	0.850798794
C97	-3.697793961	8.784882576	1.371656934
C98	-6.039398173	8.906207654	-0.137494512
C99	-3.918145056	7.837243350	0.368870620
C100	-5.088519354	7.914854913	-0.382122294
C101	3.777341894	-4.314269360	-9.010577935
C102	2.379501479	-3.995142376	-8.506484358
C103	1.033780531	-2.385790540	-7.169890864
C104	0.564398117	-1.042139081	-7.743061701
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C113	-1.179712054	-6.173224755	-6.750116200
C114	-4.246312198	-0.153372451	-8.187177817
C115	-3.673989831	1.087181434	-8.842916982
C116	-4.684536794	0.037393533	-6.714508642
C117	-3.471314156	0.055895531	-5.833399013
C118	-2.740824280	1.242130403	-5.651759455
C119	-2.945303528	-1.154524106	-5.354900429
C120	-1.463042286	1.194038072	-5.090385630
C121	-1.669220858	-1.197452858	-4.791629073
C122	-0.910825751	-0.027408877	-4.701525411
C123	7.578375882	-6.690089834	-4.668889703
C124	8.762278569	-6.821241641	-3.697709041
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C126	5.001139433	-6.681366997	-4.717169837
C127	4.580396643	-7.293303816	-5.880075052
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C129	9.931300505	-8.083277973	-1.989799344
C130	11.284128052	-7.911119889	-2.643867167
C131	0.342367401	-6.861141624	0.001805431

C132	1.834751043	-7.053169080	0.310895841
C133	2.735770097	-7.209164531	-0.949178936
C134	2.604850824	-8.657957364	-1.489483231
C135	3.633534614	-9.089934642	-2.536735110
C136	3.567355270	-10.592389415	-2.899630532
C137	4.201578702	-6.956847702	-0.583715580
C138	3.530402381	-0.934354103	-2.275090257
Fe139	3.741652100	-2.215497104	-3.792063659
Fe140	1.864213921	0.453826507	-1.304963429
Fe141	4.813130941	0.355025588	-1.434335861
Fe142	3.629583305	0.351755732	-3.747468457
Fe143	3.670972215	2.571758426	-2.242011387
Fe144	4.772584905	-2.179635894	-1.486647359
Fe145	2.215589679	-2.154535285	-1.533347246
H146	-6.628819219	-7.234972281	0.638794914
H147	-6.821946453	-6.300714140	-0.684581005
H148	-9.828481076	-4.278122694	1.556628853
H149	-9.085787417	-5.784311182	-0.099831406
H150	-8.946782907	-6.870503660	1.278020384
H151	-7.873996154	-2.354389358	2.178882317
H152	-8.881335791	-5.073234545	4.209308281
H153	-9.524864224	-2.403042634	2.836547625
H154	-8.131826074	-5.710797748	6.314230839
H155	-6.254971160	-5.416799674	3.904520443
H156	-7.887307268	-3.997952688	6.730705506
H157	-2.903831969	-1.568510363	3.209676651
H158	-5.121350656	-3.353892230	3.228332841
H159	-4.012095511	-5.893994802	3.561066103
H160	-4.487781286	0.403044290	7.170890620
H161	-5.599896663	-1.791726352	5.641675057
H162	-3.710894124	-5.932013159	5.315841785
H163	-4.616447816	-1.128933565	3.066534229
H164	-4.400527974	-3.176955284	7.769462189
H165	-5.735129921	-0.754250031	7.716184591
H166	-0.612667887	-3.178138400	3.416257531
H167	-0.708271039	-2.087014378	2.016000245
H168	0.879897112	-2.598202355	2.637722972
H169	-1.140361378	-0.800936581	4.121744159
H170	-3.488724436	-4.238730747	9.629063227
H171	-1.321135110	2.342876832	5.006504289
H172	-1.005162549	0.109892023	8.928184610
H173	-0.649502154	3.750305830	9.084271262
H174	-0.017560060	0.341711337	2.223734089
H175	1.579881529	-0.085904913	2.877475270
H176	9.273720612	1.615892589	4.471110404
H177	-1.936943228	3.911478011	5.562450370
H178	-1.550341522	4.712068853	7.885540502
H179	-0.188902499	3.686000712	5.303787675
H180	0.213867998	4.523017327	7.732857287
H181	-1.865895539	2.270357312	7.464031399
H182	1.140139471	2.230338437	6.863114467
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H192	-1.020858976	-2.542221124	5.933784400
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H195	-2.140908969	-4.161411387	7.003220669
H196	-2.844898994	-2.683613697	10.214557339
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	H212	-2.385889386	-1.204564512	-8.383256939
	H213	-5.173822134	-0.344495079	-8.767583594
	H214	-1.228454676	-2.636374794	-9.519000059
	H215	-1.499087430	-5.806792196	-2.242820479
	H216	-1.825418579	-3.624440968	-7.238713599
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	H218	-6.913218430	-3.262014604	-2.705220136
	H219	-3.532863701	-2.229230537	-0.496535321
	H220	0.498698433	-5.464855311	-7.489986789
	H221	-2.422302388	-4.202262405	-0.933759625
	H222	-3.769203086	2.794563122	3.161149777
	H223	-3.223427642	0.630869785	1.723401073
	H224	-8.192125923	1.221633196	3.839638535
	H225	-7.302922747	0.239980412	1.157563741
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	H233	-4.604792538	4.113148806	0.506001354
	H234	-9.381696751	10.946533711	3.097326812
	H235	-8.112899363	6.071968878	1.662210153
	H236	-6.072960281	2.252892629	1.425297723
	H237	-7.125620461	-0.166268432	3.611594736
	H238	-9.826459253	2.279938205	-0.240005471
	H239	-2.260151856	0.995188884	-2.351338407
	H240	-10.233178581	0.559314261	-0.114790918
	H241	10.342190072	2.759627780	2.678703862
	H242	8.749862710	2.919799508	2.351481649
	H243	1.652106877	5.776234564	-1.523330242
	H244	-0.653428101	5.474871312	0.185525996
	H245	1.956354529	7.883387381	0.152756947
	H246	-3.170036328	3.288619595	-1.547671071
	H247	-4.928704342	4.215445827	-2.753303643
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	H250	-5.376070342	1.310352440	-3.930158429
	H251	-7.166482009	1.364008978	-3.809340566
	H252	0.364367573	11.538171009	-2.158716473
	H253	-0.723207290	12.926215565	-1.948784304
	H254	-0.604366209	10.058221949	-3.493428689
	H255	-2.319173145	9.646122055	-3.435342428
	H256	-3.380362498	9.150091756	-6.193541609
	H257	-2.531763097	4.782449416	-5.809672446
	H258	-6.967246290	8.937920116	-0.714805690
	H259	-2.792287110	8.690063583	1.976779827
	H260	-4.425551665	7.819938754	-3.079590730
	H261	1.216971398	5.200561632	-3.976572427
	H262	2.547446498	6.980912822	-3.288351057
	H263	-1.244980667	4.764505218	-3.456287753
	H264	-8.363329077	0.031815363	-1.379439755
	H265	3.937622512	9.752632951	-4.317344362
	H266	-6.032280703	-0.800748624	-2.923026636
	H267	0.733839202	6.186796261	-5.353113340
	H268	-3.171509106	7.070659928	0.159938077
	H269	3.651727502	10.081317710	-2.596042555
	H270	-2.674596889	7.679907033	-6.782131540
	H271	-4.850395024	8.954267108	-4.312615767
	H272	-5.352439948	-3.467133627	-3.274831879
	H273	-5.851657504	-3.237527596	-0.651577662
	H274	-6.529085717	10.644290474	1.031344275
	H275	-5.186160644	1.497257777	-1.466592163
	H276	-0.236585745	7.901086753	-3.852089173
	H277	-1.556197157	6.224190259	-6.115646999
	H278	-0.548672370	4.086713977	-4.916586458
	H279	-3.386790251	5.889978838	-3.736243430
	H280	1.100364775	8.879386129	2.753341893
	H281	-0.068397916	9.717922995	-0.160353677
	H282	0.459441320	12.563808106	0.078321640
	H283	2.593465767	9.274717463	1.865947079
	H284	-2.089203908	10.689015980	1.360686519
	H285	4.310900661	-3.381480854	-9.245439531
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	H289	3.077590996	-5.942702858	-10.007064494
	H290	5.529871774	4.491126526	-1.026850939
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	O452 1.273882564 11.537807330 2.065575810 O453 -1.849596655 13.686095401 0.410149772 O454 -2.883665953 11.216522251 -1.594482532 O455 -4.341931060 13.997184570 3.221978640 O456 -5.272051955 6.990890577 -1.424511261 O457 1.432733325 -4.797798172 -8.693614658 O458 -0.388344340 -0.963859525 -8.546938997 O459 2.064046307 3.355475447 -8.606809185 O460 5.761681617 3.996903633 -9.268555531 O461 -5.187193206 -2.671952658 -8.842338625 O462 -1.756870377 -6.732223804 -5.824799220 O463 0.144836807 -5.923838383 -6.666998398 O464 -3.971924333 2.231237432 -8.531210219 O465 9.649197847 -5.948192913 -3.633617070 O466 12.298049190 -7.596577450 -2.036129649 O467 0.082209920 -6.214395625 -1.118911064 O468 -0.525735136 -7.243027575 0.795078811 O469 4.682219663 -11.204821616 -3.054043854 O470 2.422109027 -11.104633166 -3.050260241 O471 4.831122809 -6.027739061 -1.257907183 O472 4.743183663 -7.645173868 0.301934205 O473 2.329395198 -6.228105182 -1.922944335 O474 8.700993037 -6.891589304 1.125562836 O475 6.890350669 -4.826382609 0.343264927 O476 -4.202719734 4.834324505 -2.484064334 O477 7.276977230 -10.828716225 -2.240806719 O478 7.145935474 -8.947339883 0.114905672 S479 3.591007569 4.845739901 -2.472204492 S480 1.846598267 1.714542328 -3.355789910 S481 1.880189716 -3.445348043 -3.419527275 S482 3.573142414 1.700570095 -0.179804216 S483 0.381355902 -1.115121053 -2.022686065 S484 3.913997219 -0.923009973 -5.573992467 S485 3.220363483 -3.617500392 -0.150527177 S486 5.486008556 1.562015506 -3.180434788 S487 5.568725043 -3.356674949 -3.122223395 S488 6.246420605 -1.009772386 -0.415963673 end
N2x-Fe2-brNH2-Fe6-3b3 to 3b2 **S=1, 35** **reactant** Fe(139) -2.346 Fe(140) 0.050 Fe(141) -2.581 Fe(142) 2.636 Fe(143) 3.099 Fe(144) 1.286 Fe(145) -0.395	bm5expro2b2n2x3b32tc.car_3 C1 -7.902910492 -5.023782478 1.556926523 C2 -8.343170558 -6.170751283 0.640726146 C3 -8.610797908 -2.983848918 2.731432806 C4 -8.021798510 -3.226499158 4.118241176 C5 -7.705284141 -4.771400821 5.984990027 C6 -6.182415493 -4.937938877 5.928771683 C7 -4.221221618 -5.385583603 4.539966513 C8 -3.611994536 -3.981863576 4.486017562 C9 -3.887283415 -1.675027631 3.704073625 C10 -3.792887956 -1.012520672 5.087157332 C11 -4.769434603 -0.683780256 7.279137753 C12 -3.742170920 -1.300101863 8.240915779 C13 -2.979944305 -3.344743033 9.358458809 C14 -1.551539639 -3.750921291 8.972296929 C15 -0.085397039 -4.583006900 7.180168882 C16 0.711529595 -3.501591211 6.444777896 C17 0.639080953 -1.420513361 5.159742936 C18 1.000880151 -0.181643608 5.991260341 C19 -0.102372028 -1.086706603 3.845710211 C20 0.540781648 0.110922889 3.136788425 C21 -0.132338143 -2.315566083 2.929261496 C22 0.209066843 1.750122524 7.289787019 C23 0.565383047 1.418642469 8.750443632 C24 -0.962401663 2.751751227 7.148045864 C25 -0.738648556 3.985996697 8.031533568 C26 -1.134929555 3.169766935 5.680952148 C27 0.106922769 0.138977727 10.756876755 C28 1.546327131 -0.317246727 10.897434504 C29 5.452840909 -11.691852058 4.084452539 C30 6.086790641 -10.457586350 3.448137197 C31 6.455549073 -8.019381722 3.800011553 C32 7.701166165 -7.682037358 4.640411004 C33 5.355389919 -6.962652246 3.994188903 C34 5.806007216 -5.562009273 3.583179952 C35 4.648894970 -4.568018415 3.580820164 C36 4.759620133 -2.060490672 3.468120095 C37 10.005259664 -6.858502920 4.579995323 C38 10.321507288 -5.381043254 4.535358491 C39 -5.438489476 -2.567862823 -1.439740262 C40 -5.840131687 -1.148962351 -0.989467344 C41 -3.902366930 -2.698987460 -1.415429362

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C133	2.732550734	-7.203340643	-0.938550032
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C138	3.534501440	-0.930175140	-2.281769594
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Fe143	3.663712995	2.583206956	-2.246989895
Fe144	4.802997728	-2.146208115	-1.505785617
Fe145	2.237894263	-2.147408822	-1.511864825
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	H207	-3.366272057	-4.424378677	-7.069760529
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	H225	-7.297536337	0.237612281	1.149487024
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	H239	-2.280317797	0.983752985	-2.355392862
	H240	-10.234094258	0.578571228	-0.121812796
	H241	10.355943629	2.764476065	2.665427011
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	H247	-4.935131134	4.208695581	-2.763601804
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	H254	-0.610362353	10.061004494	-3.494802766
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	O426	-2.562650239	-3.696620707	5.090941877
	O427	-2.851226661	-0.257044289	5.376938288
	O428	-2.981700306	-0.583343438	8.913553888
	O429	-0.650060874	-3.741395485	9.822390922
	O430	1.941716874	-3.621430872	6.316749470
	O431	2.194869301	0.144085439	6.135243500
	O432	1.535840100	1.951866653	9.315746797
	O433	2.158386092	-0.296753759	11.954880574
	O434	6.641402342	-10.546180130	2.333503303
	O435	7.698435106	-7.831900211	5.875462117
	O436	11.454897336	-4.933226338	4.611502438
	O437	-5.921558688	-0.811661031	0.206300547
	O438	-3.910751805	-4.472004463	-3.815824245
	O439	-7.067642166	2.755912387	-0.409742250
	O440	-6.196675111	3.135632485	-3.327495724
	O441	-9.782837681	1.927426492	2.280420373

	O442	-5.710171874	1.870302107	4.577163595
	O443	-4.078131871	5.261599310	3.821320137
	O444	-6.117238614	7.737045243	5.104847865
	O445	10.616142234	-0.543870246	4.240737418
	O446	3.693445653	4.627027813	3.847902804
	O447	3.951159989	8.223261593	-0.805308888
	O448	1.285950379	9.890360196	-3.732681007
	O449	-1.212723950	7.221651489	-1.666040859
	O450	-0.522103654	7.205403992	2.027934729
	O451	2.515879380	5.518658606	1.316971646
	O452	1.306261438	11.533806371	2.059441110
	O453	-1.843348740	13.690062498	0.406633737
	O454	-2.875376583	11.218168625	-1.577562728
	O455	-4.340037560	13.996564937	3.229682065
	O456	-5.261480018	6.983733524	-1.422677692
	O457	1.433161827	-4.809279926	-8.681463718
	O458	-0.383415990	-0.972348921	-8.572673591
	O459	2.052303425	3.355690393	-8.615849816
	O460	5.697022696	4.037139793	-9.296291850
	O461	-5.172459368	-2.675887248	-8.865195379
	O462	-1.767537198	-6.729567094	-5.817733360
	O463	0.146790666	-5.942186692	-6.652778620
	O464	-3.943679724	2.224666664	-8.567567121
	O465	9.657695735	-5.947666205	-3.644395462
	O466	12.306469990	-7.595851436	-2.039018204
	O467	0.071244151	-6.173762997	-1.090857823
	O468	-0.524001938	-7.200228725	0.831239244
	O469	4.685203517	-11.180621395	-3.067991273
	O470	2.424215527	-11.086740623	-3.058283180
	O471	4.823325442	-6.004797032	-1.238669523
	O472	4.751888338	-7.635406458	0.303153311
	O473	2.327620687	-6.225540081	-1.922693439
	O474	8.700574671	-6.891883832	1.117909376
	O475	6.875881969	-4.817788688	0.366728272
	O476	-4.207387053	4.826535367	-2.496123067
	O477	7.285369083	-10.822930815	-2.253889487
	O478	7.144012906	-8.946053157	0.107629262
	S479	3.585622094	4.854911254	-2.486067530
	S480	1.840906731	1.721785185	-3.344766803
	S481	1.880617698	-3.430546051	-3.401919353
	S482	3.560062882	1.707625490	-0.192845009
	S483	0.400136027	-1.128074715	-2.032610198
	S484	3.888080084	-0.917901379	-5.577927129
	S485	3.271997561	-3.582032311	-0.126773458
	S486	5.446085386	1.569906301	-3.210092533
	S487	5.577498902	-3.338095389	-3.128457538
	S488	6.257241450	-0.970544878	-0.429797219
	end			
N2x-Fe2-brNH2-Fe6-3b3 to 3b2 **S=1, 35** **TS** Fe(139) -2.301 Fe(140) -0.015 Fe(141) -2.622 Fe(142) 2.622 Fe(143) 3.047 Fe(144) 1.659 Fe(145) -0.659	bm5expro2b2n2x3b32td.car_1			
	C1	-7.911196097	-5.026721429	1.549180599
	C2	-8.363452449	-6.175373231	0.640980468
	C3	-8.603837762	-2.981493340	2.724290335
	C4	-8.013226748	-3.224064436	4.110454352
	C5	-7.693240033	-4.768606712	5.976829560
	C6	-6.170481100	-4.934238522	5.915064680
	C7	-4.214651948	-5.382049752	4.519869698
	C8	-3.608239001	-3.976990131	4.472217856
	C9	-3.887479879	-1.668091584	3.693105028
	C10	-3.788927837	-1.001689350	5.073738053
	C11	-4.748826643	-0.669019402	7.270517857
	C12	-3.719910543	-1.287951224	8.228903629
	C13	-2.957102950	-3.335225416	9.341718706
	C14	-1.532090298	-3.747807661	8.949823709
	C15	-0.076263313	-4.599035885	7.160445661
	C16	0.717836172	-3.508983728	6.435344282
	C17	0.636005769	-1.421244402	5.163391676
	C18	1.001054107	-0.183383761	5.994513450
	C19	-0.108768855	-1.085587591	3.850718330
	C20	0.533554381	0.112800208	3.142647450
	C21	-0.140098412	-2.312369048	2.931724503
	C22	0.221100021	1.762044635	7.277773803
	C23	0.582138242	1.431622223	8.737666958
	C24	-0.947879557	2.766768620	7.137079802
	C25	-0.723791445	3.999668999	8.021906759
	C26	-1.117401871	3.187579414	5.670453138
	C27	0.129625302	0.140637018	10.740125150
	C28	1.570091917	-0.311555111	10.883402186
	C29	5.453068166	-11.689303274	4.097327383
	C30	6.081351331	-10.454212264	3.456890090
	C31	6.447341838	-8.015051040	3.803665980

	C32	7.692406829	-7.677317016	4.644604200
	C33	5.347612364	-6.957527684	3.994672432
	C34	5.801935736	-5.557926664	3.584339805
	C35	4.647063783	-4.561853110	3.579651086
	C36	4.765092735	-2.052859422	3.489562564
	C37	9.999846487	-6.862861085	4.583829716
	C38	10.316022537	-5.385277640	4.538853615
	C39	-5.443607674	-2.564780157	-1.431809337
	C40	-5.840391420	-1.145089112	-0.979032809
	C41	-3.907455090	-2.700445866	-1.415795815
	C42	-3.374416690	-4.147074779	-1.471624417
	C43	-3.172292027	-4.738072212	-2.866317158
	C44	-6.124322592	1.140735732	-1.924503789
	C45	-7.228563018	1.687132216	-1.013462105
	C46	-6.227453024	1.699788930	-3.350644556
	C47	-9.419612143	1.290780416	0.004932175
	C48	-9.036863556	1.343774060	1.488813931
	C49	-7.378234504	0.824985199	3.212669619
	C50	-6.170844315	1.738900549	3.435434997
	C51	-4.501138060	3.263833768	2.489299869
	C52	-4.875613001	4.612288008	3.123671464
	C53	-3.864062663	3.582025596	1.126177043
	C54	-3.359289696	2.390347498	0.385617383
	C55	-3.093183307	1.085260362	0.746429705
	C56	-2.608636488	1.211336836	-1.343057304
	C57	-6.531545926	6.423299311	3.085079687
	C58	-6.387611209	6.646002391	4.588900974
	C59	-8.017036007	6.533665908	2.664725220
	C60	-8.601610516	7.910580889	2.545558502
	C61	-8.458654551	9.031396810	3.341814843
	C62	-9.850595272	9.447079481	1.668057781
	C63	9.194697112	1.242353010	3.427753630
	C64	10.154263553	0.074170304	3.297312730
	C65	7.764752754	0.678703032	3.233096098
	C66	6.692607368	1.726027497	3.422311641
	C67	6.122704034	1.968025854	4.685615515
	C68	6.234222510	2.493528263	2.335566714
	C69	5.122427321	2.929405447	4.860801557
	C70	5.249186364	3.466543069	2.498465488
	C71	4.686717506	3.676956332	3.759940038
	C72	5.577833906	6.567328795	-1.551518813
	C73	4.588556525	7.731667517	-1.751367236
	C74	4.807778049	5.309881953	-1.166584474
	C75	3.591798780	9.308228679	-3.373398616
	C76	2.107422082	8.965224043	-3.531423806
	C77	0.424364313	7.129246328	-3.449794195
	C78	-0.078797727	6.850290462	-2.010191041
	C79	0.421264235	5.870822333	-4.343921487
	C80	-0.858165767	5.033640943	-4.452123097
	C81	-1.988594145	5.604036650	-5.322074556
	C82	-3.449876918	7.578090717	-4.873691288
	C83	0.358849538	5.901419585	0.202392620
	C84	0.283500451	7.149297679	1.090911069
	C85	1.294307166	4.890241895	0.895171926
	C86	1.501478316	9.160824429	1.772552857
	C87	0.948278019	10.532233747	1.423338038
	C88	-0.355343588	11.859146131	-0.143013239
	C89	-1.572672108	12.488964016	0.574762793
	C90	-0.555324572	11.873080270	-1.662752057
	C91	-1.775700899	11.091260171	-2.134041682
	C92	-3.572139627	12.116130695	1.920736382
	C93	-3.419084296	13.259200423	2.912519458
	C94	-4.302554348	10.924819262	2.598349743
	C95	-4.608842059	9.824966366	1.609734571
	C96	-5.786533993	9.860249364	0.847962063
	C97	-3.695718311	8.784582117	1.370971156
	C98	-6.036282569	8.905770078	-0.139418629
	C99	-3.916067939	7.836100097	0.369179904
	C100	-5.085918180	7.913635958	-0.382512702
	C101	3.774571027	-4.316281885	-9.013355546
	C102	2.377755244	-3.997778992	-8.507238648
	C103	1.032210095	-2.385829076	-7.173383420
	C104	0.561841906	-1.042877112	-7.746872832
	C105	1.013288500	1.376652637	-7.771249518
	C106	2.217675466	2.288412416	-7.994060643
	C107	4.531834642	2.867800610	-7.529943392
	C108	5.053712805	3.061309925	-8.938886547
	C109	-2.982070073	-3.655760836	-9.077606134
	C110	-3.954755837	-2.505652627	-8.792773341
	C111	-2.524841499	-4.303353089	-7.749955085

	C112	-1.879588103	-5.680729387	-7.994888155
	C113	-1.181832548	-6.176352971	-6.748351761
	C114	-4.242711207	-0.155168183	-8.196103537
	C115	-3.664491361	1.084297994	-8.849105886
	C116	-4.681146154	0.036954594	-6.722893271
	C117	-3.468986351	0.056322688	-5.839866725
	C118	-2.739829107	1.242981833	-5.655284433
	C119	-2.945362833	-1.152907871	-5.356012709
	C120	-1.466720144	1.196732766	-5.082338993
	C121	-1.674461012	-1.194211689	-4.780327372
	C122	-0.917675247	-0.023203680	-4.683331268
	C123	7.579823041	-6.692964762	-4.673047736
	C124	8.763883165	-6.822460716	-3.701027100
	C125	6.253760191	-6.959958617	-3.946154149
	C126	5.002618233	-6.678792252	-4.714940477
	C127	4.579900470	-7.289272004	-5.877566467
	C128	2.955700453	-6.000737535	-5.103857925
	C129	9.931814952	-8.082503548	-1.990893546
	C130	11.285142739	-7.911856462	-2.644532301
	C131	0.343427602	-6.843042124	0.000306557
	C132	1.839354317	-7.033279164	0.309456572
	C133	2.741306004	-7.201743352	-0.947432194
	C134	2.602667414	-8.649908210	-1.488763762
	C135	3.632796726	-9.082933738	-2.534304053
	C136	3.565430731	-10.583741210	-2.899816759
	C137	4.212055398	-6.956832353	-0.583666004
	C138	3.530228182	-0.934301606	-2.278809829
	Fe139	3.739256348	-2.216187488	-3.789880728
	Fe140	1.858030180	0.439265501	-1.323324000
	Fe141	4.819665391	0.351934007	-1.447984212
	Fe142	3.611541184	0.343984309	-3.753449705
	Fe143	3.672525251	2.569162129	-2.234175330
	Fe144	4.811885332	-2.180900546	-1.478019028
	Fe145	2.251564298	-2.162922939	-1.499764862
	H146	-6.621912208	-7.236285252	0.645505298
	H147	-6.805504084	-6.296819843	-0.676239233
	H148	-9.828400419	-4.280328564	1.555122488
	H149	-9.074058010	-5.781915818	-0.103309655
	H150	-8.941973385	-6.870610374	1.273726954
	H151	-7.880942777	-2.352325409	2.183645895
	H152	-8.887292872	-5.074436996	4.211939639
	H153	-9.532531891	-2.407135988	2.840508116
	H154	-8.139400694	-5.712400365	6.317200638
	H155	-6.258126598	-5.416230119	3.909913462
	H156	-7.895353951	-3.999857439	6.734059668
	H157	-2.904426105	-1.571120275	3.216510396
	H158	-5.121420956	-3.357682664	3.228597407
	H159	-4.015891566	-5.898439604	3.571177418
	H160	-4.503562448	0.396542872	7.178279948
	H161	-5.607143028	-1.794889183	5.640664921
	H162	-3.716676418	-5.932410415	5.326370415
	H163	-4.617034105	-1.131368790	3.071134880
	H164	-4.412393499	-3.184275902	7.776592659
	H165	-5.747848485	-0.766814677	7.717726820
	H166	-0.610381441	-3.180078709	3.415261451
	H167	-0.705311036	-2.091847105	2.012719185
	H168	0.882251670	-2.602055617	2.636008222
	H169	-1.137971657	-0.801492372	4.116133333
	H170	-3.500183211	-4.244882828	9.636000830
	H171	-1.329476933	2.333369834	5.012703811
	H172	-1.020843279	0.109681480	8.940021030
	H173	-0.658671182	3.744270323	9.089229653
	H174	-0.013411503	0.337454571	2.216942054
	H175	1.583572076	-0.086517363	2.874792107
	H176	9.273038086	1.619250117	4.465249060
	H177	-1.947519222	3.901978615	5.566645327
	H178	-1.555464323	4.707417216	7.888876016
	H179	-0.199245812	3.678527262	5.307145695
	H180	0.208510489	4.514180210	7.738578987
	H181	-1.874272382	2.264025422	7.469922305
	H182	1.132787275	2.225356705	6.871890794
	H183	-0.987937107	0.276790629	6.283233810
	H184	0.514500948	1.021173068	3.761858780
	H185	1.512092919	4.068426666	0.196783994
	H186	0.741594053	4.481459905	1.753523206
	H187	2.748514455	5.155538385	2.200714360
	H188	3.348703499	4.654765024	4.769350847
	H189	4.882699164	4.035605258	1.643697095
	H190	6.627798512	2.302525664	1.334360072
	H191	6.454356326	1.383934940	5.548759637

H192	-1.023164007	-2.534969106	5.935690421
H193	-0.210015957	-5.434414384	6.456526104
H194	0.544511896	-4.950287391	7.993704353
H195	-2.145716244	-4.148879902	7.008952703
H196	-2.860318296	-2.688688157	10.222645097
H197	4.673985996	3.086568478	5.845798370
H198	1.613143301	-1.835749612	4.882557451
H199	-0.063385919	0.955136942	11.456720714
H200	-0.506910039	-0.715883705	11.013139017
H201	2.028705707	-0.724683457	9.954225170
H202	10.843366137	-7.431912570	4.163606521
H203	-1.987142007	-6.037215466	-3.906978645
H204	1.213371599	-6.079418858	-1.664360236
H205	-2.663369400	-6.404406917	-8.260101031
H206	-1.165228977	-5.621546773	-8.829303129
H207	-3.381009395	-4.428237299	-7.068521039
H208	-2.963806699	0.879813630	-9.692605498
H209	-3.601772708	-4.393894809	-9.609690478
H210	-3.493912815	-2.110464515	-2.248405970
H211	-4.060806809	-4.825276621	-0.934203536
H212	-2.383274519	-1.208054878	-8.386553136
H213	-5.169662306	-0.344985459	-8.777911962
H214	-1.228277683	-2.640080349	-9.527137900
H215	-1.483753644	-5.798972342	-2.232870982
H216	-1.819597717	-3.624236630	-7.246143924
H217	-1.414432581	-4.056371350	-10.341242195
H218	-6.909824770	-3.261836902	-2.713151670
H219	-3.533111630	-2.225179623	-0.499206085
H220	0.499480700	-5.471690419	-7.484575585
H221	-2.419397805	-4.198247530	-0.928135575
H222	-3.768821476	2.793391957	3.160153975
H223	-3.226498307	0.629177981	1.723738996
H224	-8.192681097	1.213497293	3.839973350
H225	-7.302818738	0.239359509	1.155390314
H226	-6.711495670	4.477895049	2.213052414
H227	-7.857813913	9.227620344	4.221973041
H228	-6.590889547	5.733697743	5.201035807
H229	-8.622613258	5.910963213	3.347731491
H230	-5.921868537	7.174512783	2.558162084
H231	-10.540198600	9.999481766	1.035068528
H232	-3.044230193	4.295167001	1.317316102
H233	-4.606393198	4.112422863	0.505983946
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N2x-Fe2-brNH2-Fe6-3b3 to 3b2 **S=1, 35** **product** Fe(139) -2.332 Fe(140) 0.055 Fe(141) -2.621 Fe(142) 2.806 Fe(143) 3.151 Fe(144) 2.201 Fe(145) -1.496	bm5expro2b2n2x3b32te.car_3 C1 -7.914169203 -5.030340036 1.559142430 C2 -8.355383285 -6.175850213 0.641618156 C3 -8.612634933 -2.985594976 2.730235027 C4 -8.021847324 -3.227536460 4.116388187 C5 -7.703762343 -4.771500303 5.983821045 C6 -6.180973675 -4.938033665 5.925668503 C7 -4.221712889 -5.385561709 4.534917194 C8 -3.612348365 -3.981884824 4.482223244 C9 -3.888432428 -1.673962475 3.701231043 C10 -3.793213262 -1.010769391 5.084015423 C11 -4.765779473 -0.681272155 7.277141446 C12 -3.738012898 -1.298130124 8.238108189 C13 -2.976331167 -3.343216083 9.355415284 C14 -1.549043562 -3.752341081 8.968473676 C15 -0.086210863 -4.591039254 7.177886903 C16 0.708836956 -3.505466959 6.447444930 C17 0.633332427 -1.421997683 5.169145870 C18 0.996915794 -0.182005124 5.996904714 C19 -0.105313701 -1.088248759 3.852287643 C20 0.539764549 0.107200588 3.141311353 C21 -0.134026027 -2.316398038 2.935300678

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	C68	6.245429780	2.503641563	2.329073619
	C69	5.116250394	2.919723878	4.849831064
	C70	5.260319432	3.476367163	2.492960489
	C71	4.689668795	3.677148889	3.752313380
	C72	5.579238649	6.566820178	-1.559038407
	C73	4.590499766	7.732995220	-1.753420638
	C74	4.811934540	5.307103854	-1.179615794
	C75	3.587412436	9.309996945	-3.372820249
	C76	2.103584598	8.966487348	-3.533407187
	C77	0.422001171	7.130231481	-3.451993531
	C78	-0.078651422	6.848521897	-2.012347036
	C79	0.419483505	5.871538624	-4.346395252
	C80	-0.860442954	5.035090044	-4.455839903
	C81	-1.989406394	5.606257387	-5.327677562
	C82	-3.453464426	7.578372946	-4.877015714
	C83	0.361927890	5.897229457	0.198024435
	C84	0.282683829	7.143060036	1.089400490
	C85	1.301171830	4.888581197	0.888779294
	C86	1.496196361	9.156289854	1.775417206
	C87	0.953647399	10.531319730	1.423848834
	C88	-0.351765304	11.862744230	-0.139570314
	C89	-1.568925983	12.493846358	0.576779800
	C90	-0.551512846	11.873702311	-1.659475195
	C91	-1.773635155	11.092940003	-2.128385759
	C92	-3.568406806	12.122224891	1.924524133
	C93	-3.418610032	13.262858110	2.918917045
	C94	-4.298740869	10.928098955	2.598001042
	C95	-4.602959400	9.829015358	1.607633170
	C96	-5.779897214	9.864221675	0.844727372
	C97	-3.690501568	8.787559183	1.370744727
	C98	-6.029674837	8.908484443	-0.141363986
	C99	-3.911005037	7.837594608	0.370305698
	C100	-5.080441964	7.914726961	-0.382079780
	C101	3.772547436	-4.318443452	-9.007459544

C102	2.374748345	-4.001941891	-8.503359529
C103	1.024527774	-2.388433373	-7.176713085
C104	0.555918245	-1.045902284	-7.751816482
C105	1.005891683	1.373264335	-7.770788946
C106	2.214028754	2.278750103	-7.996546787
C107	4.530162129	2.850971545	-7.537096514
C108	5.032433556	3.066771111	-8.949022516
C109	-2.975136339	-3.662047431	-9.083113292
C110	-3.947447829	-2.510198922	-8.801727117
C111	-2.516372341	-4.304812687	-7.753853919
C112	-1.873614935	-5.684039783	-7.994137687
C113	-1.182421311	-6.178980927	-6.743606121
C114	-4.233405455	-0.157396636	-8.212438549
C115	-3.645996632	1.079858174	-8.861469860
C116	-4.683212444	0.037554544	-6.742924390
C117	-3.477291217	0.057024715	-5.851828859
C118	-2.748750401	1.243465662	-5.662560858
C119	-2.958161653	-1.153055961	-5.364802634
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C121	-1.688731971	-1.196354750	-4.786705192
C122	-0.930213368	-0.026690723	-4.692485824
C123	7.584323803	-6.697846671	-4.687767459
C124	8.768551513	-6.824523756	-3.714016252
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C129	9.932096107	-8.076530270	-1.995292319
C130	11.287493291	-7.910003672	-2.645591046
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C132	1.867918315	-6.995548943	0.297115643
C133	2.767342296	-7.186620395	-0.963986412
C134	2.616480547	-8.643339134	-1.486597221
C135	3.644357793	-9.086439510	-2.530966202
C136	3.570232307	-10.585120672	-2.904058151
C137	4.237225938	-6.967566332	-0.569763980
C138	3.523949260	-0.933858112	-2.274378436
Fe139	3.699686529	-2.231639679	-3.759148179
Fe140	1.883766330	0.464440407	-1.333792940
Fe141	4.826271947	0.319561280	-1.438028156
Fe142	3.618411268	0.357619414	-3.755284642
Fe143	3.692290394	2.560319802	-2.259919564
Fe144	4.724130754	-2.252864470	-1.399144499
Fe145	2.159488458	-2.113789250	-1.623638682
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H147	-6.781802371	-6.285153588	-0.656810641
H148	-9.831514773	-4.282765132	1.553273883
H149	-9.058487804	-5.780172112	-0.108413120
H150	-8.939119372	-6.875499722	1.264601784
H151	-7.890024021	-2.355750189	2.190015952
H152	-8.894591125	-5.078308802	4.217209347
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H158	-5.125613260	-3.361354674	3.238547005
H159	-4.021023622	-5.906889168	3.589330315
H160	-4.526234101	0.386011703	7.189901387
H161	-5.616653227	-1.799796411	5.639498332
H162	-3.726390967	-5.932541130	5.345263618
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H164	-4.430305446	-3.195576301	7.789095716
H165	-5.766159216	-0.786171556	7.719693635
H166	-0.604838713	-3.184138702	3.418453383
H167	-0.696286826	-2.096442067	2.014364852
H168	0.889581444	-2.605353294	2.642714375
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H170	-3.517316378	-4.255059685	9.646789855
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H173	-0.673153291	3.735586069	9.097508515
H174	-0.005398187	0.327109391	2.213144311
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H177	-1.962961489	3.886779901	5.574325602
H178	-1.567197204	4.699185415	7.895414312
H179	-0.214818728	3.665053298	5.313728477
H180	0.196858650	4.502645843	7.746977105
H181	-1.886233971	2.252546091	7.480755910

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H185	1.522422779	4.069555649	0.188452808
H186	0.750122800	4.475255789	1.746031360
H187	2.754356574	5.156570217	2.194306591
H188	3.346516158	4.647703975	4.761128098
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H194	0.533483014	-4.937749455	8.013811351
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H210	-3.500424004	-2.110421206	-2.248814403
H211	-4.051159273	-4.826323398	-0.927504639
H212	-2.375294139	-1.213403119	-8.395785883
H213	-5.155983861	-0.344698364	-8.801784391
H214	-1.223058080	-2.646955485	-9.539035945
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H227	-7.848174559	9.233525586	4.229010286
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H233	-4.607521255	4.115227898	0.506262889
H234	-9.358101944	10.959272435	3.104252124
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H238	-9.809553825	2.292175319	-0.237855082
H239	-2.278557138	0.983723013	-2.349170101
H240	-10.235167638	0.574917086	-0.120875673
H241	10.351775379	2.762637658	2.668691507
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H254	-0.610358867	10.061205244	-3.493445797
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H256	-3.382981099	9.154578256	-6.192203770
H257	-2.530126826	4.785966933	-5.824103582
H258	-6.956261163	8.940415843	-0.720204864
H259	-2.786314766	8.692382354	1.977577439
H260	-4.430549805	7.814696993	-3.083307711
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H263	-1.253751824	4.769478520	-3.462367322
H264	-8.367462910	0.031836221	-1.383166511
H265	3.929913977	9.760916489	-4.313938171
H266	-6.030473515	-0.807714417	-2.934953056
H267	0.731373375	6.187922089	-5.356037916
H268	-3.165444473	7.069164659	0.164752077
H269	3.641218683	10.081792461	-2.591753935
H270	-2.681758777	7.684709258	-6.787059083
H271	-4.857394383	8.951120526	-4.314496509
H272	-5.346741073	-3.477971568	-3.279724282
H273	-5.861376716	-3.244178293	-0.662049671
H274	-6.518762744	10.649480140	1.022672371
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H292	5.007317018	7.765547688	-3.766437386
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H294	7.131902595	7.672313570	-0.796130124
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H328	2.671163299	-7.161932242	-6.847538574
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H332	8.164642209	-6.106546369	0.836808747
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	H344	7.022323888	-9.531550832	0.893425261
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	H346	5.073524413	-8.012969315	-6.521653174
	H347	6.243323411	-6.356010880	-3.034210789
	H348	0.244832687	-3.130334916	-7.361426105
	H349	4.277108932	3.824440503	-7.089303144
	H350	7.630179970	-0.136344872	3.945764459
	H351	7.701859460	0.251915549	2.210613844
	H352	8.612949762	-7.335964923	-6.343306088
	H353	7.813905661	-8.543061632	-5.579652230
	H354	9.891620254	-9.093048975	-1.573685353
	H355	8.139196447	-8.688703111	-2.969167491
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	H357	9.832002327	-7.367842747	-1.157560060
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	H359	-2.408398658	13.363033570	3.381009809
	H360	9.907812248	-7.135599479	5.646738817
	H361	9.431649364	-4.709042072	4.452353997
	H362	-4.188879342	12.489786608	1.089280989
	H363	-3.679965315	10.547028609	3.425659669
	H364	-5.228547555	11.319105620	3.036113535
	H365	-6.212240072	6.986314033	-1.664757901
	H366	2.884451294	-0.906837334	0.614205168
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	N376	-5.663093653	-5.362120497	4.745468340
	N377	-4.296312849	-3.069922357	3.752769743
	N378	-4.785178746	-1.297672592	5.959501171
	N379	-3.758578762	-2.653811116	8.339790519
	N380	-1.381767994	-4.184828181	7.689866864
	N381	-0.012958695	-2.465957630	5.948906409
	N382	-0.031231640	0.537115655	6.515007442
	N383	-0.207265744	0.509679107	9.386884925
	N384	5.081349779	-11.501803928	5.498113418
	N385	5.950907634	-9.332200022	4.176265825
	N386	5.103746251	-3.268388911	3.059813469
	N387	4.245874153	-1.867359616	4.738428354
	N388	4.937026330	-0.981743304	2.706461686
	N389	8.753538923	-7.208417714	3.933573192
	N390	-5.986950391	-2.834063037	-2.780166415
	N391	-2.147329641	-5.599565953	-2.996606184
	N392	-6.106305754	-0.315032360	-2.030954629
	N393	-8.348617226	0.934583744	-0.913658230
	N394	-7.876274626	0.724588464	1.851057142
	N395	-5.657957910	2.385680064	2.350967238
	N396	-3.048061206	2.451898607	-0.958421684
	N397	-2.638702974	0.358032720	-0.322716693
	N398	-6.100620968	5.078495308	2.776047729
	N399	-9.472707717	8.189941122	1.515887201
	N400	-9.244557101	10.005799520	2.770878312
	N401	9.517868516	2.238992798	2.391403460
	N402	6.568208043	6.866180846	-0.511128224
	N403	4.467150406	8.208737640	-3.027986342
	N404	1.783815966	7.660416458	-3.452351189
	N405	-2.963933363	6.384038575	-4.555068077
	N406	-3.201477202	8.164907688	-6.061777025
	N407	-4.188317586	8.267538451	-3.969556091
	N408	0.774841206	6.196648691	-1.173996267
	N409	1.200841401	8.113466390	0.811322236
	N410	0.064370005	10.576181894	0.386101850
	N411	-1.570251768	10.301921273	-3.215205758
	N412	-2.267647666	11.696690403	1.424881956
	N413	3.709546732	-5.159709632	-10.204284315
	N414	2.247038669	-2.840122323	-7.830203125
	N415	1.270133131	0.017392384	-7.326541413
	N416	3.413408231	1.921961352	-7.472330141
	N417	-1.913298836	-3.244890297	-10.009506347
	N418	-3.393137213	-1.312776514	-8.462302705
	N419	7.733250926	-7.563856500	-5.871251480
	N420	3.971811345	-5.852652650	-4.262815179
	N421	3.294328686	-6.852108283	-6.106526281

	N422	8.849993650	-7.952404962	-2.956084238
	O423	-6.741326681	-4.891414058	1.952246474
	O424	-7.310440278	-2.361793412	4.654932440
	O425	-5.485025661	-4.715378161	6.930418534
	O426	-2.562285778	-3.698459152	5.086658317
	O427	-2.852113860	-0.254024308	5.372243638
	O428	-2.977363021	-0.581623420	8.910685151
	O429	-0.644645201	-3.737142027	9.815342136
	O430	1.938794347	-3.624005289	6.317525565
	O431	2.191657762	0.141702051	6.140529259
	O432	1.537498503	1.957530960	9.314831044
	O433	2.162561767	-0.296681197	11.952046735
	O434	6.643186582	-10.551169980	2.338611080
	O435	7.694981248	-7.831936091	5.876719476
	O436	11.452564738	-4.935867234	4.609656172
	O437	-5.927314111	-0.812486318	0.209823193
	O438	-3.932033377	-4.463164330	-3.824504183
	O439	-7.070673714	2.755989332	-0.407398210
	O440	-6.198986328	3.135435847	-3.325659926
	O441	-9.785801373	1.926893035	2.280618702
	O442	-5.710208208	1.869782946	4.576791661
	O443	-4.085150270	5.265035290	3.824165844
	O444	-6.129927412	7.735099785	5.110248412
	O445	10.609444724	-0.548225968	4.241515743
	O446	3.689282307	4.625461418	3.848982068
	O447	3.946187657	8.216317010	-0.806456912
	O448	1.285602814	9.888621363	-3.728561342
	O449	-1.209557858	7.222846992	-1.664143807
	O450	-0.522623218	7.206919327	2.027140112
	O451	2.513579951	5.516310381	1.317487499
	O452	1.299183182	11.534239605	2.060336003
	O453	-1.846081186	13.690231851	0.406242695
	O454	-2.878168241	11.218426804	-1.579727102
	O455	-4.343559423	13.997838366	3.230519462
	O456	-5.266205968	6.987222508	-1.421866223
	O457	1.431964582	-4.811720308	-8.680198903
	O458	-0.388115976	-0.971338691	-8.566621720
	O459	2.058473717	3.348576748	-8.610181271
	O460	5.705040694	4.027956589	-9.284786596
	O461	-5.177679249	-2.676859885	-8.861767398
	O462	-1.770462868	-6.726388046	-5.817971727
	O463	0.143839045	-5.943071381	-6.655452518
	O464	-3.951129319	2.225134737	-8.561784674
	O465	9.654369386	-5.950267135	-3.650186556
	O466	12.301086165	-7.595171596	-2.037754996
	O467	0.090164182	-6.180629623	-1.128822074
	O468	-0.497817347	-7.203722446	0.782156040
	O469	4.682818662	-11.199592731	-3.066372906
	O470	2.423386200	-11.093736170	-3.056268230
	O471	4.883620771	-6.041502785	-1.232047025
	O472	4.760859857	-7.669878381	0.316653511
	O473	2.387912569	-6.215559609	-1.938778174
	O474	8.699727554	-6.887691173	1.124340671
	O475	6.900680102	-4.818806541	0.332874670
	O476	-4.212323573	4.830132196	-2.495734961
	O477	7.280686679	-10.824398516	-2.251244924
	O478	7.153950942	-8.942668439	0.107668257
	S479	3.597468037	4.832117073	-2.489329928
	S480	1.836613198	1.739079502	-3.373900417
	S481	1.851081645	-3.495013219	-3.378695032
	S482	3.588923249	1.689692370	-0.198577503
	S483	0.320830337	-1.095192600	-2.022928101
	S484	3.871570368	-0.950275044	-5.562912525
	S485	3.580171356	-3.749049758	-0.012034178
	S486	5.516840269	1.520282704	-3.174918592
	S487	5.565519002	-3.360694920	-3.143345525
	S488	6.221326773	-1.030053825	-0.350147397
	end			
N2x-Fe2-brNH2-Fe6-3b2 to 6Hx **S=1, 35** **reactant** Fe(139) -2.426 Fe(140) -0.018 Fe(141) -2.534 Fe(142) 2.637 Fe(143) 2.576	9651826nh22n2x3b26hx135tc.car_3			
	C1	-9.403305187	0.828014853	1.065317340
	C2	-10.358270638	-0.063363042	0.262862238
	C3	-8.875840320	3.122900889	1.763137090
	C4	-8.595055499	2.922936408	3.249114127
	C5	-9.304129367	1.941529227	5.369714048
	C6	-8.173430732	0.931038330	5.596838632
	C7	-6.789753773	-0.840873637	4.639562280
	C8	-5.473026642	-0.080795248	4.459539068
	C9	-4.297346721	1.720510417	3.302709907
	C10	-3.910340706	2.529190908	4.549378907
	C11	-4.626824234	3.871679006	6.435783429

Fe(144) 1.872
Fe(145) -0.876

C12	-4.216429270	3.059947009	7.672930830
C13	-4.821169905	1.257159715	9.222542077
C14	-3.929466566	0.011145296	9.143748975
C15	-3.172907114	-1.865765551	7.748057373
C16	-1.822231075	-1.614832860	7.069699340
C17	-0.527959300	-0.209550697	5.531759650
C18	0.388887140	0.799436969	6.248369862
C19	-0.801325420	0.139013462	4.049947758
C20	0.490385613	0.542390797	3.327365243
C21	-1.476414301	-1.038976144	3.336000355
C22	0.776985467	3.091357387	7.014001690
C23	0.802467646	3.024765649	8.553116230
C24	0.441041482	4.499550026	6.467237734
C25	1.334081183	5.559916948	7.123717223
C26	0.601207807	4.536433223	4.941843356
C27	-0.406331372	2.892318613	10.649835093
C28	0.467139852	1.772958518	11.183838598
C29	-2.612758558	-11.370401013	6.799064358
C30	-1.332777018	-10.937256073	6.086418709
C31	0.454035138	-9.213513303	6.091254606
C32	1.629488082	-9.524075559	7.034667653
C33	0.281782947	-7.690811907	5.939727840
C34	1.542511606	-7.031103310	5.382479399
C35	1.312702751	-5.585047051	4.967212636
C36	2.995948058	-3.831590591	4.393644479
C37	4.011307776	-10.084932876	7.137617406
C38	5.056223317	-9.013997974	6.919181761
C39	-5.871808843	0.691905005	-1.860730201
C40	-5.377841539	2.145810005	-1.737125456
C41	-4.685597157	-0.264000384	-1.608504462
C42	-5.073429748	-1.727187523	-1.314079216
C43	-5.218285138	-2.636166525	-2.534361838
C44	-4.244744524	3.892115506	-3.091172577
C45	-4.836330912	5.160812291	-2.468831862
C46	-3.954342197	4.064179201	-4.589113993
C47	-6.863049211	6.326907324	-1.748207669
C48	-6.559978168	6.491588321	-0.254181969
C49	-5.600919225	5.520212776	1.777574004
C50	-4.097377746	5.633713372	2.042774563
C51	-1.814958783	5.706051872	1.159237273
C52	-1.359992543	7.135338088	1.491839111
C53	-1.043739313	5.283916393	-0.102207923
C54	-1.310352080	3.883434698	-0.538543736
C55	-1.853730912	2.784417767	0.094802309
C56	-1.376304324	2.123902434	-1.892870774
C57	-1.639997096	9.493789414	0.868649096
C58	-1.433274789	9.938771935	2.313950789
C59	-2.768190870	10.318654588	0.203351528
C60	-2.433187297	11.717773369	-0.221419530
C61	-1.745390354	12.723184711	0.429472059
C62	-2.478329766	13.438704970	-1.535425114
C63	8.224242383	-3.404684479	4.440781436
C64	8.346760667	-4.904722075	4.642132651
C65	6.727703995	-3.106502901	4.190804887
C66	6.428390368	-1.632256800	4.044754971
C67	6.073516511	-0.846218392	5.156463108
C68	6.498019238	-1.001344016	2.788601214
C69	5.789310051	0.517099236	5.023729661
C70	6.231548077	0.360274591	2.643247778
C71	5.871284688	1.117533679	3.760747255
C72	8.403519236	1.734903444	-1.750188310
C73	8.269305984	3.165251420	-2.296901202
C74	7.038461117	1.215615637	-1.298131326
C75	8.459149205	4.615577668	-4.286103655
C76	7.059310922	5.139605151	-4.613186374
C77	4.623701603	4.634893439	-4.499942268
C78	4.024216240	5.012355894	-3.120304013
C79	3.906717049	3.433872090	-5.156327152
C80	2.383248868	3.471122350	-5.317602114
C81	1.827858141	4.362683120	-6.439398651
C82	1.778767858	6.855392084	-6.557593052
C83	3.765598013	4.490772522	-0.742544436
C84	4.370294732	5.752256796	-0.114106149
C85	3.965202093	3.333787341	0.259067436
C86	6.486970309	6.849031441	0.427052991
C87	6.875694976	8.155994427	-0.240878388
C88	6.652293227	9.589509512	-2.190327314
C89	6.019879345	10.943693312	-1.782644716
C90	6.539233736	9.379260069	-3.704986197
C91	5.106697116	9.342143955	-4.222832716

C92	4.128414504	12.077684420	-0.721539392
C93	4.884643117	13.123817990	0.081641405
C94	2.827727267	11.666606140	0.024433109
C95	1.969427755	10.745643290	-0.813210145
C96	1.054003337	11.272166998	-1.736544505
C97	2.103971264	9.348952157	-0.739516358
C98	0.310023353	10.440759644	-2.575827767
C99	1.389271166	8.501678102	-1.591469013
C100	0.501702363	9.058893686	-2.507702224
C101	0.821673316	-7.626235150	-7.436055719
C102	-0.163857599	-6.489080060	-7.221015962
C103	-0.378251096	-4.137044193	-6.439447985
C104	0.060443880	-2.940981625	-7.292598160
C105	1.844565195	-1.293540073	-7.658541080
C106	3.361927675	-1.293286513	-7.813457788
C107	5.557008456	-2.070139061	-7.128814187
C108	6.122726097	-2.467817904	-8.477834499
C109	-4.251179003	-3.330151257	-8.708848884
C110	-4.365270050	-1.803922594	-8.806870748
C111	-4.304225726	-3.781575280	-7.231625933
C112	-4.589313826	-5.292460387	-7.130079805
C113	-4.370828345	-5.792251024	-5.720343391
C114	-3.227821079	0.355176648	-8.681001549
C115	-2.006218760	0.839662672	-9.436348892
C116	-3.505817646	1.105222239	-7.354994074
C117	-2.556178543	0.636000617	-6.290854102
C118	-1.273495869	1.195221985	-6.179766281
C119	-2.879114289	-0.491075815	-5.516604965
C120	-0.306694269	0.582515669	-5.377930711
C121	-1.913088409	-1.098265708	-4.713053827
C122	-0.612944713	-0.584121567	-4.675529586
C123	2.336886086	-10.727162319	-2.234847085
C124	3.200829800	-11.239649760	-1.071687876
C125	1.064438159	-10.045281972	-1.708043122
C126	0.249443074	-9.297055130	-2.712899486
C127	-0.398491149	-9.788988029	-3.826965255
C128	-0.952478022	-7.662596268	-3.541627324
C129	3.385943711	-12.455314965	1.011525146
C130	4.589889241	-13.257892023	0.570369783
C131	-3.671705156	-5.664641936	1.167427741
C132	-2.575526735	-6.542692245	1.768452019
C133	-1.931041172	-7.554309316	0.771956123
C134	-2.879854151	-8.761584231	0.555643940
C135	-2.277776182	-9.910006895	-0.255674271
C136	-3.193368960	-11.146926275	-0.392159779
C137	-0.611607884	-8.064359131	1.371966251
C138	2.391635324	-3.244342146	-1.504290959
Fe139	1.677275126	-4.694602838	-2.671901712
Fe140	1.963232800	-0.975284462	-1.142113340
Fe141	4.222933290	-2.932981701	-0.803338620
Fe142	3.238423432	-2.705604250	-3.193779516
Fe143	4.676913931	-0.730831168	-2.108762293
Fe144	2.519344303	-4.800993325	-0.280464019
Fe145	0.644405558	-3.084240118	-0.734554735
H146	-9.572840184	-1.866719213	0.805349330
H147	-9.048258932	-1.341882590	-0.646930470
H148	-10.553801362	2.471828984	0.616864476
H149	-10.632008564	0.456637311	-0.669116410
H150	-11.289737542	-0.141898695	0.849060735
H151	-7.898450303	3.116207103	1.257804909
H152	-10.375949273	1.940867701	3.503596145
H153	-9.321037492	4.117642598	1.624986602
H154	-10.232218365	1.533379971	5.791952775
H155	-8.429781441	0.149788461	3.705014384
H156	-9.037848094	2.842037935	5.938037968
H157	-3.424456345	1.116254296	3.026912688
H158	-6.275844289	0.989140091	2.895513530
H159	-6.894837760	-1.589292944	3.842602569
H160	-3.799708336	4.559724255	6.217718852
H161	-5.877843058	3.048860582	4.884801028
H162	-6.740275014	-1.362565213	5.602968916
H163	-4.511910006	2.403537918	2.469320762
H164	-5.834395694	1.796304526	7.413656575
H165	-5.517643466	4.463320840	6.687636581
H166	-2.411590139	-1.339954773	3.829557809
H167	-1.716637047	-0.771640750	2.294577255
H168	-0.807709792	-1.915622523	3.311890962
H169	-1.477562777	1.007975476	4.032511570
H170	-5.805399529	0.937052981	9.594955271
H171	-0.066628021	3.826419716	4.435395114

	H172	-1.281256167	2.969798167	8.696548746
	H173	1.180363240	5.620908908	8.210783622
	H174	0.270588485	0.806486402	2.281813518
	H175	1.222366764	-0.280775451	3.325021503
	H176	8.519337616	-2.918578497	5.390531553
	H177	0.378314289	5.541652736	4.555966726
	H178	1.125343558	6.549311650	6.690349200
	H179	1.638905858	4.290129212	4.660693142
	H180	2.397495079	5.329309920	6.948181548
	H181	-0.611509255	4.723041075	6.720350537
	H182	1.808217109	2.842424769	6.722358160
	H183	-1.001458980	2.321274333	6.057653209
	H184	0.969875101	1.417618835	3.790139536
	H185	3.744572164	2.382499527	-0.244843469
	H186	3.231688933	3.479217388	1.065901690
	H187	5.251318042	3.070758557	1.728695780
	H188	5.280114942	2.857356496	4.387473659
	H189	6.261179226	0.831162024	1.660623319
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	H209	-5.173554529	-3.687648034	-9.191914324
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Fe(144) 1.846
Fe(145) -0.685

C2	-10.371706682	-0.058793007	0.263692685
C3	-8.839340246	3.110091270	1.751351921
C4	-8.564738796	2.913028498	3.238961205
C5	-9.278132382	1.931271815	5.357280337
C6	-8.148906464	0.918471191	5.582651988
C7	-6.769737155	-0.853471684	4.620317655
C8	-5.456453688	-0.086572419	4.444639657
C9	-4.287899370	1.718469117	3.279400937
C10	-3.893285048	2.525953987	4.524474959
C11	-4.588932002	3.854893746	6.424974231
C12	-4.166652470	3.036866394	7.654112464
C13	-4.763223398	1.226328295	9.199857487
C14	-3.874363168	-0.021382364	9.116532554
C15	-3.145440444	-1.912539147	7.731228280
C16	-1.801134634	-1.641091261	7.048556634
C17	-0.532798233	-0.210805182	5.517366618
C18	0.401355486	0.788521067	6.223740847
C19	-0.825349594	0.139104693	4.038333665
C20	0.455724919	0.542828615	3.298266744
C21	-1.507309229	-1.039657937	3.332436508
C22	0.809958099	3.068786132	7.013617029
C23	0.848031475	3.006831054	8.552336483
C24	0.490485703	4.476636521	6.456565616
C25	1.389485394	5.534487392	7.107769128
C26	0.658955607	4.497466998	4.931295117
C27	-0.333861550	2.871259798	10.664208946
C28	0.527198681	1.731187431	11.176479531
C29	-2.610107273	-11.361450675	6.805669546
C30	-1.337396610	-10.912187096	6.088989682
C31	0.430163928	-9.170746045	6.085626552
C32	1.599743505	-9.484699053	7.035820022
C33	0.265329497	-7.646997841	5.936171213
C34	1.531174614	-7.000782221	5.374315750
C35	1.345245694	-5.531513361	5.028783165
C36	3.042165638	-3.799996863	4.435815999
C37	3.975507725	-10.064262449	7.158519946
C38	5.035764688	-9.010702060	6.930135060
C39	-5.865412899	0.691597783	-1.852939292
C40	-5.370226854	2.145225087	-1.725235645
C41	-4.685549194	-0.270184773	-1.594949348
C42	-5.082161103	-1.731759445	-1.306290773
C43	-5.222300048	-2.638375034	-2.529260115
C44	-4.242263521	3.897979838	-3.077819788
C45	-4.841554903	5.162494035	-2.454947791
C46	-3.954920782	4.073779946	-4.575924663
C47	-6.877398309	6.317513020	-1.739854250
C48	-6.573150294	6.490021238	-0.247318154
C49	-5.607247182	5.528844581	1.787157339
C50	-4.102481405	5.639117458	2.045069843
C51	-1.824089223	5.693671555	1.151486682
C52	-1.368898955	7.123962926	1.479761468
C53	-1.057591278	5.272293623	-0.113198788
C54	-1.320752900	3.872251624	-0.553793020
C55	-1.871238315	2.771026849	0.069136795
C56	-1.371943209	2.117354846	-1.915440161
C57	-1.655132609	9.481662577	0.855337256
C58	-1.457643087	9.928243640	2.301610231
C59	-2.780368026	10.301800215	0.180411716
C60	-2.447030729	11.702327844	-0.242746441
C61	-1.752154683	12.704960524	0.405335135
C62	-2.501654064	13.427795222	-1.550690621
C63	8.193283515	-3.403106449	4.466696006
C64	8.298408298	-4.904080343	4.672409396
C65	6.701118936	-3.091005129	4.214743507
C66	6.412717469	-1.614025212	4.067164783
C67	6.064247929	-0.823442439	5.177918716
C68	6.478032969	-0.987554289	2.808378720
C69	5.779174912	0.539100211	5.040697568
C70	6.209991167	0.373148883	2.658693654
C71	5.853566767	1.134337403	3.774573413
C72	8.403828082	1.733671669	-1.725645426
C73	8.272786971	3.164503498	-2.274515279
C74	7.039682733	1.222071650	-1.263696122
C75	8.463889239	4.610129325	-4.269158396
C76	7.065611578	5.134806399	-4.601153075
C77	4.628837882	4.634411874	-4.489974623
C78	4.022063451	5.019598537	-3.116174265
C79	3.913586751	3.432897731	-5.145627758
C80	2.390084433	3.471174264	-5.308734077
C81	1.836916216	4.357710017	-6.436002286

C82	1.779164566	6.850270737	-6.561622679
C83	3.745459793	4.514390337	-0.739210410
C84	4.367468540	5.765078197	-0.105187057
C85	3.909520011	3.354385622	0.263083765
C86	6.495886122	6.846628018	0.427376679
C87	6.876513008	8.155026191	-0.243504831
C88	6.644840893	9.586516837	-2.193158530
C89	6.006819292	10.939792981	-1.789753779
C90	6.536746236	9.372981127	-3.707605837
C91	5.105872747	9.328747604	-4.229298436
C92	4.115183413	12.072532492	-0.728922131
C93	4.871394727	13.120821881	0.072207852
C94	2.815166373	11.663166223	0.018290610
C95	1.956555539	10.742885546	-0.819139227
C96	1.042287531	11.269902847	-1.743331190
C97	2.090880776	9.346291325	-0.745516377
C98	0.299403123	10.438817851	-2.584114069
C99	1.377129300	8.499512998	-1.598726509
C100	0.491046214	9.057027425	-2.516043552
C101	0.823609822	-7.628722217	-7.447179253
C102	-0.154458314	-6.486523589	-7.223085563
C103	-0.357067840	-4.140518141	-6.422430590
C104	0.075539047	-2.941037309	-7.274269551
C105	1.864961512	-1.301142657	-7.652750447
C106	3.382363064	-1.290903152	-7.811495987
C107	5.584355583	-2.035624462	-7.114957172
C108	6.148981628	-2.475280272	-8.452350796
C109	-4.260500966	-3.315395667	-8.705171635
C110	-4.379848380	-1.789477126	-8.795757292
C111	-4.306404493	-3.775263408	-7.230144525
C112	-4.584106311	-5.287770292	-7.133956793
C113	-4.366082812	-5.791010507	-5.725250201
C114	-3.249416139	0.372593668	-8.656919678
C115	-2.026359794	0.862602019	-9.406387607
C116	-3.534941727	1.119753209	-7.330527864
C117	-2.582017614	0.648863687	-6.271120474
C118	-1.300288349	1.210893319	-6.164192228
C119	-2.895712557	-0.489175490	-5.509057460
C120	-0.322293568	0.585329331	-5.386247767
C121	-1.918088035	-1.109242918	-4.729746610
C122	-0.617801646	-0.595005040	-4.701793723
C123	2.355398738	-10.701639968	-2.222391987
C124	3.209084477	-11.218739583	-1.053574407
C125	1.072834535	-10.035081810	-1.705246748
C126	0.252963893	-9.299107143	-2.714294368
C127	-0.392436240	-9.796451813	-3.826279304
C128	-0.971874018	-7.677509919	-3.536893818
C129	3.375099395	-12.459846593	1.018137116
C130	4.582689634	-13.252206792	0.568555751
C131	-3.681096893	-5.651557541	1.184706075
C132	-2.587760197	-6.541166609	1.771434987
C133	-1.948383003	-7.540363513	0.758116623
C134	-2.905538365	-8.735230551	0.514865910
C135	-2.299871369	-9.881199802	-0.297408541
C136	-3.213015754	-11.119786577	-0.429445437
C137	-0.634658946	-8.068477724	1.356315710
C138	2.395501145	-3.251376698	-1.512568540
Fe139	1.717019687	-4.720526673	-2.684044475
Fe140	1.942384555	-1.014994687	-1.145977887
Fe141	4.208295124	-2.934157243	-0.776350397
Fe142	3.254383617	-2.723295437	-3.179732860
Fe143	4.656993853	-0.714065933	-2.088424962
Fe144	2.513122027	-4.800814251	-0.287411739
Fe145	0.615857880	-3.118786696	-0.711009342
H146	-9.582151542	-1.868545063	0.777286310
H147	-9.087218971	-1.335715775	-0.682489276
H148	-10.527804500	2.480277187	0.609741731
H149	-10.659618200	0.469927610	-0.658911041
H150	-11.292308618	-0.137269451	0.866696129
H151	-7.861005439	3.087336575	1.248114704
H152	-10.347087820	1.933576971	3.489126116
H153	-9.268259593	4.111229077	1.608193728
H154	-10.207390231	1.524079524	5.777721391
H155	-8.414650865	0.134631178	3.692957655
H156	-9.010343941	2.830381631	5.927010249
H157	-3.414424223	1.119086187	2.995157378
H158	-6.260177847	0.970732745	2.874400138
H159	-6.873563522	-1.596928108	3.818345253
H160	-3.762689537	4.542099234	6.200786627
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	H162	-6.717566755	-1.381321474	5.580144659
	H163	-4.511761683	2.402309232	2.448921482
	H164	-5.777350303	1.766963419	7.391301669
	H165	-5.475252731	4.447364223	6.690349761
	H166	-2.436343673	-1.341615992	3.836340968
	H167	-1.760602114	-0.771351228	2.294751956
	H168	-0.838338521	-1.915299543	3.298069904
	H169	-1.501583512	1.007646831	4.031006604
	H170	-5.747618085	0.910389444	9.575288929
	H171	-0.006387022	3.781835518	4.429027195
	H172	-1.233707077	2.952904278	8.719742945
	H173	1.233691530	5.602809750	8.193912067
	H174	0.219420176	0.803094555	2.255935114
	H175	1.187766604	-0.280274799	3.288071637
	H176	8.490193720	-2.918492804	5.417284372
	H177	0.439011839	5.498682114	4.532519992
	H178	1.187825941	6.522421286	6.667945256
	H179	1.698013369	4.246611923	4.658459868
	H180	2.451605595	5.295600537	6.935728829
	H181	-0.561338165	4.712689870	6.701067696
	H182	1.835584817	2.803797296	6.716843176
	H183	-0.986792002	2.315171854	6.079727738
	H184	0.940383502	1.419741499	3.751758555
	H185	3.655742882	2.410836070	-0.240036523
	H186	3.182142827	3.522830116	1.071170135
	H187	5.192319981	3.066579664	1.732344642
	H188	5.260371218	2.874799016	4.396885661
	H189	6.234407486	0.839817188	1.674443581
	H190	6.709263422	-1.582040442	1.921593270
	H191	6.002281132	-1.280407259	6.169241437
	H192	-2.595504164	-0.019218737	6.061889700
	H193	-3.698735188	-2.628577688	7.105366928
	H194	-2.923894188	-2.397656690	8.689298526
	H195	-4.520809193	-0.396856987	7.181725264
	H196	-4.302521233	1.885481025	9.945532383
	H197	5.486088692	1.132847364	5.910798841
	H198	0.058961043	-1.138387394	5.530194038
	H199	0.006504230	3.811024373	11.126834205
	H200	-1.365305089	2.679501461	10.996546650
	H201	0.650639492	0.879689990	10.466490424
	H202	4.397907315	-11.058317231	6.944132206
	H203	-5.015063574	-4.584362409	-3.124214598
	H204	-2.627712006	-5.914410145	-0.427942045
	H205	-5.632267524	-5.477882563	-7.407034012
	H206	-3.939458490	-5.837093805	-7.835628767
	H207	-5.095128136	-3.233353948	-6.685614201
	H208	-1.547264684	0.098338770	-10.062417203
	H209	-5.181123790	-3.673730256	-9.189393566
	H210	-4.006617117	-0.228705949	-2.460980703
	H211	-6.047382690	-1.767541060	-0.770664184
	H212	-2.368186274	-1.556554259	-8.331467996
	H213	-4.088154739	0.608905980	-9.343585179
	H214	-2.234902123	-3.612752651	-9.044875891
	H215	-4.514914521	-4.291630069	-1.462286404
	H216	-3.353947748	-3.514393378	-6.743420452
	H217	-3.199415960	-4.814189166	-9.624590056
	H218	-7.446006919	0.644329867	-3.188409409
	H219	-4.104535580	0.113810868	-0.745787535
	H220	-2.565186541	-6.353422611	-6.272951479
	H221	-4.344645514	-2.176696648	-0.622689417
	H222	-1.532306039	5.069071547	2.007233160
	H223	-2.256698268	2.705947355	1.082439197
	H224	-6.068012687	6.432021931	2.210777890
	H225	-5.820762754	4.553529920	-0.104993754
	H226	-2.898007750	7.827201920	0.307221166
	H227	-1.226230978	12.734341104	1.353316119
	H228	-2.189428278	9.473641282	3.012194536
	H229	-3.665454664	10.293765197	0.841478395
	H230	-0.705401454	9.613721647	0.313014247
	H231	-2.685053356	14.107382232	-2.379371266
	H232	0.013413766	5.418103204	0.105791064
	H233	-1.310623061	5.969582365	-0.929930030
	H234	-1.366537647	14.697113631	-0.270912369
	H235	-3.075838827	9.764572802	-0.734374730
	H236	-3.646377495	5.500523210	0.022934751
	H237	-5.983778070	4.676345704	2.372762315
	H238	-6.620531985	7.274606552	-2.214893329
	H239	-1.209843621	1.517439064	-2.807382120
	H240	-7.959043685	6.167593563	-1.851662955
	H241	10.000181467	-3.045058442	3.573711310

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H258	-0.421093136	10.866094737	-3.285811238
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H260	1.061811514	8.000001019	-5.017008918
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H268	1.537120870	7.421253590	-1.563720264
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H270	2.544881958	6.060479415	-8.306694201
H271	1.439639000	8.861113066	-6.466718167
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H276	4.551484855	5.531350368	-5.113569599
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H281	5.612025156	7.729257902	-1.800351237
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H288	0.811351561	-9.438152740	-8.387266908
H289	-0.669569063	-8.749149173	-8.253548574
H290	7.181636431	0.212830408	-0.853000090
H291	9.066424907	2.382667398	0.091632011
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H294	10.279745445	1.936207603	-0.911491802
H295	6.001648554	-2.704534931	-6.345645338
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H298	0.626917127	-9.601867814	5.095915075
H299	3.721568314	-2.747629022	-6.350669662
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H308	1.831381350	-7.530735289	4.459766142
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H312	-3.439925701	-11.144565352	6.115299812
H313	0.151052796	-1.090685909	-4.109872771
H314	-2.404555979	-11.176855047	8.845499291
H315	-3.841988892	-10.631678189	8.281580536
H316	2.698986087	-5.510414616	3.403531113
H317	0.680455341	1.006924668	-5.306233596
H318	-3.905344916	-0.905025403	-5.540923006
H319	-0.120386067	-12.554876983	1.508976359
H320	0.429870321	-10.803621609	-1.243431584
H321	0.166049654	-10.198094318	2.540844327

H322	-1.166900914	-12.807777023	0.384923514
H323	5.459683127	-3.094114495	-9.076677048
H324	1.954496897	-7.736017972	1.705551028
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H326	1.384915192	-5.331835024	-6.526411370
H327	-3.216076181	-9.114074351	1.500948635
H328	-1.800359142	-8.814410102	-5.106877171
H329	-1.478845541	-6.731697612	-3.686375778
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H331	3.725068414	-3.638196747	2.481586770
H332	3.038563251	-9.254915898	3.129363821
H333	3.449684270	-7.336178879	1.596567978
H334	2.792691696	-9.919098248	5.375275975
H335	2.595726796	-3.630398154	6.438569339
H336	-2.079069754	-9.524368171	-1.315256999
H337	-1.347266924	-10.201459486	0.147909113
H338	-3.810670190	-8.358146512	0.014626924
H339	-0.214404958	-3.927297675	-5.351095983
H340	-1.059859403	2.109650756	-6.737113214
H341	-3.431489662	2.196123210	-7.533496728
H342	-1.808040051	-5.850595357	2.134732495
H343	2.165241254	-10.537649016	3.281843116
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H346	-0.386738715	-10.783139794	-4.271190479
H347	1.333711483	-9.338701865	-0.897714651
H348	-1.414189949	-4.331326636	-6.616392834
H349	5.937479539	-1.016616499	-6.897723185
H350	6.126119936	-3.498320817	5.060523342
H351	6.390921592	-3.627647817	3.303939447
H352	2.937102966	-12.166273703	-3.536301640
H353	1.536748684	-12.513942303	-2.762124598
H354	2.735280572	-13.142671006	1.598869030
H355	1.589794486	-12.176067301	-0.108750472
H356	4.481832154	-13.720885051	-0.440473650
H357	3.692386612	-11.648573123	1.691960914
H358	8.326757382	-5.497596450	3.727613232
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H360	3.719597547	-10.036003346	8.233040152
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H362	3.838738911	12.531558167	-1.693383458
H363	3.086760531	11.181311590	0.970456648
H364	2.267925375	12.585975063	0.257090423
H365	-0.933777203	8.670476005	-3.788371169
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H367	-0.521007460	-3.653048867	0.363165249
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N370	1.259624376	-1.760599175	0.550519434
N371	1.603203579	0.726985939	-0.826388934
N372	1.333220375	1.787422603	-0.569407470
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N378	-4.905228258	3.055065229	5.252862334
N379	-4.954725626	1.972925909	7.964412028
N380	-3.975305971	-0.747153865	7.971608277
N381	-1.733210589	-0.515545284	6.281428869
N382	-0.069353888	2.047692851	6.443896382
N383	-0.336854660	2.935534202	9.211309597
N384	-2.842208995	-10.664419348	8.076810335
N385	-0.794462375	-9.777219185	6.575241883
N386	2.513262306	-5.023424532	4.286620550
N387	3.010215015	-3.174067486	5.634008369
N388	3.589796095	-3.156202322	3.397204446
N389	2.756490815	-9.827580687	6.415213526
N390	-6.438252398	0.472367360	-3.188456459
N391	-4.920435006	-3.937154144	-2.335355765
N392	-5.078330081	2.715876927	-2.927341644
N393	-6.194813525	5.221453007	-2.401993363
N394	-6.025965976	5.425632854	0.401556530
N395	-3.269161334	5.602256557	0.967432437
N396	-1.008356726	3.437671905	-1.828611579
N397	-1.901193691	1.688789965	-0.780013264
N398	-2.078882664	8.092762913	0.848957396
N399	-2.911178112	12.168273519	-1.463649219
N400	-1.794012668	13.791175572	-0.443280855
N401	9.011013240	-3.022461525	3.313261050

	N402	9.342792229	1.671886202	-0.593626975
	N403	8.518632231	3.318506671	-3.609156557
	N404	6.042582854	4.286075114	-4.374703510
	N405	1.468707893	5.699997365	-5.972455575
	N406	2.365284592	6.904531385	-7.772394105
	N407	1.562659824	8.017799327	-5.911223996
	N408	4.299883105	4.203194692	-2.059397136
	N409	5.690715164	5.951557685	-0.379196183
	N410	6.214695816	8.449994776	-1.403377020
	N411	4.844171282	8.324325157	-5.109035359
	N412	4.940049320	10.892246630	-0.952868806
	N413	0.312570373	-8.549400196	-8.465357631
	N414	0.393459514	-5.335980976	-6.783095222
	N415	1.277088267	-2.422484842	-6.941996765
	N416	4.135592008	-2.130372356	-7.055849457
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	N418	-3.242728582	-1.075058990	-8.564094864
	N419	2.058035932	-11.754077063	-3.210562009
	N420	-0.113055874	-7.964085097	-2.558148787
	N421	-1.152642212	-8.761593700	-4.325410165
	N422	2.594264237	-11.976015718	-0.105822557
	O423	-8.381503807	0.371449937	1.613839939
	O424	-7.512573302	3.340835810	3.744196227
	O425	-7.497307425	0.929752430	6.640824006
	O426	-4.465993760	-0.308891740	5.163041233
	O427	-2.701247397	2.676165837	4.836143221
	O428	-3.192695773	3.383689835	8.344006435
	O429	-3.163032744	-0.348103220	10.076888675
	O430	-0.863852487	-2.439449664	7.194073211
	O431	1.548278116	0.438761506	6.547963885
	O432	1.927511017	3.019388523	9.170659855
	O433	1.003732021	1.701175087	12.301431848
	O434	-0.897850663	-11.572430140	5.125308211
	O435	1.472081172	-9.375163163	8.267418658
	O436	6.226269302	-9.200691575	7.123938815
	O437	-5.247623766	2.733668312	-0.635103985
	O438	-5.623862512	-2.213182605	-3.637706738
	O439	-4.110466323	6.065081330	-2.012294074
	O440	-3.073951246	5.195608472	-4.777090419
	O441	-6.853225573	7.566333029	0.301778254
	O442	-3.690286978	5.756129642	3.206983137
	O443	-0.379425952	7.362870956	2.181266901
	O444	-0.635177822	10.751675778	2.667828718
	O445	8.326561058	-5.445484537	5.768370097
	O446	5.566572107	2.467970627	3.565195324
	O447	7.968827494	4.124780950	-1.546266772
	O448	6.940004984	6.288470163	-5.058351413
	O449	3.323558587	6.038930317	-3.008836493
	O450	3.713265935	6.494537369	0.650036004
	O451	5.241760814	3.294168754	0.782268829
	O452	7.724638255	8.902886367	0.258967995
	O453	6.496418339	12.005611816	-2.189635151
	O454	4.265326265	10.181748162	-3.909177679
	O455	4.548925221	14.298460340	0.092526996
	O456	-0.173224100	8.192890964	-3.404293145
	O457	-1.384869254	-6.650337217	-7.410948789
	O458	-0.626806662	-2.513548293	-8.214931681
	O459	3.898863056	-0.485360326	-8.604434650
	O460	7.285258532	-2.217148783	-8.816787815
	O461	-5.464331003	-1.239862441	-9.054455796
	O462	-5.205339481	-5.700147114	-4.836523109
	O463	-3.154185420	-6.321809082	-5.457553174
	O464	-1.606560099	2.010489316	-9.362672175
	O465	4.435164800	-10.999317469	-0.995543363
	O466	5.570322580	-13.443473090	1.264663325
	O467	-3.500554831	-5.311352010	-0.091648317
	O468	-4.626395922	-5.232981351	1.855296989
	O469	-2.657344019	-12.269963591	-0.308152172
	O470	-4.435263149	-10.922061229	-0.678562756
	O471	0.455021406	-7.834388410	0.672297627
	O472	-0.645426524	-8.694043611	2.435975948
	O473	-1.671898660	-6.848350562	-0.458601796
	O474	3.005331443	-10.115210705	3.616173244
	O475	2.777487269	-7.609192721	2.249934918
	O476	-0.513944568	5.633374059	-3.903976232
	O477	-0.343482580	-13.204246653	0.805782449
	O478	0.567286374	-11.083611721	2.765962401
	S479	5.813070473	1.160661669	-2.655818803
	S480	2.736132242	-0.545569549	-3.302452870
	S481	-0.483975348	-4.593709970	-2.277384755

	S482	4.025306868	-0.849904672	0.006534526
	S483	-0.277100437	-1.400858619	-1.622931263
	S484	2.683052885	-4.276166715	-4.646899941
	S485	0.561987530	-4.775955603	0.873953146
	S486	5.435504892	-2.755470164	-2.649440663
	S487	2.621809677	-6.530812756	-1.668179199
	S488	4.472538908	-4.571303521	0.691346089
	end			
N2x-Fe2-brNH2-Fe6-3b2 to 6Hx **S=1, 35** **product** Fe(139) -2.441 Fe(140) -0.400 Fe(141) -2.523 Fe(142) 2.786 Fe(143) 2.967 Fe(144) 1.948 Fe(145) -0.673	9651826nh22n2x3b26hx135tb.car_7			
	C1	-9.387280769	0.825717591	1.060558422
	C2	-10.345846282	-0.067067850	0.262295949
	C3	-8.873212719	3.122890149	1.764840300
	C4	-8.595281131	2.923660758	3.251134449
	C5	-9.306622682	1.941553169	5.370269314
	C6	-8.175801265	0.931127011	5.598646185
	C7	-6.790664350	-0.840072035	4.641744241
	C8	-5.473981950	-0.079705551	4.461454027
	C9	-4.298213395	1.720673009	3.304725645
	C10	-3.912003119	2.529844489	4.551277106
	C11	-4.630018883	3.873149214	6.437054188
	C12	-4.220928595	3.061994397	7.674960827
	C13	-4.827720352	1.259809918	9.224347070
	C14	-3.939443894	0.010839462	9.149074217
	C15	-3.170922735	-1.859491945	7.749527132
	C16	-1.820488095	-1.611954770	7.069081232
	C17	-0.524322583	-0.211701825	5.524597145
	C18	0.389554949	0.798948259	6.245713871
	C19	-0.797607406	0.138500140	4.045414007
	C20	0.494584902	0.539595324	3.322238195
	C21	-1.474139637	-1.038323679	3.331439399
	C22	0.773051019	3.092289111	7.011272846
	C23	0.797426446	3.024323496	8.550201205
	C24	0.433953705	4.500682408	6.467599316
	C25	1.324580992	5.562519195	7.125204284
	C26	0.593876632	4.539694362	4.942290004
	C27	-0.412864215	2.889808535	10.643527042
	C28	0.459907515	1.772819903	11.181967716
	C29	-2.610236824	-11.366604288	6.787523741
	C30	-1.329089056	-10.934472458	6.079303610
	C31	0.460465072	-9.215710012	6.091504957
	C32	1.636562496	-9.525327035	7.034488143
	C33	0.285688999	-7.693225283	5.940190259
	C34	1.545580988	-7.029859791	5.385819898
	C35	1.308219232	-5.588980645	4.959070431
	C36	2.994099024	-3.838723599	4.385375163
	C37	4.018857600	-10.084606608	7.134478553
	C38	5.063612547	-9.013817287	6.914681862
	C39	-5.856996195	0.688200628	-1.858795479
	C40	-5.366738471	2.143374785	-1.737004974
	C41	-4.673382545	-0.267213651	-1.609205364
	C42	-5.066961016	-1.729866209	-1.316063512
	C43	-5.213802934	-2.637107809	-2.537882187
	C44	-4.240294289	3.891423023	-3.092607474
	C45	-4.832540751	5.159641034	-2.469242202
	C46	-3.951249932	4.063690072	-4.590476327
	C47	-6.859327428	6.326894547	-1.749231525
	C48	-6.557793673	6.490864451	-0.255257172
	C49	-5.599206890	5.519091594	1.776361481
	C50	-4.095666717	5.632393588	2.041940927
	C51	-1.812439208	5.704290739	1.160835636
	C52	-1.358334660	7.134554735	1.492726868
	C53	-1.037868028	5.283507282	-0.098920821
	C54	-1.294026241	3.880560257	-0.533739470
	C55	-1.835441339	2.778869876	0.097075684
	C56	-1.362057341	2.125638397	-1.893666465
	C57	-1.638222809	9.490552865	0.869424792
	C58	-1.430698350	9.936791320	2.314454810
	C59	-2.766476594	10.319911597	0.207086135
	C60	-2.430172608	11.719242085	-0.217645488
	C61	-1.743558465	12.725534588	0.433370306
	C62	-2.475249609	13.439756256	-1.532475818
	C63	8.234173761	-3.405127915	4.445434227
	C64	8.356744377	-4.904892944	4.644145222
	C65	6.735614853	-3.107273183	4.193537033
	C66	6.434228824	-1.634899033	4.044709674
	C67	6.076975205	-0.848248363	5.154568322
	C68	6.501905392	-1.006494284	2.787251098
	C69	5.790476693	0.514182409	5.019892835
	C70	6.232965672	0.354658676	2.639236390
	C71	5.872451824	1.113768329	3.756018255

C72	8.418889233	1.740926541	-1.751840016
C73	8.280672397	3.170309820	-2.298512683
C74	7.051106094	1.217769207	-1.306819290
C75	8.462901914	4.620616766	-4.288754196
C76	7.062049600	5.143838991	-4.614637913
C77	4.627368474	4.641616144	-4.503252335
C78	4.025826385	5.014905583	-3.124043527
C79	3.909095981	3.440621748	-5.160509427
C80	2.384340001	3.475794078	-5.319900547
C81	1.825391467	4.366759622	-6.439800310
C82	1.776554950	6.858926567	-6.556627188
C83	3.760706474	4.488041647	-0.749826910
C84	4.369368027	5.745869869	-0.114915819
C85	3.942986932	3.325364563	0.247781316
C86	6.483907263	6.849720431	0.423979895
C87	6.873784088	8.158329542	-0.241971706
C88	6.654888525	9.597514908	-2.189914970
C89	6.021852208	10.950890682	-1.781879371
C90	6.542259005	9.386740717	-3.704436076
C91	5.109424732	9.347639642	-4.221068409
C92	4.129377595	12.082058461	-0.720125942
C93	4.884853520	13.128408785	0.083999105
C94	2.828895874	11.669806649	0.025333009
C95	1.971592170	10.748333665	-0.812496371
C96	1.055821489	11.273796936	-1.735959637
C97	2.107193890	9.351805832	-0.738353398
C98	0.311902339	10.441484001	-2.574381598
C99	1.392623732	8.503429527	-1.589416856
C100	0.504167923	9.059667448	-2.505419482
C101	0.820756336	-7.627132248	-7.431588267
C102	-0.164389609	-6.489129740	-7.218279263
C103	-0.376728925	-4.135402555	-6.442254919
C104	0.065637268	-2.939804370	-7.293786501
C105	1.844923185	-1.286446896	-7.652328472
C106	3.361470840	-1.289037997	-7.815158874
C107	5.558815250	-2.071652111	-7.142050435
C108	6.122773107	-2.465724571	-8.491586445
C109	-4.243549839	-3.334923930	-8.702351566
C110	-4.356963264	-1.807519246	-8.802388461
C111	-4.299874783	-3.783943177	-7.225292065
C112	-4.588443748	-5.294346374	-7.124130060
C113	-4.370894766	-5.795009771	-5.714607883
C114	-3.217158490	0.350576865	-8.682082663
C115	-1.997895449	0.836206009	-9.439742653
C116	-3.489163440	1.095640040	-7.352843223
C117	-2.544757622	0.621056308	-6.285804676
C118	-1.261325429	1.177026702	-6.163585484
C119	-2.881379945	-0.496821574	-5.504762310
C120	-0.313448292	0.579944325	-5.328301276
C121	-1.933754306	-1.089132331	-4.667822772
C122	-0.636825850	-0.569993284	-4.605037248
C123	2.335412615	-10.718332686	-2.226788970
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	H191	6.009398363	-1.307287971	6.144020396
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	H236	-3.628899284	5.514907868	0.021026600
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O425	-7.529308625	0.941633365	6.660035333
O426	-4.480327259	-0.308816943	5.173778778
O427	-2.722545592	2.674152708	4.875285963
O428	-3.249741615	3.407820920	8.369288682
O429	-3.281286467	-0.344311683	10.136720276
O430	-0.889533432	-2.413987265	7.235536826
O431	1.526726465	0.458005336	6.610499053
O432	1.869301825	3.042182073	9.181039418
O433	0.920445986	1.767918555	12.314195404
O434	-0.903909798	-11.587509796	5.103963990
O435	1.514766004	-9.426398638	8.267542865
O436	6.257597314	-9.189721091	7.098971827
O437	-5.237719983	2.732839369	-0.648254043
O438	-5.626169702	-2.213718735	-3.642913284
O439	-4.096412987	6.058237512	-2.026964545
O440	-3.066325604	5.182568212	-4.793211146
O441	-6.836751301	7.564818591	0.298660216
O442	-3.689895232	5.737805331	3.206963369
O443	-0.368859093	7.371571532	2.194991528
O444	-0.606435342	10.761600801	2.674647562
O445	8.426256278	-5.450407017	5.735690755
O446	5.589465716	2.449647737	3.548832433
O447	7.973166650	4.128313962	-1.568588749
O448	6.933845699	6.300623285	-5.064038705
O449	3.324593301	6.030953762	-3.005547223
O450	3.707542823	6.464559748	0.643990926
O451	5.278072419	3.280351283	0.761342913
O452	7.721780728	8.902284278	0.266853868
O453	6.514268509	12.016684478	-2.178289437
O454	4.273498038	10.205637741	-3.900584445
O455	4.562268998	14.305900895	0.106726860
O456	-0.162031705	8.194193167	-3.391400130
O457	-1.394498641	-6.664303745	-7.398680148
O458	-0.613826619	-2.533918491	-8.260409067
O459	3.883701038	-0.467723439	-8.587777220
O460	7.254466481	-2.182418163	-8.851258313
O461	-5.442802056	-1.255914260	-9.051419974
O462	-5.210006877	-5.701913430	-4.825875603
O463	-3.158036070	-6.323451579	-5.445417982
O464	-1.567115142	1.979687639	-9.390124798
O465	4.431461169	-11.022835379	-1.028753228
O466	5.583305617	-13.437552438	1.269067966
O467	-3.579919597	-5.323274570	-0.064900787
O468	-4.636694523	-5.255616673	1.917708491
O469	-2.629174409	-12.249516225	-0.278581283
O470	-4.410263826	-10.895402047	-0.600629306
O471	0.469967163	-7.845418654	0.599807259

	O472 -0.591457931 -8.652085843 2.407365012 O473 -1.654728613 -6.748869492 -0.435470780 O474 3.025898985 -10.119242214 3.601996882 O475 2.796303604 -7.604010378 2.249242538 O476 -0.517387221 5.637823236 -3.896964625 O477 -0.305325052 -13.204530101 0.795989427 O478 0.576472185 -11.078529863 2.760351089 S479 5.827902564 1.153344515 -2.696659007 S480 2.689427008 -0.591500958 -3.338678747 S481 -0.450997807 -4.585964577 -2.365569410 S482 3.970817615 -0.874346113 0.002670220 S483 -0.344108899 -1.550573136 -1.542019853 S484 2.685224884 -4.336359924 -4.675401487 S485 0.783082475 -4.879249479 0.997361228 S486 5.478749276 -2.759500331 -2.627997803 S487 2.591880465 -6.541741750 -1.679230759 S488 4.557608696 -4.571582363 0.635810769 end
N2x-Fe2-brNH2-Fe6-3b2 to Fe2-brNH2-Fe6-3b2 **S=1, 47** **reactant** Fe(139) 2.160 Fe(140) -0.203 Fe(141) 2.621 Fe(142) -2.623 Fe(143) 2.996 Fe(144) -2.247 Fe(145) -1.171	9651826nh23b22n22dtd.car_4 C1 -9.384937673 0.816882008 1.045184138 C2 -10.370748464 -0.057681052 0.261058461 C3 -8.819673803 3.104952467 1.742848135 C4 -8.549489305 2.908372286 3.230951696 C5 -9.266421335 1.926414069 5.347787195 C6 -8.137975806 0.912568453 5.573013662 C7 -6.760569511 -0.859002279 4.608350402 C8 -5.449367665 -0.088708059 4.433351527 C9 -4.284495814 1.717839114 3.264285240 C10 -3.885324817 2.524550774 4.508527895 C11 -4.570475139 3.848390757 6.415545471 C12 -4.143439622 3.027249762 7.641020922 C13 -4.737085914 1.212827069 9.183575052 C14 -3.850623684 -0.037365420 9.100961013 C15 -3.128272853 -1.933359229 7.719633223 C16 -1.788542015 -1.655079763 7.032610866 C17 -0.532615907 -0.213623905 5.500327156 C18 0.406518231 0.780575790 6.203786821 C19 -0.835907154 0.137425299 4.024309742 C20 0.440456266 0.538841239 3.272977341 C21 -1.526496791 -1.039230503 3.323734598 C22 0.823236033 3.054925560 7.006011485 C23 0.867538425 2.994541845 8.545574479 C24 0.509130237 4.463415505 6.444721702 C25 1.408395687 5.521070908 7.095501480 C26 0.682384390 4.478039061 4.919839491 C27 -0.301218130 2.856705370 10.662742514 C28 0.552837587 1.707059296 11.166302948 C29 -2.608334663 -11.356403038 6.800258709 C30 -1.339377907 -10.899355813 6.085263280 C31 0.418259821 -9.147531674 6.083261535 C32 1.584762478 -9.462795252 7.037415915 C33 0.253465280 -7.622806908 5.937473164 C34 1.523851118 -6.980251951 5.382632562 C35 1.359796157 -5.502851861 5.066306330 C36 3.068165270 -3.788090739 4.456312384 C37 3.956836798 -10.053615284 7.168564626 C38 5.026456779 -9.011680033 6.930668571 C39 -5.849675880 0.689279409 -1.850624320 C40 -5.356660500 2.144108143 -1.721347534 C41 -4.676014770 -0.276922454 -1.592441266 C42 -5.084525936 -1.736990051 -1.308181442 C43 -5.225362654 -2.641135085 -2.533117713 C44 -4.239998774 3.903316729 -3.074350893 C45 -4.844927516 5.165479029 -2.451839674 C46 -3.954584561 4.079659756 -4.572537782 C47 -6.885347811 6.314977822 -1.739796074 C48 -6.581286339 6.490471315 -0.247523180 C49 -5.613403177 5.534495389 1.787881488 C50 -4.107965092 5.641266197 2.044103404 C51 -1.830501558 5.682602509 1.147338433 C52 -1.377905582 7.114775697 1.475496081 C53 -1.066904467 5.264339569 -0.119945929 C54 -1.322026145 3.863050907 -0.564165148 C55 -1.879197989 2.761565275 0.052938176 C56 -1.367504888 2.110873943 -1.929678818 C57 -1.657063953 9.470878044 0.839887223 C58 -1.463196112 9.916480503 2.287270930 C59 -2.783374206 10.290869382 0.166527115 C60 -2.451606801 11.691926013 -0.254723593 C61 -1.755324317 12.693910464 0.392713292

C62	-2.513221226	13.419553053	-1.559207587
C63	8.182335205	-3.401292751	4.481563076
C64	8.277051104	-4.902529714	4.687329521
C65	6.691773865	-3.082057274	4.226829851
C66	6.407732166	-1.605292564	4.077163001
C67	6.059227354	-0.812090317	5.185854401
C68	6.469933520	-0.982488382	2.816496521
C69	5.773472331	0.549853512	5.045701976
C70	6.200359610	0.377838497	2.662960835
C71	5.846741706	1.142385075	3.778488296
C72	8.412074696	1.734916717	-1.710330961
C73	8.276944028	3.163808713	-2.265328525
C74	7.054669169	1.231541158	-1.231660159
C75	8.463796509	4.603277727	-4.265190415
C76	7.065564423	5.127129379	-4.598586326
C77	4.629559297	4.634704679	-4.490727857
C78	4.017486789	5.023013524	-3.117976083
C79	3.912734620	3.431450214	-5.143317104
C80	2.389230457	3.468440301	-5.307367727
C81	1.836416955	4.352941418	-6.436382850
C82	1.779041081	6.845475381	-6.565408146
C83	3.736750902	4.521030204	-0.742202165
C84	4.365115472	5.768744160	-0.105452458
C85	3.887921928	3.360350966	0.257600561
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C88	6.640214475	9.586135017	-2.198491701
C89	5.998754521	10.937393765	-1.795385656
C90	6.532597743	9.370469837	-3.712945320
C91	5.102048103	9.323190933	-4.234913382
C92	4.106852735	12.068115961	-0.735813372
C93	4.862962162	13.117583201	0.064064874
C94	2.806281469	11.660203167	0.011119579
C95	1.947716263	10.739292264	-0.825874406
C96	1.033663503	11.265861721	-1.750473769
C97	2.082710415	9.342791878	-0.751516670
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C102	-0.154831830	-6.485893788	-7.229535997
C103	-0.350197024	-4.140877054	-6.425368257
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C116	-3.553430911	1.132933713	-7.324671902
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C118	-1.318088453	1.229902207	-6.166058890
C119	-2.904937554	-0.480440868	-5.513888389
C120	-0.328607742	0.590395532	-5.415488504
C121	-1.915071653	-1.114473589	-4.763216839
C122	-0.613518655	-0.603692660	-4.751550233
C123	2.360342262	-10.659080995	-2.204771963
C124	3.208926650	-11.197727398	-1.040800229
C125	1.091836083	-9.970755095	-1.678629808
C126	0.273888257	-9.214494612	-2.676601494
C127	-0.373253424	-9.716084879	-3.786980174
C128	-0.969573092	-7.604920967	-3.492084989
C129	3.367158637	-12.467049737	1.015505546
C130	4.577414698	-13.253383373	0.563260299
C131	-3.706668262	-5.646369647	1.226217708
C132	-2.599473516	-6.535885301	1.790216122
C133	-1.953208128	-7.502957752	0.754326077
C134	-2.912114430	-8.692052613	0.475140677
C135	-2.304276358	-9.846532251	-0.325416360
C136	-3.218449289	-11.086531009	-0.445045257
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C138	2.409585762	-3.258157681	-1.522084569
Fe139	1.715681634	-4.726199720	-2.667494728
Fe140	1.896296163	-1.124177533	-1.104326447
Fe141	4.147675683	-2.848109833	-0.729539710

Fe142	3.342158639	-2.750535036	-3.201501647
Fe143	4.533818733	-0.625286596	-2.187359427
Fe144	2.524323117	-4.808586942	-0.230690430
Fe145	0.608049150	-3.251606552	-0.928555923
H146	-9.587893572	-1.875069581	0.759414740
H147	-9.108542552	-1.340589504	-0.705822005
H148	-10.513015181	2.479644397	0.605614727
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H150	-11.284328242	-0.131292924	0.876185678
H151	-7.840536072	3.079599078	1.241528512
H152	-10.332803738	1.929986649	3.478169476
H153	-9.245358329	4.107205880	1.597987437
H154	-10.196394188	1.519761835	5.767177924
H155	-8.408461748	0.127112275	3.684905329
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H157	-3.411176466	1.120553007	2.975645423
H158	-6.253887524	0.962257525	2.860016081
H159	-6.863229758	-1.601147389	3.805023820
H160	-3.744498672	4.535343683	6.188732074
H161	-5.849442796	3.036588679	4.878740089
H162	-6.706607463	-1.388566131	5.567138054
H163	-4.512602788	2.402171998	2.435494320
H164	-5.750043141	1.753698498	7.374967733
H165	-5.454554175	4.441752154	6.686889152
H166	-2.453486570	-1.336842967	3.832675869
H167	-1.785209125	-0.770639159	2.287462255
H168	-0.860695402	-1.917146947	3.288688235
H169	-1.510109518	1.007764765	4.020201598
H170	-5.721604452	0.899122268	9.560361495
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H172	-1.213313428	2.939568354	8.723602123
H173	1.250607651	5.591747956	8.181098402
H174	0.195046377	0.798290385	2.232455854
H175	1.173372581	-0.283564091	3.254098064
H176	8.480131498	-2.918234095	5.432272919
H177	0.461993243	5.477284035	4.516500943
H178	1.208329044	6.507802368	6.652972678
H179	1.722494626	4.227324371	4.651133715
H180	2.470244331	5.280859207	6.924945767
H181	-0.543323528	4.702565026	6.684044794
H182	1.847325845	2.785243902	6.707003637
H183	-0.978463712	2.309199774	6.078549628
H184	0.928266587	1.416554948	3.722879803
H185	3.630686603	2.415959299	-0.244335619
H186	3.162412078	3.533779945	1.067174420
H187	5.169297473	3.058579483	1.729854091
H188	5.248134012	2.882006690	4.395556126
H189	6.218694102	0.840711227	1.675835211
H190	6.697013565	-1.579186794	1.930253462
H191	5.997778035	-1.267107658	6.177918545
H192	-2.593384452	-0.029498901	6.060853548
H193	-3.680346877	-2.651262653	7.095443611
H194	-2.901549624	-2.417094516	8.676790959
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H198	0.056622999	-1.140056126	5.505453359
H199	0.050102131	3.793446925	11.126422087
H200	-1.332298193	2.673136353	11.003281658
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H206	-3.938730974	-5.832671573	-7.839346509
H207	-5.096958862	-3.233355477	-6.681695014
H208	-1.553567441	0.109519041	-10.050502482
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H210	-3.993190114	-0.238705885	-2.455285563
H211	-6.052940568	-1.765821816	-0.777274212
H212	-2.369896425	-1.549054972	-8.321418078
H213	-4.091152645	0.610323333	-9.336686391
H214	-2.235363073	-3.605880458	-9.041595633
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	H222	-1.536445454	5.059188510	2.003372974
	H223	-2.279805106	2.697776542	1.060695614
	H224	-6.071081531	6.440982181	2.207499287
	H225	-5.825659721	4.556221089	-0.104040761
	H226	-2.895269116	7.816758768	0.285201121
	H227	-1.225677911	12.722298383	1.338568286
	H228	-2.200632835	9.462836828	2.993268400
	H229	-3.667528665	10.280685292	0.828610135
	H230	-0.707352743	9.604894122	0.298348635
	H231	-2.701128450	14.100598287	-2.385897737
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	H233	-1.324069986	5.962213121	-0.934799489
	H234	-1.374311673	14.687804536	-0.281365651
	H235	-3.078433575	9.754493189	-0.748911289
	H236	-3.653742788	5.492928271	0.021600085
	H237	-5.990675252	4.685721349	2.378153480
	H238	-6.632877694	7.272473472	-2.216573091
	H239	-1.197428022	1.511380209	-2.820587793
	H240	-7.966423467	6.160093745	-1.850877617
	H241	9.992237107	-3.047256804	3.591789515
	H242	8.803322066	-2.055118927	3.070443591
	H243	4.767422532	3.297862400	-2.194231843
	H244	2.665544474	4.738782459	-0.854225707
	H245	6.187531319	5.192157961	-0.853449946
	H246	-0.613318290	4.029834814	-2.574940080
	H247	-1.448852455	5.475438403	-4.188821799
	H248	-3.065159484	5.388838275	-5.729400053
	H249	-0.489726519	6.509251785	-3.472038986
	H250	-3.488982621	3.150249568	-4.941373395
	H251	-4.900482698	4.245858324	-5.112508241
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	H253	7.014795564	10.238707577	-4.189312982
	H254	5.492157854	7.525283481	-5.183028982
	H255	3.857719183	8.175862958	-5.333501704
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N2x-Fe2-brNH2-Fe6-3b2 to Fe2-brNH2-Fe6-3b2 **S=1, 47** **TS** Fe(139) 2.414 Fe(140) -0.943 Fe(141) 2.743 Fe(142) -2.424 Fe(143) 3.043 Fe(144) -2.165 Fe(145) -1.309	9651826nh23b22n22dte_1_53198.92 C1 -9.375017096 0.810771552 1.028556985 C2 -10.392729207 -0.044629460 0.263765580 C3 -8.787192518 3.094461191 1.733032205 C4 -8.518320068 2.898519493 3.221663166 C5 -9.233884333 1.916556062 5.338158055 C6 -8.105660366 0.901088054 5.556623984 C7 -6.738997632 -0.871463370 4.578500646 C8 -5.431313191 -0.093170961 4.411547492 C9 -4.273411020 1.715859261 3.229882873 C10 -3.859533423 2.525794289 4.466533280 C11 -4.507802343 3.829046583 6.395320485 C12 -4.070831115 2.998914297 7.611295835 C13 -4.664147563 1.175191824 9.146593159 C14 -3.783691293 -0.078269086 9.071292468 C15 -3.077023463 -1.991242277 7.712805121 C16 -1.752302743 -1.686717129 7.008378479 C17 -0.544935657 -0.217435425 5.476194033 C18 0.418579549 0.759311547 6.173542732 C19 -0.867815573 0.148128049 4.007577619 C20 0.394516322 0.557400843 3.238869971 C21 -1.561164927 -1.022862332 3.299807334 C22 0.861997104 3.018268361 7.004045208 C23 0.919779484 2.965980279 8.543745524 C24 0.557206365 4.419634344 6.425083587 C25 1.445922671 5.490539631 7.066061507 C26 0.744219327 4.412154342 4.901466983 C27 -0.225725578 2.822850018 10.676953588 C28 0.609243009 1.643873127 11.144995639 C29 -2.587709704 -11.354179624 6.806018908 C30 -1.326935844 -10.876885402 6.090659425 C31 0.391621874 -9.087121690 6.083155201 C32 1.558118835 -9.388408804 7.042535658 C33 0.205444216 -7.565897039 5.942238943 C34 1.475655324 -6.914730178 5.399044158 C35 1.334148887 -5.425157542 5.129446126 C36 3.094077616 -3.769722497 4.490673854 C37 3.916820200 -10.026605008 7.193387006 C38 5.017442478 -9.019429955 6.947871089 C39 -5.834543840 0.692848457 -1.841709792 C40 -5.341720352 2.147837659 -1.705784807 C41 -4.673179920 -0.284123200 -1.569777825 C42 -5.100877435 -1.740634831 -1.293763212 C43 -5.241034561 -2.640722189 -2.522060404 C44 -4.236149251 3.916374327 -3.058587777 C45 -4.851009111 5.175547588 -2.440799174 C46 -3.948269497 4.091255984 -4.556746363 C47 -6.899188768 6.313910581 -1.735519298 C48 -6.595047331 6.495152986 -0.243526029 C49 -5.627363959 5.544238597 1.795665657 C50 -4.121168460 5.649416345 2.050214166 C51 -1.844392831 5.670745258 1.144614673

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	C86	6.507931991	6.844546656	0.422098911
	C87	6.874365441	8.157482285	-0.247709039
	C88	6.630554610	9.583391521	-2.200358672
	C89	5.983884728	10.931700658	-1.798218493
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	C91	5.092860794	9.310775750	-4.236273405
	C92	4.092997399	12.060677759	-0.740591168
	C93	4.851187075	13.112256025	0.054436652
	C94	2.789849382	11.661410496	0.005807136
	C95	1.931343238	10.740510784	-0.830204695
	C96	1.017574176	11.266431853	-1.755462593
	C97	2.068992333	9.344354981	-0.756678208
	C98	0.278693009	10.434422179	-2.598919464
	C99	1.359433532	8.496971530	-1.612211129
	C100	0.474075431	9.053296177	-2.530927543
	C101	0.818644152	-7.636412536	-7.467822149
	C102	-0.145572516	-6.484642649	-7.239184953
	C103	-0.326693586	-4.144682624	-6.420170986
	C104	0.100961017	-2.941038374	-7.268506047
	C105	1.887279369	-1.293518417	-7.632517668
	C106	3.401619348	-1.276617223	-7.813840384
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	C113	-4.358191235	-5.790521628	-5.733142780
	C114	-3.269981373	0.395836368	-8.623238253
	C115	-2.060274678	0.903142176	-9.381623324
	C116	-3.557397533	1.131141306	-7.291360241
	C117	-2.596975323	0.654926613	-6.242734548
	C118	-1.315124853	1.217556000	-6.143954827
	C119	-2.901982262	-0.494503848	-5.494184831
	C120	-0.325685091	0.577066405	-5.394347389
	C121	-1.911874512	-1.129669035	-4.745323049
	C122	-0.610924345	-0.618051347	-4.733138699
	C123	2.364227970	-10.653883551	-2.189928230
	C124	3.208137382	-11.193397725	-1.022848261
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	C126	0.263469089	-9.238437299	-2.678175396
	C127	-0.385082961	-9.745825967	-3.784718373
	C128	-0.966145633	-7.627908618	-3.511928743
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	C136	-3.235371490	-11.096288398	-0.463373650
	C137	-0.663017634	-8.073292960	1.303171031
	C138	2.419216364	-3.267787350	-1.534451832
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	Fe140	1.942758499	-1.336345132	-1.201903856
	Fe141	4.169691079	-2.874781629	-0.703221601
	Fe142	3.338174698	-2.727783882	-3.165942453
	Fe143	4.516607640	-0.606167653	-2.157686119
	Fe144	2.519529750	-4.826401107	-0.249000327
	Fe145	0.568043258	-3.322508960	-0.936327934
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	H147	-9.180748020	-1.340029854	-0.750110473
	H148	-10.496875739	2.483802008	0.614455290
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	H159	-6.841902109	-1.602223833	3.764558472
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	H169	-1.543487770	1.016149993	4.019484568
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	H186	3.142771233	3.568080901	1.065818244
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	H188	5.243279830	2.906518920	4.403844756
	H189	6.199725522	0.848605061	1.690918748
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	H193	-3.620604943	-2.725631231	7.099919685
	H194	-2.826730351	-2.464437919	8.670011679
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	H196	-4.201653684	1.833429064	9.891806195
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	H206	-3.936197146	-5.819228828	-7.845879315
	H207	-5.115662198	-3.234820211	-6.678311409
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	O452 7.716617524 8.912457651 0.253690261 O453 6.465965104 12.000442974 -2.199061998 O454 4.243939627 10.153164246 -3.909627873 O455 4.529254611 14.290032760 0.070020926 O456 -0.185392047 8.187612730 -3.420512717 O457 -1.377429352 -6.631994838 -7.429426737 O458 -0.609958062 -2.501375074 -8.196486560 O459 3.901595560 -0.485921622 -8.631335413 O460 7.314164142 -2.231619723 -8.812207077 O461 -5.483983604 -1.215800651 -8.995858232 O462 -5.193256636 -5.703732491 -4.840030786 O463 -3.144129980 -6.320684525 -5.473329502 O464 -1.646407842 2.052738202 -9.330067342 O465 4.435441859 -10.983047867 -0.957407655 O466 5.563823181 -13.437432823 1.269601375 O467 -3.540693049 -5.279867051 -0.091310155 O468 -4.673436697 -5.245515984 1.850789683 O469 -2.679954426 -12.243828848 -0.319302122 O470 -4.457139305 -10.903320112 -0.718797052 O471 0.418533560 -7.880694171 0.592285270 O472 -0.675674113 -8.706693263 2.376916058 O473 -1.676041762 -6.767305662 -0.459258105 O474 2.972909810 -10.100514184 3.641972596 O475 2.766221228 -7.651729936 2.200991776 O476 -0.504094631 5.620553143 -3.895417159 O477 -0.376494985 -13.196599625 0.819074681 O478 0.551036539 -11.083672361 2.756695682 S479 5.811976925 1.222923326 -2.572061630 S480 2.628448387 -0.602865849 -3.331545118 S481 -0.482062958 -4.623354512 -2.383204801 S482 3.804722249 -0.741097631 0.036484380 S483 -0.278039715 -1.498331501 -1.739233631 S484 2.755808910 -4.290830224 -4.637288520 S485 0.757657886 -5.103076980 1.264612583 S486 5.479945097 -2.640125835 -2.547003380 S487 2.600884334 -6.564019419 -1.631551113 S488 4.486674248 -4.554703290 0.706640040 end
N2x-Fe2-brNH2-Fe6-3b2 to Fe2-brNH2-Fe6-3b2 **S=1, 47** **product** Fe(139) 2.523 Fe(140) -0.997 Fe(141) 2.711 Fe(142) -2.335 Fe(143) 3.046 Fe(144) -2.027 Fe(145) -1.422	9651826nh23b22n22dta.car_4 C1 -9.380833132 0.814371133 1.042351059 C2 -10.371513507 -0.056842131 0.261240903 C3 -8.810908929 3.101711405 1.739883745 C4 -8.542473119 2.905704211 3.228419430 C5 -9.260448550 1.923625382 5.344847044 C6 -8.132262818 0.909451711 5.569965239 C7 -6.755152759 -0.862299428 4.604881708 C8 -5.444466372 -0.090495552 4.431594196 C9 -4.281947461 1.716545610 3.259058974 C10 -3.880828029 2.524244661 4.501809410 C11 -4.561212292 3.844471606 6.412065486 C12 -4.131526133 3.022178376 7.635870315 C13 -4.723838354 1.205855186 9.177764561 C14 -3.840186523 -0.045978293 9.096231297 C15 -3.124201780 -1.946353188 7.719892671 C16 -1.785254649 -1.664855208 7.032917237 C17 -0.533833504 -0.221760710 5.501167497 C18 0.408791452 0.775097449 6.200636549 C19 -0.841674163 0.127998700 4.028632137 C20 0.433706616 0.522104326 3.276069543 C21 -1.533800513 -1.046219967 3.325525104 C22 0.828896825 3.048033774 7.005499043 C23 0.875816992 2.990048415 8.545147156 C24 0.517809436 4.455481905 6.441642249 C25 1.417163257 5.514253163 7.090428024 C26 0.693294050 4.466441969 4.916962632 C27 -0.286194515 2.852327073 10.666378111 C28 0.563680871 1.696455822 11.163784808 C29 -2.605535523 -11.358586798 6.806457844 C30 -1.338812354 -10.897087488 6.090500236 C31 0.411993494 -9.139298286 6.086176788 C32 1.577695253 -9.453291211 7.042041148 C33 0.245836595 -7.615442012 5.940527141 C34 1.515913949 -6.972861466 5.385585819 C35 1.354547738 -5.494160047 5.073214593 C36 3.071421470 -3.790252182 4.452165342 C37 3.947072976 -10.052739985 7.179251595 C38 5.021753840 -9.017164290 6.936118358 C39 -5.843771052 0.686853173 -1.850152270 C40 -5.355446482 2.143606755 -1.720324998 C41 -4.672805455 -0.281565908 -1.590739492

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H156	-8.991911352	2.822159976	5.915246604
H157	-3.408333630	1.120679937	2.968198819
H158	-6.249414174	0.956912283	2.856454112
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N2x-Fe2-brNH2-Fe6H to Fe2-brNH2-Fe6H **S=1, 35** **reactant** Fe(139) -2.442 Fe(140) -0.417 Fe(141) -2.544 Fe(142) 2.794 Fe(143) 2.958 Fe(144) 1.967 Fe(145) -0.662	9651826nh26hx2n2xd35tc.car_3 C1 -9.381916192 0.814082164 1.049263895 C2 -10.365908248 -0.060979698 0.264303602 C3 -8.816344665 3.102042998 1.745092764 C4 -8.546718768 2.905797172 3.233720439 C5 -9.265022352 1.922811890 5.350102873 C6 -8.135807918 0.910271283 5.576771931 C7 -6.755499059 -0.860809044 4.616449418 C8 -5.444187412 -0.090631142 4.440493894 C9 -4.279843866 1.714528368 3.269192780 C10 -3.881541359 2.522379198 4.512980765 C11 -4.568558179 3.845925949 6.419263582 C12 -4.141691903 3.025013651 7.644983436 C13 -4.735355538 1.211079690 9.188855630 C14 -3.849355883 -0.038590524 9.105979076 C15 -3.127451242 -1.934407307 7.725833261 C16 -1.785164107 -1.656448662 7.041794161 C17 -0.527459130 -0.219587155 5.508349625 C18 0.412556357 0.777903101 6.210156464 C19 -0.829641627 0.131994412 4.032450007 C20 0.446231856 0.533796305 3.281083116 C21 -1.517440379 -1.045153163 3.329631070 C22 0.825407426 3.053850594 7.011971492 C23 0.868286195 2.994949911 8.550596371 C24 0.510175978 4.460871579 6.449827920 C25 1.409553883 5.519401314 7.099675678 C26 0.682995963 4.475755978 4.925059285 C27 -0.301775725 2.856986186 10.667445116 C28 0.553250959 1.707801913 11.171447824 C29 -2.608230241 -11.352007194 6.796928600 C30 -1.337467940 -10.895155807 6.084998670 C31 0.421344603 -9.148676593 6.090246172

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	C49	-5.608367913	5.531350513	1.791632522
	C50	-4.102454065	5.639912424	2.046554928
	C51	-1.825785609	5.684620062	1.148750051
	C52	-1.372598732	7.116901720	1.476786594
	C53	-1.059947256	5.262629443	-0.116210750
	C54	-1.319319248	3.861291969	-0.558852197
	C55	-1.883560334	2.761655561	0.053057378
	C56	-1.377395440	2.116574535	-1.933159097
	C57	-1.657875680	9.474759708	0.847492828
	C58	-1.464263143	9.918310541	2.295147549
	C59	-2.784902653	10.293180107	0.173801505
	C60	-2.452699538	11.693833967	-0.249061574
	C61	-1.754895845	12.695664527	0.396997587
	C62	-2.510778051	13.420341413	-1.555991782
	C63	8.186058184	-3.401491713	4.486524658
	C64	8.284277541	-4.902259935	4.693312883
	C65	6.694267002	-3.086274418	4.229186203
	C66	6.406683355	-1.610427578	4.075926244
	C67	6.058561754	-0.815839455	5.183622737
	C68	6.467042407	-0.989368042	2.814498523
	C69	5.770508262	0.545230667	5.042022879
	C70	6.195025686	0.370280829	2.659102229
	C71	5.842312643	1.135987350	3.773459551
	C72	8.414712490	1.745677997	-1.718268036
	C73	8.279014332	3.172305427	-2.272677657
	C74	7.053519412	1.235309890	-1.242992190
	C75	8.468311547	4.611556705	-4.271202602
	C76	7.069841507	5.137286963	-4.603381816
	C77	4.632434978	4.641424712	-4.491039206
	C78	4.025126839	5.026655143	-3.117267344
	C79	3.915388581	3.437611728	-5.144390636
	C80	2.391663308	3.474820413	-5.306884253
	C81	1.837385089	4.358738094	-6.435204143
	C82	1.782050735	6.851204481	-6.564710923
	C83	3.749611942	4.519890024	-0.742494033
	C84	4.374649934	5.768844997	-0.106522590
	C85	3.905688635	3.355189791	0.258527925
	C86	6.504853847	6.850973333	0.423457154
	C87	6.880388357	8.161260634	-0.244584957
	C88	6.644129125	9.593935677	-2.194056140
	C89	6.003279300	10.944569029	-1.792187522
	C90	6.536787990	9.377248492	-3.708138264
	C91	5.106207927	9.329831700	-4.229640131
	C92	4.109727791	12.075328054	-0.730349123
	C93	4.864681334	13.123410310	0.070224963
	C94	2.809112315	11.663784042	0.016057852
	C95	1.952474098	10.743511304	-0.821868812
	C96	1.038093592	11.268797463	-1.746950752
	C97	2.088001787	9.347145877	-0.747556066
	C98	0.295987837	10.436698805	-2.587623532
	C99	1.374742778	8.499164332	-1.600647976
	C100	0.488196806	9.055069040	-2.518956797
	C101	0.825088608	-7.630683337	-7.447273137
	C102	-0.146908410	-6.483943919	-7.222504199
	C103	-0.342523379	-4.137066449	-6.425713557
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	C105	1.873769854	-1.290666340	-7.646142839
	C106	3.389927453	-1.285780637	-7.820999996
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H167	-1.778060086	-0.774618226	2.293967691
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	H206	-3.933102145	-5.835413774	-7.833010293
	H207	-5.090946284	-3.235858729	-6.676315318
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	H212	-2.363392043	-1.551170736	-8.328660911
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	H214	-2.230105826	-3.606215935	-9.038047662
	H215	-4.561064864	-4.299462051	-1.457201309
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	H220	-2.557836817	-6.351685064	-6.267751347
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	H264	-6.719952895	4.401450772	-2.703216405
	H265	9.037633444	4.556044644	-5.208314990
	H266	-5.276724995	2.078985926	-3.704056337
	H267	4.382769433	3.274059290	-6.129902086
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N2x-Fe2-brNH2-Fe6H to Fe2-brNH2-Fe6H **S=1, 35** **TS** Fe(139) -2.424 Fe(140) -0.730 Fe(141) -2.577 Fe(142) 2.733 Fe(143) 3.087 Fe(144) 2.007 Fe(145) -0.515	9651826nh26hx2n2xd35td_1_53215.82 C1 -9.371100354 0.809573870 1.038458942 C2 -10.375743422 -0.053952925 0.266304894 C3 -8.794044954 3.095698143 1.739736582 C4 -8.527382581 2.900262268 3.228841258 C5 -9.245381207 1.917158220 5.344223657 C6 -8.117884896 0.901732772 5.566492573 C7 -6.743673166 -0.868846702 4.597714672 C8 -5.435266758 -0.092744698 4.428034858 C9 -4.274913739 1.713766878 3.249188937 C10 -3.868139277 2.523332050 4.488753440 C11 -4.533376065 3.834946988 6.408107958 C12 -4.099923376 3.008942708 7.628181912 C13 -4.692322294 1.188616825 9.166916675 C14 -3.810939771 -0.064548356 9.087937098 C15 -3.098587307 -1.969955075 7.718846084 C16 -1.765550543 -1.676608415 7.024212111 C17 -0.533750525 -0.219589429 5.491911296 C18 0.416917503 0.767890247 6.193056843 C19 -0.849422151 0.139260538 4.021411495 C20 0.418533054 0.546120607 3.260245783 C21 -1.541084079 -1.034673393 3.316864058

	C22	0.846424069	3.034676782	7.011279341
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C131	-3.729135219	-5.646325668	1.213718679
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C135	-2.312745659	-9.839414265	-0.337451631
C136	-3.226157031	-11.080967014	-0.445668589
C137	-0.650871613	-8.045895131	1.289460818
C138	2.426303804	-3.259530291	-1.524985335
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Fe141	4.213010544	-2.912704816	-0.744745706
Fe142	3.327714593	-2.731094595	-3.182463107
Fe143	4.587618836	-0.652139008	-2.058775772
Fe144	2.565422232	-4.820099506	-0.303465126
Fe145	0.395017166	-3.454648507	-0.661849723
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H147	-9.142930452	-1.345307736	-0.727658149
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H150	-11.278838363	-0.121255729	0.897983852
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H157	-3.402208758	1.117863157	2.955322261
H158	-6.239634708	0.947654092	2.848405158
H159	-6.841030950	-1.607888544	3.790635148
H160	-3.705792851	4.517620670	6.175108826
H161	-5.830116764	3.025288613	4.883739561
H162	-6.688559448	-1.403659880	5.553375808
H163	-4.509801056	2.396536586	2.420770452
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N2x-Fe2-brNH2-Fe6H to Fe2-brNH2-Fe6H **S=1, 35** **product** Fe(139) -2.441 Fe(140) -0.694 Fe(141) -2.522 Fe(142) 2.697	9651826nh26hx2n2xd35te.car_2 C1 -9.368705693 0.811025094 1.046502131 C2 -10.351962513 -0.066224916 0.262511677 C3 -8.814489936 3.101673608 1.745656692 C4 -8.547279771 2.905398892 3.234496077 C5 -9.268438023 1.922200255 5.349717441 C6 -8.139236512 0.910122552 5.578241734 C7 -6.757593757 -0.861331147 4.619585979 C8 -5.446382278 -0.091774935 4.441859817 C9 -4.281303825 1.712921346 3.272582296 C10 -3.883687451 2.520405861 4.516846671 C11 -4.574311648 3.846649014 6.421049075

Fe(143) 3.011 Fe(144) 1.953 Fe(145) -0.429	C12	-4.148969991	3.026675814	7.647831697
	C13	-4.742097974	1.213496683	9.191904842
	C14	-3.853374281	-0.034533186	9.108273976
	C15	-3.126622298	-1.927192430	7.723975844
	C16	-1.784091323	-1.654165583	7.039179101
	C17	-0.524397181	-0.225278187	5.499182480
	C18	0.414015835	0.774064728	6.201771965
	C19	-0.825172719	0.123574789	4.025552783
	C20	0.452970253	0.519474469	3.278256975
	C21	-1.513677236	-1.051622368	3.320867110
	C22	0.823488770	3.050919249	7.002535283
	C23	0.865146756	2.987968188	8.541981300
	C24	0.505567067	4.459865108	6.446918757
	C25	1.404141554	5.517161371	7.100191087
	C26	0.676066443	4.482013373	4.922116558
	C27	-0.309408254	2.850980786	10.657376082
	C28	0.548151770	1.707295905	11.165580490
	C29	-2.610991908	-11.350445842	6.793881368
	C30	-1.338443662	-10.898675897	6.083353566
	C31	0.426453045	-9.155949417	6.090739418
	C32	1.594690364	-9.469263687	7.042656371
	C33	0.257909997	-7.632734981	5.944193888
	C34	1.521899619	-6.986913842	5.379481238
	C35	1.339183256	-5.517710560	5.032926839
	C36	3.050304290	-3.811230826	4.406088161
	C37	3.968176249	-10.057125257	7.166252710
	C38	5.033100133	-9.009630140	6.931723725
	C39	-5.835585701	0.681946707	-1.847623411
	C40	-5.348650270	2.139264057	-1.720434085
	C41	-4.663086163	-0.285017786	-1.591419051
	C42	-5.074867338	-1.744382621	-1.309396734
	C43	-5.217885201	-2.645953049	-2.536008512
	C44	-4.243179187	3.901875222	-3.078374112
	C45	-4.847158247	5.163683175	-2.454387075
	C46	-3.956061304	4.077355222	-4.576462823
	C47	-6.884338100	6.312752190	-1.734769146
	C48	-6.578724119	6.486689271	-0.242517451
	C49	-5.612465528	5.528932023	1.792898476
	C50	-4.107239881	5.635934646	2.047301503
	C51	-1.831741766	5.675891214	1.142659628
	C52	-1.370597346	7.106105073	1.471462053
	C53	-1.074262194	5.253647959	-0.128076963
	C54	-1.348997158	3.858760697	-0.575669030
	C55	-1.928862579	2.763094288	0.033610233
	C56	-1.407593483	2.109596653	-1.944677213
	C57	-1.649156790	9.465333840	0.843730000
	C58	-1.454762275	9.910006264	2.291001910
	C59	-2.776036620	10.286187590	0.172102814
	C60	-2.445261779	11.687478557	-0.249221901
	C61	-1.751201516	12.690306152	0.399202370
	C62	-2.506186171	13.414894628	-1.554273403
	C63	8.193662091	-3.402153863	4.485247276
	C64	8.294216282	-4.903067969	4.691187524
	C65	6.701468027	-3.090946339	4.226604352
	C66	6.409352617	-1.615894726	4.071218468
	C67	6.062157135	-0.821233911	5.179305945
	C68	6.465325610	-0.995618134	2.808722914
	C69	5.772838094	0.539748471	5.037369669
	C70	6.191050546	0.363629630	2.653476411
	C71	5.840758659	1.129881876	3.768322726
	C72	8.419246207	1.744821842	-1.721113077
	C73	8.284565611	3.172385095	-2.276102840
	C74	7.055463024	1.240548927	-1.251293474
	C75	8.468659941	4.611666886	-4.275040111
	C76	7.069280586	5.134586041	-4.607420614
	C77	4.632562884	4.636808228	-4.493207611
	C78	4.031028500	5.018704233	-3.115386156
	C79	3.915259574	3.432690766	-5.144275859
	C80	2.391583049	3.468251790	-5.305590506
	C81	1.836779704	4.352781340	-6.433512188
	C82	1.782200140	6.845667705	-6.561919353
	C83	3.779295493	4.504635351	-0.735073332
	C84	4.390282533	5.765992179	-0.109126288
	C85	3.978095515	3.345546611	0.264098997
	C86	6.513543207	6.854116017	0.427238418
	C87	6.888726559	8.163792597	-0.242965820
	C88	6.646358416	9.588368420	-2.195935652
	C89	6.004253132	10.939237463	-1.791532425
	C90	6.536406432	9.372188200	-3.709837806
	C91	5.105598079	9.326687243	-4.230963794

C92	4.110766556	12.067689048	-0.731840583
C93	4.865939834	13.117081802	0.069260481
C94	2.810341021	11.657327503	0.014360027
C95	1.953012679	10.735013357	-0.822861892
C96	1.038549761	11.260141349	-1.747944446
C97	2.088615879	9.338648812	-0.747627102
C98	0.296931027	10.427716476	-2.588374321
C99	1.376244654	8.490393660	-1.600280722
C100	0.490131007	9.046240634	-2.518551466
C101	0.824516670	-7.634225290	-7.452528666
C102	-0.146339536	-6.486680065	-7.224803358
C103	-0.340179978	-4.140849516	-6.427464555
C104	0.089819636	-2.940722166	-7.279239252
C105	1.873958323	-1.293361669	-7.651138233
C106	3.389207011	-1.286806735	-7.826692742
C107	5.598506384	-2.017118497	-7.130017302
C108	6.154737491	-2.478589460	-8.462892629
C109	-4.252036881	-3.316330005	-8.695533697
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C111	-4.298758162	-3.778542693	-7.221317348
C112	-4.578092806	-5.291268623	-7.129390664
C113	-4.361610734	-5.799087136	-5.722226856
C114	-3.242760852	0.371753920	-8.645023621
C115	-2.022733049	0.865241742	-9.396423240
C116	-3.529004163	1.117200848	-7.318386258
C117	-2.574911935	0.648307237	-6.259195511
C118	-1.294139949	1.212903468	-6.151594151
C119	-2.887978097	-0.488648657	-5.495947880
C120	-0.318486858	0.593897136	-5.366336753
C121	-1.911995695	-1.102704225	-4.710257802
C122	-0.614329380	-0.582905327	-4.676607283
C123	2.361186575	-10.686586216	-2.200912178
C124	3.215358228	-11.215516770	-1.038041164
C125	1.086384825	-10.012727430	-1.672745865
C126	0.261716078	-9.264706818	-2.670589674
C127	-0.374429805	-9.768551073	-3.786546847
C128	-1.000768401	-7.668081832	-3.476064936
C129	3.380189041	-12.464837313	1.028900397
C130	4.588645406	-13.254833775	0.577555780
C131	-3.722079442	-5.648659683	1.246170496
C132	-2.577424547	-6.500298905	1.787728785
C133	-1.944970091	-7.463430876	0.740093191
C134	-2.909884052	-8.652045206	0.465742383
C135	-2.305141146	-9.819617022	-0.319286010
C136	-3.219875349	-11.059957104	-0.426723328
C137	-0.634714760	-8.035582023	1.300809340
C138	2.426614798	-3.259733570	-1.523894426
Fe139	1.801372582	-4.735645797	-2.714978577
Fe140	1.833035559	-1.452855621	-1.238216958
Fe141	4.208145697	-2.890331297	-0.742929115
Fe142	3.299079618	-2.686815438	-3.181375042
Fe143	4.570551812	-0.626194845	-2.017863261
Fe144	2.571673738	-4.809767150	-0.300922971
Fe145	0.400860819	-3.441540728	-0.645887774
H146	-9.571282735	-1.882235262	0.768203539
H147	-9.087215445	-1.352536932	-0.697028071
H148	-10.502959184	2.468150963	0.605403832
H149	-10.647164757	0.463932383	-0.656881073
H150	-11.266388327	-0.138089492	0.876182071
H151	-7.834262557	3.080577482	1.246690802
H152	-10.329841881	1.924235432	3.476902897
H153	-9.244860909	4.101870652	1.600334469
H154	-10.199184759	1.514165314	5.766030726
H155	-8.404148186	0.121954308	3.690299278
H156	-9.003263357	2.821511260	5.920491389
H157	-3.407754617	1.114772892	2.985880221
H158	-6.251126261	0.958114578	2.867189756
H159	-6.858793676	-1.608034945	3.820309591
H160	-3.748582168	4.534155884	6.195806986
H161	-5.848251516	3.032835336	4.881994907
H162	-6.704245504	-1.386166653	5.580998142
H163	-4.508584929	2.397170655	2.443434421
H164	-5.757964341	1.755203718	7.384550126
H165	-5.459823590	4.438950873	6.689605580
H166	-2.440800906	-1.353589659	3.827959151
H167	-1.771608614	-0.779189693	2.284784771
H168	-0.846475310	-1.928558987	3.279316106
H169	-1.497766781	0.995023008	4.020349141
H170	-5.726142210	0.897346770	9.568098747
H171	0.011734021	3.766608228	4.418342745

	H172	-1.216336317	2.931697390	8.715736147
	H173	1.245230239	5.586687848	8.185852048
	H174	0.209133565	0.765389445	2.235885695
	H175	1.186758999	-0.301961681	3.271878455
	H176	8.487932635	-2.917082135	5.435940300
	H177	0.456723023	5.483431934	4.523856801
	H178	1.204944408	6.505079694	6.658888115
	H179	1.715362533	4.231328450	4.650427034
	H180	2.466490653	5.276903875	6.931418480
	H181	-0.546304681	4.696451160	6.690436553
	H182	1.848566242	2.785058432	6.704838144
	H183	-0.975518578	2.300673088	6.072848813
	H184	0.937826408	1.402756405	3.718706693
	H185	3.749148007	2.391738987	-0.236790880
	H186	3.255419326	3.495485950	1.078944832
	H187	5.268393920	3.098341108	1.731934654
	H188	5.253393503	2.873559241	4.387757298
	H189	6.211240726	0.826554369	1.666929001
	H190	6.696437187	-1.592949966	1.923856337
	H191	6.005879767	-1.274304749	6.172675205
	H192	-2.584410079	-0.035623287	6.052387683
	H193	-3.680156101	-2.643694918	7.098950834
	H194	-2.903472198	-2.411915620	8.681683483
	H195	-4.502636257	-0.411835520	7.174740114
	H196	-4.280741633	1.872581423	9.937266050
	H197	5.482476999	1.136267233	5.906361544
	H198	0.067180126	-1.152782057	5.509650926
	H199	0.035608199	3.789633518	11.119969895
	H200	-1.340529881	2.663597326	10.993876357
	H201	0.668509111	0.857318523	10.454099721
	H202	4.386188684	-11.054384389	6.957318110
	H203	-5.030137795	-4.595695397	-3.129513685
	H204	-2.698157031	-5.806455991	-0.386979327
	H205	-5.626349689	-5.479190934	-7.403585743
	H206	-3.933516158	-5.838935463	-7.832458456
	H207	-5.087569001	-3.237447944	-6.675777902
	H208	-1.544238099	0.103188880	-10.055259026
	H209	-5.173355288	-3.673748128	-9.180266709
	H210	-3.981378276	-0.246864856	-2.455042493
	H211	-6.042358352	-1.772484860	-0.776765975
	H212	-2.357859807	-1.556883700	-8.325520072
	H213	-4.083403052	0.606721022	-9.330596495
	H214	-2.226239085	-3.611566729	-9.037899605
	H215	-4.557511978	-4.306061312	-1.457627887
	H216	-3.346673887	-3.520029065	-6.732524432
	H217	-3.190326950	-4.813549721	-9.617003497
	H218	-7.420720226	0.638581552	-3.178865098
	H219	-4.080038070	0.091612121	-0.740395726
	H220	-2.557963043	-6.354088182	-6.267420326
	H221	-4.343634942	-2.198567730	-0.624778714
	H222	-1.536301142	5.050380655	1.997048022
	H223	-2.325852369	2.698592989	1.042677288
	H224	-6.070985186	6.434940610	2.212631833
	H225	-5.824479730	4.551428698	-0.099764334
	H226	-2.889077702	7.812635061	0.287510599
	H227	-1.223432103	12.719695055	1.346120750
	H228	-2.191073913	9.457434834	2.998418992
	H229	-3.659795714	10.275969413	0.834774146
	H230	-0.700033479	9.600254004	0.301711412
	H231	-2.692815065	14.095577488	-2.381630137
	H232	-0.001743697	5.393950682	0.085451664
	H233	-1.325708055	5.954331029	-0.942107949
	H234	-1.371958876	14.684996139	-0.274307158
	H235	-3.073052064	9.750383782	-0.742893953
	H236	-3.659992782	5.493321092	0.023810838
	H237	-5.989767088	4.680076109	2.383183426
	H238	-6.629890515	7.270037305	-2.210848904
	H239	-1.250712342	1.516046947	-2.841022366
	H240	-7.965858300	6.160581753	-1.844901411
	H241	10.002824334	-3.047239183	3.594592367
	H242	8.814522378	-2.052654697	3.077327112
	H243	4.792679766	3.291472225	-2.205599957
	H244	2.700459998	4.698399512	-0.826709961
	H245	6.217275694	5.201452338	-0.851083271
	H246	-0.633863676	4.026199949	-2.583009148
	H247	-1.448586525	5.477786303	-4.193903474
	H248	-3.064372485	5.384155879	-5.733352818
	H249	-0.484749201	6.500739080	-3.466525639
	H250	-3.490973503	3.146981112	-4.943904320
	H251	-4.901251060	4.244547016	-5.117704526

	H252	7.104424960	8.476399621	-3.995091327
	H253	7.018969519	10.239972184	-4.186668179
	H254	5.493339992	7.528935976	-5.180175475
	H255	3.859101987	8.181847494	-5.329918901
	H256	2.824865079	7.750232773	-8.080116218
	H257	0.941518135	3.884635475	-6.871060174
	H258	-0.423376381	10.853458574	-3.290974913
	H259	2.748475625	8.880537677	-0.005512189
	H260	1.061657545	7.994562422	-5.016332171
	H261	4.156810574	2.543106794	-4.541031980
	H262	6.264360565	3.358375367	-4.000090161
	H263	1.894194781	3.718278573	-4.355376084
	H264	-6.725134556	4.401045715	-2.703402350
	H265	9.039338702	4.557972152	-5.211339519
	H266	-5.277738736	2.075170947	-3.707280261
	H267	4.381080163	3.267995244	-6.130061069
	H268	1.537973970	7.412422684	-1.564244786
	H269	8.939267228	5.375597258	-3.639026852
	H270	2.546331276	6.054071345	-8.304265502
	H271	1.438094467	8.855903796	-6.466656830
	H272	-6.240345573	-0.512257471	-3.474151215
	H273	-6.566597415	0.549898778	-1.026988311
	H274	0.891690609	12.341042912	-1.809716047
	H275	-3.288861605	3.757724585	-2.552753990
	H276	4.550973186	5.532744073	-5.116373573
	H277	2.580687962	4.428092026	-7.237374770
	H278	2.093295149	2.437226161	-5.538654642
	H279	0.802333453	5.725132411	-5.169996128
	H280	5.960859726	7.101931360	1.345878625
	H281	5.626931868	7.725497130	-1.797155504
	H282	7.713106975	9.741300561	-1.969969840
	H283	7.449647204	6.356646323	0.716673276
	H284	4.520228831	9.973497220	-0.799079355
	H285	1.799397625	-7.235274830	-7.771012576
	H286	0.978169086	-8.099061734	-6.456262187
	H287	2.988659489	-9.931841880	-2.698269341
	H288	0.803546678	-9.439809649	-8.399498766
	H289	-0.675945467	-8.748936904	-8.252762175
	H290	7.181886778	0.222299953	-0.862263396
	H291	9.088675076	2.397036035	0.095399243
	H292	8.763170780	2.499393334	-4.159942877
	H293	6.672472214	1.892232293	-0.454098181
	H294	10.296800200	1.965398363	-0.917328049
	H295	6.019441732	-2.673888740	-6.352666457
	H296	8.795278693	1.074918423	-2.509938525
	H297	-0.003134093	-7.197823605	6.923592851
	H298	0.626388993	-9.584875414	5.100650499
	H299	3.740034521	-2.725187745	-6.350619552
	H300	4.240557872	-2.411715504	3.538533056
	H301	1.425260810	-1.254180867	-8.651363065
	H302	-2.154595333	-1.986602493	-4.117039444
	H303	1.611082848	-0.347054662	-7.147525883
	H304	1.201619309	-4.912156939	5.936849215
	H305	1.716477439	-2.770499608	-6.069544886
	H306	0.438611901	-5.370250883	4.413167713
	H307	-0.589292578	-7.459066991	5.262091191
	H308	1.818808347	-7.517050402	4.463760901
	H309	2.358312476	-7.079484960	6.089154399
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	H311	-1.264569159	-9.399568784	7.411129433
	H312	-3.440858281	-11.128997033	6.105197421
	H313	0.157907472	-1.072927251	-4.082057695
	H314	-2.396757291	-11.174644334	8.833916611
	H315	-3.842674187	-10.641418088	8.280633585
	H316	2.652217957	-5.511057264	3.379418837
	H317	0.684010485	1.015490350	-5.283260716
	H318	-3.895620859	-0.908530788	-5.530082659
	H319	-0.127022539	-12.551619634	1.516609131
	H320	0.439563849	-10.780864083	-1.214468746
	H321	0.160285601	-10.195366985	2.514789819
	H322	-1.170844071	-12.784054258	0.388570823
	H323	5.460201811	-3.102710994	-9.075285366
	H324	1.943155462	-7.748949863	1.673037169
	H325	-2.925961229	-7.051928956	2.668997963
	H326	1.399151494	-5.336346624	-6.531545252
	H327	-3.248879185	-9.020965523	1.446839044
	H328	-1.805632898	-8.807872368	-5.057758353
	H329	-1.532603397	-6.737437984	-3.625094274
	H330	-2.550475013	-12.449607719	6.870682060
	H331	3.733374745	-3.670157129	2.447099832

	H332	3.021255451	-9.256072090	3.132026095
	H333	3.433611962	-7.322775647	1.609526813
	H334	2.783904092	-9.915410251	5.383417592
	H335	2.606030018	-3.614796215	6.406476298
	H336	-2.076119308	-9.492837235	-1.344895556
	H337	-1.356580365	-10.136660533	0.135721546
	H338	-3.798302049	-8.268728793	-0.058587473
	H339	-0.194158477	-3.925456676	-5.357671479
	H340	-1.053036929	2.109115242	-6.727904398
	H341	-3.429044159	2.194149022	-7.520413891
	H342	-1.804926928	-5.788257279	2.124655949
	H343	2.149502049	-10.538454661	3.286759440
	H344	0.073237620	-11.296144014	3.597879457
	H345	3.101844711	-2.161693623	5.632112360
	H346	-0.353061241	-10.754952549	-4.233841074
	H347	1.356204456	-9.326512108	-0.861157871
	H348	-1.398090204	-4.331545205	-6.617112329
	H349	5.953596800	-0.994503586	-6.929055615
	H350	6.124118569	-3.495693130	5.071870150
	H351	6.396402837	-3.632811315	3.317272400
	H352	2.936433570	-12.140613927	-3.528974512
	H353	1.544958659	-12.499680356	-2.745312771
	H354	2.740997723	-13.151889959	1.605449754
	H355	1.594339332	-12.171549112	-0.094971717
	H356	4.487998898	-13.724260073	-0.431092692
	H357	3.696197309	-11.656327540	1.707015233
	H358	8.326661319	-5.495809336	3.745909585
	H359	5.718920070	12.732155488	0.675818322
	H360	3.713449308	-10.022497108	8.241224632
	H361	4.657008090	-8.019192456	6.575523639
	H362	3.834685179	12.526074455	-1.696790199
	H363	3.081500224	11.176694830	0.967458069
	H364	2.261411767	12.579738706	0.251721601
	H365	-0.935599826	8.654529723	-3.788774593
	H366	1.754325229	-2.203899209	1.236832269
	H367	-1.002419101	-3.385632686	-0.094438791
	H368	0.332069864	-1.393796896	0.884892171
	Mo369	0.359405964	-6.223331307	-0.920896251
	N370	1.066955980	-1.992953452	0.507528315
	N371	1.193240430	1.531936014	-0.613502495
	N372	1.080681271	2.188957702	0.276355015
	N373	-9.897922944	-1.403851451	-0.075281142
	N374	-9.716002106	2.126097892	1.151532291
	N375	-9.492499218	2.252666464	3.952102202
	N376	-7.922025691	0.011829988	4.585042970
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	N378	-4.893781961	3.048452083	5.248734188
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	N380	-3.957262002	-0.762302796	7.964867441
	N381	-1.720354877	-0.529199173	6.271066611
	N382	-0.057428277	2.031263330	6.433346840
	N383	-0.317906053	2.916871213	9.204692318
	N384	-2.843557575	-10.662176938	8.070264777
	N385	-0.797458936	-9.766247571	6.576174435
	N386	2.498559427	-5.025400391	4.269020126
	N387	3.038628620	-3.176198206	5.601197743
	N388	3.595352361	-3.180546727	3.358597470
	N389	2.749682760	-9.819619689	6.423011076
	N390	-6.412853266	0.466658147	-3.182939982
	N391	-4.934641855	-3.948633811	-2.340985193
	N392	-5.069680298	2.714122105	-2.923888439
	N393	-6.200314996	5.217493841	-2.397044895
	N394	-6.032683530	5.422084718	0.407430151
	N395	-3.277657703	5.588063960	0.966696626
	N396	-1.021313391	3.424056003	-1.845495336
	N397	-1.965673707	1.685678666	-0.820336395
	N398	-2.072221695	8.076562397	0.833382576
	N399	-2.912637071	12.154278389	-1.468445246
	N400	-1.797026126	13.777941937	-0.447543698
	N401	9.013993595	-3.023733647	3.332989332
	N402	9.364979547	1.690319939	-0.594038032
	N403	8.528800125	3.322491009	-3.611270186
	N404	6.046120583	4.286419181	-4.382202420
	N405	1.467790076	5.694903305	-5.971821895
	N406	2.367387582	6.897894532	-7.772424127
	N407	1.560694762	8.013511643	-5.910571253
	N408	4.321239775	4.203538557	-2.061785596
	N409	5.712736070	5.958616597	-0.383134844
	N410	6.224111673	8.452244217	-1.402776081
	N411	4.844605167	8.323613432	-5.111883170

	N412	4.937221207	10.888533580	-0.955164473
	N413	0.305160199	-8.550172273	-8.470536131
	N414	0.407699955	-5.337771373	-6.787300293
	N415	1.289693386	-2.419728927	-6.944672002
	N416	4.149700757	-2.109177386	-7.059500570
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	N418	-3.233783916	-1.075677699	-8.553086246
	N419	2.058155686	-11.734141335	-3.193501058
	N420	-0.134918737	-7.938603272	-2.498844897
	N421	-1.158507424	-8.747848965	-4.276115608
	N422	2.599877196	-11.977488288	-0.094038129
	O423	-8.348412619	0.360694594	1.598986446
	O424	-7.498281600	3.335359410	3.744765855
	O425	-7.487832410	0.923718183	6.636356584
	O426	-4.455438568	-0.310478584	5.160625831
	O427	-2.690814850	2.671913001	4.824412111
	O428	-3.174492091	3.373695949	8.336868484
	O429	-3.140023085	-0.359665671	10.067704453
	O430	-0.845185262	-2.450826220	7.183039740
	O431	1.563784281	0.424481335	6.516038465
	O432	1.946457121	3.000680993	9.157247122
	O433	1.025851095	1.673035753	12.289798840
	O434	-0.896358600	-11.555044106	5.118165539
	O435	1.467026213	-9.354098914	8.273714549
	O436	6.222369036	-9.203207522	7.130091980
	O437	-5.228904805	2.729222054	-0.630589576
	O438	-5.601585347	-2.213470298	-3.647473592
	O439	-4.118565573	6.069069814	-2.012626413
	O440	-3.073623496	5.198999484	-4.777355228
	O441	-6.857712042	7.563529281	0.305327670
	O442	-3.689809204	5.757410000	3.206586273
	O443	-0.383776011	7.340649378	2.177818915
	O444	-0.631012819	10.730650369	2.660139277
	O445	8.312454530	-5.445909064	5.786830789
	O446	5.555841882	2.463642700	3.556280399
	O447	7.982644226	4.135106036	-1.549988739
	O448	6.944398014	6.288081756	-5.066172587
	O449	3.326324068	6.033534616	-3.003818293
	O450	3.730986465	6.496111168	0.640894828
	O451	5.313435492	3.319503177	0.779637368
	O452	7.733602594	8.916508576	0.257720119
	O453	6.490908781	12.007147742	-2.189510403
	O454	4.264211419	10.178932412	-3.909979606
	O455	4.543084866	14.294649277	0.088472761
	O456	-0.172825166	8.179959571	-3.405592736
	O457	-1.378001777	-6.643455533	-7.409350467
	O458	-0.613615944	-2.513519758	-8.219293374
	O459	3.898387931	-0.497126451	-8.639896112
	O460	7.290577296	-2.230332512	-8.835117782
	O461	-5.456843138	-1.240140277	-9.036551010
	O462	-5.203969240	-5.714873832	-4.835534965
	O463	-3.148486443	-6.326235504	-5.453121206
	O464	-1.604566349	2.013637410	-9.351042592
	O465	4.442437466	-11.001375251	-0.980406593
	O466	5.576274735	-13.446853652	1.273620477
	O467	-3.589810243	-5.281473920	-0.032297477
	O468	-4.667877760	-5.281078342	1.942218097
	O469	-2.660702946	-12.207904970	-0.303063517
	O470	-4.445787987	-10.866484767	-0.661732073
	O471	0.441434325	-7.841091713	0.585725908
	O472	-0.637446458	-8.671713419	2.373621553
	O473	-1.668607275	-6.708476530	-0.440556523
	O474	2.988525895	-10.114705849	3.622144106
	O475	2.750020583	-7.622537360	2.238319442
	O476	-0.511877475	5.619349798	-3.900792055
	O477	-0.357355028	-13.196281738	0.810826756
	O478	0.552404468	-11.078473450	2.759415376
	S479	5.807372733	1.214796800	-2.618584680
	S480	2.596566857	-0.536263647	-3.232952211
	S481	-0.423998241	-4.607690273	-2.430137485
	S482	3.756080670	-0.824747907	0.023488197
	S483	-0.311249517	-1.596034456	-1.689863377
	S484	2.763376946	-4.269299411	-4.660156853
	S485	0.751664452	-4.868003243	0.988193904
	S486	5.488900612	-2.650912195	-2.540610124
	S487	2.588111366	-6.559488578	-1.674331985
	S488	4.530548114	-4.563350046	0.666479601
	end			
N2x-Fe2-brNH2-Fe6-3b2 to N2x-	965182n2x3btonh335th.car_5			
	C1	-9.382518244	0.815882698	1.041259191

Fe2NH3
S=1, 35
reactant

Fe(139) -2.138
Fe(140) 0.019
Fe(141) -2.513
Fe(142) 2.631
Fe(143) 2.542
Fe(144) 2.082
Fe(145) -1.045

C2	-10.382164892	-0.048686769	0.264569407
C3	-8.804632074	3.101947238	1.739310028
C4	-8.535818527	2.906274924	3.227907672
C5	-9.251817849	1.924350937	5.345000284
C6	-8.123701941	0.909713261	5.567788537
C7	-6.748911795	-0.861408902	4.598306983
C8	-5.438947353	-0.087953546	4.426825517
C9	-4.278061950	1.720027479	3.251772229
C10	-3.874081950	2.527602680	4.493649094
C11	-4.545854843	3.843079217	6.408798014
C12	-4.113672163	3.017872030	7.629849511
C13	-4.705738845	1.198593602	9.169371234
C14	-3.823150111	-0.053663831	9.088861415
C15	-3.108405363	-1.956133694	7.715564719
C16	-1.773063367	-1.668172642	7.023169720
C17	-0.532712639	-0.216116317	5.491676191
C18	0.414436291	0.773739056	6.192765403
C19	-0.845574991	0.142524819	4.019641447
C20	0.424274501	0.548223696	3.260715313
C21	-1.537419308	-1.031945642	3.316520324
C22	0.839735099	3.043264925	7.004409099
C23	0.890048025	2.985509462	8.543415914
C24	0.529495894	4.449249744	6.437532759
C25	1.425967178	5.510952869	7.084834729
C26	0.708277688	4.454938837	4.913191087
C27	-0.268266665	2.840701573	10.666802742
C28	0.579120063	1.680833813	11.158785056
C29	-2.602030472	-11.355698901	6.817242564
C30	-1.338091011	-10.889347607	6.100246265
C31	0.401519608	-9.120735930	6.091371747
C32	1.567269468	-9.431513787	7.048122799
C33	0.229055258	-7.598178544	5.946500732
C34	1.498435848	-6.953324163	5.393676304
C35	1.340736935	-5.473309860	5.084081522
C36	3.063829141	-3.789234974	4.428605557
C37	3.933276009	-10.043269035	7.188299111
C38	5.014473732	-9.015628678	6.940903783
C39	-5.842922480	0.694067892	-1.846170856
C40	-5.349475308	2.148381198	-1.712676259
C41	-4.674379432	-0.277517093	-1.584004573
C42	-5.092158650	-1.736190235	-1.304023564
C43	-5.234084813	-2.636162558	-2.531612501
C44	-4.233709596	3.910705798	-3.064285517
C45	-4.842935573	5.172027370	-2.443913036
C46	-3.947827495	4.086567927	-4.562704094
C47	-6.888164028	6.315586885	-1.736220977
C48	-6.585423337	6.494250191	-0.243924770
C49	-5.619077300	5.541366197	1.794498711
C50	-4.113630609	5.646489437	2.051563420
C51	-1.834711777	5.674525176	1.153789574
C52	-1.386214055	7.106483130	1.483873519
C53	-1.076171574	5.261677561	-0.118217968
C54	-1.329735252	3.859860890	-0.557478146
C55	-1.886827031	2.759506757	0.060365290
C56	-1.362113398	2.103139824	-1.916983864
C57	-1.654928675	9.457977480	0.830214625
C58	-1.463671263	9.906233696	2.276589689
C59	-2.781962746	10.277686687	0.156271881
C60	-2.453819670	11.680823390	-0.262548648
C61	-1.756458187	12.682494933	0.384337571
C62	-2.523099736	13.411870685	-1.562833607
C63	8.160990366	-3.397966218	4.495858202
C64	8.245531244	-4.900077052	4.703281205
C65	6.673176503	-3.072065915	4.237198795
C66	6.392780018	-1.594488595	4.084931049
C67	6.042803948	-0.800167447	5.192644597
C68	6.459508777	-0.971516215	2.824608030
C69	5.757160241	0.561794050	5.051205306
C70	6.190769832	0.388985479	2.670290659
C71	5.831943416	1.153469452	3.783345590
C72	8.389367820	1.743514084	-1.714387674
C73	8.256184389	3.167648053	-2.272672133
C74	7.030482204	1.238748520	-1.224941419
C75	8.451458426	4.597301881	-4.274491842
C76	7.053288126	5.122501809	-4.604398888
C77	4.616829022	4.624441576	-4.488529113
C78	4.008687515	5.023766383	-3.119544570
C79	3.902124050	3.417506474	-5.135101765
C80	2.379999073	3.457497824	-5.303105614
C81	1.833507686	4.342558357	-6.434181295

C82	1.780258032	6.834409450	-6.561156056
C83	3.722313083	4.536061830	-0.740024727
C84	4.358315043	5.779719645	-0.106714592
C85	3.865718146	3.377287261	0.265456295
C86	6.498922871	6.836357096	0.427147186
C87	6.873779847	8.145333711	-0.244936398
C88	6.634102433	9.572143477	-2.196583784
C89	5.992425366	10.922370174	-1.791149050
C90	6.524022276	9.358627243	-3.710742706
C91	5.093227852	9.314947155	-4.232358769
C92	4.100255218	12.052891351	-0.735818308
C93	4.857972714	13.104123526	0.059938857
C94	2.797516478	11.652709752	0.010465589
C95	1.937672532	10.734155767	-0.826910352
C96	1.025681497	11.261632502	-1.753078134
C97	2.071710589	9.337708636	-0.752557758
C98	0.284385849	10.430795943	-2.595638691
C99	1.359040154	8.491490599	-1.606744099
C100	0.474957980	9.048952144	-2.526044667
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C114	-3.261962099	0.389709882	-8.631317075
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H157	-3.404804226	1.124795216	2.958434033
H158	-6.244703593	0.958117427	2.851615497
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H160	-3.719204898	4.527715479	6.177959997
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	H167	-1.797183179	-0.759501626	2.281179722
	H168	-0.870406695	-1.909089756	3.277253064
	H169	-1.521352695	1.011285269	4.025279340
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	H171	0.053026494	3.727102979	4.414884848
	H172	-1.190098816	2.932891523	8.730930032
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	H175	1.156109386	-0.274619110	3.234253939
	H176	8.459252937	-2.916705743	5.447391328
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	H180	2.488493851	5.275343985	6.911722715
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	H182	1.861079760	2.766838148	6.703266228
	H183	-0.971031880	2.304364423	6.091632725
	H184	0.914926645	1.423666899	3.710739255
	H185	3.592389445	2.437926836	-0.234622972
	H186	3.143437076	3.563107046	1.074245736
	H187	5.146476577	3.073664884	1.733949864
	H188	5.244644320	2.897083253	4.401102349
	H189	6.214689986	0.852647742	1.684082338
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	H191	5.978739318	-1.254194573	6.185181583
	H192	-2.588280565	-0.040820050	6.063256685
	H193	-3.657565744	-2.680222390	7.095252997
	H194	-2.873567978	-2.436341086	8.673052359
	H195	-4.498185766	-0.452197994	7.168758001
	H196	-4.241839044	1.856503138	9.914026306
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	H200	-1.298568768	2.665328199	11.011988220
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	H203	-5.030984436	-4.580508230	-3.132352164
	H204	-2.635335399	-5.851254286	-0.421185831
	H205	-5.630329182	-5.474997865	-7.415623946
	H206	-3.936088549	-5.823527574	-7.846404335
	H207	-5.104925094	-3.232652093	-6.682252708
	H208	-1.570336831	0.130290270	-10.050216373
	H209	-5.187915692	-3.655710854	-9.187917969
	H210	-3.985528633	-0.242081822	-2.442257370
	H211	-6.061824074	-1.760188085	-0.775045261
	H212	-2.374105144	-1.540319913	-8.325663445
	H213	-4.103896464	0.626247357	-9.314503792
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	H220	-2.562286726	-6.347519676	-6.286257006
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	H236	-3.659892411	5.480728101	0.031914254
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	H239	-1.188121677	1.500954525	-2.805663985
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	H241	9.974570663	-3.052355259	3.610114069

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	H247	-1.441334100	5.469072959	-4.182728728
	H248	-3.062715590	5.396156959	-5.721263584
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	H261	4.138108646	2.530073371	-4.526413595
	H262	6.250034789	3.349219410	-3.989278759
	H263	1.879326429	3.711088310	-4.355584051
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	H265	9.020658834	4.537658605	-5.210988277
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	H267	4.372158034	3.247971068	-6.118111117
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	H273	-6.578852946	0.561976734	-1.030516691
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	H280	5.958665157	7.085399426	1.352743725
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	H319	-0.144487807	-12.556168033	1.522099300
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N385	-0.820601925	-9.737146204	6.574883111
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N392	-5.060509870	2.722805400	-2.913388093
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N394	-6.038689692	5.431914380	0.408928819
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N396	-1.000418532	3.423727890	-1.827124017
N397	-1.905212165	1.675433766	-0.787063262
N398	-2.078105351	8.069228310	0.823635898
N399	-2.928828866	12.151003623	-1.477673267
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	N403	8.502256909	3.309523241	-3.607972190
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	N408	4.278670454	4.213658001	-2.056239663
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	N410	6.210152393	8.435069245	-1.404986269
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	N412	4.925061337	10.871669801	-0.954828854
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	N415	1.293442230	-2.426132151	-6.948251043
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	N418	-3.250929935	-1.058301691	-8.547468795
	N419	2.072271254	-11.702868241	-3.195686058
	N420	-0.093220676	-7.901148473	-2.528548702
	N421	-1.143237542	-8.709990535	-4.289573280
	N422	2.588677995	-11.972863622	-0.093417226
	O423	-8.363500942	0.355005605	1.586835608
	O424	-7.484835106	3.333731363	3.735933273
	O425	-7.467286237	0.921464309	6.622758651
	O426	-4.450457353	-0.304255936	5.149804331
	O427	-2.679351966	2.685072165	4.791217035
	O428	-3.140974042	3.368045623	8.319926969
	O429	-3.094831925	-0.368827599	10.040328165
	O430	-0.829212576	-2.461658700	7.151451714
	O431	1.567161725	0.418128468	6.490511253
	O432	1.975628945	2.994981803	9.151198342
	O433	1.066955589	1.630937523	12.277078902
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	O435	1.437835108	-9.302080171	8.277654315
	O436	6.201099398	-9.225115029	7.140379572
	O437	-5.235503079	2.736122308	-0.620887913
	O438	-5.629143866	-2.204147719	-3.639479682
	O439	-4.118853910	6.080053828	-2.000200589
	O440	-3.070574341	5.211203396	-4.765231823
	O441	-6.866672289	7.572024906	0.301000444
	O442	-3.700308299	5.779864393	3.211337071
	O443	-0.419460253	7.355375615	2.213402423
	O444	-0.641606121	10.730540779	2.643855778
	O445	8.240067221	-5.442562419	5.799211530
	O446	5.542578638	2.485641353	3.568790088
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	O448	6.927943764	6.273673390	-5.067855052
	O449	3.313738506	6.046544350	-3.021885580
	O450	3.710711386	6.521403519	0.642627947
	O451	5.197391604	3.292172984	0.782015422
	O452	7.719923576	8.896913934	0.255334448
	O453	6.479146231	11.990675292	-2.188297302
	O454	4.250671543	10.163783230	-3.905935455
	O455	4.535686427	14.282460773	0.075107948
	O456	-0.187076058	8.183668887	-3.413778369
	O457	-1.382883892	-6.632226918	-7.427144822
	O458	-0.620887005	-2.507198885	-8.208015963
	O459	3.898344963	-0.496075132	-8.636275441
	O460	7.299411920	-2.230515941	-8.807435662
	O461	-5.474111839	-1.222100882	-9.031868622
	O462	-5.200977637	-5.701623447	-4.844875367
	O463	-3.150258325	-6.320627693	-5.470132640
	O464	-1.631903768	2.038570120	-9.341186999
	O465	4.437487004	-10.991063433	-0.961393399
	O466	5.564764516	-13.446876244	1.267611180
	O467	-3.520845452	-5.273620914	-0.082954164
	O468	-4.642677024	-5.234573961	1.865926606
	O469	-2.669382299	-12.233879115	-0.320339769
	O470	-4.447650433	-10.888361983	-0.698036089
	O471	0.443141780	-7.866004949	0.622812734
	O472	-0.665197084	-8.704519397	2.390024407
	O473	-1.654479228	-6.762055935	-0.453077296
	O474	2.980478012	-10.112411210	3.640082330
	O475	2.782975453	-7.653450092	2.211294929
	O476	-0.505521642	5.617106435	-3.891533773
	O477	-0.376942573	-13.206887519	0.822524166
	O478	0.547431488	-11.090189418	2.767484417
	S479	5.762568521	1.172680890	-2.575212005
	S480	2.743356113	-0.462779693	-3.232516401
	S481	-0.463925103	-4.589004987	-2.324163119

	S482	3.909681508	-0.905118216	0.079867652
	S483	-0.277338274	-1.401303299	-1.769173349
	S484	2.732188863	-4.268447780	-4.628676800
	S485	0.800002785	-5.055273417	1.232571902
	S486	5.445639916	-2.708068059	-2.611468199
	S487	2.613192965	-6.539315214	-1.662721136
	S488	4.549275412	-4.580817253	0.660231028
	end			
N2x-Fe2-brNH2-Fe6-3b2 to N2x-Fe2NH3 **S=1, 35** **TS** Fe(139) -2.321 Fe(140) -0.033 Fe(141) -2.423 Fe(142) 2.894 Fe(143) 3.143 Fe(144) 2.460 Fe(145) -1.999	965182n2x3btonh335tl.car_1			
	C1	-9.368038057	0.810715767	1.011408660
	C2	-10.416406321	-0.028762608	0.267882311
	C3	-8.781803364	3.094983704	1.733558622
	C4	-8.501825818	2.890686510	3.219077832
	C5	-9.208696019	1.913863793	5.339946028
	C6	-8.073626432	0.904301012	5.547219987
	C7	-6.720863693	-0.873070555	4.562049002
	C8	-5.413794663	-0.096073059	4.389971795
	C9	-4.257450170	1.717977063	3.208380208
	C10	-3.830294552	2.528627629	4.439949376
	C11	-4.455904182	3.817369173	6.383298178
	C12	-4.010861730	2.973622759	7.587040080
	C13	-4.616436422	1.153329049	9.120620090
	C14	-3.734829745	-0.098976581	9.051659942
	C15	-3.029031844	-2.024493590	7.715606809
	C16	-1.714709592	-1.702089733	7.001836545
	C17	-0.553235567	-0.229393758	5.445329946
	C18	0.440018764	0.720846252	6.130933187
	C19	-0.892419433	0.155038367	3.982304968
	C20	0.361957394	0.581174293	3.207934157
	C21	-1.585811255	-1.003768207	3.253368786
	C22	0.905045695	2.970504019	6.979580632
	C23	0.968742360	2.919318212	8.526128122
	C24	0.592747137	4.365859795	6.389545038
	C25	1.457061682	5.453120286	7.032629904
	C26	0.785620828	4.368406361	4.865047882
	C27	-0.193562585	2.779251561	10.672757631
	C28	0.645692340	1.591466286	11.112848722
	C29	-2.561542751	-11.347706314	6.807570151
	C30	-1.309277064	-10.856424180	6.088315460
	C31	0.379796292	-9.035474299	6.074641802
	C32	1.551654174	-9.314986315	7.035929989
	C33	0.161637725	-7.519559597	5.932610458
	C34	1.427856610	-6.853763687	5.406595586
	C35	1.305175611	-5.357484257	5.172498323
	C36	3.131523515	-3.759492732	4.554612397
	C37	3.897281531	-9.997187586	7.198477822
	C38	5.023100573	-9.014545380	6.966420485
	C39	-5.828664806	0.695225152	-1.838968708
	C40	-5.344892958	2.152829680	-1.698971753
	C41	-4.673705963	-0.284365565	-1.552068956
	C42	-5.117588299	-1.737026654	-1.277999494
	C43	-5.262259294	-2.639007678	-2.504573630
	C44	-4.245696654	3.928092036	-3.046136389
	C45	-4.866815533	5.188395468	-2.435552714
	C46	-3.948051719	4.099868152	-4.542852150
	C47	-6.914779434	6.327095037	-1.732371499
	C48	-6.605277891	6.508895462	-0.241544310
	C49	-5.635937335	5.552221937	1.794927249
	C50	-4.129409881	5.649592956	2.048318707
	C51	-1.852013528	5.671489060	1.143951268
	C52	-1.407608727	7.100786561	1.480407360
	C53	-1.101833427	5.283084647	-0.140729798
	C54	-1.323908796	3.875082317	-0.573255540
	C55	-1.883249320	2.777784107	0.047073002
	C56	-1.341193192	2.110854383	-1.921500360
	C57	-1.664366352	9.443185912	0.816927013
	C58	-1.496518430	9.898607080	2.264570574
	C59	-2.782926184	10.270766433	0.136892287
	C60	-2.455034858	11.674490642	-0.282485786
	C61	-1.751816460	12.678496664	0.355057587
	C62	-2.554894731	13.408374801	-1.577842602
	C63	8.081893700	-3.399076610	4.546989298
	C64	8.162941316	-4.899629078	4.769714968
	C65	6.608658006	-3.064107656	4.275693742
	C66	6.347186602	-1.582227490	4.125032834
	C67	6.001559838	-0.778905360	5.228260559
	C68	6.422443803	-0.968628432	2.861189205
	C69	5.725212296	0.584104563	5.075952296
	C70	6.165972056	0.391852929	2.697173608
	C71	5.809565824	1.166373289	3.804389350

C72	8.405655670	1.739458061	-1.687101213
C73	8.273683984	3.164095284	-2.253600076
C74	7.048779355	1.246226453	-1.198462088
C75	8.462953981	4.586911528	-4.266399466
C76	7.066252974	5.120156939	-4.594998528
C77	4.626231105	4.638373269	-4.482445346
C78	4.014461936	5.040975430	-3.116891739
C79	3.907264320	3.433676163	-5.130269678
C80	2.384268860	3.474315553	-5.297905487
C81	1.836748211	4.356966461	-6.430293904
C82	1.782395510	6.848273867	-6.561860914
C83	3.711522458	4.557644155	-0.741024416
C84	4.362994819	5.788819602	-0.096656681
C85	3.818079354	3.391491709	0.258439486
C86	6.508591591	6.845355837	0.423892689
C87	6.864548941	8.160146183	-0.249039676
C88	6.618434479	9.580158777	-2.204985848
C89	5.966543140	10.924479306	-1.802552649
C90	6.512064798	9.362601588	-3.718646698
C91	5.082157689	9.304362504	-4.240306991
C92	4.085101830	12.051276014	-0.739501826
C93	4.845372591	13.108301718	0.047348673
C94	2.776728921	11.670872171	0.005502165
C95	1.917333597	10.749691249	-0.827638713
C96	1.003107000	11.274082444	-1.752923071
C97	2.060797163	9.354301365	-0.755458836
C98	0.269276674	10.440263172	-2.599046106
C99	1.358273026	8.505563962	-1.614977044
C100	0.472280633	9.060305910	-2.534133878
C101	0.813893199	-7.649716611	-7.490893220
C102	-0.140535449	-6.489897301	-7.255386692
C103	-0.303454179	-4.155032563	-6.417060727
C104	0.124546541	-2.948252133	-7.261035661
C105	1.898779472	-1.283339770	-7.609987201
C106	3.412229946	-1.257252953	-7.807492792
C107	5.643200716	-1.945616686	-7.119253799
C108	6.213409861	-2.495371929	-8.412615452
C109	-4.295040633	-3.280835673	-8.699557181
C110	-4.420731251	-1.753650319	-8.761197530
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C112	-4.589181972	-5.273193800	-7.138291113
C113	-4.349919543	-5.777949373	-5.733055685
C114	-3.292528339	0.410894834	-8.619390875
C115	-2.083880374	0.921959841	-9.378046928
C116	-3.556767386	1.126422396	-7.271993582
C117	-2.588983696	0.639071249	-6.234023809
C118	-1.307872846	1.202994575	-6.128524585
C119	-2.898102787	-0.506681250	-5.481886300
C120	-0.327673603	0.574407194	-5.356428759
C121	-1.916753480	-1.130297691	-4.711338852
C122	-0.619143526	-0.611015125	-4.681173749
C123	2.358173637	-10.645340400	-2.176676855
C124	3.202752698	-11.186596413	-1.010308601
C125	1.057190865	-10.004042910	-1.671843162
C126	0.246630377	-9.259033436	-2.684877680
C127	-0.396220221	-9.780969997	-3.787911565
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C130	4.579566920	-13.239621344	0.584371836
C131	-3.743906484	-5.638675849	1.132244295
C132	-2.651265422	-6.531187183	1.716749033
C133	-1.985726379	-7.498214536	0.690949774
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C137	-0.675352807	-8.043500644	1.275658424
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Fe139	1.802447886	-4.782095849	-2.732762245
Fe140	1.862849945	-1.271114190	-1.044994569
Fe141	4.152333984	-2.888041996	-0.732468224
Fe142	3.350373386	-2.721160624	-3.209842905
Fe143	4.582282729	-0.631748548	-1.991015333
Fe144	2.575839365	-4.883638813	-0.270557754
Fe145	0.529682048	-3.434719930	-0.934984123
H146	-9.691459565	-1.890358008	0.693973038
H147	-9.253476187	-1.341715592	-0.781659500
H148	-10.509226967	2.481142670	0.645620944
H149	-10.745328627	0.530017174	-0.622882650
H150	-11.296635016	-0.081204300	0.932804383
H151	-7.806500956	3.073660773	1.225072076

	H152	-10.296938197	1.934714058	3.481862869
	H153	-9.209550364	4.097951706	1.599341298
	H154	-10.132705574	1.499475575	5.764657819
	H155	-8.395255599	0.101289786	3.675676457
	H156	-8.939454665	2.811010181	5.912237445
	H157	-3.391320124	1.119311529	2.901486958
	H158	-6.230869781	0.967295774	2.834745361
	H159	-6.828502555	-1.603894865	3.748889001
	H160	-3.626360707	4.494789973	6.142362508
	H161	-5.785437094	3.020215478	4.878674504
	H162	-6.655551205	-1.416022221	5.512455201
	H163	-4.500257564	2.400516260	2.382011232
	H164	-5.615234716	1.704720237	7.307883213
	H165	-5.323394334	4.419096864	6.687491748
	H166	-2.516637321	-1.315463970	3.747390500
	H167	-1.839193958	-0.705314575	2.222673783
	H168	-0.921397978	-1.881684107	3.189163288
	H169	-1.567978363	1.021528131	4.010065221
	H170	-5.608000591	0.845332597	9.483137529
	H171	0.155708992	3.623664392	4.359425007
	H172	-1.103353478	2.909790346	8.729198575
	H173	1.331831335	5.494239622	8.124045571
	H174	0.084508339	0.854443624	2.178828860
	H175	1.101078307	-0.234111116	3.156092586
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	O472 -0.681133993 -8.677218422 2.348545834 O473 -1.689736503 -6.761546823 -0.500442900 O474 2.946907656 -10.085664346 3.647998194 O475 2.718364327 -7.607510938 2.238610720 O476 -0.497561478 5.623125656 -3.886112858 O477 -0.387285817 -13.192832311 0.829430456 O478 0.531346492 -11.074295586 2.752546935 S479 5.794261711 1.223439677 -2.557327980 S480 2.633536346 -0.556658192 -3.253968350 S481 -0.450438965 -4.650274332 -2.510122548 S482 3.881518659 -0.877009284 0.127868350 S483 -0.344846439 -1.628934591 -1.685697881 S484 2.838772952 -4.334489737 -4.653934851 S485 0.713298472 -5.004758378 1.129276087 S486 5.513281920 -2.666680350 -2.479428580 S487 2.593589961 -6.620230035 -1.655536590 S488 4.512791203 -4.545214754 0.696714527 end
N2x-Fe2-brNH2-Fe6-3b2 to N2x-Fe2NH3 **S=1, 35** **product** Fe(139) -2.288 Fe(140) 0.014 Fe(141) -2.716 Fe(142) 2.742 Fe(143) 3.173 Fe(144) 2.291 Fe(145) -1.725	965182n2x26nh26htonh335tc.car_7 C1 -9.409010853 0.821786622 1.055909927 C2 -10.382380914 -0.057292764 0.262074778 C3 -8.847294706 3.110212643 1.750114475 C4 -8.568771512 2.910796398 3.236434549 C5 -9.277583170 1.928639665 5.356233961 C6 -8.146490182 0.917898063 5.580787859 C7 -6.764343213 -0.852735295 4.620802016 C8 -5.451665333 -0.085149815 4.441920520 C9 -4.292760863 1.726659298 3.276575498 C10 -3.899615598 2.535804332 4.520940322 C11 -4.595445863 3.856860931 6.425858625 C12 -4.168889556 3.035012953 7.651210704 C13 -4.762712580 1.222332902 9.195479376 C14 -3.873036487 -0.025117775 9.113354473 C15 -3.144757196 -1.921525235 7.733502763 C16 -1.797881396 -1.655431838 7.052861432 C17 -0.529458099 -0.213829574 5.521891517 C18 0.397884598 0.780064045 6.247822523 C19 -0.839298214 0.181073465 4.062361121 C20 0.422759978 0.687020208 3.357371477 C21 -1.476658718 -0.998183685 3.315973600 C22 0.808997340 3.066294979 7.019589914 C23 0.848645232 3.006489040 8.557956150 C24 0.486133632 4.473201379 6.461580581 C25 1.386046337 5.532080783 7.110065315 C26 0.650265413 4.495547309 4.936042404 C27 -0.336106174 2.865688149 10.665356513 C28 0.524336252 1.726487194 11.179004328 C29 -2.611744165 -11.361977904 6.820223935 C30 -1.346329992 -10.907614699 6.096507032 C31 0.425322728 -9.169024617 6.093491411 C32 1.596220211 -9.480059588 7.043083422 C33 0.256783263 -7.645726075 5.941857845 C34 1.514443375 -6.994067333 5.366618204 C35 1.305298323 -5.529426140 5.006812187 C36 3.002356209 -3.816157718 4.346323880 C37 3.970661445 -10.065748062 7.162931720 C38 5.030732071 -9.011909438 6.935633813 C39 -5.870765725 0.697961128 -1.852948341 C40 -5.369300962 2.149288946 -1.726330373 C41 -4.693768871 -0.265855300 -1.598542404 C42 -5.093169240 -1.728473955 -1.317747405 C43 -5.238826666 -2.627585471 -2.546081380 C44 -4.239973221 3.898163466 -3.080816454 C45 -4.837449480 5.163730086 -2.457818036 C46 -3.952617458 4.071270208 -4.579032693 C47 -6.873080013 6.320048625 -1.742473026 C48 -6.569709541 6.490734860 -0.249328670 C49 -5.606906070 5.526939743 1.784804444 C50 -4.102338395 5.635854804 2.044665407 C51 -1.822522431 5.690074464 1.155093584 C52 -1.370753201 7.122189129 1.481938812 C53 -1.052203769 5.267974106 -0.106857551 C54 -1.302278806 3.862543523 -0.538627174 C55 -1.828117351 2.755850217 0.096718385 C56 -1.365670820 2.106033946 -1.897972588 C57 -1.656628433 9.477419000 0.851656728 C58 -1.460036147 9.924248498 2.298161432 C59 -2.782602218 10.298225112 0.177545119 C60 -2.449254089 11.698931909 -0.245117133 C61 -1.754914956 12.701739594 0.403261342

C62	-2.504438928	13.424730567	-1.552757728
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C65	6.690218254	-3.094490449	4.211612679
C66	6.397267361	-1.618905705	4.062122262
C67	6.046669943	-0.827633506	5.171956133
C68	6.463665977	-0.993314550	2.803178149
C69	5.763480352	0.535412747	5.033771737
C70	6.197197082	0.367622461	2.652109895
C71	5.840384990	1.130035486	3.767055983
C72	8.393922669	1.721663935	-1.735691896
C73	8.267542335	3.154500146	-2.279384669
C74	7.021184858	1.208698655	-1.307878319
C75	8.456204810	4.605537850	-4.269879852
C76	7.054942738	5.123569294	-4.601696808
C77	4.620574908	4.621432682	-4.498429162
C78	4.012811096	5.011876206	-3.127372109
C79	3.902299680	3.416891225	-5.147895832
C80	2.378763949	3.459024546	-5.312338372
C81	1.830516309	4.349575883	-6.438568975
C82	1.778939595	6.842269697	-6.561844570
C83	3.714800021	4.512833753	-0.754683287
C84	4.350285615	5.753564620	-0.112131020
C85	3.840794805	3.351747849	0.248812917
C86	6.482829465	6.825349658	0.425676629
C87	6.866655494	8.134802845	-0.242593213
C88	6.642666131	9.574863681	-2.188548343
C89	6.007084659	10.927519501	-1.782882550
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C91	5.103489407	9.324233314	-4.225925111
C92	4.114440565	12.062725090	-0.728260507
C93	4.871229644	13.111561981	0.071346854
C94	2.811812194	11.657203985	0.017197357
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C96	1.040132616	11.266256236	-1.745957664
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C98	0.296587919	10.436028301	-2.586811557
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C121	-2.005731606	-1.089039748	-4.626059712
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C126	0.253737409	-9.339605664	-2.716887630
C127	-0.389894487	-9.890674180	-3.805154713
C128	-1.034178660	-7.787555983	-3.563469781
C129	3.385616232	-12.462300449	1.031308023
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C131	-3.671143319	-5.618090666	1.180996541
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C134	-2.889185765	-8.659588249	0.450329309
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C136	-3.218676092	-11.070805595	-0.420322688
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Fe139	1.850593632	-4.836768351	-2.797686053
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Fe141	4.240986406	-2.953000745	-0.809884810

Fe142	3.303173035	-2.756562193	-3.201818208
Fe143	4.612008137	-0.700232565	-2.192900362
Fe144	2.579156566	-4.886382207	-0.338637122
Fe145	0.501621510	-3.601805275	-1.149947079
H146	-9.592667157	-1.867607940	0.773488026
H147	-9.097804610	-1.332738785	-0.685721158
H148	-10.537473368	2.481659613	0.609211734
H149	-10.670502414	0.472645378	-0.659730784
H150	-11.302890249	-0.136318346	0.865673060
H151	-7.870257519	3.088659762	1.244309169
H152	-10.350906042	1.932106959	3.490717606
H153	-9.276886183	4.111333609	1.609633157
H154	-10.205509604	1.519619222	5.777767370
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H156	-9.010991159	2.828147688	5.926031508
H157	-3.418047652	1.129906489	2.990951636
H158	-6.264015284	0.975050667	2.878480323
H159	-6.867482664	-1.598511718	3.820954709
H160	-3.770799562	4.546165183	6.202279690
H161	-5.865847820	3.042188673	4.883738496
H162	-6.711454698	-1.378012349	5.582057035
H163	-4.519859713	2.408812664	2.445710177
H164	-5.780305452	1.765546690	7.390016233
H165	-5.482483634	4.446642730	6.694471613
H166	-2.411195014	-1.320340652	3.797592260
H167	-1.711632415	-0.722320574	2.275901530
H168	-0.797439250	-1.866338299	3.288954526
H169	-1.552547659	1.018320042	4.087842605
H170	-5.746906540	0.905461827	9.570705055
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H178	1.182893209	6.519326779	6.669394975
H179	1.686094175	4.236322109	4.658857742
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H181	-0.565135646	4.708034007	6.709108051
H182	1.834465186	2.802040995	6.721180662
H183	-0.986128579	2.310535166	6.087388091
H184	0.829686448	1.592143080	3.828278591
H185	3.545161481	2.415373796	-0.247300938
H186	3.127607480	3.552840354	1.062685428
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H188	5.259396256	2.874308462	4.388788432
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H192	-2.591757566	-0.033473917	6.067981764
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	H224	-6.066969793	6.430864680	2.207576731
	H225	-5.818216932	4.553347357	-0.107770056
	H226	-2.893178687	7.820419078	0.297797784
	H227	-1.229256038	12.731742906	1.351299544
	H228	-2.193548608	9.470913026	3.007743403
	H229	-3.667343859	10.289882567	0.839198764
	H230	-0.707217519	9.610397302	0.309291643
	H231	-2.687707803	14.104528573	-2.381492454
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	H233	-1.313294340	5.957133345	-0.927679353
	H234	-1.370169156	14.694507192	-0.272615349
	H235	-3.078667123	9.761477479	-0.737314584
	H236	-3.642669157	5.494534423	0.023233388
	H237	-5.984740699	4.674131040	2.368960256
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	H239	-1.220107343	1.509946629	-2.795393896
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	H246	-0.637825422	4.028091179	-2.565023297
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	H249	-0.495071220	6.512046161	-3.469715981
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	H251	-4.898274775	4.236222324	-5.119924427
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	H255	3.852907261	8.182509548	-5.323514578
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	H257	0.935366342	3.885862015	-6.881021310
	H258	-0.422235125	10.863761677	-3.289698096
	H259	2.743605879	8.881019361	-0.004134309
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	H266	-5.293017683	2.083162809	-3.713365065
	H267	4.370596224	3.250128670	-6.132213140
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	H269	8.923894913	5.369286344	-3.631499004
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	H271	1.433419491	8.851923574	-6.467185003
	H272	-6.274222328	-0.496251655	-3.479219412
	H273	-6.600703224	0.567974385	-1.031001934
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	H275	-3.287026331	3.745866353	-2.553498761
	H276	4.544376931	5.514975365	-5.125800393
	H277	2.578099573	4.426878974	-7.238839933
	H278	2.075393241	2.429881683	-5.547760882
	H279	0.798301435	5.722188580	-5.170250907
	H280	5.932541051	7.077298257	1.344443735
	H281	5.604647154	7.718289505	-1.804709426
	H282	7.709568560	9.718381635	-1.957868448
	H283	7.416498869	6.323925338	0.715820466
	H284	4.515767909	9.967412527	-0.796717563
	H285	1.800255601	-7.234347783	-7.773253589
	H286	0.976203332	-8.095431112	-6.458928972
	H287	2.993055634	-9.960176769	-2.717697235
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	H290	7.142881781	0.195582312	-0.904206854
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	H292	8.745866836	2.492513850	-4.165645937
	H293	6.598714627	1.859537757	-0.529214463
	H294	10.256151300	1.927558675	-0.896252603
	H295	5.996779127	-2.697332548	-6.330361507
	H296	8.788019571	1.061727399	-2.524006059
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	H298	0.622055628	-9.601906855	5.104365485
	H299	3.720429660	-2.733570667	-6.343569739
	H300	4.255834933	-2.465138611	3.494615515
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	O449	3.321689898	6.036445809	-3.021584222
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N2x-Fe2-brNH2-Fe6H to N2x-Fe2NH3 **S=1, 35** **reactant** Fe(139) -2.437 Fe(140) -0.418 Fe(141) -2.540 Fe(142) 2.795 Fe(143) 2.956 Fe(144) 1.970 Fe(145) -0.660	965182n2x26nh26htonh335te.car_5 C1 -9.377364547 0.813972169 1.043811421 C2 -10.365531193 -0.058737040 0.261717133 C3 -8.814650808 3.102988658 1.742194338 C4 -8.546135260 2.906929583 3.231183875 C5 -9.264563368 1.923719766 5.346983842 C6 -8.135632817 0.910831917 5.572916869 C7 -6.755313131 -0.859749190 4.611559672 C8 -5.444336776 -0.088781957 4.436768723 C9 -4.280541180 1.716714520 3.265016040 C10 -3.881876722 2.524909244 4.508320798 C11 -4.567341360 3.847082648 6.415956206 C12 -4.139964668 3.025475173 7.641014446 C13 -4.733437191 1.210271590 9.183622902 C14 -3.847847629 -0.039765521 9.101113993 C15 -3.126390705 -1.936359588 7.721609520 C16 -1.784273254 -1.657988767 7.036444219 C17 -0.527250436 -0.218826335 5.503874028 C18 0.412005878 0.777404780 6.208217420 C19 -0.830547891 0.136592601 4.028273619 C20 0.443244113 0.544538136 3.277184664 C21 -1.517788098 -1.039610859 3.323808369 C22 0.825952790 3.053530727 7.009423921 C23 0.869637333 2.994880763 8.547509047 C24 0.511185474 4.460542380 6.447089056 C25 1.409906262 5.519910617 7.096025471 C26 0.684699342 4.473661580 4.922287432 C27 -0.299096237 2.855308450 10.664645198 C28 0.554372991 1.704550733 11.167395960 C29 -2.607340760 -11.354090822 6.802624325 C30 -1.338617159 -10.895508804 6.087344256 C31 0.417686261 -9.143944329 6.090086570 C32 1.584623753 -9.456099636 7.044100610 C33 0.247236189 -7.620913132 5.943658753 C34 1.512383170 -6.974539158 5.382015233 C35 1.337800789 -5.500666598 5.051290722 C36 3.047840558 -3.801304177 4.400700840 C37 3.955305280 -10.053718367 7.175096819 C38 5.026121950 -9.013023843 6.937696201 C39 -5.839628705 0.689750718 -1.846464571 C40 -5.345218239 2.143401375 -1.716854905 C41 -4.666437228 -0.280134971 -1.589311127 C42 -5.078939728 -1.738268553 -1.307161543 C43 -5.223094419 -2.639129148 -2.534358147 C44 -4.231959315 3.903987071 -3.071414751 C45 -4.838018461 5.165633162 -2.449338703 C46 -3.947033619 4.079353466 -4.570004715 C47 -6.879956916 6.312412890 -1.738136495 C48 -6.576746730 6.488293001 -0.245618132 C49 -5.609221937 5.532710305 1.790579691 C50 -4.104225979 5.640309207 2.048297939 C51 -1.824942955 5.682251577 1.156058955

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	C131	-3.717123986	-5.636551493	1.243533932

C132	-2.576374064	-6.496365216	1.786038514
C133	-1.938918577	-7.454177823	0.737559371
C134	-2.905673203	-8.638619402	0.453156762
C135	-2.301401321	-9.809436603	-0.328078243
C136	-3.218231328	-11.049197053	-0.432971033
C137	-0.632020902	-8.032616428	1.300234311
C138	2.418701001	-3.259688172	-1.518556498
Fe139	1.796787434	-4.744205872	-2.706714992
Fe140	1.819041860	-1.257906297	-1.155293143
Fe141	4.233006332	-2.931658232	-0.786761649
Fe142	3.303777320	-2.742292356	-3.196290545
Fe143	4.619018027	-0.681491566	-2.058539958
Fe144	2.601758764	-4.808561678	-0.313516597
Fe145	0.472366542	-3.423573534	-0.611817117
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H157	-3.407128303	1.119060725	2.976920919
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O442	-3.691927749	5.768202999	3.209000282
O443	-0.405416976	7.363330633	2.205451149
O444	-0.641720452	10.737987523	2.654557141
O445	8.291346657	-5.443766819	5.792483148
O446	5.551961401	2.472378034	3.558087511
O447	7.971421382	4.134657762	-1.546142482
O448	6.936035148	6.284757012	-5.064558861
O449	3.320880997	6.047973710	-3.021567946
O450	3.708107346	6.505632906	0.646590432
O451	5.177834592	3.262112948	0.761006714

	O452 7.719413283 8.896998588 0.259139141 O453 6.487726640 12.005467053 -2.187242684 O454 4.261476367 10.178185975 -3.907020638 O455 4.537705350 14.295005342 0.085300097 O456 -0.178571572 8.187112044 -3.409015919 O457 -1.385121721 -6.643345351 -7.411802957 O458 -0.614112128 -2.506978706 -8.223038648 O459 3.894686571 -0.493808596 -8.633132298 O460 7.292806019 -2.228060747 -8.819640013 O461 -5.461042287 -1.235767369 -9.028740882 O462 -5.201861903 -5.711112170 -4.833528573 O463 -3.147114687 -6.322993665 -5.453092110 O464 -1.607328912 2.021247972 -9.343840617 O465 4.441207215 -10.997296711 -0.978054349 O466 5.573359014 -13.445264825 1.271127667 O467 -3.581557172 -5.260974251 -0.033308442 O468 -4.664974484 -5.271230450 1.937101598 O469 -2.659589027 -12.197257244 -0.308775676 O470 -4.444203648 -10.854191475 -0.666504190 O471 0.443414502 -7.842474612 0.581885871 O472 -0.639548637 -8.668097999 2.373408780 O473 -1.657638805 -6.689656365 -0.436881874 O474 2.987100154 -10.113684857 3.628069056 O475 2.758850820 -7.622923448 2.241679840 O476 -0.506677232 5.623534014 -3.896165848 O477 -0.364114041 -13.198002427 0.810016169 O478 0.548934939 -11.081130481 2.761760676 S479 5.817416463 1.175336504 -2.637930782 S480 2.683275586 -0.574127965 -3.325225549 S481 -0.417505884 -4.582953838 -2.388079566 S482 3.942026918 -0.883321953 0.038275934 S483 -0.362006955 -1.580074443 -1.556723686 S484 2.757976674 -4.332257081 -4.662459815 S485 0.795468855 -4.878136775 1.013224658 S486 5.502014664 -2.713614313 -2.591511214 S487 2.592357884 -6.560145190 -1.667287468 S488 4.563573578 -4.582964917 0.645290243 end
N2x-Fe2-brNH2-Fe6H to N2x-Fe2NH3 **S=1, 35** **TS** Fe(139) -2.442 Fe(140) -0.072 Fe(141) -2.565 Fe(142) 2.582 Fe(143) 3.158 Fe(144) 2.110 Fe(145) -1.147	965182n2x26nh26htonh335te_1_53201.98 C1 -9.379758987 0.812206774 1.035520746 C2 -10.388879322 -0.047824570 0.265222168 C3 -8.792224209 3.095856821 1.736165768 C4 -8.523903186 2.900211215 3.224880470 C5 -9.240172927 1.917679581 5.340957752 C6 -8.112741133 0.901650202 5.560647264 C7 -6.742729843 -0.869465449 4.586876360 C8 -5.434896557 -0.092102167 4.418911297 C9 -4.275523403 1.715787477 3.238682826 C10 -3.864984742 2.524779808 4.477287931 C11 -4.520877432 3.832648693 6.401209799 C12 -4.085420207 3.004344128 7.619007744 C13 -4.678103730 1.182288360 9.155953052 C14 -3.797826408 -0.071468411 9.079107853 C15 -3.089306442 -1.981403999 7.715878341 C16 -1.761300833 -1.680893582 7.016286123 C17 -0.542310161 -0.214048781 5.488623027 C18 0.415390060 0.767412560 6.185985817 C19 -0.861075766 0.147135750 4.017655699 C20 0.404045504 0.557826572 3.253421048 C21 -1.553527342 -1.025933750 3.312015993 C22 0.853003226 3.029289704 7.010436099 C23 0.908693710 2.976655393 8.550226332 C24 0.548053124 4.431664410 6.433032741 C25 1.441073939 5.498721969 7.075027659 C26 0.732786450 4.426229962 4.909186338 C27 -0.238594519 2.834145780 10.680866694 C28 0.598304612 1.658525755 11.154767620 C29 -2.591905031 -11.356943166 6.808987461 C30 -1.330342898 -10.881393419 6.092371013 C31 0.397487832 -9.099679430 6.086034798 C32 1.563404084 -9.404708881 7.045078070 C33 0.217577549 -7.577557476 5.942964711 C34 1.485907760 -6.928129594 5.392910343 C35 1.332664433 -5.443054751 5.106863338 C36 3.078636941 -3.773574514 4.463479764 C37 3.925117026 -10.033210708 7.193142285 C38 5.018802622 -9.018687733 6.946328434 C39 -5.839174173 0.693182855 -1.840853376 C40 -5.343671292 2.147145556 -1.706277251 C41 -4.674406830 -0.281414644 -1.572008700

C42	-5.096793757	-1.739193260	-1.295554735
C43	-5.236254434	-2.638942989	-2.524270841
C44	-4.232386641	3.911941961	-3.058539858
C45	-4.845582503	5.171788693	-2.439616876
C46	-3.947033897	4.087789875	-4.557126201
C47	-6.893575240	6.311853101	-1.734544644
C48	-6.590410098	6.492641873	-0.242517363
C49	-5.621236205	5.541806375	1.795884827
C50	-4.115480146	5.647399502	2.050835655
C51	-1.837400866	5.675139961	1.149995064
C52	-1.390513853	7.108250620	1.482307520
C53	-1.080700511	5.265155586	-0.124574535
C54	-1.320136925	3.859058802	-0.561149932
C55	-1.872645131	2.756030043	0.056538373
C56	-1.349985158	2.103280936	-1.922444175
C57	-1.662902608	9.462071296	0.831955755
C58	-1.475632814	9.909814693	2.279305577
C59	-2.788520960	10.277672189	0.151709125
C60	-2.460176692	11.680076697	-0.268575515
C61	-1.757350446	12.679908025	0.375244460
C62	-2.531292545	13.411024498	-1.568428354
C63	8.152959615	-3.401097933	4.513188143
C64	8.228490341	-4.903090782	4.722806346
C65	6.667676604	-3.068894844	4.253350159
C66	6.391123589	-1.590467909	4.099194897
C67	6.042486789	-0.793172513	5.205443586
C68	6.454424829	-0.972041055	2.836358844
C69	5.754980111	0.567922982	5.059514168
C70	6.182758398	0.386999380	2.677613325
C71	5.826525030	1.155119497	3.789210287
C72	8.410523136	1.739048056	-1.695057286
C73	8.273649794	3.165028469	-2.256300496
C74	7.052140000	1.237280613	-1.214558438
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C77	4.627522960	4.634310952	-4.484843517
C78	4.013113988	5.030826927	-3.118560679
C79	3.912072447	3.429301536	-5.135209233
C80	2.389019821	3.467246342	-5.302091561
C81	1.838585847	4.349943618	-6.433175676
C82	1.783083182	6.841665881	-6.563508830
C83	3.716492634	4.544562643	-0.742554657
C84	4.360786193	5.782092929	-0.102904912
C85	3.836813303	3.381848116	0.260292291
C86	6.502961065	6.841947326	0.423382021
C87	6.872634410	8.154650985	-0.246338383
C88	6.633015256	9.584874824	-2.196878450
C89	5.988017990	10.934678417	-1.795752213
C90	6.526650864	9.367319163	-3.710776829
C91	5.096577932	9.314522470	-4.233346293
C92	4.096403175	12.064008523	-0.737710725
C93	4.853593610	13.115257260	0.059149609
C94	2.794294183	11.661774940	0.008916969
C95	1.935807589	10.741437130	-0.827890375
C96	1.022379372	11.267674651	-1.753278394
C97	2.072630837	9.345227177	-0.754098349
C98	0.282573935	10.435848114	-2.596081016
C99	1.361895857	8.497953431	-1.608834517
C100	0.476495325	9.054434699	-2.527479358
C101	0.821385761	-7.633839670	-7.458855549
C102	-0.146010536	-6.483286520	-7.232276339
C103	-0.331997699	-4.140309446	-6.422722826
C104	0.098114573	-2.937653600	-7.271530893
C105	1.884929831	-1.290506011	-7.634838249
C106	3.400037503	-1.279216629	-7.812406654
C107	5.614332979	-1.986540909	-7.107818068
C108	6.176766162	-2.483747612	-8.424869354
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C110	-4.388100870	-1.770251258	-8.766133176
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C113	-4.358865919	-5.792274782	-5.729088039
C114	-3.264827998	0.392454542	-8.623945637
C115	-2.052777535	0.897097499	-9.380303780
C116	-3.555161976	1.131668669	-7.294925532
C117	-2.596365943	0.657722500	-6.243966686
C118	-1.314028243	1.219954718	-6.145632870
C119	-2.902288289	-0.490483956	-5.494896113
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C122	-0.612960389	-0.610945521	-4.726249482
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C124	3.209479579	-11.197816939	-1.025335277
C125	1.071659987	-10.011475969	-1.674518910
C126	0.252506002	-9.263524132	-2.676976827
C127	-0.381410033	-9.767212871	-3.793935619
C128	-0.993050605	-7.660173437	-3.500542192
C129	3.364791110	-12.468622908	1.031835665
C130	4.578484000	-13.247714507	0.575479813
C131	-3.729072801	-5.638678366	1.195047540
C132	-2.614014120	-6.521739212	1.755031674
C133	-1.967572525	-7.482151379	0.712736953
C134	-2.924043922	-8.678639852	0.438462012
C135	-2.317039036	-9.844416819	-0.346987664
C136	-3.231323258	-11.086312099	-0.454465299
C137	-0.657198549	-8.047943718	1.274881413
C138	2.415870771	-3.264072793	-1.524687092
Fe139	1.791754963	-4.765528302	-2.739014425
Fe140	1.805525522	-1.242229104	-1.128795357
Fe141	4.210729809	-2.916244389	-0.751173941
Fe142	3.310154553	-2.767303038	-3.163756555
Fe143	4.587881924	-0.665950155	-2.083087455
Fe144	2.627617871	-4.852552811	-0.337375937
Fe145	0.499724030	-3.413414779	-0.666089124
H146	-9.617433447	-1.878342688	0.733954370
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H148	-10.498404230	2.484792025	0.611585265
H149	-10.698445548	0.495281773	-0.641668761
H150	-11.289422848	-0.115076351	0.900614695
H151	-7.813319014	3.061612876	1.234814813
H152	-10.309394157	1.924892218	3.472587770
H153	-9.209406374	4.101392368	1.590015160
H154	-10.170016742	1.512806576	5.762276760
H155	-8.398463366	0.114290721	3.675654898
H156	-8.968384178	2.815081422	5.911519815
H157	-3.403591677	1.120519383	2.941415266
H158	-6.239417829	0.948112451	2.839874775
H159	-6.841098016	-1.604954480	3.776635017
H160	-3.692365395	4.513274163	6.165679287
H161	-5.825314092	3.025466415	4.881365736
H162	-6.686052043	-1.408304710	5.540135013
H163	-4.512482500	2.398814978	2.411054430
H164	-5.681275367	1.722925133	7.341653709
H165	-5.395966558	4.432386712	6.687108336
H166	-2.479942372	-1.328824769	3.819969245
H167	-1.816419518	-0.751032760	2.277787534
H168	-0.888058953	-1.904890766	3.267175762
H169	-1.536862187	1.015109287	4.025474675
H170	-5.666129069	0.874263331	9.528256925
H171	0.083346749	3.691310311	4.413831137
H172	-1.169607752	2.930379408	8.747916188
H173	1.295639760	5.564852754	8.162815894
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H175	1.139844137	-0.261915476	3.222459194
H176	8.450861212	-2.920484974	5.465458235
H177	0.502360982	5.415861021	4.487924454
H178	1.221776997	6.483901362	6.637459457
H179	1.778168976	4.185199945	4.652019752
H180	2.504108614	5.273795829	6.890889902
H181	-0.506000554	4.674330153	6.660827184
H182	1.871329208	2.743453426	6.707574536
H183	-0.966436821	2.300234222	6.109441518
H184	0.896928180	1.433128166	3.700413828
H185	3.545086571	2.445610772	-0.238878780
H186	3.119786922	3.580611228	1.071087894
H187	5.119896793	3.056525333	1.724596101
H188	5.244706554	2.901652273	4.403352683
H189	6.202540699	0.846084451	1.689354288
H190	6.683963620	-1.571307436	1.952457478
H191	5.980909245	-1.243810373	6.199773552
H192	-2.595359973	-0.055175683	6.068909882
H193	-3.634240152	-2.712016867	7.099763607
H194	-2.843995389	-2.457418849	8.672845212
H195	-4.489883251	-0.487773423	7.169037109
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	H204	-2.675868319	-5.838937468	-0.425363780
	H205	-5.628971646	-5.478083452	-7.408025553
	H206	-3.934266612	-5.822987085	-7.841038290
	H207	-5.108152473	-3.235279958	-6.674916150
	H208	-1.578621940	0.141556116	-10.049921688
	H209	-5.185909433	-3.652595599	-9.182341727
	H210	-3.980774472	-0.246088279	-2.426092569
	H211	-6.069176042	-1.761578828	-0.771685644
	H212	-2.370885207	-1.536029999	-8.324594863
	H213	-4.108104944	0.627071273	-9.307086646
	H214	-2.239245649	-3.596476709	-9.025447655
	H215	-4.554266223	-4.299508680	-1.455550634
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	H217	-3.205355542	-4.784133952	-9.630717959
	H218	-7.404477697	0.665595888	-3.195370317
	H219	-4.101356941	0.089933459	-0.711999676
	H220	-2.557259688	-6.347936893	-6.283510539
	H221	-4.374548105	-2.198167725	-0.604659542
	H222	-1.535928701	5.049299055	2.001867240
	H223	-2.271874811	2.692640812	1.064485414
	H224	-6.078451391	6.449775813	2.212906730
	H225	-5.833700426	4.559462680	-0.093694273
	H226	-2.873979846	7.799103505	0.244978029
	H227	-1.217750290	12.704681391	1.315541702
	H228	-2.216104757	9.461310698	2.984480766
	H229	-3.676898429	10.264349925	0.808224647
	H230	-0.710783894	9.598368356	0.294916858
	H231	-2.724721281	14.094252652	-2.392055943
	H232	-0.009533474	5.436330388	0.075008322
	H233	-1.364465933	5.954566010	-0.937866403
	H234	-1.380864620	14.675307928	-0.297092626
	H235	-3.076558825	9.739763215	-0.765160538
	H236	-3.664004546	5.479581411	0.030859982
	H237	-5.999461109	4.694517252	2.388208550
	H238	-6.647864410	7.269924336	-2.213401645
	H239	-1.177609475	1.503948933	-2.813069410
	H240	-7.973554622	6.149350350	-1.845810801
	H241	9.969227695	-3.055010526	3.635947901
	H242	8.786658689	-2.063470791	3.101019183
	H243	4.753059976	3.307360991	-2.181733388
	H244	2.649914958	4.782034867	-0.866012224
	H245	6.178687544	5.188010917	-0.849475100
	H246	-0.602235852	4.024408193	-2.569068723
	H247	-1.441034211	5.474633565	-4.184414677
	H248	-3.066517590	5.401162218	-5.715122108
	H249	-0.482145418	6.508430282	-3.470518754
	H250	-3.477461605	3.159834326	-4.924471912
	H251	-4.893954708	4.249836662	-5.096826982
	H252	7.098955472	8.473755491	-3.994431490
	H253	7.006054117	10.236693369	-4.187822809
	H254	5.496297219	7.522975287	-5.188327179
	H255	3.859267314	8.166199673	-5.336976730
	H256	2.826456414	7.747660790	-8.081101159
	H257	0.944201135	3.882425186	-6.873193532
	H258	-0.436725179	10.861374685	-3.299920337
	H259	2.732489838	8.886596531	-0.012190337
	H260	1.059120375	7.995829749	-5.022108171
	H261	4.148901119	2.540871056	-4.528386103
	H262	6.253580822	3.354871052	-3.968674524
	H263	1.889502693	3.721713161	-4.354116815
	H264	-6.718644406	4.400373066	-2.699944120
	H265	9.029184976	4.531199007	-5.202160899
	H266	-5.260202552	2.082008323	-3.691121102
	H267	4.381853515	3.262582865	-6.118809649
	H268	1.524277717	7.420049240	-1.575217053
	H269	8.941188124	5.361588992	-3.635415440
	H270	2.552023482	6.050824233	-8.304821388
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N2x-Fe2-brNH2-Fe6H to N2x-Fe2NH3 **S=1, 35** **product** Fe(139) -2.288 Fe(140) 0.014 Fe(141) -2.716 Fe(142) 2.742 Fe(143) 3.173 Fe(144) 2.291 Fe(145) -1.725	965182n2x26nh26htonh335tc.car_7 C1 -9.409010853 0.821786622 1.055909927 C2 -10.382380914 -0.057292764 0.262074778 C3 -8.847294706 3.110212643 1.750114475 C4 -8.568771512 2.910796398 3.236434549 C5 -9.277583170 1.928639665 5.356233961 C6 -8.146490182 0.917898063 5.580787859 C7 -6.764343213 -0.852735295 4.620802016 C8 -5.451665333 -0.085149815 4.441920520 C9 -4.292760863 1.726659298 3.276575498 C10 -3.899615598 2.535804332 4.520940322 C11 -4.595445863 3.856860931 6.425858625 C12 -4.168889556 3.035012953 7.651210704 C13 -4.762712580 1.222332902 9.195479376 C14 -3.873036487 -0.025117775 9.113354473 C15 -3.144757196 -1.921525235 7.733502763 C16 -1.797881396 -1.655431838 7.052861432 C17 -0.529458099 -0.213829574 5.521891517 C18 0.397884598 0.780064045 6.247822523 C19 -0.839298214 0.181073465 4.062361121 C20 0.422759978 0.687020208 3.357371477 C21 -1.476658718 -0.998183685 3.315973600 C22 0.808997340 3.066294979 7.019589914 C23 0.848645232 3.006489040 8.557956150 C24 0.486133632 4.473201379 6.461580581 C25 1.386046337 5.532080783 7.110065315 C26 0.650265413 4.495547309 4.936042404 C27 -0.336106174 2.865688149 10.665356513 C28 0.524336252 1.726487194 11.179004328 C29 -2.611744165 -11.361977904 6.820223935 C30 -1.346329992 -10.907614699 6.096507032 C31 0.425322728 -9.169024617 6.093491411

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	C98	0.296587919	10.436028301	-2.586811557
	C99	1.370840213	8.495651242	-1.599538781
	C100	0.485957281	9.053900409	-2.517914752
	C101	0.824191334	-7.630421247	-7.455285643
	C102	-0.143634344	-6.479933704	-7.228125794
	C103	-0.334350270	-4.136450886	-6.427314646
	C104	0.095526374	-2.935162145	-7.274502072
	C105	1.870908073	-1.276624220	-7.631243217
	C106	3.386574877	-1.272980861	-7.801563572
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C113	-4.367461385	-5.788359614	-5.735597614
C114	-3.237681888	0.367291340	-8.674050660
C115	-2.015139422	0.859684948	-9.422401407
C116	-3.512899256	1.099495811	-7.338914135
C117	-2.579631829	0.614209783	-6.266488905
C118	-1.293318863	1.160630839	-6.129847668
C119	-2.934159686	-0.498727898	-5.486068260
C120	-0.365111850	0.564171244	-5.271970886
C121	-2.005731606	-1.089039748	-4.626059712
C122	-0.710234410	-0.573856999	-4.539838844
C123	2.371255759	-10.716552492	-2.215968825
C124	3.223707507	-11.226397208	-1.044530077
C125	1.086989539	-10.051146612	-1.701497286
C126	0.253737409	-9.339605664	-2.716887630
C127	-0.389894487	-9.890674180	-3.805154713
C128	-1.034178660	-7.787555983	-3.563469781
C129	3.385616232	-12.462300449	1.031308023
C130	4.592306366	-13.257137244	0.583183829
C131	-3.671143319	-5.618090666	1.180996541
C132	-2.538025784	-6.479952995	1.720186281
C133	-1.923047379	-7.467295567	0.683737976
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Fe141	4.240986406	-2.953000745	-0.809884810
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Fe144	2.579156566	-4.886382207	-0.338637122
Fe145	0.501621510	-3.601805275	-1.149947079
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H147	-9.097804610	-1.332738785	-0.685721158
H148	-10.537473368	2.481659613	0.609211734
H149	-10.670502414	0.472645378	-0.659730784
H150	-11.302890249	-0.136318346	0.865673060
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H153	-9.276886183	4.111333609	1.609633157
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H160	-3.770799562	4.546165183	6.202279690
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H183	-0.986128579	2.310535166	6.087388091
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H186	3.127607480	3.552840354	1.062685428
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	H194	-2.928109440	-2.405003142	8.693451044
	H195	-4.517737942	-0.403865616	7.178538690
	H196	-4.302900998	1.881720110	9.941574641
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	H203	-5.035557013	-4.573469537	-3.148089363
	H204	-2.682613873	-5.812888784	-0.466021014
	H205	-5.629703467	-5.478711005	-7.420502846
	H206	-3.935413229	-5.837707468	-7.844223723
	H207	-5.095071316	-3.232656613	-6.701637248
	H208	-1.541649066	0.099652236	-10.087158749
	H209	-5.178063068	-3.677377163	-9.204537433
	H210	-4.013087485	-0.222165734	-2.462856127
	H211	-6.056274667	-1.765101288	-0.778216295
	H212	-2.359821548	-1.563246061	-8.353413275
	H213	-4.079978424	0.611687455	-9.354480534
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	H220	-2.561900989	-6.349486502	-6.273377311
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	H226	-2.893178687	7.820419078	0.297797784
	H227	-1.229256038	12.731742906	1.351299544
	H228	-2.193548608	9.470913026	3.007743403
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N422	2.606741302	-11.978415534	-0.093595486
O423	-8.391429852	0.371077794	1.613293309
O424	-7.514949225	3.337354557	3.739564263
O425	-7.494704258	0.930517569	6.638877672
O426	-4.457673370	-0.308793160	5.155403052
O427	-2.707511974	2.690572623	4.831127070
O428	-3.192597517	3.379892116	8.338725597
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	O432 1.927642380 3.021316744 9.176741824 O433 0.997761763 1.695791259 12.305141938 O434 -0.916620016 -11.561029662 5.123712965 O435 1.470502118 -9.365104916 8.274311389 O436 6.221435438 -9.201631988 7.128237150 O437 -5.239174612 2.736366047 -0.635929326 O438 -5.636382752 -2.195634814 -3.652842321 O439 -4.105184194 6.064476077 -2.013203984 O440 -3.073132188 5.194259393 -4.781944172 O441 -6.849409650 7.566601248 0.300606037 O442 -3.691583163 5.754668333 3.206878271 O443 -0.384424251 7.363767578 2.187027149 O444 -0.637474012 10.747451910 2.665225946 O445 8.317136510 -5.446764377 5.763114728 O446 5.554305485 2.463481735 3.555041661 O447 7.959903186 4.111785529 -1.547856290 O448 6.926633773 6.277881319 -5.058074890 O449 3.321689898 6.036445809 -3.021584222 O450 3.699086894 6.485814869 0.643550725 O451 5.174657734 3.245533904 0.755308993 O452 7.715140589 8.879698832 0.263886279 O453 6.499078261 11.993533948 -2.179456074 O454 4.265054951 10.179685378 -3.905218940 O455 4.549169833 14.289516596 0.089825694 O456 -0.178944801 8.190223739 -3.405686478 O457 -1.375902852 -6.633319310 -7.413404206 O458 -0.598728907 -2.516495845 -8.225590314 O459 3.903157557 -0.473523091 -8.601033958 O460 7.285174714 -2.215425874 -8.805064918 O461 -5.458610280 -1.241103995 -9.063844123 O462 -5.209699456 -5.695136152 -4.849204676 O463 -3.157932394 -6.319691183 -5.463093305 O464 -1.589444942 2.004788244 -9.366785256 O465 4.450505245 -11.011567470 -0.987145517 O466 5.580081925 -13.447634117 1.279385947 O467 -3.541374979 -5.261201403 -0.101687593 O468 -4.606315884 -5.226521935 1.877249293 O469 -2.664712040 -12.221367138 -0.299275436 O470 -4.445280215 -10.870343786 -0.645216769 O471 0.474950235 -7.802708328 0.555218476 O472 -0.604762127 -8.650380741 2.330151810 O473 -1.663656069 -6.751923851 -0.524487037 O474 2.970900255 -10.122699127 3.620369322 O475 2.747977025 -7.617692841 2.251910047 O476 -0.515393465 5.629261243 -3.900837616 O477 -0.362599043 -13.209156723 0.813499265 O478 0.528290096 -11.086494270 2.765085674 S479 5.833119594 1.168898345 -2.729765641 S480 2.549823355 -0.635736229 -3.293860823 S481 -0.407465840 -4.779794175 -2.748580786 S482 4.086968123 -0.867573725 -0.040114654 S483 -0.413982123 -1.685136882 -1.320108836 S484 2.838469922 -4.338983128 -4.711250493 S485 0.623508575 -4.737298700 0.778179505 S486 5.509478785 -2.771969934 -2.642909531 S487 2.608324344 -6.649269075 -1.698159230 S488 4.554426993 -4.636672730 0.603002320 end
N2x-Fe2NH3 to Fe2NH3 **S=1, 35** **reactant** Fe(139) -2.245 Fe(140) 0.013 Fe(141) -2.699 Fe(142) 2.706 Fe(143) 3.159 Fe(144) 2.293 Fe(145) -1.700	965182nh32n2xd35td.car_4 C1 -9.408141991 0.821280939 1.053745388 C2 -10.383380628 -0.056969077 0.260990016 C3 -8.851616611 3.110788482 1.750633529 C4 -8.573140225 2.911357273 3.236975337 C5 -9.280409015 1.927935482 5.356620571 C6 -8.148285711 0.918220126 5.580939586 C7 -6.763427465 -0.850310995 4.620345499 C8 -5.451089272 -0.082116206 4.441026475 C9 -4.296333283 1.733579527 3.277792602 C10 -3.904160042 2.541260490 4.523568282 C11 -4.602652558 3.858764027 6.430255669 C12 -4.174430726 3.035668700 7.654158910 C13 -4.763757699 1.217732745 9.194109246 C14 -3.874191775 -0.029599460 9.110489155 C15 -3.144100253 -1.923873701 7.728614622 C16 -1.796832477 -1.656487855 7.048934363 C17 -0.526789311 -0.210482924 5.524249937 C18 0.395128574 0.786345912 6.252851153 C19 -0.835665635 0.182024140 4.062974599 C20 0.422712881 0.696104563 3.355036503 C21 -1.464467793 -1.000989929 3.316238135

	C22	0.802222622	3.071797658	7.025260092
	C23	0.841747613	3.007119852	8.563228061
	C24	0.478523911	4.480913805	6.473311125
	C25	1.385126678	5.535194977	7.120315996
	C26	0.634470405	4.508299926	4.946783721
	C27	-0.343500625	2.860363153	10.670005343
	C28	0.522691210	1.724972233	11.183703261
	C29	-2.620258786	-11.354668068	6.818712794
	C30	-1.353938067	-10.901896214	6.096119477
	C31	0.419346732	-9.163975203	6.100492035
	C32	1.592977344	-9.471257728	7.048185910
	C33	0.240415068	-7.641933903	5.951059852
	C34	1.493065982	-6.979339103	5.378995835
	C35	1.260407501	-5.528059883	4.978842991
	C36	2.990173457	-3.829351963	4.354988699
	C37	3.966172794	-10.065544286	7.163815012
	C38	5.026301988	-9.011951326	6.935523440
	C39	-5.869209366	0.697788643	-1.853732392
	C40	-5.369893606	2.150143564	-1.725803529
	C41	-4.694874043	-0.270012737	-1.605951836
	C42	-5.101046531	-1.731573276	-1.328492810
	C43	-5.258165418	-2.627740728	-2.557842802
	C44	-4.246066202	3.901664936	-3.081998414
	C45	-4.844802547	5.167483681	-2.460368130
	C46	-3.959910931	4.072708306	-4.580823132
	C47	-6.879728912	6.325294111	-1.746337904
	C48	-6.576823409	6.497227781	-0.253359896
	C49	-5.615275017	5.533377592	1.781644807
	C50	-4.110947392	5.644029339	2.043475002
	C51	-1.829742307	5.695855156	1.157546041
	C52	-1.373499411	7.125797108	1.483468312
	C53	-1.060147667	5.272311942	-0.103277142
	C54	-1.319580319	3.868871048	-0.535648114
	C55	-1.864984779	2.769349995	0.095624722
	C56	-1.373177723	2.107306260	-1.887878327
	C57	-1.655375148	9.480940074	0.852773133
	C58	-1.457259004	9.930781292	2.297979980
	C59	-2.779450460	10.303764735	0.177639968
	C60	-2.445078809	11.704329009	-0.245416097
	C61	-1.752236426	12.708262254	0.402881216
	C62	-2.501208034	13.429305955	-1.553971025
	C63	8.192267682	-3.407706600	4.461602733
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	C67	6.050713648	-0.833801727	5.175534867
	C68	6.468810627	-0.999328285	2.806776368
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	C70	6.203098728	0.361804838	2.655967487
	C71	5.847651078	1.124475000	3.771224024
	C72	8.398750355	1.722963377	-1.753637152
	C73	8.273057684	3.156707558	-2.295391868
	C74	7.021184338	1.186884647	-1.368907464
	C75	8.454160101	4.609154758	-4.284413565
	C76	7.052614945	5.125023124	-4.616891233
	C77	4.618848239	4.620180201	-4.513596444
	C78	4.021368386	5.000761709	-3.133240981
	C79	3.894948058	3.417740581	-5.162033129
	C80	2.370633924	3.460275370	-5.318386373
	C81	1.819023110	4.349066262	-6.444311656
	C82	1.772317286	6.842538659	-6.565632575
	C83	3.750634246	4.479223623	-0.758961716
	C84	4.370615712	5.729272898	-0.118298508
	C85	3.905875052	3.312503900	0.236320643
	C86	6.489522814	6.829099052	0.417798458
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	C88	6.642343313	9.579636787	-2.194301445
	C89	6.007591510	10.933157143	-1.788414498
	C90	6.531978527	9.366873786	-3.708570210
	C91	5.099447223	9.325520339	-4.226728420
	C92	4.115798739	12.067111680	-0.729542383
	C93	4.871744322	13.115365674	0.072630537
	C94	2.814308531	11.658162400	0.015538415
	C95	1.956570735	10.737365780	-0.822072591
	C96	1.042447585	11.264216855	-1.746361257
	C97	2.090418349	9.340748822	-0.747890887
	C98	0.299336943	10.433075988	-2.586617345
	C99	1.376724557	8.493493541	-1.600646525
	C100	0.490520312	9.051119403	-2.518064943
	C101	0.820128823	-7.620011892	-7.455658783

C102	-0.147035783	-6.467523222	-7.236712032
C103	-0.335598571	-4.120684707	-6.442658486
C104	0.096521309	-2.917263031	-7.284949049
C105	1.861088894	-1.237851764	-7.612094162
C106	3.378453540	-1.228355776	-7.777086326
C107	5.577482405	-2.020258956	-7.106650729
C108	6.155421231	-2.460211317	-8.437417352
C109	-4.241601665	-3.322012348	-8.728205722
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C112	-4.581182376	-5.288837816	-7.153977924
C113	-4.369812042	-5.789549456	-5.743617309
C114	-3.226123759	0.365494714	-8.680955973
C115	-2.002756050	0.871327562	-9.417791366
C116	-3.515139464	1.070373373	-7.334976050
C117	-2.599933848	0.575320326	-6.249846332
C118	-1.311643348	1.110505137	-6.087308994
C119	-2.982450471	-0.524988935	-5.464252180
C120	-0.413777243	0.524363905	-5.191397105
C121	-2.083559762	-1.107167027	-4.568277438
C122	-0.789038137	-0.596118441	-4.446714957
C123	2.385933433	-10.721620158	-2.208059827
C124	3.240306747	-11.230586734	-1.037242213
C125	1.099319610	-10.059143667	-1.693709583
C126	0.262595421	-9.350978778	-2.709251918
C127	-0.392962325	-9.905887576	-3.789656800
C128	-1.001402255	-7.788561630	-3.571744945
C129	3.400509373	-12.453544868	1.046437815
C130	4.603826436	-13.257231541	0.605988314
C131	-3.662665768	-5.615609331	1.132507263
C132	-2.533792771	-6.474407456	1.689294493
C133	-1.918277273	-7.470083160	0.661721824
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C135	-2.296654683	-9.838817653	-0.347959342
C136	-3.220093333	-11.073881938	-0.430652936
C137	-0.605146030	-8.022369543	1.236374664
C138	2.386446697	-3.255879398	-1.509853870
Fe139	1.838157610	-4.831924997	-2.798179947
Fe140	1.872763889	-1.285537250	-0.917231267
Fe141	4.248694686	-2.938861007	-0.841275683
Fe142	3.264991674	-2.746341347	-3.218501723
Fe143	4.617633716	-0.708667054	-2.245775492
Fe144	2.614516483	-4.889692792	-0.344320183
Fe145	0.523073208	-3.578252656	-1.098083767
H146	-9.597123087	-1.869543967	0.770070878
H147	-9.103022045	-1.334862821	-0.689555868
H148	-10.540550049	2.479350687	0.610698779
H149	-10.672168960	0.473729722	-0.660166057
H150	-11.303238426	-0.134693501	0.865901139
H151	-7.874390698	3.091562593	1.245192968
H152	-10.354056028	1.930015335	3.491019968
H153	-9.283781356	4.110960021	1.610508489
H154	-10.207905447	1.518603625	5.778829922
H155	-8.412475675	0.131835591	3.691858378
H156	-9.013960938	2.827919829	5.925759697
H157	-3.420527136	1.139099634	2.990610254
H158	-6.266975208	0.979816285	2.880897828
H159	-6.866370157	-1.596228289	3.820708762
H160	-3.779498050	4.550349774	6.208169373
H161	-5.871109642	3.045898592	4.885836855
H162	-6.710485591	-1.375503059	5.581612896
H163	-4.525367801	2.416669367	2.448173686
H164	-5.781917615	1.762045969	7.389061574
H165	-5.490905667	4.446221625	6.699955022
H166	-2.396712328	-1.332818796	3.795121419
H167	-1.703404488	-0.723894556	2.277442066
H168	-0.778744957	-1.863694680	3.286991100
H169	-1.555428776	1.013667271	4.087408133
H170	-5.747622764	0.900363656	9.569888038
H171	-0.052256105	3.812930493	4.445294164
H172	-1.239383309	2.943111113	8.725200735
H173	1.236772324	5.602464092	8.207540067
H174	0.194985483	0.933073044	2.304834179
H175	1.232732010	-0.047960401	3.384051063
H176	8.490264692	-2.924409460	5.411911772
H177	0.430464901	5.516414236	4.557180132
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H179	1.665861014	4.238954018	4.662777128
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H181	-0.570758266	4.717700117	6.727581964

	H182	1.828176091	2.810207162	6.725391019
	H183	-0.989653568	2.316215582	6.083554984
	H184	0.806999423	1.616834515	3.816399559
	H185	3.626136037	2.375249431	-0.266737280
	H186	3.190499050	3.491799228	1.052122795
	H187	5.196919238	3.039658046	1.702176660
	H188	5.271405099	2.870691780	4.393703813
	H189	6.228647935	0.826779402	1.670257674
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	H191	5.986055898	-1.291197574	6.166613562
	H192	-2.590626106	-0.033616585	6.066009638
	H193	-3.698153051	-2.638958257	7.102383977
	H194	-2.927421212	-2.408299208	8.688114269
	H195	-4.516827208	-0.405930611	7.174463547
	H196	-4.303450445	1.876493221	9.940450549
	H197	5.475276189	1.123244029	5.906724248
	H198	0.071439847	-1.133866144	5.516059718
	H199	-0.009643500	3.802155148	11.135803048
	H200	-1.374962253	2.663176873	11.000999415
	H201	0.650867825	0.874694185	10.473287230
	H202	4.385849327	-11.058993880	6.942977259
	H203	-5.053529066	-4.569972124	-3.169973731
	H204	-2.654881200	-5.831255645	-0.502523516
	H205	-5.628511747	-5.477639884	-7.430948900
	H206	-3.934161701	-5.840088000	-7.851722471
	H207	-5.092857155	-3.231703351	-6.716932478
	H208	-1.543607657	0.129173633	-10.112866452
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	H210	-4.015345184	-0.225577709	-2.470871364
	H211	-6.062873625	-1.763628720	-0.786391315
	H212	-2.337577946	-1.566375538	-8.391257272
	H213	-4.066233466	0.616624200	-9.362711522
	H214	-2.213603397	-3.623446940	-9.057412757
	H215	-4.543321915	-4.286385693	-1.508494943
	H216	-3.352121437	-3.516371215	-6.756845578
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	H219	-4.111787702	0.102775561	-0.753067835
	H220	-2.562081624	-6.344449574	-6.276457899
	H221	-4.361848430	-2.188434314	-0.654163113
	H222	-1.542011135	5.073196015	2.016210369
	H223	-2.243384393	2.708626137	1.111671970
	H224	-6.077010966	6.435739711	2.205765144
	H225	-5.825866563	4.559898719	-0.111439344
	H226	-2.900247494	7.827539209	0.306841059
	H227	-1.227457898	12.739413304	1.351375463
	H228	-2.190631566	9.478643416	3.008591630
	H229	-3.664897988	10.296898344	0.838383749
	H230	-0.706200504	9.609936764	0.308686666
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	H234	-1.369574217	14.700669934	-0.273613176
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	H353	1.606289157	-12.556121633	-2.731322275
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N2x-Fe2NH3 to Fe2NH3 **S=1, 35** **TS** Fe(139) -2.378 Fe(140) 0.033 Fe(141) -2.560 Fe(142) 2.727 Fe(143) 3.176	965182nh32n2xd35tc.car_1 C1 -9.402033334 0.817115496 1.044265021 C2 -10.397209721 -0.049199537 0.263714261 C3 -8.819771066 3.101608335 1.740267959 C4 -8.545568134 2.903947370 3.227587635 C5 -9.255746746 1.921873204 5.346404422 C6 -8.126364213 0.908275141 5.568035425 C7 -6.749483809 -0.861682021 4.599472883 C8 -5.440014548 -0.087135702 4.426784626 C9 -4.288367568 1.727484143 3.251988041 C10 -3.886529939 2.538561297 4.492265797 C11 -4.559340596 3.844046276 6.412990052

Fe(144) 2.406
Fe(145) -1.957

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C16	-1.777279863	-1.679215320	7.032492553
C17	-0.538131786	-0.213171461	5.507924192
C18	0.403584010	0.772688414	6.223973932
C19	-0.864599543	0.180181177	4.050662642
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C21	-1.505895570	-0.999063720	3.307687127
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C27	-0.276553667	2.844940638	10.679948290
C28	0.571863219	1.685638426	11.171207024
C29	-2.601288844	-11.358917126	6.827343920
C30	-1.343722510	-10.889720550	6.102293113
C31	0.400600448	-9.125997847	6.094367136
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C33	0.223706125	-7.604349304	5.945374925
C34	1.486120852	-6.951567573	5.384889005
C35	1.296248146	-5.479873083	5.049120491
C36	3.033931352	-3.799563291	4.407664852
C37	3.932609374	-10.049701488	7.185155602
C38	5.012998428	-9.020332484	6.942055721
C39	-5.860031963	0.697825122	-1.847314216
C40	-5.364636855	2.151918705	-1.716393710
C41	-4.692167890	-0.273416437	-1.584754290
C42	-5.106344401	-1.734305322	-1.313717128
C43	-5.252325142	-2.628375002	-2.546183318
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C46	-3.957363510	4.080639129	-4.570541083
C47	-6.892235907	6.320326420	-1.737339603
C48	-6.586950739	6.496187755	-0.245160054
C49	-5.623318453	5.539580109	1.792126920
C50	-4.118398995	5.648522106	2.049157104
C51	-1.840268079	5.681216757	1.149769952
C52	-1.385142744	7.112163301	1.479233142
C53	-1.083688418	5.261528803	-0.121175173
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C55	-1.914295645	2.764893228	0.054921032
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C58	-1.468197633	9.915084266	2.283584156
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C61	-1.757399395	12.687254241	0.384328979
C62	-2.520735078	13.414844912	-1.564758028
C63	8.163538970	-3.405794219	4.487838079
C64	8.249353252	-4.907639044	4.695097260
C65	6.674030179	-3.083128124	4.234799119
C66	6.389092705	-1.605986046	4.083076596
C67	6.042702773	-0.811831876	5.192259066
C68	6.450650624	-0.983734375	2.821968121
C69	5.757723831	0.550297984	5.051648673
C70	6.182607515	0.376817338	2.668675211
C71	5.829643209	1.141690418	3.783330915
C72	8.392939506	1.726304113	-1.726445326
C73	8.279254320	3.159312787	-2.270156232
C74	7.008565978	1.219070941	-1.324026335
C75	8.458062734	4.599787850	-4.269020425
C76	7.056366280	5.116471639	-4.603132708
C77	4.619958330	4.619622149	-4.495769001
C78	4.014630809	5.010397296	-3.122790131
C79	3.899779622	3.412965462	-5.142149845
C80	2.376040434	3.452736536	-5.308492857
C81	1.829717162	4.341651715	-6.437211770
C82	1.778928024	6.835453741	-6.564958067
C83	3.746881270	4.509912813	-0.742471193
C84	4.370703726	5.762459674	-0.112999114
C85	3.917680865	3.353737529	0.264747682
C86	6.503331928	6.832463761	0.423764378
C87	6.876090402	8.144794617	-0.243574222
C88	6.636885379	9.572545664	-2.195521110
C89	5.995492938	10.923991273	-1.793210656
C90	6.526842451	9.352967642	-3.709025916
C91	5.095916377	9.306061062	-4.230385016

C92	4.104042633	12.058321281	-0.736822034
C93	4.862366297	13.106453599	0.062388874
C94	2.801816751	11.652840961	0.009080894
C95	1.942826473	10.732480726	-0.827937008
C96	1.029313336	11.259650625	-1.752807596
C97	2.076177661	9.335772278	-0.753302587
C98	0.286884004	10.428940329	-2.594261441
C99	1.362712620	8.489285495	-1.606851247
C100	0.477858136	9.047124558	-2.525361973
C101	0.822249394	-7.631520051	-7.460657921
C102	-0.140489261	-6.475777967	-7.238903644
C103	-0.325497632	-4.129735921	-6.447147630
C104	0.103622717	-2.924221907	-7.288349012
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C106	3.397268157	-1.245249567	-7.792657981
C107	5.600510237	-1.999040308	-7.095182750
C108	6.176224909	-2.473372415	-8.414758817
C109	-4.258941292	-3.306391677	-8.714484805
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C113	-4.366485390	-5.789160108	-5.741107916
C114	-3.247190008	0.381268976	-8.653624552
C115	-2.033865307	0.889765174	-9.405583230
C116	-3.514524620	1.086000608	-7.302976451
C117	-2.589756858	0.580480305	-6.231839003
C118	-1.299493995	1.114126017	-6.081133948
C119	-2.964730305	-0.525649773	-5.450930325
C120	-0.391043551	0.518015719	-5.202807648
C121	-2.055327441	-1.116186293	-4.571304569
C122	-0.758514381	-0.608925281	-4.465221432
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C124	3.228178622	-11.225455307	-1.031690259
C125	1.082150704	-10.070316778	-1.701742989
C126	0.249422867	-9.368987248	-2.724308074
C127	-0.400976061	-9.930525120	-3.803992583
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C132	-2.551462377	-6.489686733	1.669145466
C133	-1.932570078	-7.483125361	0.640692412
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C137	-0.618898689	-8.029946889	1.221496956
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Fe140	1.937256879	-1.450341657	-0.995306809
Fe141	4.212505688	-2.878998326	-0.816490604
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Fe143	4.591664269	-0.660715233	-2.240691435
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H148	-10.520646981	2.486888558	0.608728967
H149	-10.698607746	0.490095243	-0.648202985
H150	-11.305482081	-0.122654254	0.887113728
H151	-7.842095422	3.070313152	1.235895774
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H153	-9.240147640	4.106209862	1.596928338
H154	-10.184360416	1.515852765	5.769388120
H155	-8.403400826	0.120522442	3.681585870
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H157	-3.413395478	1.134853507	2.958453782
H158	-6.253145655	0.960504437	2.856776593
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H160	-3.734751507	4.531150568	6.182437566
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H162	-6.694301860	-1.396318501	5.555261693
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H167	-1.751135478	-0.718630687	2.270855023
H168	-0.822398686	-1.863107942	3.267970978
H169	-1.577257798	1.017140987	4.082029227
H170	-5.696780290	0.884018131	9.544165090
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	H172	-1.195670524	2.933526066	8.742892472
	H173	1.274229421	5.583212527	8.182954024
	H174	0.136999924	0.926557178	2.281289927
	H175	1.186755066	-0.074496165	3.331596078
	H176	8.463304290	-2.923732517	5.438383382
	H177	0.483472050	5.461761286	4.520812495
	H178	1.219104294	6.498772419	6.654755419
	H179	1.729683388	4.197656055	4.658499932
	H180	2.485260144	5.273464176	6.918560496
	H181	-0.529658299	4.696469286	6.692832280
	H182	1.852933258	2.770227247	6.716803869
	H183	-0.977568547	2.307117056	6.105578378
	H184	0.793617674	1.595630474	3.779808881
	H185	3.681597957	2.403470977	-0.236770019
	H186	3.184007131	3.518163840	1.068160555
	H187	5.194084933	3.078259963	1.741394491
	H188	5.254198544	2.889139945	4.403956177
	H189	6.206703842	0.839716732	1.681959166
	H190	6.680000376	-1.579581495	1.935731870
	H191	5.985260597	-1.264937254	6.185603949
	H192	-2.595026818	-0.053763069	6.072742577
	H193	-3.663695681	-2.689226246	7.100318170
	H194	-2.883535381	-2.445275377	8.680011350
	H195	-4.503738855	-0.461158088	7.170253830
	H196	-4.246264144	1.852337669	9.913222925
	H197	5.467791142	1.147314170	5.920481756
	H198	0.059063045	-1.136851923	5.483803198
	H199	0.085731462	3.775250329	11.146034354
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	H203	-5.045972585	-4.568460358	-3.160698587
	H204	-2.663364843	-5.838742587	-0.521757762
	H205	-5.627968065	-5.477717943	-7.426084292
	H206	-3.932048858	-5.829184519	-7.850259690
	H207	-5.102185985	-3.233313515	-6.698269556
	H208	-1.581192503	0.148644884	-10.105585957
	H209	-5.179374677	-3.662589872	-9.202407171
	H210	-4.000146893	-0.230817027	-2.439558483
	H211	-6.073672859	-1.764216111	-0.781107504
	H212	-2.357024940	-1.550454199	-8.371791702
	H213	-4.097112127	0.635080148	-9.321149020
	H214	-2.232049671	-3.609897980	-9.047043225
	H215	-4.547168562	-4.290535496	-1.495393167
	H216	-3.359779144	-3.507700555	-6.749073043
	H217	-3.199380201	-4.802076967	-9.639009779
	H218	-7.435266884	0.667052950	-3.190151190
	H219	-4.119017753	0.097456884	-0.724753670
	H220	-2.561076964	-6.349066144	-6.279576136
	H221	-4.375676615	-2.193887858	-0.631971742
	H222	-1.542342164	5.055121656	2.002575168
	H223	-2.294492217	2.698584456	1.069880115
	H224	-6.082642676	6.445509754	2.211215746
	H225	-5.835132891	4.560116841	-0.099629565
	H226	-2.877657397	7.807744392	0.258001014
	H227	-1.223837200	12.714084925	1.328103645
	H228	-2.206294437	9.464314263	2.989840385
	H229	-3.673106936	10.272853500	0.819663539
	H230	-0.709426795	9.605182447	0.296504267
	H231	-2.709976765	14.096402326	-2.390573528
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	H233	-1.343018197	5.960910805	-0.933935458
	H234	-1.377299178	14.681333932	-0.289447592
	H235	-3.078266731	9.747202958	-0.755837297
	H236	-3.666136601	5.487977263	0.028718986
	H237	-6.000906822	4.690187379	2.381781326
	H238	-6.641219363	7.278061304	-2.214094771
	H239	-1.273625541	1.517413558	-2.829796255
	H240	-7.973239237	6.164492249	-1.847401446
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	H242	8.789060295	-2.061455125	3.077194898
	H243	4.759372554	3.282662340	-2.211151941
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	H245	6.193486103	5.180768828	-0.853582299
	H246	-0.653728584	4.028614452	-2.578784898
	H247	-1.452538294	5.476699763	-4.195128915
	H248	-3.070869527	5.387306771	-5.731137217
	H249	-0.490835622	6.502898544	-3.472746515
	H250	-3.487631274	3.150772074	-4.933331046
	H251	-4.902246482	4.241973196	-5.114021650

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H256	2.826139141	7.738463930	-8.081689475
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H258	-0.432354786	10.855272184	-3.297680223
H259	2.735119103	8.875739170	-0.011410285
H260	1.057550461	7.985844159	-5.020607387
H261	4.135646106	2.526140845	-4.533011625
H262	6.246437693	3.337956269	-3.990475776
H263	1.877035258	3.704725322	-4.359533200
H264	-6.728749740	4.409220413	-2.705706092
H265	9.028526075	4.547296544	-5.205589333
H266	-5.283320045	2.083871517	-3.701573184
H267	4.368718358	3.242094995	-6.125383739
H268	1.522560059	7.410900738	-1.572211282
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H271	1.435466913	8.846381685	-6.470515129
H272	-6.261471983	-0.493257308	-3.477156338
H273	-6.596927845	0.568146788	-1.031483720
H274	0.883826358	12.340858697	-1.813982522
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H284	4.507547093	9.962461199	-0.802144974
H285	1.801642668	-7.241668267	-7.775355767
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	H337	-1.356271754	-10.165164584	0.086063014
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	H340	-1.004854886	1.980097349	-6.680196539
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	H348	-1.383957574	-4.318994162	-6.636009145
	H349	5.951095701	-0.973871849	-6.899977978
	H350	6.096877295	-3.487516782	5.080410665
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	H354	2.737632550	-13.157018998	1.610326613
	H355	1.599443057	-12.167374177	-0.091205197
	H356	4.487114322	-13.726306483	-0.418204869
	H357	3.691838687	-11.661545432	1.724474760
	H358	8.292253323	-5.500717146	3.750436141
	H359	5.714714506	12.719910905	0.668844562
	H360	3.674587937	-9.997277195	8.258157958
	H361	4.651549260	-8.027072816	6.578524103
	H362	3.829904589	12.514896927	-1.703202032
	H363	3.069974131	11.172592869	0.963015633
	H364	2.256092311	12.577522112	0.244249310
	H365	-0.945608856	8.659257883	-3.799013077
	H366	2.319175002	-1.326601719	1.634535095
	H367	1.253063163	-2.544353641	1.258546849
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	N392	-5.076036881	2.723824326	-2.918328751
	N393	-6.205428605	5.226437367	-2.398714020
	N394	-6.042127525	5.431981875	0.406247197
	N395	-3.285801696	5.590447459	0.971689272
	N396	-1.044688558	3.429911889	-1.840727747
	N397	-1.956188763	1.685994447	-0.798431368
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	N402	9.296961773	1.652848849	-0.567001571
	N403	8.526133421	3.312894043	-3.603432886
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	N422	2.604915716	-11.975631378	-0.083620849
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	O454	4.252704420	10.155415071	-3.906553683
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	O460	7.316619245	-2.227799809	-8.774489885
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	S479	5.840936219	1.192271773	-2.765577386
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C6	-8.147016608	0.916871295	5.580690056
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C13	-4.762345285	1.217125717	9.193920924
C14	-3.873633447	-0.031390914	9.111004175
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C16	-1.799548597	-1.660842415	7.055008210
C17	-0.526576983	-0.216298297	5.530664525
C18	0.395149352	0.783242363	6.255672737
C19	-0.836637879	0.171093554	4.071827103
C20	0.422421171	0.674391197	3.360418405
C21	-1.466624441	-1.010329596	3.321847108
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C31	0.419581861	-9.165461331	6.102773938
C32	1.592915676	-9.472299655	7.051027060
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C40	-5.369437794	2.147720659	-1.727583429
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C43	-5.254706690	-2.634703073	-2.557396570
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C45	-4.853115135	5.169089082	-2.464248499
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C47	-6.885926841	6.325075329	-1.744518561
C48	-6.581086704	6.496506666	-0.251798517
C49	-5.622194253	5.534055692	1.784353406
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C51	-1.839896413	5.694964876	1.147194759
C52	-1.371732436	7.121743217	1.474013305
C53	-1.091250980	5.267290369	-0.125376716
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C56	-1.435230834	2.106771025	-1.912160987
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C80	2.371680613	3.454378896	-5.317294275
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C82	1.773400094	6.835259745	-6.563457557
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C85	4.007176521	3.313862844	0.243766854
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C93	4.871079380	13.113057583	0.070618905
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C99	1.378492372	8.488137422	-1.599821631
C100	0.491296168	9.043920917	-2.517439972
C101	0.820526674	-7.618216119	-7.447170802
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	H184	0.821276151	1.589541899	3.821984477
	H185	3.775967360	2.362664325	-0.260674186
	H186	3.286921053	3.463714510	1.061459188
	H187	5.296840901	3.064204738	1.708289307
	H188	5.273349440	2.868136561	4.388710610
	H189	6.231389475	0.818703162	1.668495931
	H190	6.704577490	-1.600232164	1.922705590
	H191	5.991789894	-1.289248177	6.169784570
	H192	-2.591540031	-0.038899929	6.068074857
	H193	-3.700199208	-2.642562407	7.104330684
	H194	-2.931824258	-2.412718267	8.690958676
	H195	-4.517792927	-0.408913488	7.175830427
	H196	-4.301219638	1.875524743	9.940017085
	H197	5.476932083	1.123634692	5.904486246
	H198	0.070144475	-1.138317868	5.524667821
	H199	-0.005128779	3.806757680	11.139822063
	H200	-1.374328896	2.667577953	11.006029923
	H201	0.649615873	0.877226424	10.475471910
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	H203	-5.050198285	-4.576521910	-3.167620693
	H204	-2.650800395	-5.843616431	-0.517275085
	H205	-5.628206094	-5.477198506	-7.425739421
	H206	-3.935127899	-5.844168782	-7.847079679
	H207	-5.086102132	-3.233969584	-6.707744620
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	H209	-5.153366409	-3.679507082	-9.205737262
	H210	-4.010571242	-0.234728741	-2.473931548
	H211	-6.059572378	-1.768182229	-0.786484837
	H212	-2.329094518	-1.571091445	-8.385229064
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	H214	-2.206463726	-3.624017659	-9.054312420
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	S484	2.807719425	-4.250708230	-4.740950549
	S485	0.642346952	-4.760233856	0.742153896
	S486	5.384614738	-2.752467575	-2.717057324
	S487	2.625477384	-6.690183650	-1.724353282
	S488	4.579645204	-4.604712336	0.575105051
	end			
Fe2-brNH2-Fe6-3b2 to Fe2NH3 **S=1, 35** **reactant** Fe(139) -2.338 Fe(140) 0.969 Fe(141) -2.447 Fe(142) 2.223 Fe(143) 2.975 Fe(144) 2.392 Fe(145) -1.328	9651826nh23b2t35tc.car_5			
	C1	-8.048847165	-4.997017915	-0.543868807
	C2	-8.420698110	-5.774534945	-1.811048357
	C3	-8.855585703	-3.462698095	1.199590719
	C4	-8.335358027	-4.152606415	2.456576562
	C5	-8.094327513	-6.237697661	3.713875680
	C6	-6.571172961	-6.405854577	3.707912946
	C7	-4.506674803	-6.384730182	2.401184183
	C8	-3.915395042	-5.051695760	2.871796881
	C9	-4.187514367	-2.617876336	2.901851128
	C10	-4.251512198	-2.480690760	4.428961464
	C11	-5.447825957	-2.902108714	6.487462280
	C12	-4.488142509	-3.794917449	7.288374008
	C13	-3.661650339	-6.075059625	7.657152027
	C14	-2.193015442	-6.346342950	7.300347179
	C15	-0.528550254	-6.545143769	5.496990834
	C16	0.266904012	-5.283025512	5.148781899
	C17	0.174765679	-2.859233761	4.731713052
	C18	0.324995874	-2.001458991	6.003270765
	C19	-0.461492900	-2.134583581	3.523232762
	C20	0.166379884	-0.755189520	3.297151657
	C21	-0.344366259	-3.001044192	2.262359150
	C22	-0.744184583	-0.639366399	7.734135636
	C23	-0.469021149	-1.417516842	9.033534962
	C24	-2.002894929	0.257237868	7.810533112
	C25	-2.019188088	1.088999063	9.097316613
	C26	-2.074569694	1.171991564	6.580776177
	C27	-1.043382892	-3.249801321	10.510641735
	C28	0.402017094	-3.626930876	10.769702576
	C29	4.929824689	-12.601663441	0.362799710
	C30	5.704510544	-11.293837230	0.258451589
	C31	6.173539909	-9.177567935	1.465795300
	C32	7.392861415	-9.141191498	2.403906819
	C33	5.077523555	-8.224846634	1.973156307
	C34	5.536151569	-6.772051600	1.938765646
	C35	4.440573346	-5.788888056	2.332010710
	C36	4.999924385	-3.417979829	2.932254245
	C37	9.657021186	-8.267896889	2.721417549
	C38	9.900210673	-6.830124305	3.124331822
	C39	-5.375912216	-1.724490651	-2.457056623
	C40	-5.736566241	-0.490157167	-1.611138887
	C41	-3.847838009	-1.932709205	-2.406099457
	C42	-3.352075509	-3.311952791	-2.885760408
	C43	-3.091347993	-3.457620983	-4.384537700
	C44	-5.923823145	1.978914397	-1.813349230
	C45	-7.058070454	2.240695652	-0.815539917
	C46	-5.969333504	2.954744839	-2.997962323
	C47	-9.308049689	1.620100976	-0.072165384
	C48	-9.002508361	1.175208890	1.363378307
	C49	-7.447436422	0.054413768	2.886194271
	C50	-6.247037047	0.823359033	3.446330562
	C51	-4.538802858	2.553292584	3.126718093
	C52	-4.958957547	3.620075183	4.150137425
	C53	-3.845873529	3.300844113	1.976388724
	C54	-3.227387630	2.409701302	0.952715397
	C55	-2.956019132	1.057402019	0.915235654
	C56	-2.265629590	1.832394339	-0.967668419
	C57	-6.601056717	5.385589687	4.597742952
	C58	-6.515549519	5.132037330	6.100816194
	C59	-8.067554880	5.653594115	4.178435238
	C60	-8.608154902	7.027714993	4.443380611
	C61	-8.538766203	7.826129011	5.568712300
	C62	-9.711906177	8.832027327	3.980963530
	C63	9.229877021	0.115648172	3.961418670
	C64	10.221922416	-0.936976743	3.505857480
	C65	7.827423685	-0.403838926	3.579181450
	C66	6.701088261	0.505295763	4.018933864
	C67	6.073077749	0.349171398	5.268320086
	C68	6.248493862	1.544816084	3.184456252
	C69	5.022860774	1.185320125	5.668325390
	C70	5.217239135	2.398221053	3.576662209
	C71	4.598147058	2.213273208	4.816603975

C72	5.794954239	6.605713061	0.774061522
C73	4.822775147	7.791366220	0.891102704
C74	5.015016505	5.297206092	0.651696921
C75	3.956828340	9.830057896	-0.207901602
C76	2.486440442	9.596564212	-0.566489633
C77	0.782538905	7.873902393	-1.145996933
C78	0.183281916	7.173400617	0.099044310
C79	0.820588354	6.955352211	-2.386986505
C80	-0.460551987	6.230345637	-2.815433301
C81	-1.538077306	7.079633959	-3.507260666
C82	-2.964323740	8.873020086	-2.524803086
C83	0.442381355	5.562189141	1.915100999
C84	0.371245549	6.450977646	3.167676929
C85	1.247634040	4.299494753	2.267001531
C86	1.565254049	8.111541440	4.517055860
C87	1.062719047	9.545473326	4.613857390
C88	-0.154558430	11.362697692	3.525543232
C89	-1.411275700	11.783252897	4.322519484
C90	-0.242224490	11.850945219	2.075020373
C91	-1.423828857	11.278635038	1.298852156
C92	-3.474553078	11.066399403	5.426275458
C93	-3.376680730	11.826337513	6.739107590
C94	-4.243500753	9.730540062	5.635195133
C95	-4.497350301	9.020648041	4.325725141
C96	-5.626259983	9.338514896	3.556331654
C97	-3.584452134	8.087199195	3.808701022
C98	-5.826590566	8.767090503	2.298998019
C99	-3.755639887	7.524644376	2.541388915
C100	-4.876498541	7.877974619	1.795046167
C101	4.273505897	-1.499643847	-9.642707217
C102	2.847984973	-1.296252915	-9.160735429
C103	1.419132307	-0.091367378	-7.521598592
C104	1.022493044	1.383420319	-7.672913442
C105	1.530966265	3.673021885	-6.934783693
C106	2.778984377	4.546081579	-6.816947980
C107	5.080726968	4.828107195	-6.086434189
C108	5.650932148	5.438432238	-7.351193017
C109	-2.456567195	-0.537347471	-9.873045583
C110	-3.426226804	0.500906150	-9.296723289
C111	-2.101731078	-1.592831594	-8.801065560
C112	-1.449277139	-2.829101036	-9.445460130
C113	-0.879101694	-3.753944853	-8.393327017
C114	-3.713409144	2.558917007	-8.012744908
C115	-3.089416924	3.920256185	-8.241639778
C116	-4.218527866	2.307218983	-6.572142013
C117	-3.058145796	1.958759535	-5.687217743
C118	-2.255546979	2.966860646	-5.129169902
C119	-2.651223027	0.617304835	-5.579981418
C120	-1.024047075	2.642710100	-4.554283908
C121	-1.420714482	0.297997457	-5.005427818
C122	-0.588110622	1.316564407	-4.534912949
C123	7.751408636	-5.197278277	-6.154891461
C124	8.884201711	-5.631461517	-5.208383429
C125	6.381355104	-5.596202941	-5.581588026
C126	5.177083835	-5.074561573	-6.300255945
C127	4.809306013	-5.314561037	-7.607839132
C128	3.165643237	-4.244781401	-6.578582744
C129	9.941978820	-7.360259735	-3.873110723
C130	11.328861072	-7.027164088	-4.374321060
C131	0.253007759	-6.457795590	-2.123587547
C132	1.714138863	-6.752953321	-1.792328641
C133	2.692561542	-6.624105515	-2.998523270
C134	2.541343592	-7.854575827	-3.931401879
C135	3.603553655	-7.975449057	-5.025970743
C136	3.533338768	-9.285764066	-5.840467776
C137	4.140156683	-6.588879204	-2.475928537
C138	3.667158956	-0.283961683	-2.226100156
Fe139	3.834766907	-1.087952870	-4.015410021
Fe140	2.326717544	0.658054027	-1.168026138
Fe141	4.972748054	0.603905240	-1.000252999
Fe142	3.912920649	1.377997911	-3.212583404
Fe143	3.896865591	3.034078186	-1.252067976
Fe144	4.833943771	-1.863715871	-1.779064604
Fe145	2.226978280	-1.636861417	-1.940306258
H146	-6.686099396	-6.828782843	-2.012582140
H147	-6.749907196	-5.497502855	-2.953833324
H148	-9.979562842	-4.297198383	-0.410705051
H149	-9.061925482	-5.136568511	-2.440790070
H150	-9.052304627	-6.621649699	-1.491677586
H151	-8.125300814	-2.679808222	0.946785588

H152	-9.153995420	-5.932701847	1.866621846
H153	-9.804915455	-2.969529085	1.448455039
H154	-8.559626478	-7.231905353	3.701207671
H155	-6.500163823	-6.172673559	1.661187481
H156	-8.353602422	-5.754225034	4.665220740
H157	-3.164409919	-2.369985994	2.596367302
H158	-5.333327624	-4.040553040	1.778792797
H159	-4.223905338	-6.563735042	1.354568416
H160	-5.249894759	-1.866275378	6.793422833
H161	-6.118736346	-3.362567128	4.491356933
H162	-4.069148206	-7.176724913	3.020389426
H163	-4.863776720	-1.890266161	2.433731026
H164	-4.933106396	-5.401764738	6.072106102
H165	-6.477628469	-3.161498435	6.770159490
H166	-0.806722042	-3.988425272	2.402438798
H167	-0.835910871	-2.512208879	1.406546776
H168	0.714187956	-3.154923042	1.993104284
H169	-1.524994942	-1.981349078	3.760297505
H170	-4.202481902	-7.030676509	7.578589727
H171	-2.108072494	0.603821371	5.641476037
H172	-2.000461407	-2.781692446	8.660574182
H173	-2.037951965	0.461444399	10.000182215
H174	1.237838689	-0.835640790	3.053943364
H175	0.067637982	-0.103661376	4.178309573
H176	9.287651714	0.164528040	5.066793871
H177	-2.974803312	1.801703543	6.617353955
H178	-2.909386587	1.735063519	9.111671889
H179	-1.196979204	1.839004702	6.550109197
H180	-1.129578390	1.736805214	9.153129453
H181	-2.887720638	-0.404693263	7.811882799
H182	0.139987483	0.004820707	7.611764250
H183	-1.716976608	-1.679290465	6.116164249
H184	-0.334026761	-0.250784584	2.456394255
H185	1.409711919	3.704429702	1.351247655
H186	0.633601179	3.708521104	2.962699073
H187	2.672298025	4.042191470	3.612782756
H188	3.175301042	2.804715728	5.993898724
H189	4.862100467	3.183840684	2.909791131
H190	6.687042397	1.673448924	2.192011033
H191	6.401345895	-0.448434502	5.940388254
H192	-1.472119905	-4.196715716	5.030393467
H193	-0.546991486	-7.186869231	4.603206914
H194	0.036695176	-7.069882968	6.277492258
H195	-2.588134800	-6.071709834	5.280833883
H196	-3.669057316	-5.760201209	8.707514784
H197	4.530778900	1.027766769	6.632016722
H198	1.214094386	-3.103835406	4.468252790
H199	-1.420517567	-2.676904939	11.373547909
H200	-1.616738679	-4.187258523	10.441333578
H201	1.021205594	-3.781419293	9.855123091
H202	10.549405742	-8.656884485	2.207901079
H203	-1.892069148	-4.437518283	-5.720580163
H204	1.073166290	-5.293202273	-3.433285163
H205	-2.210556198	-3.383503904	-10.013692232
H206	-0.658313920	-2.516522953	-10.142365870
H207	-3.009731187	-1.905183816	-8.262642288
H208	-2.404350618	3.966396447	-9.121160323
H209	-3.059374341	-1.045443573	-10.642440113
H210	-3.361005464	-1.133410055	-2.985743067
H211	-4.083888040	-4.093407272	-2.612911732
H212	-1.861427546	1.558169475	-8.432684151
H213	-4.611227370	2.579087118	-8.667017805
H214	-0.659692642	0.505525484	-9.904080414
H215	-1.470463068	-4.728863442	-4.037154803
H216	-1.435234440	-1.138564212	-8.051699397
H217	-0.837690640	-0.576804830	-11.134663952
H218	-6.780202367	-1.932907699	-3.960178958
H219	-3.515475307	-1.794985440	-1.367778052
H220	0.884061910	-2.970399037	-8.753656660
H221	-2.432423208	-3.569397518	-2.340566415
H222	-3.830972095	1.888954062	3.641267487
H223	-3.175543627	0.316140481	1.678936381
H224	-8.284236196	0.230352653	3.576088895
H225	-7.282471168	0.168751741	0.758096473
H226	-6.726601060	3.832635773	3.129477557
H227	-8.045347857	7.695320604	6.525036268
H228	-6.748650391	4.078963992	6.391024522
H229	-8.713072372	4.882659375	4.635515973
H230	-5.968414655	6.252603291	4.347659495
H231	-10.310355585	9.596143451	3.490473384

	H232	-3.083324625	3.952750251	2.435578588
	H233	-4.583216929	3.965493872	1.494679959
	H234	-9.378888532	9.771100334	5.863036612
	H235	-8.130053391	5.502842809	3.089267766
	H236	-6.044390996	1.953040271	1.715001826
	H237	-7.213481057	-1.019438626	2.938575772
	H238	-9.673600010	2.653254216	0.003532592
	H239	-1.831488369	1.935820165	-1.959855158
	H240	-10.133317150	1.004037536	-0.453947217
	H241	10.357916328	1.802028330	3.701263176
	H242	8.761130050	2.033507737	3.428986744
	H243	1.858359757	5.939289695	0.322932938
	H244	-0.593903413	5.258102926	1.706195158
	H245	2.085853220	7.421774279	2.585817836
	H246	-2.908581560	3.860148797	-0.590825012
	H247	-4.634865146	5.096650449	-1.599146189
	H248	-6.128070813	4.887768631	-3.267674306
	H249	-4.346781837	6.019780676	-0.347792777
	H250	-5.115786634	2.734028026	-3.660340002
	H251	-6.906140942	2.807056185	-3.559484720
	H252	0.712964284	11.664537617	1.564699594
	H253	-0.389514965	12.941751230	2.112480873
	H254	-0.176660305	10.760753480	-0.276888185
	H255	-1.891471111	10.391866374	-0.452533422
	H256	-2.889571858	10.756787890	-3.335946907
	H257	-2.071990677	6.466452578	-4.249837173
	H258	-6.716091403	9.015668066	1.714727229
	H259	-2.718949185	7.771941384	4.398209616
	H260	-4.006567344	8.602571558	-0.770404223
	H261	1.583308282	6.182795095	-2.201870072
	H262	2.885376179	7.621078664	-0.910150270
	H263	-0.906125386	5.673704960	-1.976136112
	H264	-8.211523211	0.831477674	-1.740626648
	H265	4.371463451	10.540770215	-0.934664671
	H266	-5.838127480	0.434570841	-3.368851579
	H267	1.194871269	7.560436944	-3.229566378
	H268	-3.007414748	6.846451022	2.130807413
	H269	3.959338809	10.317828218	0.777555573
	H270	-2.231998080	9.508714808	-4.344492573
	H271	-4.358619255	10.063174853	-1.624087849
	H272	-5.194563343	-2.023251320	-4.485299331
	H273	-5.854367800	-2.581800633	-1.945051412
	H274	-6.366759568	10.041729264	3.943716386
	H275	-4.996415209	2.146552137	-1.244419242
	H276	0.155903374	8.753688599	-1.322783121
	H277	-1.058497860	7.902659349	-4.052935787
	H278	-0.145406129	5.469409972	-3.542896410
	H279	-3.004798751	6.916432564	-1.963080031
	H280	1.087732372	7.541894000	5.328135917
	H281	0.062020366	9.326381489	2.841053021
	H282	0.657765421	11.925164686	4.010970061
	H283	2.646868349	8.136822664	4.709737239
	H284	-1.935619469	9.840940803	4.588697688
	H285	4.848205996	-0.570079404	-9.519410256
	H286	4.717956355	-2.246069771	-8.952300382
	H287	7.818247421	-4.100146189	-6.197696868
	H288	5.203567791	-2.292848861	-11.275297159
	H289	3.613418511	-2.672014882	-11.168850165
	H290	5.739669317	4.478089286	0.557622648
	H291	6.119559575	6.536203062	2.789239577
	H292	5.396536426	8.451939599	-0.968894275
	H293	4.394037281	5.138074617	1.543784369
	H294	7.279652614	7.355873612	1.977871781
	H295	5.861372724	4.194003433	-5.637705047
	H296	6.421470836	6.733645537	-0.122584540
	H297	4.783853377	-8.523250359	2.993891162
	H298	6.470573560	-8.874597627	0.453543957
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	H301	1.035109425	3.930394263	-7.878710455
	H302	-1.102124171	-0.743100195	-4.915203435
	H303	0.853000393	3.985704027	-6.122204533
	H304	4.184050594	-5.899776743	3.392407253
	H305	2.348789276	1.807470089	-6.190649877
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	H307	4.200978926	-8.354938527	1.318461692
	H308	5.871088699	-6.525636342	0.921252812
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	H310	-4.950893613	1.487903280	-6.607032047
	H311	5.126348333	-10.939653357	2.144045738

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H320	6.312894219	-6.697628930	-5.568701918
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	N396	-6.161040124	4.194383983	3.893821097
	N397	-9.345173591	7.668078102	3.459150690
	N398	-9.243281518	8.969010397	5.253745457
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	N402	2.146314706	8.334972957	-0.898515148
	N403	-2.527451641	7.618040642	-2.568747828
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	N420	8.907983065	-6.929069180	-4.799393899
	O421	-6.901016116	-4.989318123	-0.064147772
	O422	-7.687145031	-3.508680731	3.299731999
	O423	-5.956208025	-6.552566412	4.778228880
	O424	-2.926780897	-4.994575859	3.625182913
	O425	-3.358418327	-1.895139921	5.059194169
	O426	-3.909848822	-3.355263337	8.297964711
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	O432	6.294460326	-11.001688822	-0.801876368
	O433	7.355833006	-9.683444426	3.522379884
	O434	10.994962482	-6.397244193	3.449534463
	O435	-5.834785036	-0.518054456	-0.369997195
	O436	-3.782522332	-2.868335339	-5.247352478
	O437	-6.914143756	3.047854767	0.118573295
	O438	-5.899648624	4.310687647	-2.517278017
	O439	-9.777445815	1.505781043	2.273542824
	O440	-5.842187728	0.569324576	4.588234680
	O441	-4.221156851	3.990224681	5.070712058
	O442	-6.290944954	5.992737967	6.935951128
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	O445	4.105269681	7.962380220	1.892234763
	O446	1.696105904	10.561675791	-0.540225225
	O447	-0.962302734	7.459326049	0.482399662
	O448	-0.472514194	6.228985718	4.044888272
	O449	2.499552274	4.648676447	2.865907064
	O450	1.407012565	10.272351879	5.554099883
	O451	-1.680388808	12.984122774	4.475847693
	O452	-2.558860632	11.216308293	1.793523984
	O453	-4.318684372	12.431993637	7.226954331
	O454	-5.006653241	7.345635235	0.501038729
	O455	1.913112579	-1.992741705	-9.626427823
	O456	0.131461323	1.745119168	-8.471099614
	O457	2.704993582	5.750617329	-7.114878802
	O458	6.409837124	6.395272385	-7.349813899
	O459	-4.653173893	0.404418586	-9.469992672
	O460	-1.559420742	-4.538914975	-7.741687355
	O461	0.445354408	-3.649619948	-8.155263773
	O462	-3.337447346	4.919258885	-7.581611892
	O463	9.783475255	-4.839692328	-4.862353207
	O464	12.306590987	-6.921904007	-3.645948774
	O465	0.066857076	-5.514589444	-3.049681965
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	O471	2.400869926	-5.403445536	-3.679786077

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	O474	-3.917272158	5.577747825	-1.112876710
	O475	7.210070288	-9.816809522	-5.143117796
	O476	6.978288814	-8.770333530	-2.326160168
	S477	3.893256810	5.283716018	-0.823899238
	S478	2.093249577	2.495679065	-2.541352811
	S479	1.951881801	-2.315350513	-4.121317447
	S480	3.605009003	1.618348824	0.465961602
	S481	0.477481771	-0.327955145	-1.998301254
	S482	4.133101556	0.715691774	-5.310870206
	S483	3.540213630	-3.638704416	-1.039753843
	S484	5.775849429	2.255923683	-2.262046242
	S485	5.676901641	-2.401985099	-3.765344936
	S486	6.310801976	-1.045158034	-0.369068433
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Fe2-brNH2-Fe6-3b2 to Fe2NH3 **S=1, 35** **TS** Fe(139) -2.330 Fe(140) 0.926 Fe(141) -2.473 Fe(142) 2.212 Fe(143) 3.048 Fe(144) 2.483 Fe(145) -1.293	9651826nh23b2t35te_1_52971.25			
	C1	-8.052755068	-4.987586549	-0.547749645
	C2	-8.438924938	-5.762026092	-1.812555684
	C3	-8.834625513	-3.445149718	1.198829425
	C4	-8.315533896	-4.134780808	2.456255253
	C5	-8.076343967	-6.218113257	3.716535608
	C6	-6.553522339	-6.388487105	3.709979252
	C7	-4.490365423	-6.375264614	2.402554581
	C8	-3.901292912	-5.040254740	2.870783791
	C9	-4.184224516	-2.603568048	2.885936320
	C10	-4.245288376	-2.454988566	4.412284882
	C11	-5.424689195	-2.878057098	6.478602723
	C12	-4.458133228	-3.765713521	7.277006354
	C13	-3.622068673	-6.045195990	7.638463116
	C14	-2.152602386	-6.319829523	7.285854306
	C15	-0.491533450	-6.577559558	5.487335856
	C16	0.305071938	-5.316306849	5.135854506
	C17	0.186838854	-2.889260955	4.711840027
	C18	0.344603575	-2.033031689	5.983560665
	C19	-0.496676353	-2.183186453	3.520180124
	C20	0.046848512	-0.768479124	3.292006050
	C21	-0.362901816	-3.030787435	2.248397988
	C22	-0.713181515	-0.654615686	7.708556690
	C23	-0.433434507	-1.425232104	9.010971875
	C24	-1.972448523	0.241191125	7.786319895
	C25	-1.991099197	1.067980755	9.076196555
	C26	-2.045517644	1.160199022	6.559738285
	C27	-1.018540789	-3.238320121	10.507677347
	C28	0.424106010	-3.627104518	10.763502268
	C29	4.943528779	-12.590726405	0.381515835
	C30	5.705030364	-11.275652531	0.267908771
	C31	6.153552677	-9.149903119	1.471032375
	C32	7.366132593	-9.105985424	2.418254327
	C33	5.045343556	-8.209102791	1.971205596
	C34	5.499527359	-6.755174067	1.962377505
	C35	4.406743445	-5.781609005	2.386032962
	C36	5.036396684	-3.426749231	2.972501887
	C37	9.640170199	-8.258244456	2.735555589
	C38	9.903550520	-6.824071937	3.139281899
	C39	-5.379137422	-1.721483762	-2.452321257
	C40	-5.741546537	-0.487222835	-1.606713895
	C41	-3.852961958	-1.939916874	-2.397505222
	C42	-3.369496170	-3.320980958	-2.885032344
	C43	-3.099115867	-3.455032599	-4.383336090
	C44	-5.943778555	1.980282291	-1.810692119
	C45	-7.081779208	2.235865121	-0.815145457
	C46	-5.991563093	2.957051875	-2.994322711
	C47	-9.326585110	1.598485934	-0.070965647
	C48	-9.014161470	1.163797909	1.366473892
	C49	-7.450317258	0.058239935	2.891194252
	C50	-6.247658925	0.828467019	3.444333314
	C51	-4.536018219	2.552524941	3.112444745
	C52	-4.954882517	3.617415583	4.137705174
	C53	-3.853436788	3.306929962	1.960382894
	C54	-3.244295684	2.422847483	0.925241983
	C55	-2.987604065	1.068098134	0.869847467
	C56	-2.295929110	1.859406615	-1.005334514
	C57	-6.607117499	5.368829460	4.592858719
	C58	-6.538868826	5.108563467	6.096194724
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	C60	-8.610835555	7.016729828	4.425757577
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	C62	-9.730343103	8.812962316	3.969479933
	C63	9.197302530	0.073450096	3.975672845

C64	10.170922271	-0.995652209	3.513172687
C65	7.787293872	-0.428883031	3.595793134
C66	6.672928590	0.490149062	4.039689173
C67	6.044959535	0.335513454	5.289466458
C68	6.228837105	1.532593556	3.206055949
C69	5.007051657	1.184429072	5.693688141
C70	5.209915799	2.397391537	3.602636858
C71	4.594174836	2.219707376	4.845270169
C72	5.802818381	6.596283673	0.777682931
C73	4.832083023	7.784974300	0.888507339
C74	5.024498620	5.288338977	0.663616356
C75	3.976773114	9.826449139	-0.213709646
C76	2.502907636	9.596848132	-0.560433788
C77	0.793607605	7.877024243	-1.133226412
C78	0.201380659	7.183583643	0.119244093
C79	0.822469001	6.953948930	-2.370810504
C80	-0.464474567	6.235454853	-2.793419620
C81	-1.533536838	7.087811364	-3.495646918
C82	-2.964779699	8.877426207	-2.514472976
C83	0.474034249	5.576874479	1.939017934
C84	0.399794541	6.467941562	3.189131896
C85	1.291535753	4.321662144	2.290992842
C86	1.585740272	8.139244203	4.531014920
C87	1.065939000	9.567000041	4.617558677
C88	-0.162639748	11.361827009	3.512570031
C89	-1.424067846	11.781589534	4.303802809
C90	-0.247674304	11.846146673	2.061265440
C91	-1.425962353	11.271022127	1.283120156
C92	-3.480331987	11.061496447	5.418361280
C93	-3.386286009	11.824464383	6.730385388
C94	-4.246477961	9.724780417	5.628736924
C95	-4.501319771	9.014136085	4.319869437
C96	-5.635205757	9.325223157	3.555002242
C97	-3.584476707	8.086834733	3.799099388
C98	-5.837045559	8.752731018	2.298264565
C99	-3.757205950	7.522951955	2.532723567
C100	-4.883497024	7.869081278	1.790999353
C101	4.272581248	-1.509192761	-9.655920392
C102	2.846639693	-1.300428408	-9.176231137
C103	1.418690975	-0.095298785	-7.536370525
C104	1.024828202	1.381748795	-7.675660368
C105	1.540600482	3.665646861	-6.924836668
C106	2.784018254	4.546359991	-6.809434527
C107	5.084320324	4.845987474	-6.078381589
C108	5.674599335	5.434767836	-7.344015567
C109	-2.474333006	-0.532386484	-9.876222960
C110	-3.446356663	0.498807490	-9.292575465
C111	-2.114965629	-1.588111035	-8.805123109
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N418	4.130508147	-4.433511340	-5.707298025
N419	3.569811606	-4.832944479	-7.800380129
N420	8.915347752	-6.925339500	-4.791038575
O421	-6.900765194	-4.984984722	-0.078164493
O422	-7.666293850	-3.490335185	3.298167880
O423	-5.937264539	-6.529424060	4.780307125
O424	-2.915660404	-4.981518450	3.627320262
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O428	1.534792813	-5.387570049	4.971506229
O429	1.472122352	-1.811022279	6.452234710
O430	0.435509527	-1.047352588	9.816054174
O431	0.875814379	-3.824914402	11.882112006
O432	6.293365042	-10.985661879	-0.793913845
O433	7.319242417	-9.638033119	3.541225729
O434	11.007132711	-6.404734130	3.452726570
O435	-5.841672397	-0.515666179	-0.365500696
O436	-3.782945208	-2.856353764	-5.245681650
O437	-6.943637145	3.045011319	0.118049601
O438	-5.920302118	4.312627368	-2.511928914
O439	-9.789395298	1.493763858	2.276639984
O440	-5.842647938	0.582898141	4.587866044
O441	-4.211388208	4.000617798	5.048171328
O442	-6.329250507	5.966073490	6.938042267
O443	10.618306933	-1.875576567	4.235124324
O444	3.572912914	3.088702652	5.170941960
O445	4.113978815	7.961568853	1.888334359
O446	1.713143433	10.562065178	-0.523833949
O447	-0.943564251	7.469071719	0.505368637
O448	-0.443443290	6.246992273	4.067293352
O449	2.540551029	4.679066641	2.891721118
O450	1.399459671	10.304723197	5.553448996
O451	-1.703303063	12.981843470	4.443100991
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O453	-4.330216480	12.428533181	7.216344194
O454	-5.015784608	7.334986680	0.497466265
O455	1.909535438	-1.991007914	-9.646109991
O456	0.122753787	1.748260894	-8.459120463
O457	2.700325182	5.750902792	-7.104865765
O458	6.428413304	6.395350448	-7.348379728
O459	-4.674049662	0.387802111	-9.448875142
O460	-1.561302727	-4.524742536	-7.738189494
O461	0.442204231	-3.638793494	-8.163924435
O462	-3.384733162	4.917448029	-7.573731080
O463	9.780984885	-4.830813417	-4.833271165

O464	12.306423395	-6.908879071	-3.618927287
O465	0.042796496	-5.520442545	-3.060356167
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O467	4.640929293	-9.854762110	-6.137105665
O468	2.385566241	-9.706482587	-6.207414436
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O471	2.382779008	-5.398625684	-3.697652176
O472	8.474352398	-7.210310064	-0.613108967
O473	6.702900359	-4.954633753	-0.749050446
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O475	7.207100919	-9.818974772	-5.144987624
O476	6.969885299	-8.770633232	-2.332818564
S477	3.889705126	5.283215658	-0.801005719
S478	2.077797646	2.454373923	-2.564796240
S479	1.967067610	-2.303572990	-4.192860320
S480	3.548073956	1.600423325	0.459971813
S481	0.461743735	-0.410906681	-1.999488330
S482	4.154611403	0.739029042	-5.323611146
S483	3.485775464	-3.563765490	-1.068112508
S484	5.754535166	2.275833342	-2.229810007
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S=1, 35
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Fe(139) -2.474
Fe(140) 0.207
Fe(141) -2.519
Fe(142) 2.597
Fe(143) 3.210
Fe(144) 2.446
Fe(145) -2.063

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C5	-8.097528942	-6.242000319	3.714808779
C6	-6.574167613	-6.408675588	3.708095861
C7	-4.508988043	-6.386539845	2.402816353
C8	-3.917142780	-5.053736206	2.873904950
C9	-4.190994663	-2.620362470	2.905208594
C10	-4.256482717	-2.484574139	4.432300511
C11	-5.454026415	-2.907669379	6.489393661
C12	-4.494306639	-3.801172273	7.289740556
C13	-3.670765026	-6.081993968	7.660634793
C14	-2.202482672	-6.354396385	7.303328204
C15	-0.536992671	-6.547470449	5.499933697
C16	0.260299471	-5.285665653	5.154254727
C17	0.171642896	-2.859473535	4.743519362
C18	0.320571419	-2.005353414	6.018497834
C19	-0.471970644	-2.128750143	3.546541467
C20	0.142026434	-0.738316547	3.358801972
C21	-0.345942801	-2.983039805	2.278759459
C22	-0.751932158	-0.639511590	7.745471544
C23	-0.479478640	-1.415738314	9.046153655
C24	-2.010132892	0.258435349	7.818578815
C25	-2.026728117	1.092995052	9.103676494
C26	-2.080974974	1.171396846	6.587525846
C27	-1.052097837	-3.251601243	10.518221846
C28	0.394044388	-3.627721122	10.775488261
C29	4.932349109	-12.609374037	0.366963715
C30	5.701656185	-11.298359245	0.260330831
C31	6.175243276	-9.181432846	1.463717676
C32	7.394604599	-9.146952080	2.401719727
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C34	5.536217898	-6.769723337	1.923438510
C35	4.425817210	-5.788396605	2.282421378
C36	4.971868254	-3.415219932	2.877666977
C37	9.659137996	-8.273841743	2.718959028
C38	9.899608739	-6.835848070	3.122222630
C39	-5.384798057	-1.727605076	-2.460157653
C40	-5.742243848	-0.492481333	-1.614489671
C41	-3.855923087	-1.934401458	-2.404341061
C42	-3.354639027	-3.311351163	-2.884011814
C43	-3.096125012	-3.454841928	-4.383989963
C44	-5.920348552	1.976214418	-1.816071885
C45	-7.052610294	2.240734246	-0.816749080
C46	-5.964467422	2.953138252	-2.999791173
C47	-9.303998204	1.625337573	-0.072521740
C48	-8.999874783	1.178607731	1.362842031
C49	-7.446745034	0.053405972	2.884338548
C50	-6.246238361	0.821813213	3.445230704
C51	-4.541740954	2.556209498	3.129733713
C52	-4.961988809	3.623702299	4.152661599
C53	-3.845675430	3.300677991	1.979318688
C54	-3.217132139	2.405876154	0.964862091
C55	-2.927706698	1.057051976	0.943192710

	C56	-2.237745085	1.820370787	-0.944411025
	C57	-6.603782601	5.389769704	4.601854973
	C58	-6.514994252	5.135909810	6.104770041
	C59	-8.071273202	5.656189794	4.184683713
	C60	-8.611185789	7.030520133	4.448861969
	C61	-8.542880319	7.827874964	5.574887388
	C62	-9.709002120	8.837831965	3.984603329
	C63	9.238263359	0.128413158	3.951184360
	C64	10.223627368	-0.928458807	3.488820116
	C65	7.832549075	-0.406593343	3.579774106
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	C67	6.075193415	0.340002186	5.264716947
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	C71	4.601743499	2.206629260	4.816339565
	C72	5.793314845	6.599474918	0.770572043
	C73	4.824096383	7.788450864	0.892154631
	C74	5.004058316	5.300453825	0.647095378
	C75	3.954488215	9.826716225	-0.204420757
	C76	2.485155170	9.591205338	-0.567142690
	C77	0.781717722	7.869511921	-1.150180401
	C78	0.179884995	7.169033842	0.093751798
	C79	0.821119291	6.951005801	-2.391446236
	C80	-0.459951844	6.226087376	-2.821284761
	C81	-1.538648411	7.076529116	-3.509712731
	C82	-2.963619305	8.870855481	-2.526930192
	C83	0.436444031	5.556893967	1.909300094
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	C90	-0.240017916	11.849095910	2.077145450
	C91	-1.422640742	11.278540367	1.301099783
	C92	-3.472198926	11.067445693	5.428393297
	C93	-3.372674646	11.827152325	6.741436493
	C94	-4.242195406	9.732039404	5.637470594
	C95	-4.496389404	9.021878242	4.327942397
	C96	-5.624640069	9.340878576	3.558079408
	C97	-3.584610300	8.087147792	3.811153126
	C98	-5.825214929	8.769931371	2.300604875
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	C100	-4.875809185	7.879996048	1.796774691
	C101	4.273177458	-1.502197184	-9.636803604
	C102	2.846203724	-1.291473983	-9.159746490
	C103	1.411247467	-0.076002304	-7.538908804
	C104	1.015821986	1.398226640	-7.682522901
	C105	1.522124697	3.682942003	-6.928634202
	C106	2.771065622	4.554711322	-6.804615133
	C107	5.077986398	4.818318612	-6.080039638
	C108	5.650708812	5.434721043	-7.341037501
	C109	-2.453833916	-0.536059202	-9.875969506
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	C119	-2.644915425	0.590808384	-5.567703599
	C120	-1.016163717	2.580938607	-4.482589545
	C121	-1.450499185	0.244559997	-4.933117691
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	Fe140	2.366941249	0.517093432	-1.086514630
	Fe141	4.989264575	0.585558766	-1.043808134
	Fe142	3.850915293	1.328952236	-3.275279854
	Fe143	3.897748101	3.052112942	-1.264953887
	Fe144	4.818761673	-1.892588902	-1.883849901
	Fe145	2.293900375	-1.718050189	-2.498073540
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	H147	-6.752728831	-5.494959385	-2.947204964
	H148	-9.987107492	-4.302038228	-0.412204709
	H149	-9.066855562	-5.143693219	-2.440665756
	H150	-9.055015336	-6.630248743	-1.495356186
	H151	-8.135810793	-2.686575943	0.944708998
	H152	-9.160855041	-5.938738374	1.869369979
	H153	-9.814453901	-2.976826090	1.449192625
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	H156	-8.356639631	-5.758946845	4.666485184
	H157	-3.167786971	-2.372330749	2.600264346
	H158	-5.337851821	-4.043130277	1.783849917
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	H160	-5.256067148	-1.872051967	6.796070257
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	H162	-4.072462238	-7.179295562	3.021717673
	H163	-4.866793254	-1.892561821	2.436747215
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	H179	-1.202335145	1.836911122	6.555020612
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	H181	-2.895551430	-0.402643685	7.820747290
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	H184	-0.304505087	-0.249608854	2.479093560
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	H186	0.623502113	3.702267342	2.955704767
	H187	2.662610356	4.031929170	3.608591837
	H188	3.177842736	2.800143417	5.992441758
	H189	4.870310981	3.180837883	2.911218736
	H190	6.689389617	1.668025972	2.190876629
	H191	6.401968675	-0.456333734	5.939224883
	H192	-1.476925211	-4.195639681	5.040742349
	H193	-0.555967081	-7.187113331	4.604658300
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	H196	-3.677566797	-5.766397484	8.710859358
	H197	4.533641817	1.022154386	6.629663162
	H198	1.210022836	-3.102017815	4.475829328
	H199	-1.429364096	-2.682518346	11.383847932
	H200	-1.623863370	-4.190065199	10.446514624
	H201	1.012949487	-3.779728251	9.860227336
	H202	10.552080489	-8.660982156	2.204334828
	H203	-1.892448421	-4.428461074	-5.721657906
	H204	1.049630382	-5.290786631	-3.488360646
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	H206	-0.657908351	-2.514874746	-10.143238530
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	H209	-3.055104640	-1.045965318	-10.644155111
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	H216	-1.435090785	-1.137972699	-8.052315333
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	H218	-6.788707023	-1.937011305	-3.962929540
	H219	-3.534065104	-1.794917225	-1.362768089
	H220	0.883087886	-2.975361083	-8.752164398
	H221	-2.431889873	-3.564238586	-2.341668027
	H222	-3.835784896	1.892031690	3.647187059
	H223	-3.145013947	0.320267157	1.712071809
	H224	-8.283453430	0.228833316	3.574512866
	H225	-7.282191155	0.169035328	0.756522561
	H226	-6.728445974	3.839426950	3.130898232
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	H229	-8.715628407	4.885277471	4.643242711
	H230	-5.972789949	6.257777399	4.350914092
	H231	-10.304175614	9.603855706	3.493192077
	H232	-3.087324932	3.957157115	2.438934161
	H233	-4.582442596	3.960362313	1.490097054
	H234	-9.378613766	9.774849312	5.868172772
	H235	-8.135156665	5.504368452	3.095831047
	H236	-6.046822146	1.957144583	1.716997294
	H237	-7.212969948	-1.020512539	2.935615421
	H238	-9.667104129	2.659327225	0.003607565
	H239	-1.805203054	1.917754706	-1.937629692
	H240	-10.130619129	1.011325124	-0.454671234
	H241	10.359166704	1.821223927	3.686692203
	H242	8.761023518	2.047649005	3.423053702
	H243	1.854676109	5.934788243	0.318151933
	H244	-0.600352426	5.254386831	1.700238517
	H245	2.080967597	7.414567609	2.582089855
	H246	-2.903469530	3.845277890	-0.590251031
	H247	-4.634635172	5.096624494	-1.598638956
	H248	-6.124543908	4.886218047	-3.268119490
	H249	-4.348611339	6.020861248	-0.346466136
	H250	-5.109441266	2.734085952	-3.660677565
	H251	-6.900117918	2.804604977	-3.562872413
	H252	0.714741666	11.661550603	1.566393739
	H253	-0.385791552	12.940088991	2.114983585
	H254	-0.176196779	10.756474191	-0.274211034
	H255	-1.891996740	10.391706050	-0.450179222
	H256	-2.889169306	10.753470821	-3.341271465
	H257	-2.074385218	6.464032160	-4.251542659
	H258	-6.714280431	9.019812527	1.716236240
	H259	-2.719888607	7.770484055	4.401014946
	H260	-4.000930956	8.602657710	-0.769444562
	H261	1.583185429	6.178187956	-2.205266358
	H262	2.883204369	7.613057856	-0.907165830
	H263	-0.904011851	5.667107999	-1.982673617
	H264	-8.210451343	0.835548238	-1.742239258
	H265	4.369149622	10.540807081	-0.927846102
	H266	-5.843508290	0.431604226	-3.372545102
	H267	1.196420689	7.556122254	-3.233644954
	H268	-3.008291878	6.845907687	2.133329760
	H269	3.953202305	10.311715583	0.782312689
	H270	-2.234306371	9.503772147	-4.349428329
	H271	-4.357185065	10.060900105	-1.625422019
	H272	-5.202743805	-2.025088802	-4.488389486
	H273	-5.862077590	-2.584551335	-1.947510927
	H274	-6.364150229	10.045078209	3.945339933
	H275	-4.991516937	2.139916251	-1.247971617
	H276	0.155266341	8.749598727	-1.328002585
	H277	-1.059188905	7.899113167	-4.056069392
	H278	-0.145247030	5.467120971	-3.551568831
	H279	-3.001416419	6.915378593	-1.961336758
	H280	1.083415366	7.533846722	5.324605266
	H281	0.061755745	9.324785684	2.839552952
	H282	0.661890950	11.921100329	4.012356049
	H283	2.643494455	8.126221747	4.706463162
	H284	-1.937357598	9.840600505	4.585965222
	H285	4.852032916	-0.575156395	-9.511769811
	H286	4.712197217	-2.251601579	-8.945595918
	H287	7.837351966	-4.123896768	-6.223735742
	H288	5.203774779	-2.297413394	-11.267170824
	H289	3.612614328	-2.671972466	-11.163585247
	H290	5.718740168	4.473322480	0.547827484
	H291	6.124110094	6.526747685	2.785629702
	H292	5.389021816	8.445765985	-0.970629702
	H293	4.384698724	5.143113397	1.540388131
	H294	7.284968594	7.341863724	1.971295571
	H295	5.855002574	4.175474419	-5.637325095

	H296	6.418084387	6.727444898	-0.127155743
	H297	4.788039355	-8.517602186	2.989550806
	H298	6.473785453	-8.882664498	0.450702107
	H299	3.960706418	3.004769323	-6.061715718
	H300	5.373227280	-1.427510363	3.105986977
	H301	1.028290726	3.944573213	-7.872445072
	H302	-1.158067858	-0.803507910	-4.834257438
	H303	0.843838828	3.991453148	-6.114771789
	H304	4.149179128	-5.890900319	3.338843691
	H305	2.342903245	1.814376837	-6.199090621
	H306	3.518474092	-5.988169486	1.690961012
	H307	4.204087113	-8.358932008	1.313887954
	H308	5.886483759	-6.534919386	0.908779031
	H309	6.385240380	-6.601668059	2.603872403
	H310	-4.924285594	1.492476331	-6.600222546
	H311	5.128677612	-10.942455215	2.147478140
	H312	4.038103442	-12.480640722	-0.261926878
	H313	0.312826101	0.974348125	-3.921926423
	H314	5.237665100	-13.494072109	2.201271152
	H315	3.671705050	-13.507910683	1.721814786
	H316	5.221396851	-4.259825388	1.054662713
	H317	-0.376789140	3.341720551	-4.028918119
	H318	-3.288167345	-0.191010492	-5.978110281
	H319	7.112931215	-9.573981962	-4.199043276
	H320	6.366254899	-6.747019102	-5.616760512
	H321	6.133453692	-8.245558653	-2.240815020
	H322	6.266787840	-9.774507140	-5.488412505
	H323	5.354482292	4.929717368	-8.291257399
	H324	6.078028281	-5.187756537	-1.486745814
	H325	1.806175813	-7.692169930	-1.341655612
	H326	3.508875114	0.064354635	-7.772705602
	H327	2.591979403	-8.727319922	-3.279504188
	H328	3.065619238	-4.994352784	-8.733813724
	H329	2.212763210	-3.971573463	-6.580611009
	H330	5.552076521	-13.381192389	-0.120372138
	H331	5.720083411	-2.026259127	1.506826915
	H332	7.947588355	-6.386411580	-0.640217163
	H333	7.053328587	-4.098445500	-0.968400363
	H334	8.428121516	-8.026312549	0.973508321
	H335	3.927366399	-4.295307822	4.425449769
	H336	3.496342678	-7.153353148	-5.749155547
	H337	4.615957683	-7.895247685	-4.598963106
	H338	1.543331391	-7.835228550	-4.395016338
	H339	1.486312297	-0.356552195	-6.476785280
	H340	-2.512556656	3.979713797	-5.195622005
	H341	-4.689878854	3.221769210	-6.229071141
	H342	2.011360480	-5.953352952	-1.062136298
	H343	8.019091390	-7.803922882	-1.279882304
	H344	6.767067152	-9.583772857	-1.786891654
	H345	4.570412059	-2.747312593	4.763045208
	H346	5.453890351	-5.911489778	-8.492005818
	H347	6.332692485	-5.319344923	-4.592683143
	H348	0.641833821	-0.684254905	-8.019596849
	H349	4.860602495	5.622114569	-5.358861614
	H350	7.712723040	-1.395326193	4.050477343
	H351	7.798991177	-0.546689925	2.487017488
	H352	8.929865551	-5.410773598	-7.879594813
	H353	8.048440725	-6.748890189	-7.545496728
	H354	9.882448918	-8.453674884	-3.768069058
	H355	8.202688295	-7.616589943	-5.062294411
	H356	11.423620678	-6.962248903	-5.478043548
	H357	9.804850593	-6.929161058	-2.856745082
	H358	10.454819849	-0.892922638	2.400005038
	H359	-2.383695603	11.768136101	7.253970662
	H360	9.528045257	-8.852236493	3.651340029
	H361	8.993109423	-6.182884937	3.123997905
	H362	-4.042103798	11.697700025	4.724963706
	H363	-3.668924829	9.090774196	6.324891845
	H364	-5.193125201	9.979399168	6.130483962
	H365	2.888739802	-0.632245592	1.269264691
	H366	-5.927050775	7.481705502	0.207107771
	H367	2.250953691	-1.749218032	0.214894518
	H368	1.262742382	-0.663268700	0.968501368
	Mo369	3.722965044	-3.730039146	-3.601777968
	N370	2.184516125	-0.776956249	0.539052595
	N371	-7.312946321	-6.278435239	-2.602319071
	N372	-9.092691744	-4.357027890	0.069013336
	N373	-8.622206206	-5.475472400	2.597256390
	N374	-5.963385632	-6.410959963	2.497514333
	N375	-4.559186589	-3.946074979	2.432743752

	N376	-5.329776958	-3.035507378	5.047201445
	N377	-4.375706337	-5.086640570	6.865261488
	N378	-1.890732224	-6.331428980	5.978803242
	N379	-0.461129794	-4.142454852	5.022692828
	N380	-0.819073762	-1.526757306	6.584414056
	N381	-1.215725949	-2.534601681	9.266131358
	N382	4.517238696	-12.935762220	1.737623754
	N383	5.646743634	-10.529759961	1.365671159
	N384	4.861705616	-4.417158590	2.001442467
	N385	4.595831271	-3.572389900	4.170561216
	N386	5.472913932	-2.233451276	2.493501801
	N387	8.460298529	-8.454778950	1.925678241
	N388	-5.853069199	-1.542686357	-3.841313535
	N389	-2.094920932	-4.287450654	-4.727415757
	N390	-5.932072505	0.627479779	-2.362593061
	N391	-8.197840966	1.541230655	-1.009259067
	N392	-7.887238792	0.418508522	1.550947528
	N393	-5.675309629	1.770809389	2.651400985
	N394	-2.765315831	2.883888376	-0.254215144
	N395	-2.324851915	0.700524824	-0.242005713
	N396	-6.163432322	4.199200417	3.896566537
	N397	-9.343765992	7.673345517	3.462918787
	N398	-9.243497655	8.972771421	5.258779403
	N399	9.530888399	1.390718953	3.266910113
	N400	6.692063899	6.507813861	1.932402277
	N401	4.804259029	8.651873469	-0.164778078
	N402	2.145674878	8.329859747	-0.900250981
	N403	-2.525280485	7.616090778	-2.568709437
	N404	-2.610020010	9.784037859	-3.450906957
	N405	-3.716642855	9.284792773	-1.478144814
	N406	0.960275686	6.252409289	0.732644118
	N407	1.308082952	7.428734039	3.252738392
	N408	0.207130132	9.953727450	3.629351080
	N409	-1.149442528	10.906051929	0.022225379
	N410	-2.149519298	10.791047225	4.880383948
	N411	4.284859045	-1.908222089	-11.044719947
	N412	2.679233857	-0.355561898	-8.201996907
	N413	1.719871674	2.245425032	-6.904955498
	N414	3.913382591	3.991811398	-6.340273844
	N415	-1.334226415	0.110160147	-10.570806416
	N416	-2.871534596	1.523740023	-8.590355299
	N417	8.011454534	-5.724720961	-7.553367797
	N418	4.152841422	-4.499446614	-5.791398031
	N419	3.623148668	-4.927653889	-7.887353990
	N420	8.918083896	-6.935716366	-4.794629114
	O421	-6.910745211	-4.998113537	-0.058557595
	O422	-7.691196120	-3.512947998	3.296693200
	O423	-5.959279226	-6.556148629	4.778449977
	O424	-2.927749637	-4.995749218	3.626527317
	O425	-3.363336902	-1.900359987	5.064207679
	O426	-3.913332638	-3.361105964	8.297630480
	O427	-1.392162723	-6.635745434	8.198218634
	O428	1.490967401	-5.360023068	4.996963343
	O429	1.446321880	-1.769623936	6.485578453
	O430	0.378067977	-1.036307248	9.862036151
	O431	0.844952852	-3.828044466	11.894005003
	O432	6.288353976	-11.005812664	-0.801815740
	O433	7.357712934	-9.690438281	3.519611512
	O434	10.993218895	-6.400281655	3.447506251
	O435	-5.838070588	-0.518909340	-0.373013528
	O436	-3.790199149	-2.866683698	-5.245466809
	O437	-6.905799374	3.047322338	0.117441487
	O438	-5.897544012	4.308599693	-2.517703506
	O439	-9.774178112	1.510042187	2.273161340
	O440	-5.839017193	0.563921802	4.585513247
	O441	-4.224116321	3.991804052	5.074052141
	O442	-6.286879959	5.996247191	6.939391557
	O443	10.705121697	-1.787232721	4.212877280
	O444	3.565634555	3.060773162	5.136548068
	O445	4.107778722	7.957244205	1.894721459
	O446	1.694815570	10.556596085	-0.542369065
	O447	-0.965987220	7.455795728	0.475935720
	O448	-0.477780807	6.221794402	4.040143135
	O449	2.491027879	4.639289923	2.862326188
	O450	1.408572398	10.262661386	5.554180880
	O451	-1.672216077	12.983186960	4.483303240
	O452	-2.557983388	11.219401220	1.795721003
	O453	-4.313872978	12.433772071	7.229467428
	O454	-5.005829927	7.348048987	0.502800372
	O455	1.911069347	-1.987802675	-9.625467900

	O456	0.125039823	1.765369655	-8.479190376
	O457	2.696757737	5.763589037	-7.085075025
	O458	6.410945645	6.390268436	-7.335766120
	O459	-4.651316465	0.401688693	-9.470753584
	O460	-1.568746871	-4.535241469	-7.744101472
	O461	0.440478336	-3.657660331	-8.160442183
	O462	-3.321697319	4.920776489	-7.579509426
	O463	9.806930087	-4.853050237	-4.877198448
	O464	12.314336208	-6.923359149	-3.642438215
	O465	0.052340246	-5.518933768	-3.092436810
	O466	-0.668586587	-6.949147029	-1.515021286
	O467	4.644456322	-9.872645168	-6.119628158
	O468	2.390488803	-9.705662538	-6.181864652
	O469	4.832950716	-5.484420210	-2.826166250
	O470	4.599794762	-7.493714018	-1.845479309
	O471	2.385283378	-5.395443352	-3.747158922
	O472	8.482863177	-7.217499366	-0.620021712
	O473	6.687807614	-4.972434782	-0.731504279
	O474	-3.918674065	5.579171415	-1.111530564
	O475	7.211058962	-9.818793935	-5.146559239
	O476	6.968316438	-8.779271837	-2.329187903
	S477	3.882468415	5.309347240	-0.827226917
	S478	2.018630405	2.371397929	-2.443671713
	S479	2.090076387	-2.305925368	-4.612214956
	S480	3.688379842	1.663333463	0.463538194
	S481	0.547460427	-0.638154881	-1.841729166
	S482	4.206861024	0.768652331	-5.403444346
	S483	3.218871430	-3.365117578	-1.275547439
	S484	5.733017074	2.227578497	-2.350830836
	S485	5.725642447	-2.457008720	-3.850544033
	S486	6.305533242	-1.112016461	-0.455596883
	end			
Fe2-brNH2-Fe6H to Fe2NH3 **S=1, 35** **reactant** Fe(139) -2.453 Fe(140) -0.652 Fe(141) -2.507 Fe(142) 2.679 Fe(143) 3.036 Fe(144) 1.916 Fe(145) -0.408	9651826nh26hxton35ti.car_4			
	1	-9.356131447	0.820980362	1.039841690
	2	-10.332073313	-0.063329223	0.253623430
	3	-8.823866800	3.115154554	1.744310405
	4	-8.556367040	2.917970124	3.233148603
	5	-9.278579389	1.933689445	5.347735923
	6	-8.147986006	0.923580181	5.578132123
	7	-6.764190333	-0.848483697	4.621338996
	8	-5.451273695	-0.082054914	4.441962702
	9	-4.282037220	1.719763030	3.275063714
	10	-3.887991341	2.527967769	4.520106944
	11	-4.587470812	3.860021153	6.418559514
	12	-4.167627456	3.043265548	7.649340401
	13	-4.764621529	1.234784696	9.196471491
	14	-3.872016352	-0.010454478	9.113028318
	15	-3.134134599	-1.896549354	7.722986310
	16	-1.789327667	-1.630568046	7.038509242
	17	-0.517291147	-0.211813721	5.496828308
	18	0.414483600	0.790262136	6.204015817
	19	-0.808075021	0.136656694	4.018316872
	20	0.475199346	0.535341025	3.277459842
	21	-1.494519769	-1.039940100	3.313747186
	22	0.813791761	3.071515275	6.998827904
	23	0.848754973	3.006328382	8.537638790
	24	0.488598449	4.480306918	6.447139183
	25	1.384674498	5.539013656	7.101395379
	26	0.655222306	4.508221920	4.921819998
	27	-0.338845229	2.869317907	10.644955626
	28	0.524997079	1.734578012	11.162506214
	29	-2.614156547	-11.344271151	6.788084816
	30	-1.337835269	-10.900365281	6.077712148
	31	0.438441828	-9.168563863	6.088222360
	32	1.608162432	-9.481293527	7.038348951
	33	0.269637360	-7.645673515	5.938063881
	34	1.532170819	-6.998466276	5.371675785
	35	1.339112990	-5.533931952	5.009832455
	36	3.037672622	-3.812595471	4.388223047
	37	3.982989487	-10.065385243	7.158778914
	38	5.041332706	-9.009180993	6.933635509
	39	-5.819505486	0.693490219	-1.842142127
	40	-5.309789113	2.141722786	-1.718804792
	41	-4.646399190	-0.276479188	-1.589783216
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	55	-1.711149225	2.749288376	0.140542350
	56	-1.155511812	2.062256240	-1.819081841
	57	-1.642170902	9.469923417	0.841961084
	58	-1.441009351	9.919860052	2.287430695
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	62	-2.492996941	13.423459762	-1.554716695
	63	8.215417216	-3.389833547	4.480953668
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	67	6.068875456	-0.814617967	5.160829172
	68	6.472521533	-1.003036069	2.791373702
	69	5.769075426	0.543214066	5.008448610
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	93	4.872341202	13.124720975	0.072922069
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358	8.349528117	-5.480837940	3.735126253
359	5.724534727	12.741095817	0.681287343
360	3.728045439	-10.042278159	8.233635777
361	4.656926123	-8.017335346	6.590596672
362	3.843668264	12.530981909	-1.693397468
363	3.084803408	11.184568642	0.970293893
364	2.268505259	12.589223785	0.253587554
365	-0.930505211	8.672132051	-3.792144910
366	1.906490710	-2.247924214	1.260291880
367	-0.899146166	-3.301167603	0.075304487

	368	0.527988383	-1.343658925	0.955201523
	369	0.375777571	-6.198430811	-0.901871625
	370	1.202963821	-1.997548707	0.559033779
	371	-9.872897999	-1.401928644	-0.073133792
	372	-9.716375224	2.132707924	1.147885812
	373	-9.501242722	2.263207118	3.949672780
	374	-7.927544178	0.025989687	4.585053850
	375	-5.444398215	0.866203187	3.476706597
	376	-4.900696707	3.058964159	5.246475604
	377	-4.957799249	1.981584924	7.961550350
	378	-3.961342842	-0.729018990	7.962718048
	379	-1.720309600	-0.512185414	6.261368979
	380	-0.060231695	2.048151942	6.425107143
	381	-0.337850068	2.933257946	9.193028029
	382	-2.843971634	-10.653456213	8.063272865
	383	-0.785511409	-9.776191638	6.576723563
	384	2.504551352	-5.035640685	4.259265262
	385	2.995331003	-3.160057684	5.571972721
	386	3.601894646	-3.193194385	3.342875259
	387	2.763459881	-9.827753510	6.416998079
	388	-6.403055509	0.478888051	-3.173958450
	389	-4.923516439	-3.939772700	-2.339055658
	390	-5.025812802	2.709598694	-2.923032353
	391	-6.152739066	5.211923540	-2.404142940
	392	-6.005650686	5.419087406	0.398595531
	393	-3.249110455	5.580467039	0.972437426
	394	-0.868228446	3.404311980	-1.772188149
	395	-1.669299773	1.639719870	-0.674543960
	396	-2.070010041	8.083296220	0.839683604
	397	-2.898000265	12.162271255	-1.470959230
	398	-1.789693319	13.787399089	-0.444748826
	399	9.033882470	-3.005195575	3.329284334
	400	9.351466253	1.694456605	-0.590518923
	401	8.530491727	3.345449059	-3.610646400
	402	6.038910048	4.297676382	-4.374545471
	403	1.469490698	5.696155867	-5.977584260
	404	2.363596674	6.903139009	-7.777811869
	405	1.569973927	8.014689238	-5.909348300
	406	4.240262940	4.209449718	-2.089761379
	407	5.647031325	5.921978234	-0.385489202
	408	6.210141198	8.448399166	-1.410885200
	409	4.852147410	8.342568947	-5.098483388
	410	4.944158003	10.894208453	-0.946042486
	411	0.311517085	-8.541149107	-8.467568466
	412	0.404379244	-5.324018391	-6.795250411
	413	1.278753602	-2.396839895	-6.949583395
	414	4.140093547	-2.106055805	-7.072402924
	415	-3.111560963	-3.808800844	-9.498963944
	416	-3.214873253	-1.080677951	-8.558051513
	417	2.032997344	-11.724444747	-3.196012672
	418	-0.120390667	-7.902317256	-2.474743555
	419	-1.150917492	-8.692492250	-4.255162752
	420	2.600890409	-11.979033432	-0.106330670
	421	-8.332781803	0.378776666	1.592286154
	422	-7.508531501	3.349270819	3.744509811
	423	-7.498660457	0.937696301	6.637514292
	424	-4.459219126	-0.304052555	5.158347845
	425	-2.696210791	2.676916865	4.833113599
	426	-3.193019855	3.388771680	8.338985531
	427	-3.168567426	-0.341020591	10.077838229
	428	-0.852889660	-2.428952553	7.189857374
	429	1.561660004	0.443154542	6.530270026
	430	1.926636959	3.019445229	9.158731559
	431	0.997809766	1.709340545	12.289209187
	432	-0.903696951	-11.554964098	5.107590443
	433	1.481643027	-9.369395163	8.269794248
	434	6.232387278	-9.197526073	7.125617933
	435	-5.166811351	2.729031844	-0.630091149
	436	-5.589794074	-2.202194080	-3.644272853
	437	-4.071265482	6.057880902	-2.002285978
	438	-3.045474359	5.199399839	-4.779853881
	439	-6.833655800	7.559260600	0.291744361
	440	-3.676203143	5.754962129	3.209097875
	441	-0.388658477	7.372165521	2.202027999
	442	-0.617071880	10.742407303	2.650103369
	443	8.360593925	-5.436470331	5.776536260
	444	5.525679665	2.451646062	3.509440586
	445	7.980547323	4.146313304	-1.544305597
	446	6.930971084	6.297648190	-5.073475137
	447	3.307162476	6.057697995	-3.053917291

	448	3.680081123	6.467485884	0.661052440
	449	5.029941948	3.138115264	0.682769252
	450	7.708779511	8.861102715	0.269566032
	451	6.509486928	12.013713504	-2.165776640
	452	4.279282269	10.203637595	-3.902255265
	453	4.549053252	14.302149683	0.089754930
	454	-0.169910565	8.195677717	-3.406913148
	455	-1.379596899	-6.638907734	-7.404829698
	456	-0.609771973	-2.513548544	-8.241752823
	457	3.897402001	-0.483581387	-8.642779439
	458	7.282499620	-2.212950664	-8.846091946
	459	-5.438650220	-1.241761921	-9.039595780
	460	-5.200678258	-5.712505071	-4.829035524
	461	-3.144025615	-6.321242755	-5.446395237
	462	-1.574666406	2.001935324	-9.357568550
	463	4.442110541	-11.000603150	-0.993136730
	464	5.578224746	-13.443483867	1.263935298
	465	-3.571723712	-5.255826851	-0.007751431
	466	-4.651312217	-5.268304864	1.965604632
	467	-2.656659386	-12.183206484	-0.303962374
	468	-4.437694511	-10.831798419	-0.643577031
	469	0.456977258	-7.830829628	0.596849379
	470	-0.621278526	-8.656969319	2.388873503
	471	-1.648102306	-6.677271505	-0.414791038
	472	2.996809435	-10.117412572	3.615253649
	473	2.785660860	-7.624138215	2.231609735
	474	-0.490769751	5.630011641	-3.887856982
	475	-0.358082719	-13.189619958	0.802135762
	476	0.557204921	-11.076134442	2.753354787
	477	5.835228954	1.219054775	-2.681417647
	478	2.560137717	-0.471525698	-3.206202448
	479	-0.428878375	-4.555927031	-2.368304178
	480	3.825708771	-0.788943972	-0.005931485
	481	-0.254524490	-1.536490389	-1.579224672
	482	2.712424082	-4.230275167	-4.666718887
	483	0.826998614	-4.874648978	1.020976961
	484	5.447144549	-2.648720472	-2.622224998
	485	2.589891618	-6.546442497	-1.688112057
	486	4.585830034	-4.537095037	0.630016695
	end			
Fe2-brNH2-Fe6H to Fe2NH3 **S=1, 35** **TS** Fe(139) -2.407 Fe(140) -0.940 Fe(141) -2.535 Fe(142) 2.718 Fe(143) 3.040 Fe(144) 1.937 Fe(145) -0.283	9651826nh26hxton35ti_1_52967.57			
	1	-9.370514715	0.820466501	1.040159736
	2	-10.355811873	-0.056000279	0.257519569
	3	-8.812255559	3.109670279	1.739243503
	4	-8.543898621	2.913185862	3.227966070
	5	-9.264148325	1.929819220	5.343413955
	6	-8.134994291	0.917367963	5.570540816
	7	-6.754949773	-0.854248696	4.609988174
	8	-5.443826811	-0.084121157	4.433309424
	9	-4.279031225	1.720416941	3.262511298
	10	-3.880012067	2.527693477	4.506409074
	11	-4.566214115	3.852262318	6.412835636
	12	-4.140072620	3.031463239	7.638837548
	13	-4.733945326	1.218045050	9.182895292
	14	-3.846359997	-0.030697155	9.099786656
	15	-3.121615060	-1.924763680	7.717475193
	16	-1.781245950	-1.646817111	7.030246553
	17	-0.524464504	-0.208965685	5.496653581
	18	0.415352656	0.787390039	6.200216747
	19	-0.825207527	0.141833103	4.020559291
	20	0.452300276	0.543151149	3.271266021
	21	-1.514258244	-1.035054978	3.318900978
	22	0.827838765	3.062305523	7.003599488
	23	0.870384050	3.001255462	8.542656957
	24	0.512205257	4.469478252	6.443016707
	25	1.410695918	5.528238725	7.093166271
	26	0.684873273	4.484679958	4.918149867
	27	-0.300844243	2.860925594	10.658218981
	28	0.553914663	1.712291829	11.162125667
	29	-2.606668364	-11.351424946	6.801509025
	30	-1.337918752	-10.894725433	6.086496862
	31	0.423153109	-9.146477956	6.088363587
	32	1.591066284	-9.457765784	7.042125131
	33	0.253901551	-7.623096075	5.940093835
	34	1.519072453	-6.976758775	5.377597290
	35	1.340555621	-5.504861854	5.039931738
	36	3.048997048	-3.796884479	4.405960539
	37	3.962401854	-10.054162561	7.172997449
	38	5.031343055	-9.011066566	6.936508671
	39	-5.831689956	0.696072876	-1.843949108

	40	-5.325222499	2.145879200	-1.716414880
	41	-4.660304493	-0.273874195	-1.587367323
	42	-5.070280490	-1.734103703	-1.307830026
	43	-5.214602091	-2.633333511	-2.536320027
	44	-4.208128182	3.900830914	-3.071583821
	45	-4.815410526	5.161767506	-2.446500114
	46	-3.930577583	4.080444699	-4.571010241
	47	-6.861499520	6.309905466	-1.744583673
	48	-6.564480754	6.487595915	-0.251100858
	49	-5.599965794	5.533667161	1.787934801
	50	-4.094636173	5.637813238	2.045905230
	51	-1.815428957	5.683897412	1.152096150
	52	-1.374016321	7.118136866	1.482991224
	53	-1.049536635	5.277603235	-0.117473151
	54	-1.249106100	3.859473111	-0.531968314
	55	-1.755800703	2.748206730	0.109221646
	56	-1.190618674	2.069798648	-1.850888945
	57	-1.648816363	9.467892214	0.836314251
	58	-1.453523604	9.916362485	2.282648757
	59	-2.774900189	10.289859108	0.163445328
	60	-2.443827317	11.691830072	-0.256924230
	61	-1.749538552	12.694551417	0.391651495
	62	-2.505852447	13.420219162	-1.560807684
	63	8.192756957	-3.392713892	4.486847251
	64	8.291614489	-4.893682075	4.692064173
	65	6.700461659	-3.079550190	4.228430174
	66	6.408896977	-1.604977577	4.068215371
	67	6.063064540	-0.805207835	5.173176928
	68	6.462371007	-0.990687225	2.802582034
	69	5.769015297	0.554219503	5.024088803
	70	6.182825682	0.366529777	2.640231239
	71	5.829432712	1.137366863	3.751136593
	72	8.414286455	1.746375975	-1.719041646
	73	8.280226965	3.176001849	-2.267779923
	74	7.047057677	1.238165634	-1.264918607
	75	8.465460759	4.616981687	-4.266698122
	76	7.064218056	5.134802485	-4.599280682
	77	4.628711734	4.633398811	-4.497749904
	78	4.005880484	5.028410805	-3.135520779
	79	3.917178910	3.427883415	-5.151333643
	80	2.393479181	3.464050752	-5.314387961
	81	1.838341646	4.351146517	-6.439846371
	82	1.785670963	6.843061863	-6.563313930
	83	3.676782558	4.535733266	-0.768226115
	84	4.338099091	5.752792034	-0.102180839
	85	3.734417573	3.354607625	0.217356120
	86	6.478403720	6.823730095	0.419120493
	87	6.863437825	8.133876193	-0.250792131
	88	6.646521644	9.586766263	-2.191290660
	89	6.006946274	10.936691922	-1.784856480
	90	6.542315097	9.379008633	-3.707374310
	91	5.112068495	9.333660304	-4.231291287
	92	4.111414842	12.066942868	-0.733170123
	93	4.866585098	13.118732774	0.064429309
	94	2.809492980	11.662097415	0.012495526
	95	1.951326411	10.742624510	-0.825662690
	96	1.038805869	11.269984962	-1.751290003
	97	2.086171660	9.346177127	-0.752024110
	98	0.297201539	10.439214150	-2.593376234
	99	1.373894604	8.499847117	-1.606523597
	100	0.488663298	9.057453825	-2.524725901
	101	0.826286745	-7.625916589	-7.456890648
	102	-0.144833674	-6.478691526	-7.228671975
	103	-0.339260149	-4.131262689	-6.433124898
	104	0.090311109	-2.931122820	-7.285677836
	105	1.875643193	-1.285155458	-7.658855287
	106	3.391977521	-1.278252612	-7.827970579
	107	5.599623106	-2.005147228	-7.121307996
	108	6.156053179	-2.470645612	-8.451729810
	109	-4.249576050	-3.308512581	-8.697290446
	110	-4.367959578	-1.781809235	-8.782620332
	111	-4.296850521	-3.771884404	-7.224056453
	112	-4.576779884	-5.284481225	-7.132021499
	113	-4.359206164	-5.791807547	-5.724791180
	114	-3.238852152	0.378554297	-8.643349233
	115	-2.017579090	0.872366405	-9.392329424
	116	-3.534481661	1.128976582	-7.321872639
	117	-2.587822118	0.657651947	-6.257787046
	118	-1.302422109	1.211525823	-6.151118205
	119	-2.909533154	-0.478625730	-5.497439380

	120	-0.329923085	0.579917824	-5.371865147
	121	-1.937456292	-1.103696464	-4.715287691
	122	-0.635109702	-0.596217531	-4.683988353
	123	2.360832181	-10.677893546	-2.204877013
	124	3.213341929	-11.208722511	-1.040545666
	125	1.085076513	-10.004186009	-1.679562341
	126	0.263277619	-9.251932584	-2.676924696
	127	-0.374410428	-9.751384834	-3.793764558
	128	-0.994822381	-7.649362335	-3.479181298
	129	3.376208394	-12.468391554	1.021975958
	130	4.587308398	-13.253068709	0.568331005
	131	-3.707307451	-5.637280824	1.237200570
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	133	-1.935151824	-7.456553903	0.734560726
	134	-2.902352982	-8.642924243	0.455205797
	135	-2.301481059	-9.812921553	-0.329123045
	136	-3.219156337	-11.051875406	-0.433815297
	137	-0.628267376	-8.037128453	1.293168397
	138	2.423485154	-3.260313299	-1.520387845
	139	1.813184259	-4.733878476	-2.729841849
	140	1.880261878	-1.431115330	-1.242940405
	141	4.205243931	-2.829015310	-0.750714405
	142	3.275196717	-2.656383101	-3.190052095
	143	4.559298445	-0.575013518	-2.067954537
	144	2.656176380	-4.842177170	-0.337961202
	145	0.514231261	-3.430211418	-0.612686644
	146	-9.573022828	-1.871724090	0.761669092
	147	-9.091690209	-1.341658304	-0.704463053
	148	-10.503439533	2.479798157	0.600380865
	149	-10.651021595	0.474782930	-0.661519514
	150	-11.270106761	-0.128403641	0.872051701
	151	-7.832078221	3.086700218	1.239766615
	152	-10.327075746	1.933355070	3.471758912
	153	-9.240427447	4.110768073	1.594022414
	154	-10.194687470	1.521887884	5.760299452
	155	-8.402500907	0.129363128	3.682864889
	156	-8.998317317	2.828626782	5.914561746
	157	-3.406241333	1.121556208	2.975200449
	158	-6.249314730	0.965909567	2.859313218
	159	-6.856307146	-1.599305007	3.809173286
	160	-3.739916326	4.538739766	6.186553685
	161	-5.843927159	3.039717891	4.875937019
	162	-6.701362314	-1.380933938	5.570384476
	163	-4.505624461	2.403988188	2.432542635
	164	-5.748085146	1.759367242	7.374552236
	165	-5.450305654	4.445806602	6.683412082
	166	-2.442007064	-1.333469754	3.826839441
	167	-1.771467525	-0.767059320	2.281967502
	168	-0.847818827	-1.912677899	3.283099450
	169	-1.499180605	1.011906600	4.016870920
	170	-5.718579661	0.903390397	9.558760832
	171	0.022374209	3.765249041	4.417455767
	172	-1.210757142	2.948457324	8.718697209
	173	1.254179213	5.597845063	8.179146209
	174	0.207686227	0.799087720	2.228785746
	175	1.186413312	-0.278014701	3.264168979
	176	8.486551476	-2.908402860	5.437675793
	177	0.464141579	5.483670002	4.514371452
	178	1.208942557	6.515566624	6.651911721
	179	1.725132935	4.234342182	4.649387092
	180	2.472905725	5.289253515	6.921846507
	181	-0.539987001	4.707826434	6.683618638
	182	1.852007384	2.793041121	6.705454016
	183	-0.975316525	2.312983919	6.080907795
	184	0.937736801	1.424232536	3.715913559
	185	3.381538422	2.439487162	-0.289253256
	186	3.041728254	3.586174053	1.040736231
	187	5.027610578	2.994721603	1.670582620
	188	5.243046698	2.882094953	4.363045777
	189	6.197000111	0.823517875	1.650843543
	190	6.694340024	-1.591752313	1.920427910
	191	6.011291588	-1.252670469	6.169394470
	192	-2.584623437	-0.023441872	6.053314875
	193	-3.673567761	-2.643688544	7.093851273
	194	-2.894303837	-2.408224083	8.674973399
	195	-4.503139273	-0.413770478	7.169988054
	196	-4.272047990	1.876977520	9.928022058
	197	5.478771524	1.154712029	5.890550335
	198	0.067719378	-1.136154874	5.504664117
	199	0.050006769	3.797008395	11.122690895

	200	-1.332169747	2.677196576	10.997430534
	201	0.668021182	0.863514973	10.447559411
	202	4.376611156	-11.053468193	6.967427244
	203	-5.030473658	-4.583201404	-3.132322865
	204	-2.671068819	-5.802060807	-0.390616735
	205	-5.625274420	-5.472302660	-7.405305934
	206	-3.932978250	-5.832626140	-7.835399495
	207	-5.085049452	-3.230690149	-6.677927628
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	209	-5.171387482	-3.664518128	-9.183276039
	210	-3.976949341	-0.234541327	-2.449840610
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	212	-2.354389992	-1.549981301	-8.323833207
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	215	-4.554796975	-4.296630614	-1.460775782
	216	-3.344841940	-3.513998604	-6.735222182
	217	-3.188154293	-4.805316157	-9.619375551
	218	-7.415600883	0.655514647	-3.177918746
	219	-4.082406250	0.098557613	-0.730756706
	220	-2.555203401	-6.346777654	-6.270969375
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	223	-2.160997651	2.691108351	1.115389614
	224	-6.056883841	6.441996583	2.204598422
	225	-5.806978689	4.554875042	-0.103467349
	226	-2.877215526	7.810743282	0.268474061
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	228	-2.191434349	9.468337545	2.991067025
	229	-3.659131050	10.279427120	0.825712541
	230	-0.699210662	9.600929648	0.294397748
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	236	-3.637649306	5.488490278	0.024522985
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	239	-1.002771420	1.460538570	-2.731531019
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	241	10.002628016	-3.033259856	3.601131692
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	243	4.736095590	3.301649560	-2.196786989
	244	2.620656766	4.808750671	-0.912868569
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	246	-0.537606679	4.010417725	-2.544885400
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	256	2.827837447	7.750692870	-8.080357079
	257	0.942149948	3.884606114	-6.877210511
	258	-0.421874664	10.865905919	-3.296716279
	259	2.744893592	8.887064814	-0.009388960
	260	1.065875858	7.994051254	-5.018132328
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	276	4.557675426	5.524999602	-5.128917828
	277	2.581605835	4.428756126	-7.244238285
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	285	1.801448540	-7.226939643	-7.773473530
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	287	2.989697417	-9.922366213	-2.699002321
	288	0.809154188	-9.430724997	-8.404478887
	289	-0.671363955	-8.742513418	-8.259727591
	290	7.169174305	0.214074201	-0.888211865
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	306	0.438342419	-5.350490826	4.424140294
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	316	2.653569114	-5.499256737	3.386506545
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	320	0.436478636	-10.772464542	-1.224191537
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	323	5.463063422	-3.097958621	-9.062114262
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	329	-1.525560056	-6.717577753	-3.626942411
	330	-2.541880118	-12.450500765	6.880799125
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	336	-2.072554436	-9.488960588	-1.355577533
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	339	-0.191072510	-3.913859980	-5.363882153
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	346	-0.355726068	-10.737077984	-4.242830860
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	348	-1.397524816	-4.321581035	-6.621312910
	349	5.955808383	-0.982649367	-6.922510048
	350	6.124021264	-3.481587458	5.075680783
	351	6.393846242	-3.623669155	3.320896365
	352	2.938233185	-12.129171890	-3.535035794
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	447	3.313070562	6.053677302	-3.041985144
	448	3.696178468	6.482276779	0.664401186
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	450	7.713124172	8.874868844	0.259417804
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	453	4.542561898	14.295997193	0.080362428
	454	-0.174463808	8.192841148	-3.412552807
	455	-1.376752320	-6.637637382	-7.410661570
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	471	-1.650664239	-6.694918907	-0.440238080
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	475	-0.362300530	-13.197612176	0.808966030
	476	0.550891999	-11.081324157	2.759481838
	477	5.819953476	1.241676050	-2.652750470
	478	2.545211486	-0.489242974	-3.221974338
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	481	-0.288802368	-1.595461003	-1.644587277
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	483	0.870615119	-4.917711091	0.979779953
	484	5.468094994	-2.607724644	-2.564571669
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	1	-9.392435686	0.830165548	1.053660867
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	5	-9.287345173	1.937975762	5.355413764
	6	-8.155248614	0.929096230	5.583022111
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	16	-1.804287008	-1.630619917	7.060211453
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	18	0.399146492	0.794824980	6.247330703
	19	-0.821817918	0.174351032	4.059581791
	20	0.453394228	0.647777268	3.354571600
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	22	0.798251672	3.084611565	7.015506363
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	25	1.366141230	5.551987436	7.111471133
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	37	3.991190677	-10.078250706	7.156830000
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Fe2-brNH2-Fe6H to Fe6NH3 **S=1, 47** **reactant** Fe(139) 2.431 Fe(140) -1.113 Fe(141) 2.489 Fe(142) -2.540 Fe(143) 2.915 Fe(144) -2.159 Fe(145) -0.273	9651826nh26hxtontm.car_4 1 -9.355258120 0.819819685 1.038887683 2 -10.334338690 -0.062075677 0.254372648 3 -8.817933397 3.113211783 1.743034299 4 -8.551858128 2.916826846 3.232167657 5 -9.274296715 1.932392696 5.346295583 6 -8.144006009 0.921821560 5.576253934 7 -6.760141612 -0.849759464 4.619608949 8 -5.447778220 -0.082182430 4.441260421 9 -4.279516308 1.719968927 3.273034719 10 -3.884814067 2.528377745 4.517540160 11 -4.581941342 3.858062189 6.417888236 12 -4.160349174 3.040584951 7.647593315 13 -4.756396127 1.230558365 9.193854382 14 -3.865554933 -0.015961055 9.110308156 15 -3.132222197 -1.904503573 7.722630009 16 -1.787711086 -1.635391678 7.039055894 17 -0.516959476 -0.212323570 5.500371845 18 0.415499452 0.789347101 6.207123857 19 -0.810238592 0.137249972 4.022114143 20 0.470697631 0.535527309 3.277699218 21 -1.497447162 -1.038938703 3.317652960 22 0.817496194 3.069727293 7.002544011 23 0.854282231 3.006907730 8.541490624

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Fe2-brNH2-Fe6H to Fe6NH3 **S=1, 47** **TS** Fe(139) 2.497 Fe(140) -1.097 Fe(141) 2.693 Fe(142) -2.473 Fe(143) 3.080 Fe(144) -2.021 Fe(145) -1.245	9651826nh26hxtontn_1_52966.47 !DATE Jan 02 11:14:07 2025 1 -9.366312084 0.818363505 1.037617800 2 -10.357193178 -0.054487484 0.258297890 3 -8.803822364 3.107140123 1.737479850 4 -8.537265472 2.911304830 3.226560559 5 -9.257971248 1.927772265 5.341463098 6 -8.129654851 0.914258337 5.567939644 7 -6.750488735 -0.856655362 4.605687561 8 -5.440482359 -0.084552422 4.430459230 9 -4.276760419 1.720403379 3.257703001 10 -3.875763764 2.528076185 4.500657675 11 -4.556662518 3.849262399 6.410521088 12 -4.128344814 3.027035766 7.634830862 13 -4.720982731 1.211302432 9.177233787 14 -3.835125261 -0.038654015 9.094827603

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	262	6.258987362	3.361048839	-3.971988948
	263	1.897419246	3.716916726	-4.361143517
	264	-6.696763488	4.400956332	-2.711224095
	265	9.034505943	4.554186611	-5.203853476
	266	-5.259343428	2.083893901	-3.702364437
	267	4.387053816	3.267397218	-6.132829265
	268	1.534024380	7.421514802	-1.573771589
	269	8.940688619	5.379065035	-3.635035973
	270	2.551760384	6.054699772	-8.307477513
	271	1.441627491	8.853352055	-6.471817416
	272	-6.229810413	-0.494676327	-3.474542173
	273	-6.560252172	0.566342763	-1.024970455
	274	0.891496023	12.350762507	-1.814370877
	275	-3.255612876	3.759427851	-2.544854694
	276	4.560659597	5.527707750	-5.125108143
	277	2.583852733	4.429770689	-7.241856160
	278	2.095785406	2.435872056	-5.544431987
	279	0.807786541	5.724145628	-5.169408453
	280	5.944585066	7.082916191	1.342942383
	281	5.603432316	7.732345481	-1.815849221
	282	7.711497013	9.733725296	-1.958931795
	283	7.421820867	6.328385542	0.702005309
	284	4.516366496	9.973307545	-0.802246018
	285	1.803062726	-7.228084984	-7.771941817
	286	0.978806596	-8.092922656	-6.460520381
	287	2.989978724	-9.915891025	-2.693515351
	288	0.810462497	-9.429875837	-8.407034182
	289	-0.670292330	-8.741955178	-8.261468026
	290	7.179656505	0.213849915	-0.863991250
	291	9.098834333	2.405039373	0.100616313
	292	8.760654107	2.500954947	-4.145618229
	293	6.668313971	1.880456401	-0.441900044
	294	10.302612631	1.968219590	-0.915541494
	295	6.025950604	-2.647851517	-6.335604553
	296	8.795101523	1.079147619	-2.501113307
	297	-0.015142917	-7.178243957	6.919511906
	298	0.623030597	-9.563917024	5.097254577
	299	3.748401837	-2.702636649	-6.334464639
	300	4.248495168	-2.397746726	3.544246895
	301	1.435159531	-1.247808941	-8.656528415
	302	-2.173627539	-1.995586567	-4.141296548
	303	1.614454359	-0.339874926	-7.153024740
	304	1.218360363	-4.894869715	5.963037745
	305	1.729057636	-2.775053687	-6.081014049
	306	0.435117190	-5.329525195	4.441993443
	307	-0.596432083	-7.438853392	5.256512809
	308	1.807180772	-7.487132009	4.457840060
	309	2.352084055	-7.070638873	6.086813615
	310	-4.584820924	0.929647238	-7.040275825
	311	-1.270622242	-9.384633400	7.406916974
	312	-3.435949969	-11.133767748	6.113247021
	313	0.138412080	-1.105275865	-4.119093008
	314	-2.382207131	-11.167116371	8.838634799
	315	-3.835656356	-10.648902579	8.290325065
	316	2.642849895	-5.485174046	3.389012633
	317	0.679071505	0.994207148	-5.307479096
	318	-3.919674062	-0.889359249	-5.530787260
	319	-0.129825656	-12.549966247	1.513622655
	320	0.435434481	-10.775927786	-1.225966282
	321	0.161877621	-10.198441070	2.508697380
	322	-1.173289218	-12.783439581	0.385209108
	323	5.468471603	-3.102175319	-9.056423292
	324	1.951549367	-7.759685057	1.665984292
	325	-2.936294231	-7.054257710	2.654721603
	326	1.404417696	-5.326285392	-6.541761456
	327	-3.246028045	-9.021181123	1.433919312
	328	-1.799911277	-8.796801582	-5.071828268
	329	-1.528855280	-6.726063065	-3.638886147
	330	-2.536311357	-12.449198036	6.877549116
	331	3.751406635	-3.658200076	2.456543484
	332	3.020422166	-9.254981114	3.138265886
	333	3.439602352	-7.323080438	1.615134075
	334	2.779486468	-9.906696921	5.389399759

	335	2.622295423	-3.596404250	6.417837851
	336	-2.076340802	-9.492979129	-1.358415915
	337	-1.357105298	-10.136611597	0.122769316
	338	-3.799258052	-8.267961208	-0.068644836
	339	-0.188893545	-3.915013151	-5.361638834
	340	-1.064555574	2.118375322	-6.720879225
	341	-3.437445804	2.208971620	-7.520560929
	342	-1.805194170	-5.793127570	2.122335669
	343	2.148578286	-10.536863195	3.290490639
	344	0.072138260	-11.290925256	3.599688779
	345	3.132789239	-2.146429893	5.646856780
	346	-0.353139673	-10.745141894	-4.243631230
	347	1.346385796	-9.320792098	-0.865167880
	348	-1.394147219	-4.321680912	-6.620289311
	349	5.960198342	-0.974760012	-6.929932289
	350	6.119920257	-3.476743437	5.081029406
	351	6.391449570	-3.618764125	3.326732699
	352	2.948124013	-12.120489715	-3.533609529
	353	1.555423955	-12.488070103	-2.755847054
	354	2.735180343	-13.159894399	1.594075821
	355	1.591152357	-12.164814257	-0.100693902
	356	4.488778004	-13.714996230	-0.442500488
	357	3.688899781	-11.664202473	1.708108053
	358	8.316650775	-5.486455275	3.754099866
	359	5.717882661	12.737395675	0.670413010
	360	3.698959581	-10.004135011	8.251375564
	361	4.661047707	-8.020376268	6.574288059
	362	3.834711232	12.523860318	-1.701544670
	363	3.076108926	11.182483160	0.964703746
	364	2.262442342	12.587542488	0.245653177
	365	-0.937080820	8.665883514	-3.797977154
	366	1.775190318	-2.203864368	1.337223597
	367	-0.089286729	-2.894689583	0.744657838
	368	0.510271327	-1.180311184	0.893966585
	369	0.383672448	-6.227546539	-0.918653502
	370	1.122040389	-1.941195415	0.588479778
	371	-9.909327357	-1.392634957	-0.085275069
	372	-9.708902959	2.134687101	1.144017042
	373	-9.482847213	2.259180131	3.944265900
	374	-7.915528487	0.015700160	4.574190950
	375	-5.435091383	0.862327141	3.463840409
	376	-4.882878123	3.053641080	5.238319507
	377	-4.911173625	1.957938189	7.941424345
	378	-3.950098987	-0.774738012	7.957651777
	379	-1.717703088	-0.521079648	6.266952137
	380	-0.052388722	2.039475490	6.439036002
	381	-0.300997089	2.928034418	9.209984879
	382	-2.837289843	-10.661021869	8.075710741
	383	-0.803110461	-9.750104889	6.571655415
	384	2.497759289	-5.002821585	4.281183775
	385	3.055335365	-3.159681948	5.611771343
	386	3.598352981	-3.163073772	3.364014433
	387	2.742161288	-9.806564853	6.428478146
	388	-6.400651418	0.483907501	-3.180700561
	389	-4.933748288	-3.937823829	-2.344450884
	390	-5.038816279	2.717130962	-2.917190753
	391	-6.174562454	5.216670532	-2.398352799
	392	-6.022748758	5.427257735	0.403937194
	393	-3.263008130	5.578538706	0.969611006
	394	-0.899864785	3.411820098	-1.798128740
	395	-1.742656251	1.648932349	-0.729457709
	396	-2.073454541	8.077837164	0.826924529
	397	-2.916591613	12.157972626	-1.476785982
	398	-1.797567949	13.780305127	-0.457651585
	399	9.012470782	-3.017663049	3.343324880
	400	9.372308899	1.694577660	-0.586210201
	401	8.530858103	3.325524461	-3.597391706
	402	6.043856501	4.287201647	-4.363280961
	403	1.470444834	5.692940232	-5.974341603
	404	2.372588624	6.897066828	-7.773644129
	405	1.565096498	8.012382651	-5.913497960
	406	4.258814758	4.211635804	-2.070011323
	407	5.670478752	5.929513965	-0.374633188
	408	6.210326107	8.445305287	-1.411269642
	409	4.852779873	8.329030232	-5.115408984
	410	4.935765164	10.887911029	-0.954499850
	411	0.310796022	-8.540810188	-8.476839277
	412	0.411024325	-5.330021510	-6.790625140
	413	1.295311088	-2.412850283	-6.949408196
	414	4.156836624	-2.091349905	-7.049553779

	415	-3.119215436	-3.786787815	-9.501079637
	416	-3.230872739	-1.064720201	-8.543828426
	417	2.067128690	-11.718961962	-3.199538847
	418	-0.136017220	-7.930015889	-2.506800429
	419	-1.154475164	-8.736583386	-4.288566185
	420	2.596759087	-11.971977872	-0.097329658
	421	-8.346046844	0.364281771	1.586881681
	422	-7.488124448	3.340698867	3.736894298
	423	-7.476004420	0.927275957	6.624629844
	424	-4.450632741	-0.301410501	5.151406981
	425	-2.681824491	2.682064383	4.803128546
	426	-3.154783345	3.375670689	8.324323603
	427	-3.113556411	-0.358529943	10.049788789
	428	-0.833145200	-2.447562055	7.160458356
	429	1.569688803	0.431995156	6.497442641
	430	1.963292451	3.006428335	9.153986817
	431	1.051028739	1.658091373	12.280613843
	432	-0.889533484	-11.546669890	5.122365130
	433	1.457128557	-9.323331114	8.272467834
	434	6.217638415	-9.212191561	7.134514111
	435	-5.189338273	2.731582916	-0.624052745
	436	-5.599845907	-2.198581725	-3.646616219
	437	-4.096011883	6.070334141	-1.998437095
	438	-3.057694712	5.209126521	-4.771103839
	439	-6.852535431	7.566634918	0.295082000
	440	-3.684125867	5.771700078	3.205803491
	441	-0.406691508	7.365645816	2.207219988
	442	-0.634328766	10.737400039	2.647394513
	443	8.290233281	-5.438434314	5.795079883
	444	5.535552414	2.471953448	3.537340701
	445	7.973064498	4.135436454	-1.537675460
	446	6.942854347	6.282933624	-5.066106642
	447	3.315829768	6.054154207	-3.037040357
	448	3.703083860	6.487882401	0.663980162
	449	5.081371874	3.180765215	0.717453523
	450	7.715695314	8.882366911	0.257418109
	451	6.492557301	12.006365638	-2.185386905
	452	4.267442079	10.181019158	-3.910532543
	453	4.540693933	14.296820450	0.079250444
	454	-0.174826461	8.191263393	-3.413825629
	455	-1.375052467	-6.636175316	-7.412175110
	456	-0.611130002	-2.501138450	-8.219537543
	457	3.905216569	-0.493791928	-8.645226883
	458	7.297425452	-2.225386574	-8.824034456
	459	-5.453483774	-1.228505354	-9.030626880
	460	-5.200072469	-5.707868274	-4.838160539
	461	-3.145352797	-6.319669804	-5.458308563
	462	-1.607575902	2.028441843	-9.343927674
	463	4.439928715	-10.989445101	-0.975626656
	464	5.574985996	-13.442210271	1.264838231
	465	-3.576211959	-5.270876269	-0.044561211
	466	-4.662003639	-5.267434366	1.925397543
	467	-2.661576861	-12.206837776	-0.310891545
	468	-4.445431952	-10.866244340	-0.678626977
	469	0.439296078	-7.855062723	0.563793724
	470	-0.633863511	-8.670443291	2.360836445
	471	-1.664647613	-6.701632040	-0.445431506
	472	2.985622110	-10.112619216	3.629183288
	473	2.751544649	-7.626597207	2.237270900
	474	-0.496455142	5.624975224	-3.890921035
	475	-0.361299480	-13.196130311	0.809535411
	476	0.551120470	-11.080070242	2.758959663
	477	5.831656693	1.235800107	-2.620632551
	478	2.541235256	-0.613611235	-3.287890892
	479	-0.470765164	-4.551415041	-2.344032618
	480	3.696062341	-0.657954789	-0.018281240
	481	-0.271528167	-1.534990187	-1.661301409
	482	2.765348181	-4.242217508	-4.679517894
	483	0.883471793	-4.933595891	0.980658215
	484	5.476775031	-2.578263284	-2.574117360
	485	2.586868151	-6.571982855	-1.764089866
	486	4.577024630	-4.500403115	0.654742842
	end			
Fe2-brNH2-Fe6H to Fe6NH3 **S=1, 47** **product** Fe(139) 2.357 Fe(140) -2.330	9651826nh26hxtontl.car_7			
	1	-9.378015751	0.826198025	1.049189230
	2	-10.345953724	-0.060189016	0.256154346
	3	-8.837925197	3.118429264	1.748183747
	4	-8.564416421	2.919237088	3.235512317
	5	-9.281157510	1.935997276	5.352501264
	6	-8.149583030	0.926568105	5.580626703

Fe(141) 2.776	7	-6.766081478	-0.845676010	4.624295890
Fe(142) -2.386	8	-5.452250304	-0.080715248	4.443939437
Fe(143) 2.932	9	-4.286896882	1.724630133	3.277420207
Fe(144) -2.279	10	-3.893383170	2.531313486	4.523457650
Fe(145) 0.849	11	-4.593367820	3.862876327	6.421442650
	12	-4.173432912	3.045310881	7.651636774
	13	-4.771208553	1.238374121	9.199948891
	14	-3.877369457	-0.005959344	9.117154442
	15	-3.135824645	-1.890757417	7.726709968
	16	-1.791260055	-1.626706390	7.041288316
	17	-0.519974037	-0.202519639	5.499234359
	18	0.411931166	0.795169726	6.212475652
	19	-0.821703007	0.156240260	4.030105616
	20	0.458370244	0.553714130	3.283632805
	21	-1.533935438	-1.018032729	3.349246247
	22	0.812868022	3.077659012	7.000822377
	23	0.846011546	3.011070068	8.539736300
	24	0.484701363	4.485608940	6.449572187
	25	1.379994135	5.544629958	7.104008178
	26	0.648975027	4.515209909	4.924082517
	27	-0.346954912	2.870762115	10.643968721
	28	0.518523975	1.738369762	11.163736274
	29	-2.614421377	-11.352892618	6.802802532
	30	-1.342370058	-10.907871612	6.086109215
	31	0.438197729	-9.180637345	6.091305886
	32	1.610177065	-9.491743314	7.039358844
	33	0.271324028	-7.657714965	5.938502237
	34	1.533262879	-7.010547487	5.370177678
	35	1.331292576	-5.549326932	5.000675658
	36	3.020378702	-3.817170171	4.389006556
	37	3.986857925	-10.068820920	7.154847272
	38	5.041894206	-9.009079745	6.931657260
	39	-5.841415708	0.699848615	-1.844584915
	40	-5.326188408	2.145778253	-1.721366647
	41	-4.665233972	-0.266813539	-1.590364786
	42	-5.066301349	-1.728492699	-1.307128009
	43	-5.212843150	-2.629049255	-2.534379351
	44	-4.195189073	3.889625318	-3.077352205
	45	-4.795322750	5.153385474	-2.450602636
	46	-3.918846643	4.068537177	-4.576999603
	47	-6.837117258	6.310304276	-1.749499991
	48	-6.544333851	6.483358261	-0.254536933
	49	-5.586725004	5.521975439	1.784493497
	50	-4.081972269	5.627474865	2.047062742
	51	-1.800724041	5.690246388	1.158684667
	52	-1.363046174	7.124421301	1.489718879
	53	-1.031572696	5.287039858	-0.109605568
	54	-1.215544895	3.863287545	-0.509033341
	55	-1.712321005	2.755724196	0.146063139
	56	-1.159580082	2.062750884	-1.812211012
	57	-1.639945742	9.471684078	0.844522532
	58	-1.437070375	9.920621086	2.289665629
	59	-2.765785539	10.294837398	0.172627486
	60	-2.433765418	11.696655557	-0.247331399
	61	-1.744833632	12.700417140	0.405078625
	62	-2.488599646	13.424134189	-1.552690093
	63	8.205675643	-3.392440257	4.461721590
	64	8.323198975	-4.892790000	4.664926084
	65	6.709420451	-3.095238420	4.203321333
	66	6.405073491	-1.623640205	4.040677340
	67	6.062781471	-0.823756906	5.146412117
	68	6.446154756	-1.011119287	2.773064581
	69	5.764535033	0.534851421	4.997729988
	70	6.160840776	0.344997499	2.610461021
	71	5.815173862	1.116871751	3.723599893
	72	8.406096071	1.740386531	-1.723722434
	73	8.276626599	3.173617591	-2.265533646
	74	7.035808353	1.228641380	-1.280934621
	75	8.456778292	4.620136512	-4.261564062
	76	7.054876344	5.133062199	-4.599739898
	77	4.620554220	4.627673162	-4.507918716
	78	3.990740417	5.024561397	-3.149621308
	79	3.912593968	3.421337108	-5.163010344
	80	2.389235091	3.455925339	-5.328807748
	81	1.833729228	4.350704261	-6.447665724
	82	1.785098575	6.843163851	-6.563234192
	83	3.648770966	4.533209506	-0.784332041
	84	4.314318913	5.744077301	-0.111700139
	85	3.691791777	3.349130903	0.197800743
	86	6.457232859	6.805754990	0.417274750

	87	6.854935510	8.115707236	-0.246587682
	88	6.654241918	9.579561586	-2.182666252
	89	6.019472774	10.930714795	-1.772046163
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	91	5.117407208	9.337988274	-4.222517659
	92	4.121853185	12.062831429	-0.725778157
	93	4.878760828	13.113520465	0.071908998
	94	2.819194208	11.658931906	0.019197426
	95	1.960367613	10.741032735	-0.819999533
	96	1.049279064	11.270493079	-1.745734661
	97	2.092397263	9.344276463	-0.747026822
	98	0.306321007	10.441665732	-2.588331024
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	102	-0.144124585	-6.479610078	-7.227961713
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	116	-3.522641514	1.116655292	-7.350253562
	117	-2.588687797	0.644595273	-6.274905171
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	119	-2.929661991	-0.477998375	-5.502543086
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	122	-0.678469884	-0.582005853	-4.628896263
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	394	-0.863927241	3.403228260	-1.766455418
	395	-1.677856374	1.645332891	-0.667648179
	396	-2.067907578	8.085355256	0.842745127
	397	-2.894480050	12.163189163	-1.469304558
	398	-1.786610064	13.787937074	-0.441837683
	399	9.021051754	-3.006287012	3.308551787
	400	9.343801579	1.670943785	-0.590394325
	401	8.526637689	3.331901687	-3.598472802
	402	6.033924629	4.283802346	-4.368043960
	403	1.470964643	5.691304300	-5.976410867
	404	2.362499672	6.900417658	-7.777945340
	405	1.569460527	8.010385523	-5.907661215
	406	4.229962214	4.205921899	-2.086872407

	407	5.640705120	5.914124265	-0.382999847
	408	6.208806415	8.433221731	-1.409105337
	409	4.850360380	8.332737168	-5.098434643
	410	4.946014342	10.881104637	-0.943846649
	411	0.303256411	-8.543645071	-8.476457108
	412	0.412369684	-5.331794920	-6.790605355
	413	1.288180846	-2.404968576	-6.934424443
	414	4.137682328	-2.115776170	-7.068341261
	415	-3.123194476	-3.808783809	-9.514094634
	416	-3.224921608	-1.083013859	-8.570509082
	417	2.043589591	-11.747559228	-3.203151039
	418	-0.101894132	-7.911332356	-2.514387948
	419	-1.154700240	-8.715241557	-4.275357694
	420	2.600142724	-11.983093782	-0.109794365
	421	-8.357202251	0.383321502	1.606955279
	422	-7.513213885	3.347279798	3.742692612
	423	-7.499647850	0.939913851	6.639712337
	424	-4.458392423	-0.304713075	5.157916412
	425	-2.701742357	2.678357634	4.838533688
	426	-3.197182900	3.388825764	8.339849154
	427	-3.176672028	-0.337792404	10.083337361
	428	-0.856107965	-2.427397822	7.188105864
	429	1.555486081	0.444413679	6.546664831
	430	1.922641326	3.023989835	9.162591109
	431	0.988785640	1.714751425	12.291422846
	432	-0.914467644	-11.560295288	5.111789690
	433	1.485232052	-9.380651743	8.270975011
	434	6.233418004	-9.194556376	7.122629043
	435	-5.183499651	2.732340603	-0.632159537
	436	-5.601659529	-2.195444295	-3.643288452
	437	-4.065114407	6.053233086	-2.001114636
	438	-3.046650621	5.196140984	-4.780397525
	439	-6.827852817	7.559395526	0.292591191
	440	-3.673441545	5.748675960	3.209679360
	441	-0.386196170	7.374871974	2.204947491
	442	-0.612396390	10.744142808	2.651407602
	443	8.364211964	-5.436776747	5.759220985
	444	5.516669366	2.446008701	3.503990720
	445	7.969441487	4.130982885	-1.533703075
	446	6.927891737	6.282863393	-5.068568667
	447	3.297424617	6.050011906	-3.060223302
	448	3.674253531	6.472223997	0.657870981
	449	5.020172895	3.146097053	0.689425760
	450	7.706333803	8.849281354	0.271554306
	451	6.514339545	11.998056835	-2.161503445
	452	4.280744673	10.196442567	-3.904533429
	453	4.557011780	14.291613430	0.086986261
	454	-0.172480557	8.196798035	-3.406462555
	455	-1.376754515	-6.636203974	-7.406862223
	456	-0.602406918	-2.521094223	-8.223662256
	457	3.898600806	-0.488830776	-8.635746703
	458	7.283246581	-2.206674965	-8.831040126
	459	-5.447137245	-1.240422618	-9.061517175
	460	-5.200955668	-5.697582099	-4.835783169
	461	-3.146675485	-6.313918798	-5.453128296
	462	-1.578677671	1.995982999	-9.371439809
	463	4.443481656	-11.009197466	-0.996329283
	464	5.577347274	-13.447420814	1.261433801
	465	-3.524549670	-5.228042903	-0.042469999
	466	-4.607842859	-5.248529755	1.931106907
	467	-2.659690443	-12.184472517	-0.301778104
	468	-4.437830650	-10.826453905	-0.632705865
	469	0.482648841	-7.849158837	0.531762165
	470	-0.589225664	-8.649545121	2.335296331
	471	-1.625385829	-6.673209178	-0.469136705
	472	2.989407491	-10.123896073	3.612905985
	473	2.776529250	-7.631133537	2.229010865
	474	-0.492383754	5.631386411	-3.889396484
	475	-0.363719234	-13.201962331	0.807123298
	476	0.545027935	-11.083685729	2.758994523
	477	5.824958687	1.250163193	-2.678631896
	478	2.759857074	-0.750214588	-3.739965187
	479	-0.385628956	-4.491720100	-2.370185029
	480	3.479858702	-0.513946420	-0.244111262
	481	-0.170119629	-1.409420910	-1.478565033
	482	2.815793901	-4.359209936	-4.670392780
	483	0.864491835	-4.934290964	0.951640114
	484	5.554777622	-2.557898067	-2.469049917
	485	2.643321959	-6.574511685	-1.737501246
	486	4.633241170	-4.400238476	0.637562720

	end
N2x-Fe2NH3 to N2x-core **S=1, 35** **reactant** Fe(139) -2.245 Fe(140) 0.013 Fe(141) -2.699 Fe(142) 2.706 Fe(143) 3.159 Fe(144) 2.293 Fe(145) -1.700	965182nh32n2xd35td.car_4

C1	-9.408141991	0.821280939	1.053745388
C2	-10.383380628	-0.056969077	0.260990016
C3	-8.851616611	3.110788482	1.750633529
C4	-8.573140225	2.911357273	3.236975337
C5	-9.280409015	1.927935482	5.356620571
C6	-8.148285711	0.918220126	5.580939586
C7	-6.763427465	-0.850310995	4.620345499
C8	-5.451089272	-0.082116206	4.441026475
C9	-4.296333283	1.733579527	3.277792602
C10	-3.904160042	2.541260490	4.523568282
C11	-4.602652558	3.858764027	6.430255669
C12	-4.174430726	3.035668700	7.654158910
C13	-4.763757699	1.217732745	9.194109246
C14	-3.874191775	-0.029599460	9.110489155
C15	-3.144100253	-1.923873701	7.728614622
C16	-1.796832477	-1.656487855	7.048934363
C17	-0.526789311	-0.210482924	5.524249937
C18	0.395128574	0.786345912	6.252851153
C19	-0.835665635	0.182024140	4.062974599
C20	0.422712881	0.696104563	3.355036503
C21	-1.464467793	-1.000989929	3.316238135
C22	0.802222622	3.071797658	7.025260092
C23	0.841747613	3.007119852	8.563228061
C24	0.478523911	4.480913805	6.473311125
C25	1.385126678	5.535194977	7.120315996
C26	0.634470405	4.508299926	4.946783721
C27	-0.343500625	2.860363153	10.670005343
C28	0.522691210	1.724972233	11.183703261
C29	-2.620258786	-11.354668068	6.818712794
C30	-1.353938067	-10.901896214	6.096119477
C31	0.419346732	-9.163975203	6.100492035
C32	1.592977344	-9.471257728	7.048185910
C33	0.240415068	-7.641933903	5.951059852
C34	1.493065982	-6.979339103	5.378995835
C35	1.260407501	-5.528059883	4.978842991
C36	2.990173457	-3.829351963	4.354988699
C37	3.966172794	-10.065544286	7.163815012
C38	5.026301988	-9.011951326	6.935523440
C39	-5.869209366	0.697788643	-1.853732392
C40	-5.369893606	2.150143564	-1.725803529
C41	-4.694874043	-0.270012737	-1.605951836
C42	-5.101046531	-1.731573276	-1.328492810
C43	-5.258165418	-2.627740728	-2.557842802
C44	-4.246066202	3.901664936	-3.081998414
C45	-4.844802547	5.167483681	-2.460368130
C46	-3.959910931	4.072708306	-4.580823132
C47	-6.879728912	6.325294111	-1.746337904
C48	-6.576823409	6.497227781	-0.253359896
C49	-5.615275017	5.533377592	1.781644807
C50	-4.110947392	5.644029339	2.043475002
C51	-1.829742307	5.695855156	1.157546041
C52	-1.373499411	7.125797108	1.483468312
C53	-1.060147667	5.272311942	-0.103277142
C54	-1.319580319	3.868871048	-0.535648114
C55	-1.864984779	2.769349995	0.095624722
C56	-1.373177723	2.107306260	-1.887878327
C57	-1.655375148	9.480940074	0.852773133
C58	-1.457259004	9.930781292	2.297979980
C59	-2.779450460	10.303764735	0.177639968
C60	-2.445078809	11.704329009	-0.245416097
C61	-1.752236426	12.708262254	0.402881216
C62	-2.501208034	13.429305955	-1.553971025
C63	8.192267682	-3.407706600	4.461602733
C64	8.300660486	-4.908954447	4.663034160
C65	6.697628077	-3.100554122	4.214226870
C66	6.401602614	-1.625111652	4.065771280
C67	6.050713648	-0.833801727	5.175534867
C68	6.468810627	-0.999328285	2.806776368
C69	5.768196541	0.529148084	5.037150481
C70	6.203098728	0.361804838	2.655967487
C71	5.847651078	1.124475000	3.771224024
C72	8.398750355	1.722963377	-1.753637152
C73	8.273057684	3.156707558	-2.295391868
C74	7.021184338	1.186884647	-1.368907464
C75	8.454160101	4.609154758	-4.284413565
C76	7.052614945	5.125023124	-4.616891233
C77	4.618848239	4.620180201	-4.513596444
C78	4.021368386	5.000761709	-3.133240981

C79	3.894948058	3.417740581	-5.162033129
C80	2.370633924	3.460275370	-5.318386373
C81	1.819023110	4.349066262	-6.444311656
C82	1.772317286	6.842538659	-6.565632575
C83	3.750634246	4.479223623	-0.758961716
C84	4.370615712	5.729272898	-0.118298508
C85	3.905875052	3.312503900	0.236320643
C86	6.489522814	6.829099052	0.417798458
C87	6.866710623	8.140935290	-0.248533433
C88	6.642343313	9.579636787	-2.194301445
C89	6.007591510	10.933157143	-1.788414498
C90	6.531978527	9.366873786	-3.708570210
C91	5.099447223	9.325520339	-4.226728420
C92	4.115798739	12.067111680	-0.729542383
C93	4.871744322	13.115365674	0.072630537
C94	2.814308531	11.658162400	0.015538415
C95	1.956570735	10.737365780	-0.822072591
C96	1.042447585	11.264216855	-1.746361257
C97	2.090418349	9.340748822	-0.747890887
C98	0.299336943	10.433075988	-2.586617345
C99	1.376724557	8.493493541	-1.600646525
C100	0.490520312	9.051119403	-2.518064943
C101	0.820128823	-7.620011892	-7.455658783
C102	-0.147035783	-6.467523222	-7.236712032
C103	-0.335598571	-4.120684707	-6.442658486
C104	0.096521309	-2.917263031	-7.284949049
C105	1.861088894	-1.237851764	-7.612094162
C106	3.378453540	-1.228355776	-7.777086326
C107	5.577482405	-2.020258956	-7.106650729
C108	6.155421231	-2.460211317	-8.437417352
C109	-4.241601665	-3.322012348	-8.728205722
C110	-4.358052847	-1.795633964	-8.818595392
C111	-4.300157925	-3.777083371	-7.252039218
C112	-4.581182376	-5.288837816	-7.153977924
C113	-4.369812042	-5.789549456	-5.743617309
C114	-3.226123759	0.365494714	-8.680955973
C115	-2.002756050	0.871327562	-9.417791366
C116	-3.515139464	1.070373373	-7.334976050
C117	-2.599933848	0.575320326	-6.249846332
C118	-1.311643348	1.110505137	-6.087308994
C119	-2.982450471	-0.524988935	-5.464252180
C120	-0.413777243	0.524363905	-5.191397105
C121	-2.083559762	-1.107167027	-4.568277438
C122	-0.789038137	-0.596118441	-4.446714957
C123	2.385933433	-10.721620158	-2.208059827
C124	3.240306747	-11.230586734	-1.037242213
C125	1.099319610	-10.059143667	-1.693709583
C126	0.262595421	-9.350978778	-2.709251918
C127	-0.392962325	-9.905887576	-3.789656800
C128	-1.001402255	-7.788561630	-3.571744945
C129	3.400509373	-12.453544868	1.046437815
C130	4.603826436	-13.257231541	0.605988314
C131	-3.662665768	-5.615609331	1.132507263
C132	-2.533792771	-6.474407456	1.689294493
C133	-1.918277273	-7.470083160	0.661721824
C134	-2.888290757	-8.658576082	0.425546851
C135	-2.296654683	-9.838817653	-0.347959342
C136	-3.220093333	-11.073881938	-0.430652936
C137	-0.605146030	-8.022369543	1.236374664
C138	2.386446697	-3.255879398	-1.509853870
Fe139	1.838157610	-4.831924997	-2.798179947
Fe140	1.872763889	-1.285537250	-0.917231267
Fe141	4.248694686	-2.938861007	-0.841275683
Fe142	3.264991674	-2.746341347	-3.218501723
Fe143	4.617633716	-0.708667054	-2.245775492
Fe144	2.614516483	-4.889692792	-0.344320183
Fe145	0.523073208	-3.578252656	-1.098083767
H146	-9.597123087	-1.869543967	0.770070878
H147	-9.103022045	-1.334862821	-0.689555868
H148	-10.540550049	2.479350687	0.610698779
H149	-10.672168960	0.473729722	-0.660166057
H150	-11.303238426	-0.134693501	0.865901139
H151	-7.874390698	3.091562593	1.245192968
H152	-10.354056028	1.930015335	3.491019968
H153	-9.283781356	4.110960021	1.610508489
H154	-10.207905447	1.518603625	5.778829922
H155	-8.412475675	0.131835591	3.691858378
H156	-9.013960938	2.827919829	5.925759697
H157	-3.420527136	1.139099634	2.990610254
H158	-6.266975208	0.979816285	2.880897828

	H159	-6.866370157	-1.596228289	3.820708762
	H160	-3.779498050	4.550349774	6.208169373
	H161	-5.871109642	3.045898592	4.885836855
	H162	-6.710485591	-1.375503059	5.581612896
	H163	-4.525367801	2.416669367	2.448173686
	H164	-5.781917615	1.762045969	7.389061574
	H165	-5.490905667	4.446221625	6.699955022
	H166	-2.396712328	-1.332818796	3.795121419
	H167	-1.703404488	-0.723894556	2.277442066
	H168	-0.778744957	-1.863694680	3.286991100
	H169	-1.555428776	1.013667271	4.087408133
	H170	-5.747622764	0.900363656	9.569888038
	H171	-0.052256105	3.812930493	4.445294164
	H172	-1.239383309	2.943111113	8.725200735
	H173	1.236772324	5.602464092	8.207540067
	H174	0.194985483	0.933073044	2.304834179
	H175	1.232732010	-0.047960401	3.384051063
	H176	8.490264692	-2.924409460	5.411911772
	H177	0.430464901	5.516414236	4.557180132
	H178	1.183277091	6.524218108	6.683054766
	H179	1.665861014	4.238954018	4.662777128
	H180	2.445500714	5.293653165	6.941122175
	H181	-0.570758266	4.717700117	6.727581964
	H182	1.828176091	2.810207162	6.725391019
	H183	-0.989653568	2.316215582	6.083554984
	H184	0.806999423	1.616834515	3.816399559
	H185	3.626136037	2.375249431	-0.266737280
	H186	3.190499050	3.491799228	1.052122795
	H187	5.196919238	3.039658046	1.702176660
	H188	5.271405099	2.870691780	4.393703813
	H189	6.228647935	0.826779402	1.670257674
	H190	6.700417665	-1.592439248	1.919256972
	H191	5.986055898	-1.291197574	6.166613562
	H192	-2.590626106	-0.033616585	6.066009638
	H193	-3.698153051	-2.638958257	7.102383977
	H194	-2.927421212	-2.408299208	8.688114269
	H195	-4.516827208	-0.405930611	7.174463547
	H196	-4.303450445	1.876493221	9.940450549
	H197	5.475276189	1.123244029	5.906724248
	H198	0.071439847	-1.133866144	5.516059718
	H199	-0.009643500	3.802155148	11.135803048
	H200	-1.374962253	2.663176873	11.000999415
	H201	0.650867825	0.874694185	10.473287230
	H202	4.385849327	-11.058993880	6.942977259
	H203	-5.053529066	-4.569972124	-3.169973731
	H204	-2.654881200	-5.831255645	-0.502523516
	H205	-5.628511747	-5.477639884	-7.430948900
	H206	-3.934161701	-5.840088000	-7.851722471
	H207	-5.092857155	-3.231703351	-6.716932478
	H208	-1.543607657	0.129173633	-10.112866452
	H209	-5.161299126	-3.679791952	-9.217086010
	H210	-4.015345184	-0.225577709	-2.470871364
	H211	-6.062873625	-1.763628720	-0.786391315
	H212	-2.337577946	-1.566375538	-8.391257272
	H213	-4.066233466	0.616624200	-9.362711522
	H214	-2.213603397	-3.623446940	-9.057412757
	H215	-4.543321915	-4.286385693	-1.508494943
	H216	-3.352121437	-3.516371215	-6.756845578
	H217	-3.176852805	-4.827215855	-9.632031815
	H218	-7.459851469	0.667063746	-3.178725094
	H219	-4.111787702	0.102775561	-0.753067835
	H220	-2.562081624	-6.344449574	-6.276457899
	H221	-4.361848430	-2.188434314	-0.654163113
	H222	-1.542011135	5.073196015	2.016210369
	H223	-2.243384393	2.708626137	1.111671970
	H224	-6.077010966	6.435739711	2.205765144
	H225	-5.825866563	4.559898719	-0.111439344
	H226	-2.900247494	7.827539209	0.306841059
	H227	-1.227457898	12.739413304	1.351375463
	H228	-2.190631566	9.478643416	3.008591630
	H229	-3.664897988	10.296898344	0.838383749
	H230	-0.706200504	9.609936764	0.308686666
	H231	-2.685291379	14.108353779	-2.382812775
	H232	0.010262076	5.421575400	0.115594043
	H233	-1.313987611	5.965090155	-0.923418304
	H234	-1.369574217	14.700669934	-0.273613176
	H235	-3.075898789	9.767328773	-0.737357100
	H236	-3.648478019	5.502195431	0.023047264
	H237	-5.992353901	4.680151886	2.365638325
	H238	-6.620838710	7.282017733	-2.220877138

	H239	-1.214709814	1.504811704	-2.778426261
	H240	-7.961498401	6.177536354	-1.858898878
	H241	9.994713314	-3.043121042	3.562324582
	H242	8.799719411	-2.052745352	3.052497674
	H243	4.758349023	3.261576123	-2.237547074
	H244	2.677300928	4.691955948	-0.866721249
	H245	6.200171690	5.177517605	-0.869498265
	H246	-0.620309563	4.021274590	-2.550552824
	H247	-1.458147972	5.475439196	-4.189195847
	H248	-3.066434788	5.372624897	-5.742997972
	H249	-0.500907740	6.508788304	-3.470097036
	H250	-3.495174342	3.141151576	-4.946029225
	H251	-4.906237688	4.237983345	-5.121023089
	H252	7.096149235	8.469063077	-3.995163586
	H253	7.016420276	10.233332077	-4.185605174
	H254	5.478096740	7.524301902	-5.174566574
	H255	3.845881275	8.182651274	-5.320914065
	H256	2.818507277	7.749422073	-8.080599719
	H257	0.921973544	3.886056015	-6.883383108
	H258	-0.421101307	10.859781200	-3.288871359
	H259	2.749791283	8.881864168	-0.005796048
	H260	1.055332459	7.991021976	-5.017919598
	H261	4.134312368	2.528808911	-4.557766461
	H262	6.249756195	3.336760211	-4.030663374
	H263	1.877576347	3.714535333	-4.366957694
	H264	-6.725826175	4.413474482	-2.713750990
	H265	9.027368578	4.565013768	-5.219655681
	H266	-5.295527921	2.084708710	-3.712952650
	H267	4.357728859	3.250659615	-6.148621798
	H268	1.536313795	7.415102649	-1.565119878
	H269	8.918862752	5.372324491	-3.643252921
	H270	2.536078147	6.054439095	-8.310183279
	H271	1.433298318	8.853314136	-6.466962667
	H272	-6.289623920	-0.492718685	-3.479108739
	H273	-6.596313463	0.565891785	-1.029542575
	H274	0.897057942	12.345344567	-1.808069977
	H275	-3.292381549	3.751161986	-2.555451596
	H276	4.537146215	5.517887597	-5.134142651
	H277	2.563750114	4.424710185	-7.247434334
	H278	2.063606432	2.430875869	-5.549219782
	H279	0.789340527	5.723635333	-5.175637937
	H280	5.931318985	7.076174628	1.333302433
	H281	5.608815086	7.721127057	-1.812062155
	H282	7.709531938	9.723650164	-1.965206146
	H283	7.425711427	6.334767015	0.712860446
	H284	4.519773026	9.972819686	-0.798184054
	H285	1.797517174	-7.226618408	-7.772529367
	H286	0.969017823	-8.080173449	-6.456509765
	H287	3.006652334	-9.965077119	-2.710749606
	H288	0.795229338	-9.431801620	-8.389447765
	H289	-0.681537536	-8.732178748	-8.255317789
	H290	7.146933897	0.170601593	-0.975029990
	H291	8.965764796	2.367883786	0.098528023
	H292	8.748169881	2.496149797	-4.183095746
	H293	6.574606786	1.822684868	-0.591302642
	H294	10.228005238	1.938870771	-0.847667412
	H295	5.980309343	-2.693080176	-6.333379021
	H296	8.831721623	1.072699199	-2.529950819
	H297	-0.024327919	-7.207109464	6.929191289
	H298	0.616686416	-9.594913398	5.110541730
	H299	3.706033445	-2.749603951	-6.383963845
	H300	4.285243541	-2.496883963	3.529532096
	H301	1.420159561	-1.199852063	-8.616187471
	H302	-2.387177892	-1.960237023	-3.956286007
	H303	1.593573891	-0.292279810	-7.110163549
	H304	1.093631662	-4.892270133	5.856677016
	H305	1.685751559	-2.705104476	-6.029785960
	H306	0.357599789	-5.443317959	4.351692643
	H307	-0.610495591	-7.479319081	5.270806941
	H308	1.812444000	-7.529280840	4.482927478
	H309	2.326260080	-7.022870244	6.096846117
	H310	-4.563284329	0.861884301	-7.073613630
	H311	-1.258565295	-9.415644511	7.436098164
	H312	-3.455050993	-11.137109237	6.134889443
	H313	-0.085290051	-1.045798286	-3.746152360
	H314	-2.407255237	-11.182657714	8.859614380
	H315	-3.843912058	-10.627257325	8.303438901
	H316	2.583083592	-5.533762707	3.330065443
	H317	0.593238065	0.926217234	-5.058647440
	H318	-3.993934936	-0.927246941	-5.555275146

H319	-0.136739905	-12.559386109	1.513860219
H320	0.466406363	-10.829546570	-1.220356045
H321	0.141886447	-10.200222138	2.498050490
H322	-1.175787119	-12.796659000	0.383150974
H323	5.470397642	-3.074831275	-9.070641538
H324	1.951748548	-7.726640361	1.668712189
H325	-2.888714461	-7.004961362	2.580574377
H326	1.402071421	-5.315943472	-6.547319252
H327	-3.214356056	-9.008062282	1.416993593
H328	-1.836449077	-8.997688498	-5.085551463
H329	-1.532228178	-6.863024175	-3.752557827
H330	-2.557307612	-12.453441628	6.897962692
H331	3.761079528	-3.731024529	2.425297992
H332	2.981522995	-9.257191839	3.140538840
H333	3.459783188	-7.363155899	1.646239864
H334	2.773604138	-9.923165857	5.385113936
H335	2.505363887	-3.606853286	6.346588227
H336	-2.074487059	-9.527001754	-1.379658566
H337	-1.345871032	-10.154405548	0.103150947
H338	-3.782548171	-8.281192242	-0.091442644
H339	-0.191447397	-3.916669406	-5.370741000
H340	-1.009630433	1.971653682	-6.689618112
H341	-3.408541170	2.152448676	-7.503968373
H342	-1.750421921	-5.767989530	2.013335785
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H346	-0.381473983	-10.910393062	-4.194024315
H347	1.355928194	-9.350438880	-0.897384434
H348	-1.393712556	-4.309560266	-6.634394211
H349	5.932631077	-1.003134633	-6.880888897
H350	6.126529129	-3.511872352	5.060585759
H351	6.392655841	-3.640530154	3.303663508
H352	2.984455612	-12.174418934	-3.527591827
H353	1.606289157	-12.556121633	-2.731322275
H354	2.757630717	-13.126271532	1.635139427
H355	1.616963711	-12.171710681	-0.085473649
H356	4.501216393	-13.736549438	-0.397931258
H357	3.721775314	-11.636085404	1.711109882
H358	8.332875461	-5.498364728	3.715514373
H359	5.724489780	12.729501257	0.678995461
H360	3.714747393	-10.042653507	8.239112636
H361	4.643648701	-8.020490377	6.589838900
H362	3.841888827	12.526116849	-1.694939567
H363	3.084905332	11.177383953	0.968373507
H364	2.266864543	12.581119814	0.252974052
H365	-0.935986995	8.665362807	-3.788196800
H366	2.301890378	-1.210645051	1.694986080
H367	1.450491197	-2.565522404	1.285935239
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Mo369	0.373923803	-6.272494163	-1.038420418
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N381	-1.728740314	-0.532395697	6.281367144
N382	-0.076441174	2.048354974	6.457939444
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N384	-2.844946073	-10.664056846	8.095012819
N385	-0.799948094	-9.778043724	6.594372122
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N387	2.959259838	-3.187151109	5.543378929
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N390	-6.453099454	0.487932406	-3.186991756
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N392	-5.081755190	2.720436509	-2.928579475
N393	-6.198250372	5.228122279	-2.407627642
N394	-6.031516224	5.431633172	0.395069821
N395	-3.274033883	5.605911006	0.968467010
N396	-1.011293225	3.428617146	-1.808899279
N397	-1.896497080	1.682676415	-0.747728075
N398	-2.082756694	8.093632336	0.850702739

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N401	9.004452785	-3.023252222	3.306074910
N402	9.279990995	1.663216666	-0.576452945
N403	8.521879930	3.317248943	-3.627987682
N404	6.032778431	4.269834428	-4.403889593
N405	1.454499492	5.691492141	-5.978771819
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N408	4.303457036	4.176988661	-2.082013769
N409	5.692969118	5.926467162	-0.390512698
N410	6.208035887	8.441076516	-1.408451288
N411	4.832399323	8.321610721	-5.104576421
N412	4.940654350	10.886492614	-0.951746496
N413	0.301584081	-8.540271100	-8.470183048
N414	0.411765573	-5.315534124	-6.811947086
N415	1.272686014	-2.366447382	-6.913008918
N416	4.127065414	-2.105127100	-7.060774056
N417	-3.108406160	-3.812925946	-9.524503165
N418	-3.213440607	-1.084864598	-8.619377190
N419	2.099985456	-11.783929507	-3.189835889
N420	-0.123691782	-8.015592670	-2.594272610
N421	-1.177196204	-8.904334526	-4.317031291
N422	2.622235060	-11.977416296	-0.082387859
O423	-8.389262901	0.371063537	1.609220750
O424	-7.519920777	3.339399335	3.740223234
O425	-7.497041075	0.930771286	6.639364910
O426	-4.455588341	-0.306435683	5.152278009
O427	-2.712386085	2.696448840	4.834334147
O428	-3.200075463	3.382471363	8.343437500
O429	-3.164718508	-0.356472049	10.072047157
O430	-0.859577875	-2.454789576	7.195675867
O431	1.535291834	0.437110237	6.598978586
O432	1.920461582	3.023748071	9.182332706
O433	0.997746541	1.697326528	12.309331534
O434	-0.928157006	-11.550581527	5.118513145
O435	1.470921532	-9.350523744	8.279301633
O436	6.216971480	-9.202040917	7.127613884
O437	-5.243285512	2.738527566	-0.635759849
O438	-5.674945033	-2.195602209	-3.657908690
O439	-4.113269197	6.069598498	-2.017496906
O440	-3.079244668	5.194162089	-4.785825496
O441	-6.856071222	7.573302792	0.296153012
O442	-3.702134700	5.762107017	3.206448841
O443	-0.382851537	7.365146960	2.183174949
O444	-0.633377239	10.753307051	2.663415357
O445	8.325751789	-5.454456360	5.757005402
O446	5.565994585	2.458828261	3.560333826
O447	7.965576008	4.112973397	-1.562551348
O448	6.922566295	6.282129845	-5.065631313
O449	3.325568070	6.020520007	-3.014812161
O450	3.712664401	6.450722500	0.642045326
O451	5.240392191	3.224043098	0.742950647
O452	7.711382108	8.888452980	0.260397333
O453	6.498984324	11.998792546	-2.186685157
O454	4.261467319	10.180777805	-3.904050762
O455	4.549299564	14.293037854	0.093663856
O456	-0.174753922	8.187557283	-3.405800545
O457	-1.379381815	-6.622911200	-7.418151869
O458	-0.583159849	-2.510739273	-8.251152845
O459	3.893672981	-0.391862739	-8.537868957
O460	7.296591981	-2.205700280	-8.788261531
O461	-5.448123399	-1.243646319	-9.047241427
O462	-5.216286838	-5.700942019	-4.860761082
O463	-3.158876167	-6.315789790	-5.466797158
O464	-1.560362957	2.007359309	-9.323393039
O465	4.467363830	-11.016220631	-0.980519809
O466	5.590125910	-13.446585270	1.304597168
O467	-3.523008767	-5.270769968	-0.150999273
O468	-4.602520331	-5.218117619	1.819883626
O469	-2.667200092	-12.224422992	-0.304578673
O470	-4.447652897	-10.874072075	-0.651060900
O471	0.478881059	-7.810865068	0.539770193
O472	-0.606276708	-8.649792271	2.314181603
O473	-1.646899889	-6.757437275	-0.546245461
O474	2.955269966	-10.118503994	3.625214270
O475	2.741948556	-7.609185027	2.260457748
O476	-0.521662989	5.628577819	-3.903975468
O477	-0.362122757	-13.206148046	0.808317874
O478	0.519297939	-11.084083604	2.759229700

	S479	5.855968246	1.144533204	-2.809848714
	S480	2.521974294	-0.616271587	-3.264491308
	S481	-0.411617600	-4.747157846	-2.706454573
	S482	4.160519112	-0.850462178	-0.081430169
	S483	-0.392086243	-1.656593163	-1.181211197
	S484	2.820976511	-4.358220765	-4.701879907
	S485	0.672745921	-4.761249650	0.799252581
	S486	5.474394155	-2.792773577	-2.710029483
	S487	2.616611827	-6.638636692	-1.719679111
	S488	4.593963079	-4.611377216	0.578536849
	end			
N2x-Fe2NH3 to N2x-core **S=1, 35** **TS** Fe(139) -2.089 Fe(140) -0.307 Fe(141) -2.357 Fe(142) 2.649 Fe(143) 2.610 Fe(144) 2.369 Fe(145) -1.256	965182n2x2nh3d35tj_1_53231.48			
	C1	-9.381596117	0.817039020	1.026450663
	C2	-10.404174864	-0.035078119	0.264146108
	C3	-8.791396735	3.100350389	1.732412365
	C4	-8.519412644	2.902793935	3.220148120
	C5	-9.231583066	1.921340186	5.337943740
	C6	-8.101178082	0.908182468	5.555927531
	C7	-6.731441835	-0.862985070	4.579994284
	C8	-5.425842040	-0.080276737	4.416144358
	C9	-4.275897648	1.732423128	3.226881666
	C10	-3.864027863	2.548598161	4.460157646
	C11	-4.507697386	3.837271722	6.397111279
	C12	-4.064494155	3.001809934	7.607701324
	C13	-4.654689298	1.175008187	9.140615217
	C14	-3.771277726	-0.077097247	9.066697602
	C15	-3.062085459	-1.994780966	7.714188141
	C16	-1.737825370	-1.690902616	7.006752798
	C17	-0.546049186	-0.214043526	5.455461238
	C18	0.423217080	0.748305512	6.165486737
	C19	-0.907763472	0.206832820	4.017068643
	C20	0.332641542	0.724378202	3.280708672
	C21	-1.610237880	-0.951773580	3.297455247
	C22	0.872549830	3.009631871	6.995026906
	C23	0.930457847	2.956761685	8.533956824
	C24	0.562364175	4.412956130	6.420653576
	C25	1.446285778	5.487151088	7.062849944
	C26	0.745857671	4.415290201	4.897066147
	C27	-0.222102152	2.808430122	10.661440977
	C28	0.617035947	1.633447412	11.132118694
	C29	-2.587313464	-11.351183139	6.815808505
	C30	-1.331695449	-10.869632469	6.095810147
	C31	0.382764519	-9.075663008	6.086571856
	C32	1.552472625	-9.369942154	7.044257920
	C33	0.188180543	-7.556253363	5.943872494
	C34	1.455813916	-6.901571881	5.402719082
	C35	1.307662693	-5.415273656	5.122928806
	C36	3.086164405	-3.777170483	4.484094538
	C37	3.908930342	-10.014895682	7.193454781
	C38	5.013397556	-9.011932000	6.949053170
	C39	-5.842353871	0.699757268	-1.840876889
	C40	-5.349090808	2.154372879	-1.705694401
	C41	-4.681930582	-0.276388988	-1.560089215
	C42	-5.109756862	-1.732775929	-1.281954670
	C43	-5.244894859	-2.637033451	-2.507772693
	C44	-4.239794695	3.920902256	-3.056431976
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	C46	-3.949027093	4.095737071	-4.554096273
	C47	-6.903005106	6.322024811	-1.737274709
	C48	-6.598393587	6.503285697	-0.245493035
	C49	-5.631094621	5.550854688	1.793206186
	C50	-4.125306220	5.654129113	2.048526005
	C51	-1.846236381	5.667760104	1.149385374
	C52	-1.399337692	7.099162356	1.481660330
	C53	-1.092224485	5.266317493	-0.129038361
	C54	-1.325178212	3.860434612	-0.565335597
	C55	-1.880826372	2.757949456	0.049831152
	C56	-1.350543228	2.106300730	-1.927084438
	C57	-1.657319491	9.446419110	0.816516201
	C58	-1.472924361	9.898975441	2.262817344
	C59	-2.780673558	10.267420368	0.137550335
	C60	-2.454871647	11.671917809	-0.279244718
	C61	-1.755896105	12.674062630	0.365306348
	C62	-2.540300728	13.406703524	-1.573772655
	C63	8.116797212	-3.396739912	4.504773743
	C64	8.192891876	-4.898174632	4.720321854
	C65	6.635447841	-3.061473735	4.244945679
	C66	6.365599960	-1.581154316	4.095409349
	C67	6.019133126	-0.784235252	5.202680122
	C68	6.435009778	-0.960511940	2.834213161

C69	5.737947662	0.578522544	5.058828531
C70	6.170891119	0.400114788	2.677870547
C71	5.814612728	1.167525088	3.789934326
C72	8.384294241	1.733986456	-1.701339736
C73	8.252789477	3.158381956	-2.261065546
C74	7.025121393	1.232038598	-1.212055862
C75	8.452991798	4.587375481	-4.266240845
C76	7.055618090	5.115481613	-4.597177008
C77	4.617467411	4.624109686	-4.485444134
C78	4.005793866	5.027907147	-3.120205466
C79	3.900981127	3.418547755	-5.133338398
C80	2.378058480	3.460354370	-5.301652771
C81	1.833528581	4.347376347	-6.432468814
C82	1.780790518	6.838511247	-6.561228963
C83	3.703668915	4.549345021	-0.742690545
C84	4.355611611	5.780312233	-0.098715040
C85	3.809264377	3.384304605	0.258071244
C86	6.501522879	6.832888924	0.426922196
C87	6.866197030	8.143279068	-0.249426570
C88	6.622465724	9.565121772	-2.203113902
C89	5.976833881	10.912350848	-1.796719208
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C91	5.084207484	9.304251915	-4.240469819
C92	4.089426172	12.042279061	-0.741875653
C93	4.849352837	13.097757219	0.047039630
C94	2.783172587	11.655837196	0.004467556
C95	1.922387782	10.737175424	-0.830550674
C96	1.010245731	11.264599409	-1.756302536
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C98	0.272530131	10.433643959	-2.601721151
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C116	-3.524866251	1.100020701	-7.275273118
C117	-2.568118911	0.596570188	-6.230571588
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C119	-2.907492935	-0.525476467	-5.456664503
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	H152	-10.305595301	1.929568543	3.471994763
	H153	-9.209736386	4.105899026	1.589356783
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	H160	-3.678822640	4.516218786	6.158080689
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	H166	-2.552015218	-1.212635475	3.800406090
	H167	-1.846345750	-0.681561824	2.254355615
	H168	-0.984963390	-1.857572693	3.280638005
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	H183	-0.950846161	2.288042331	6.103365620
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	H191	5.954349039	-1.235811207	6.196480132
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	H194	-2.811957112	-2.465270141	8.672568481
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	H206	-3.941273151	-5.809263042	-7.856296987
	H207	-5.131107242	-3.227135252	-6.693989883
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	H219	-4.114500432	0.096067911	-0.696899835
	H220	-2.561522964	-6.332671139	-6.299806001
	H221	-4.395631760	-2.192383588	-0.583228102
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	H261	4.137653853	2.530611169	-4.525619777
	H262	6.246382353	3.346091866	-3.976695776
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	H305	1.756276640	-2.785569402	-6.092565318
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	H319	-0.162349332	-12.552231322	1.527570574
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	H331	3.756478599	-3.648750035	2.521578495
	H332	2.967244646	-9.242541186	3.153720188
	H333	3.391165675	-7.295522541	1.656874705
	H334	2.739744484	-9.870188121	5.398544633
	H335	2.609229011	-3.543832658	6.471834278
	H336	-2.099076137	-9.537739764	-1.408200311
	H337	-1.372672621	-10.165941870	0.077862767
	H338	-3.821094316	-8.304057437	-0.108821028
	H339	-0.150453916	-3.938116649	-5.371353513
	H340	-1.015518514	2.027412063	-6.691378473
	H341	-3.420861739	2.182872735	-7.442525418
	H342	-1.818266878	-5.812575712	2.046130177
	H343	2.109966028	-10.533031130	3.302002653
	H344	0.039290871	-11.268310276	3.608294672
	H345	3.259297141	-2.150422120	5.719688342
	H346	-0.399673687	-10.890380159	-4.242635540
	H347	1.271974560	-9.359843353	-0.895831390
	H348	-1.368926492	-4.329937694	-6.616831336
	H349	5.962877963	-0.920019588	-6.965124355
	H350	6.051627535	-3.462276688	5.087458988
	H351	6.325211993	-3.594491454	3.332713227
	H352	3.017589001	-12.109106532	-3.529094186
	H353	1.619877648	-12.520561923	-2.781825755
	H354	2.718863145	-13.181508571	1.591909189
	H355	1.576638962	-12.162793160	-0.092751435
	H356	4.482145601	-13.708726435	-0.437793207
	H357	3.663099541	-11.680532880	1.729791408
	H358	8.246456254	-5.498904436	3.781150781
	H359	5.703710906	12.718164211	0.654576342
	H360	3.646416818	-9.946298406	8.264518384
	H361	4.676607433	-8.002862522	6.605680603
	H362	3.817558026	12.493539834	-1.711505295
	H363	3.040323075	11.184856715	0.965842704
	H364	2.246952146	12.590257774	0.222818950
	H365	-0.953330969	8.659931456	-3.809851385
	H366	1.974963790	-2.590400658	1.174743076
	H367	0.411580825	-2.134774469	1.306624539
	H368	1.576197828	-1.709454945	2.465888191
	Mo369	0.399028891	-6.283188280	-1.113388934
	N370	1.377540470	-1.822913677	1.471014683
	N371	1.488533337	0.517399123	-0.702198084
	N372	1.211131161	1.564787457	-0.409788781
	N373	-9.988686501	-1.375583899	-0.106678193
	N374	-9.708429654	2.137350408	1.143502343
	N375	-9.463676726	2.253404104	3.942121870
	N376	-7.899198476	0.006480383	4.562644333
	N377	-5.424068591	0.863566486	3.446448343
	N378	-4.860741783	3.052751580	5.225773055
	N379	-4.836968613	1.922405572	7.903688609
	N380	-3.915936689	-0.845333686	7.953799203
	N381	-1.710773268	-0.550627561	6.259745099
	N382	-0.032751809	2.000624653	6.447676620
	N383	-0.245867605	2.902565579	9.209928147
	N384	-2.819729610	-10.671229992	8.096184476
	N385	-0.828878330	-9.711700250	6.570442451
	N386	2.455299046	-4.948216473	4.328802178
	N387	3.122274792	-3.157563051	5.687180732
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	N389	2.704104650	-9.750006026	6.435907883
	N390	-6.391467124	0.486564680	-3.188062037
	N391	-4.942035320	-3.934181426	-2.316867371
	N392	-5.061815851	2.729994076	-2.906247624
	N393	-6.208869343	5.229646216	-2.394317708
	N394	-6.052702846	5.440956334	0.408265280
	N395	-3.292138148	5.572766268	0.973051792
	N396	-0.989136700	3.426647003	-1.834402775
	N397	-1.895009345	1.675216977	-0.799378832
	N398	-2.084520167	8.060019449	0.812193715
	N399	-2.940678272	12.144189431	-1.489408491
	N400	-1.817100507	13.766214954	-0.474937020
	N401	8.952430065	-3.028046666	3.361291913
	N402	9.344534324	1.682681861	-0.585427989
	N403	8.503163654	3.301389953	-3.595495631
	N404	6.029502083	4.273021340	-4.359942336
	N405	1.466016315	5.689149871	-5.970114578
	N406	2.370468061	6.890371091	-7.769939347
	N407	1.556431363	8.008699755	-5.914476261
	N408	4.266662010	4.219198351	-2.053900806
	N409	5.683317693	5.937312533	-0.365106487
	N410	6.202731630	8.426506593	-1.411194611
	N411	4.831964343	8.309087360	-5.133435606
	N412	4.912664192	10.860046000	-0.956361312
	N413	0.275972460	-8.548876519	-8.515089118
	N414	0.430168468	-5.342489360	-6.815446570
	N415	1.312458177	-2.413360365	-6.948878031
	N416	4.171883901	-2.054790905	-7.045597120
	N417	-3.153493811	-3.760181755	-9.514890808
	N418	-3.266880942	-1.046990567	-8.586478244
	N419	2.118945020	-11.735153586	-3.211212869
	N420	-0.144533680	-8.008233165	-2.624663715
	N421	-1.189155632	-8.882058186	-4.357926666
	N422	2.582515861	-11.973643190	-0.085977681
	O423	-8.358644504	0.348750728	1.556775298
	O424	-7.466838551	3.328145641	3.726509460
	O425	-7.435903278	0.924659083	6.605131559
	O426	-4.441083069	-0.288141027	5.147041274
	O427	-2.667233659	2.729975828	4.733876838
	O428	-3.090312476	3.350698368	8.296633747
	O429	-3.026825987	-0.375047460	10.011352897
	O430	-0.782161945	-2.472927696	7.117771086
	O431	1.578216760	0.381579030	6.436464403
	O432	2.019430334	2.954771881	9.136061957
	O433	1.115158055	1.565215249	12.245505607
	O434	-0.871433338	-11.524560474	5.138382812
	O435	1.426363005	-9.219543442	8.271872754
	O436	6.195925385	-9.257239346	7.131057431
	O437	-5.235048300	2.742339981	-0.613789452
	O438	-5.644984220	-2.207467096	-3.616786237
	O439	-4.134005437	6.092618420	-1.997582715
	O440	-3.072782926	5.221362746	-4.754474857
	O441	-6.877903560	7.582203731	0.297943337
	O442	-3.710607040	5.798148688	3.206280942
	O443	-0.437451050	7.349802648	2.216944147
	O444	-0.651347651	10.721816883	2.632587361
	O445	8.168780067	-5.432757653	5.819858660
	O446	5.529164629	2.499613814	3.571826046
	O447	7.948334675	4.124554189	-1.540299423
	O448	6.933612664	6.265354481	-5.064458923
	O449	3.313912585	6.053244067	-3.026973141
	O450	3.713105487	6.524213857	0.653004276
	O451	5.140366831	3.256317905	0.767273597
	O452	7.707406854	8.900872083	0.249962649
	O453	6.458279454	11.982001007	-2.196715933
	O454	4.236901485	10.147296945	-3.911708365
	O455	4.526886305	14.275509302	0.057076547
	O456	-0.189730499	8.187433926	-3.425911465
	O457	-1.374292816	-6.616490487	-7.446567466
	O458	-0.604387991	-2.491886046	-8.207386206
	O459	3.898146163	-0.465199704	-8.647776457
	O460	7.317512926	-2.225141328	-8.806648255
	O461	-5.505926959	-1.204706440	-8.988495127
	O462	-5.197000176	-5.688955800	-4.850095051
	O463	-3.147997586	-6.304631847	-5.483768720
	O464	-1.646111297	2.059114341	-9.320422818
	O465	4.430409713	-10.995344594	-0.958641438
	O466	5.565353634	-13.435373685	1.271185525
	O467	-3.523509987	-5.262043872	-0.175413296
	O468	-4.628638427	-5.194942979	1.792229561

	O469	-2.688378965	-12.237751481	-0.313465539
	O470	-4.465568198	-10.896295822	-0.710209417
	O471	0.442874956	-7.808930383	0.491417045
	O472	-0.632259805	-8.652039028	2.273433895
	O473	-1.691039076	-6.755394347	-0.580896089
	O474	2.942415892	-10.101754840	3.643056167
	O475	2.688666770	-7.603296570	2.260640974
	O476	-0.503380528	5.617626131	-3.889173355
	O477	-0.392662565	-13.205808055	0.829688177
	O478	0.515440176	-11.082962770	2.759637441
	S479	5.763113093	1.175399043	-2.570108824
	S480	2.638309785	-0.583961358	-3.192662754
	S481	-0.306221784	-4.723084652	-2.778130876
	S482	3.925321742	-0.875309492	0.070694457
	S483	-0.314385135	-1.659145248	-1.226520397
	S484	2.928630101	-4.282825207	-4.724680060
	S485	0.638881870	-4.790048922	0.729799693
	S486	5.493870524	-2.678606498	-2.533261004
	S487	2.660593239	-6.655833863	-1.743344321
	S488	4.498335906	-4.561541627	0.696692893
	end			
N2x-Fe2NH3 to N2x-core **S=1, 35** **product** Fe(139) -2.059 Fe(140) -0.956 Fe(141) -2.356 Fe(142) 2.839 Fe(143) 2.786 Fe(144) 2.380 Fe(145) -1.014	965182n2x2nh3d35ti.car_2			
	C1	-9.379760948	0.816975753	1.031645634
	C2	-10.386187009	-0.043712135	0.259296025
	C3	-8.801323787	3.103344517	1.732547667
	C4	-8.535231195	2.908586560	3.221841071
	C5	-9.249753789	1.924624207	5.338227292
	C6	-8.120067695	0.912028490	5.564191327
	C7	-6.733950404	-0.853019860	4.597780801
	C8	-5.426999032	-0.071005808	4.431957751
	C9	-4.284965782	1.746366856	3.245427907
	C10	-3.886150605	2.565683645	4.481049189
	C11	-4.552732317	3.853901694	6.412463006
	C12	-4.108041376	3.021448914	7.624892180
	C13	-4.686490326	1.191016459	9.157370672
	C14	-3.800348095	-0.059982122	9.079281337
	C15	-3.081847260	-1.967831332	7.711765356
	C16	-1.748336788	-1.683548730	7.012827706
	C17	-0.527008818	-0.216097542	5.459945575
	C18	0.423446335	0.758568995	6.180328353
	C19	-0.903270513	0.229092643	4.027307950
	C20	0.300031624	0.799942113	3.268188407
	C21	-1.585751260	-0.933465160	3.282122425
	C22	0.855556791	3.031612271	6.990564866
	C23	0.907466509	2.970854126	8.527713829
	C24	0.537950529	4.441229498	6.435427472
	C25	1.432798302	5.502734915	7.084896879
	C26	0.708364168	4.461819792	4.911341209
	C27	-0.253959903	2.815950566	10.645848181
	C28	0.594320646	1.658141615	11.139016932
	C29	-2.604874705	-11.347753340	6.810548313
	C30	-1.345164440	-10.877317324	6.091665202
	C31	0.392522523	-9.109582927	6.092294847
	C32	1.561369418	-9.413679165	7.046475135
	C33	0.208068944	-7.589705283	5.950329990
	C34	1.472000814	-6.934884124	5.402249785
	C35	1.300889699	-5.456910212	5.088061862
	C36	3.080557164	-3.803776042	4.487088509
	C37	3.926786602	-10.028714203	7.179663433
	C38	5.011301317	-9.004855705	6.930576795
	C39	-5.842749512	0.697569923	-1.845258141
	C40	-5.349881830	2.151816589	-1.713690566
	C41	-4.677655461	-0.274193766	-1.571405529
	C42	-5.100219404	-1.731673234	-1.294052602
	C43	-5.239360875	-2.630449385	-2.523607261
	C44	-4.235659424	3.912356398	-3.066833080
	C45	-4.845509600	5.174602268	-2.448377450
	C46	-3.948369574	4.087170192	-4.565102001
	C47	-6.891444574	6.318825078	-1.742723026
	C48	-6.589021035	6.498979055	-0.250437456
	C49	-5.623957400	5.547804812	1.789305231
	C50	-4.118860675	5.655194827	2.047233555
	C51	-1.837594890	5.665862053	1.155361390
	C52	-1.391161319	7.098680909	1.483015781
	C53	-1.076244357	5.257360406	-0.116430432
	C54	-1.315527928	3.853610084	-0.556690551
	C55	-1.872398919	2.749666096	0.054658903
	C56	-1.346007129	2.105519713	-1.925488141
	C57	-1.649637117	9.444731818	0.814937292
	C58	-1.458322850	9.896520013	2.260403660

	C59	-2.775894396	10.267467747	0.142527775
	C60	-2.449491266	11.672199806	-0.273344771
	C61	-1.755155847	12.675179689	0.374890498
	C62	-2.526778582	13.406052881	-1.569829519
	C63	8.149858341	-3.395936710	4.468993901
	C64	8.226786224	-4.897617781	4.682625519
	C65	6.667779802	-3.062490518	4.220515209
	C66	6.390276408	-1.583381599	4.073561481
	C67	6.038993433	-0.791599330	5.182605089
	C68	6.452390847	-0.959839466	2.813217089
	C69	5.750929129	0.570142817	5.042734353
	C70	6.180107627	0.399420981	2.660478580
	C71	5.823588362	1.162761633	3.775496679
	C72	8.384797097	1.727202253	-1.708408416
	C73	8.248475173	3.152590696	-2.269622550
	C74	7.025317418	1.230590102	-1.224429810
	C75	8.446318048	4.589204618	-4.270437012
	C76	7.048298116	5.113713686	-4.604695324
	C77	4.610909579	4.619094472	-4.494285406
	C78	4.002366063	5.020718620	-3.126215934
	C79	3.895358554	3.411244228	-5.139488931
	C80	2.372480063	3.451827970	-5.308891665
	C81	1.829595112	4.341805012	-6.438304914
	C82	1.778088621	6.833788684	-6.565014539
	C83	3.700385760	4.538562485	-0.749138486
	C84	4.350864548	5.770976901	-0.105862241
	C85	3.809957774	3.375920818	0.253954197
	C86	6.495117437	6.823506482	0.425776808
	C87	6.868593315	8.131151816	-0.251300704
	C88	6.629519969	9.558175670	-2.202815823
	C89	5.987194987	10.906844013	-1.794209086
	C90	6.519101564	9.348163982	-3.717537548
	C91	5.088763659	9.305416800	-4.240314119
	C92	4.096386017	12.036926571	-0.742979045
	C93	4.855864402	13.090936822	0.048249352
	C94	2.791591834	11.645096656	0.003307736
	C95	1.930040082	10.728025672	-0.833213934
	C96	1.019127853	11.257079206	-1.759345019
	C97	2.063687456	9.331627440	-0.759628657
	C98	0.278536199	10.427527327	-2.603521654
	C99	1.352353013	8.486624031	-1.615839576
	C100	0.469382236	9.045841823	-2.535157325
	C101	0.809143463	-7.637991338	-7.506735904
	C102	-0.144593480	-6.478553729	-7.269173253
	C103	-0.315040104	-4.137933002	-6.455974703
	C104	0.104878056	-2.928798153	-7.297894224
	C105	1.879340898	-1.262768562	-7.651456027
	C106	3.394939048	-1.246030570	-7.831437029
	C107	5.608691393	-1.966279756	-7.123825941
	C108	6.175277496	-2.465256439	-8.439292297
	C109	-4.282200279	-3.293044450	-8.725862927
	C110	-4.403221311	-1.766231517	-8.800060576
	C111	-4.326057905	-3.759159594	-7.252238661
	C112	-4.590377391	-5.274303487	-7.158107896
	C113	-4.367395693	-5.775486220	-5.749169953
	C114	-3.268469834	0.395537263	-8.652358431
	C115	-2.061319224	0.907262571	-9.413240435
	C116	-3.507910228	1.084997381	-7.287145163
	C117	-2.561464651	0.575556792	-6.234681578
	C118	-1.273746683	1.118111304	-6.093055346
	C119	-2.919083987	-0.534144382	-5.451020122
	C120	-0.353230167	0.530138274	-5.220957517
	C121	-1.997693378	-1.119742420	-4.579566353
	C122	-0.704487020	-0.600854885	-4.479077654
	C123	2.370202748	-10.703026293	-2.210116147
	C124	3.212744360	-11.222655763	-1.034133316
	C125	1.067609087	-10.059676143	-1.712244825
	C126	0.247154568	-9.336805634	-2.732766245
	C127	-0.409533817	-9.883275220	-3.816156508
	C128	-0.997737976	-7.760264424	-3.600136647
	C129	3.362762656	-12.482635679	1.029563504
	C130	4.578938594	-13.258683002	0.574201370
	C131	-3.651986986	-5.589363421	1.086316524
	C132	-2.548087860	-6.478704019	1.650447651
	C133	-1.918841403	-7.465644500	0.617853915
	C134	-2.891621657	-8.653602266	0.381463650
	C135	-2.307536743	-9.840569362	-0.386470239
	C136	-3.233368396	-11.076491583	-0.458298629
	C137	-0.605055459	-8.015184879	1.191242353
	C138	2.399705522	-3.287961395	-1.557033951

Fe139	1.890214741	-4.802450134	-2.821090625
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Fe141	4.168464229	-2.880727280	-0.758335639
Fe142	3.368615648	-2.726523778	-3.216340850
Fe143	4.586177222	-0.668703759	-2.065777026
Fe144	2.599857894	-4.895989795	-0.342024048
Fe145	0.579390489	-3.552521194	-1.098848277
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H147	-9.154378846	-1.334958768	-0.735614220
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H157	-3.404916497	1.161361447	2.953433874
H158	-6.238372410	0.953467096	2.847814669
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H160	-3.728626293	4.540810389	6.179564320
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H173	1.284453286	5.566441619	8.172125682
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H176	8.453554062	-2.916741258	5.420483646
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H191	5.974205352	-1.247483003	6.174594771
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	H236	-3.660907371	5.467017412	0.030564161
	H237	-6.002052542	4.699752067	2.380672431
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	O442	-3.707053757	5.804406071	3.205259425
	O443	-0.429193432	7.351811671	2.217288774
	O444	-0.635738777	10.720179310	2.626322908
	O445	8.208832285	-5.434124288	5.781364837
	O446	5.533972354	2.494539891	3.562552075
	O447	7.935648015	4.115385467	-1.547891804
	O448	6.924709918	6.264482975	-5.070108198
	O449	3.313257256	6.047816415	-3.030012028
	O450	3.706583654	6.514389070	0.644872785
	O451	5.140954966	3.252679876	0.764055015
	O452	7.714065140	8.883929863	0.248309307
	O453	6.472802945	11.976349492	-2.189590934
	O454	4.245572973	10.153020253	-3.912402233
	O455	4.534608395	14.269036451	0.059340301
	O456	-0.191747705	8.181837334	-3.425025609
	O457	-1.378890860	-6.619080403	-7.443852854
	O458	-0.603446950	-2.495468125	-8.230660844

	O459	3.895897467	-0.451805987	-8.644716305
	O460	7.312449334	-2.225679248	-8.813062896
	O461	-5.495906379	-1.212400094	-9.008326016
	O462	-5.204206227	-5.683556938	-4.858161771
	O463	-3.154528168	-6.304663122	-5.483165847
	O464	-1.620583028	2.044011545	-9.321885050
	O465	4.439829078	-11.010294632	-0.968506101
	O466	5.567691656	-13.447140064	1.269764751
	O467	-3.501288403	-5.244865525	-0.196475092
	O468	-4.590391669	-5.165940623	1.757324906
	O469	-2.680782004	-12.225227231	-0.317067203
	O470	-4.460175346	-10.879518934	-0.685146086
	O471	0.477335239	-7.789320966	0.496061922
	O472	-0.608179243	-8.652534805	2.262615754
	O473	-1.635312834	-6.753934747	-0.590959985
	O474	2.942729267	-10.109669816	3.635029183
	O475	2.707989312	-7.603568819	2.260478207
	O476	-0.505311180	5.612914110	-3.893225934
	O477	-0.388009133	-13.212795002	0.822614131
	O478	0.513691060	-11.088002235	2.755089857
	S479	5.785462780	1.185002785	-2.602071526
	S480	2.679537779	-0.594415069	-3.341943667
	S481	-0.343730797	-4.665186481	-2.756134719
	S482	3.816615827	-0.844750943	0.023821795
	S483	-0.266230498	-1.605028826	-1.101718763
	S484	2.919572957	-4.318174213	-4.721256680
	S485	0.651659835	-4.756489519	0.749372682
	S486	5.519013102	-2.685061028	-2.521628323
	S487	2.630874539	-6.626691885	-1.760926597
	S488	4.523737306	-4.533590816	0.664313777
	end			
Fe2NH3 to core **S=0, 47** **reactant** Fe(139) 2.361 Fe(140) -1.209 Fe(141) 2.680 Fe(142) -2.571 Fe(143) 2.943 Fe(144) -2.272 Fe(145) -2.309	96518262nh3dth_3_53013.22			
	C1	-8.056357204	-4.996782105	-0.543140119
	C2	-8.426409212	-5.772592299	-1.811543175
	C3	-8.860103507	-3.460443116	1.199109614
	C4	-8.339083381	-4.149812499	2.456022046
	C5	-8.096479563	-6.234490655	3.713871376
	C6	-6.573271957	-6.401908151	3.708950768
	C7	-4.507305761	-6.378357455	2.405059122
	C8	-3.919654892	-5.044045185	2.876373775
	C9	-4.200246632	-2.610454849	2.905397320
	C10	-4.264768416	-2.472836032	4.432565368
	C11	-5.455944898	-2.902851755	6.491702028
	C12	-4.491105213	-3.793421089	7.289160854
	C13	-3.657574036	-6.070529618	7.656881894
	C14	-2.187589672	-6.338099838	7.300598547
	C15	-0.519522235	-6.534919335	5.499085931
	C16	0.274221538	-5.272454528	5.145630999
	C17	0.163879881	-2.846934001	4.720254881
	C18	0.323511035	-1.995220069	5.994988009
	C19	-0.506759142	-2.125492137	3.532331580
	C20	0.078326112	-0.723360218	3.338783672
	C21	-0.382028726	-2.978163266	2.264431442
	C22	-0.741787786	-0.634055819	7.729749857
	C23	-0.464578052	-1.414040023	9.027238130
	C24	-2.001763445	0.260847130	7.808481176
	C25	-2.017944730	1.090635301	9.096316703
	C26	-2.077411728	1.177770130	6.580490386
	C27	-1.038645513	-3.250656129	10.499487362
	C28	0.407155580	-3.624109819	10.761261890
	C29	4.930535573	-12.606249800	0.369506588
	C30	5.699162435	-11.294527613	0.260807296
	C31	6.170043666	-9.175652216	1.464636586
	C32	7.388327652	-9.136758052	2.404391766
	C33	5.071879740	-8.222798775	1.967089094
	C34	5.524442576	-6.767694270	1.927749062
	C35	4.411169892	-5.790741179	2.288301286
	C36	4.981009213	-3.433205972	2.908085800
	C37	9.653923710	-8.265355311	2.721514120
	C38	9.897155810	-6.827330700	3.123965676
	C39	-5.384261365	-1.722016223	-2.455760708
	C40	-5.743350343	-0.487289221	-1.610246300
	C41	-3.855456176	-1.930138426	-2.402353128
	C42	-3.357385625	-3.307386729	-2.884961427
	C43	-3.097601824	-3.449933822	-4.384325261
	C44	-5.925079735	1.981770518	-1.812783173
	C45	-7.059025591	2.245227493	-0.814907552
	C46	-5.968885080	2.958381512	-2.996843948
	C47	-9.309505912	1.626362571	-0.071413416
	C48	-9.004097929	1.181250736	1.364189911

	C49	-7.450479432	0.058389521	2.886524873
	C50	-6.249420020	0.825752077	3.447668103
	C51	-4.536301723	2.551046175	3.129625335
	C52	-4.956402904	3.617081189	4.152680094
	C53	-3.842611829	3.301251577	1.981502444
	C54	-3.226440850	2.410170500	0.957062826
	C55	-2.959696652	1.056801035	0.918876291
	C56	-2.275726379	1.827890680	-0.966213292
	C57	-6.591775165	5.389266713	4.591587407
	C58	-6.505566211	5.139628228	6.095293799
	C59	-8.058913202	5.657329352	4.173630802
	C60	-8.601170840	7.030552994	4.440145423
	C61	-8.534329239	7.827100446	5.566928851
	C62	-9.707844256	8.833782860	3.979949796
	C63	9.222505721	0.123716025	3.944286268
	C64	10.216766832	-0.927005319	3.483564731
	C65	7.816036820	-0.403271582	3.570107369
	C66	6.694173851	0.508150774	4.011036143
	C67	6.070719404	0.349523471	5.262209848
	C68	6.233698084	1.541654843	3.174965806
	C69	5.020346066	1.183320720	5.664896762
	C70	5.201595431	2.391643550	3.570039763
	C71	4.589956830	2.208451624	4.813338681
	C72	5.788850416	6.587287783	0.775488794
	C73	4.817501968	7.774045041	0.891512472
	C74	5.014368003	5.274480921	0.699487066
	C75	3.957401141	9.815291186	-0.207760344
	C76	2.486993020	9.584131681	-0.567459347
	C77	0.780549610	7.862236405	-1.143001992
	C78	0.174670794	7.165215189	0.101408629
	C79	0.820791739	6.944872505	-2.384902410
	C80	-0.460504742	6.222796854	-2.818758333
	C81	-1.535482907	7.077127225	-3.508686176
	C82	-2.960290700	8.870394141	-2.524980982
	C83	0.430150789	5.559809171	1.923864491
	C84	0.363454864	6.450438017	3.174653065
	C85	1.236110190	4.297259070	2.277354308
	C86	1.569428635	8.105519151	4.519205124
	C87	1.068125824	9.539557239	4.612338604
	C88	-0.146421329	11.352309070	3.517676130
	C89	-1.402525422	11.773017012	4.316375949
	C90	-0.236116381	11.842494136	2.068178559
	C91	-1.420019121	11.274611215	1.292590176
	C92	-3.465788163	11.058626519	5.418848611
	C93	-3.367180401	11.822978840	6.729547958
	C94	-4.239344740	9.726491582	5.631492881
	C95	-4.496081468	9.016500442	4.322922197
	C96	-5.625309694	9.335908718	3.554645516
	C97	-3.583929907	8.083232883	3.804578213
	C98	-5.826623586	8.766044446	2.296717086
	C99	-3.755956563	7.522532526	2.536583359
	C100	-4.877019154	7.877287904	1.791298814
	C101	4.271393102	-1.500278722	-9.661253109
	C102	2.847676040	-1.288813560	-9.176755001
	C103	1.424655908	-0.075866090	-7.542532891
	C104	1.025596255	1.397947019	-7.678161616
	C105	1.528360502	3.682667983	-6.919715685
	C106	2.773561139	4.560552741	-6.800075942
	C107	5.081996791	4.834139699	-6.079311006
	C108	5.658316284	5.445472834	-7.341512400
	C109	-2.465328847	-0.526730675	-9.888661315
	C110	-3.435537046	0.509935156	-9.311176606
	C111	-2.111872427	-1.581852933	-8.814791436
	C112	-1.456424977	-2.818069526	-9.455963506
	C113	-0.890588945	-3.740892417	-8.399652720
	C114	-3.717429372	2.569099792	-8.022250557
	C115	-3.100416616	3.933522130	-8.254116378
	C116	-4.177233420	2.304936191	-6.568856603
	C117	-3.014121511	1.925260236	-5.694558767
	C118	-2.193035483	2.906394628	-5.115505324
	C119	-2.656112669	0.572337103	-5.561624752
	C120	-1.013942159	2.540764512	-4.458781772
	C121	-1.478609653	0.209738582	-4.904265242
	C122	-0.642070502	1.195396949	-4.373969573
	C123	7.791471987	-5.215609067	-6.184202799
	C124	8.911145445	-5.641561271	-5.221263677
	C125	6.418510773	-5.635450474	-5.639774521
	C126	5.223467375	-5.143140894	-6.391723312
	C127	4.888658423	-5.407111470	-7.704239328
	C128	3.206177800	-4.363584207	-6.713900572

C129	9.953675533	-7.360878727	-3.864865744
C130	11.341652908	-7.029260104	-4.363970539
C131	0.255995906	-6.422044535	-2.145828023
C132	1.721380021	-6.706379436	-1.832657617
C133	2.684642309	-6.592224806	-3.053940515
C134	2.537052478	-7.843075404	-3.961297463
C135	3.600850675	-7.981107975	-5.052698441
C136	3.531061106	-9.301329039	-5.849080339
C137	4.135073873	-6.539181521	-2.540499489
C138	3.661294669	-0.294288296	-2.243371479
Fe139	3.972022946	-1.029375995	-4.136546770
Fe140	2.313003851	0.460164282	-1.013737410
Fe141	4.970825132	0.572138212	-1.049492777
Fe142	3.909861176	1.371015632	-3.272406521
Fe143	3.753291326	3.021790348	-1.284451026
Fe144	4.772787093	-1.915030952	-1.875090319
Fe145	2.243108504	-1.779798708	-2.371397228
H146	-6.690474576	-6.824983892	-2.012640880
H147	-6.754403079	-5.492625351	-2.952360200
H148	-9.985988895	-4.294163257	-0.410436483
H149	-9.067404934	-5.134093782	-2.441019990
H150	-9.057424533	-6.620583204	-1.493636721
H151	-8.129491329	-2.678101740	0.945171618
H152	-9.155702725	-5.930742149	1.866253984
H153	-9.808679766	-2.966379449	1.448886242
H154	-8.561173080	-7.228969283	3.701238951
H155	-6.500181780	-6.169442287	1.662042509
H156	-8.356418580	-5.751086193	4.665087177
H157	-3.178809645	-2.358338932	2.598187047
H158	-5.337662108	-4.037445886	1.780008712
H159	-4.222629624	-6.557031340	1.358915845
H160	-5.260325958	-1.866935855	6.798728260
H161	-6.127632683	-3.363081548	4.495358383
H162	-4.069332659	-7.169580871	3.024940967
H163	-4.879686203	-1.886011776	2.437180547
H164	-4.934492995	-5.402301374	6.074251956
H165	-6.484664426	-3.165389507	6.775567943
H166	-0.855222368	-3.960398183	2.398352432
H167	-0.859041548	-2.481309228	1.406235672
H168	0.675100365	-3.150377327	2.003763480
H169	-1.571584876	-2.005043272	3.781019326
H170	-4.194684713	-7.028832368	7.576304109
H171	-2.115988828	0.611478294	5.640280387
H172	-1.993956761	-2.778765731	8.649657025
H173	-2.035112005	0.461571934	9.998050511
H174	1.174002333	-0.761897420	3.240946668
H175	-0.151253701	-0.068309548	4.191346686
H176	9.283183895	0.178641741	5.047358384
H177	-2.977364179	1.807722414	6.620924269
H178	-2.908947147	1.735399300	9.112674387
H179	-1.199944011	1.844838115	6.547143167
H180	-1.129278192	1.739617688	9.152356895
H181	-2.885666749	-0.402279057	7.809649222
H182	0.141677131	0.010953544	7.606129283
H183	-1.717917481	-1.670979376	6.113152740
H184	-0.337828493	-0.259382904	2.432430682
H185	1.404172329	3.703294737	1.361872596
H186	0.620226568	3.705262102	2.970736978
H187	2.658646842	4.037781825	3.624915165
H188	3.176655895	2.807296281	5.999572482
H189	4.842701121	3.173987394	2.902324868
H190	6.667195659	1.665750378	2.179871257
H191	6.401961879	-0.446108407	5.935406167
H192	-1.468878508	-4.194969951	5.032237132
H193	-0.538176921	-7.179034083	4.606841889
H194	0.045202473	-7.057257950	6.281839304
H195	-2.580496635	-6.062340587	5.281411820
H196	-3.665904069	-5.756793763	8.707631059
H197	4.533840872	1.028946820	6.631609653
H198	1.200378658	-3.079485207	4.437139524
H199	-1.419994156	-2.682110713	11.363226819
H200	-1.607582897	-4.190564148	10.425642002
H201	1.027949742	-3.776926809	9.847629612
H202	10.545915206	-8.653662337	2.206653428
H203	-1.898370080	-4.424283760	-5.723606603
H204	1.062703455	-5.290815425	-3.499327178
H205	-2.215567826	-3.373772359	-10.025861618
H206	-0.663142949	-2.505973123	-10.150375748
H207	-3.020857214	-1.894947677	-8.278335959
H208	-2.432516138	3.987899838	-9.146195004

H209	-3.065472247	-1.035330902	-10.659052169
H210	-3.368210490	-1.128752858	-2.978579342
H211	-4.087191715	-4.091012310	-2.613012691
H212	-1.867571452	1.574836207	-8.462523739
H213	-4.630412672	2.584327626	-8.652717034
H214	-0.665497995	0.512844619	-9.914100912
H215	-1.473119505	-4.719831029	-4.041257395
H216	-1.447128928	-1.126580511	-8.064039799
H217	-0.844280211	-0.565238246	-11.147307953
H218	-6.786204990	-1.928924346	-3.960894815
H219	-3.523978334	-1.792676589	-1.363625961
H220	0.877735447	-2.966467813	-8.757491328
H221	-2.436456738	-3.563549511	-2.341323345
H222	-3.829684771	1.885563818	3.644332960
H223	-3.178216589	0.316588817	1.684039128
H224	-8.287260736	0.234798739	3.576353142
H225	-7.285052819	0.173293993	0.758436947
H226	-6.719295628	3.835645969	3.124773329
H227	-8.041371328	7.696123997	6.523451099
H228	-6.744949407	4.088692405	6.388103131
H229	-8.703379012	4.885475525	4.630726516
H230	-5.958586886	6.254836247	4.338052334
H231	-10.307137308	9.597782531	3.490243491
H232	-3.079752938	3.951889679	2.442233051
H233	-4.579998871	3.966780592	1.500846171
H234	-9.379311851	9.769562205	5.864439909
H235	-8.121914811	5.507452750	3.084330777
H236	-6.039627053	1.951399501	1.714598389
H237	-7.217990711	-1.015855656	2.938405408
H238	-9.674772606	2.659631482	0.004251676
H239	-1.850059020	1.927809800	-1.961868206
H240	-10.134912327	1.010264913	-0.452856107
H241	10.347210868	1.813230584	3.676407894
H242	8.751375828	2.044150032	3.413029508
H243	1.853656163	5.933463309	0.341293497
H244	-0.606508887	5.256596849	1.716181592
H245	2.084679807	7.407939226	2.589703169
H246	-2.911915068	3.858777154	-0.589254399
H247	-4.631130099	5.097474785	-1.599365181
H248	-6.128343143	4.891905493	-3.264556174
H249	-4.344770866	6.022693011	-0.349690903
H250	-5.114893289	2.737669118	-3.658632729
H251	-6.905049609	2.811497579	-3.559401478
H252	0.717946721	11.655989541	1.555932012
H253	-0.381546018	12.933539382	2.108200870
H254	-0.175737618	10.757174442	-0.284907342
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	C89	-1.411691344	11.773820403	4.306710606
	C90	-0.241743200	11.843642319	2.061338876
	C91	-1.423290365	11.274016081	1.284060400
	C92	-3.470585359	11.057441755	5.415362299
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	C98	-5.832351153	8.761050011	2.295727081
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	C102	2.847707818	-1.291445855	-9.183989272
	C103	1.424804756	-0.080724036	-7.547143630
	C104	1.027893641	1.393947582	-7.680143341
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	C108	5.666035018	5.444403922	-7.343833693
	C109	-2.477703751	-0.527565923	-9.888611728
	C110	-3.449169648	0.506076854	-9.307592056
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	C112	-1.460497717	-2.816908472	-9.455595974
	C113	-0.890030726	-3.736987021	-8.399016386
	C114	-3.734626210	2.563208282	-8.016200863
	C115	-3.123403873	3.930164360	-8.250261168
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	C118	-2.205402309	2.929673066	-5.123408269
	C119	-2.643341441	0.587760230	-5.559628075
	C120	-1.013374211	2.580247714	-4.481426614

	C121	-1.452970387	0.241940424	-4.916818757
	C122	-0.623198148	1.240047712	-4.399528156
	C123	7.783712160	-5.206511827	-6.175696060
	C124	8.902205232	-5.633689906	-5.210842766
	C125	6.409449143	-5.635720286	-5.641508039
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	C131	0.249436823	-6.440241773	-2.150582725
	C132	1.715373207	-6.717801613	-1.834834389
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	C137	4.127345657	-6.537121466	-2.544728924
	C138	3.660127086	-0.289387304	-2.252493352
	Fe139	3.986252439	-1.034604345	-4.179177443
	Fe140	2.300493454	0.591904514	-1.210477998
	Fe141	4.957152016	0.549513758	-0.984836507
	Fe142	3.920453688	1.372495302	-3.254270097
	Fe143	3.727142543	3.015127861	-1.263012088
	Fe144	4.764866839	-1.922988085	-1.878249619
	Fe145	2.277396950	-1.740782345	-2.401878875
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	H147	-6.766114556	-5.493854976	-2.957609162
	H148	-9.984618812	-4.281118208	-0.404559474
	H149	-9.075173672	-5.123534348	-2.441050158
	H150	-9.070942656	-6.609360134	-1.493475504
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	H153	-9.792992832	-2.948727974	1.450091856
	H154	-8.552589200	-7.216840589	3.703118300
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	H165	-6.468328950	-3.147866021	6.772236791
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	H167	-0.878068605	-2.518746686	1.404757052
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	H175	-0.145701226	-0.098925075	4.211485967
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	H188	3.180312243	2.824939096	6.014086694
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	H194	0.058089882	-7.075888555	6.275520559
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	H196	-3.649287097	-5.740524434	8.697390196
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Fe2NH3 to core **S=0, 47** **product** Fe(139) 2.490 Fe(140) -2.012 Fe(141) 2.769 Fe(142) -2.407 Fe(143) 2.799 Fe(144) -2.252 Fe(145) -1.663	96518262nh3dtgb.car_5 C1 -8.036631538 -4.989549992 -0.543379763 C2 -8.398895099 -5.771627046 -1.811004011 C3 -8.870157961 -3.467687991 1.200168688 C4 -8.352862822 -4.158461565 2.458044884 C5 -8.107772714 -6.246134413 3.710179624 C6 -6.584231995 -6.411519534 3.712627057 C7 -4.511273342 -6.377995782 2.417821521 C8 -3.924957863 -5.042722025 2.888700079 C9 -4.208051482 -2.611449596 2.925978449 C10 -4.282083458 -2.477297436 4.452959483 C11 -5.480180071 -2.920980372 6.505259218 C12 -4.514007186 -3.812589124 7.300471356 C13 -3.675006363 -6.089341710 7.659238509 C14 -2.200564081 -6.340268995 7.307252133 C15 -0.521473541 -6.482496685 5.505631525 C16 0.274354770 -5.226497906 5.130225056 C17 0.168087131 -2.800149472 4.681684513 C18 0.327212884 -1.958628334 5.964807565 C19 -0.525489480 -2.076561565 3.511376195 C20 0.067019224 -0.677605719 3.304286407 C21 -0.444459737 -2.937817357 2.243775919 C22 -0.747655582 -0.613032750 7.710643815 C23 -0.467810832 -1.406793703 8.998617825 C24 -2.014816939 0.271464076 7.802676918 C25 -2.031683962 1.091915535 9.097425593 C26 -2.103130930 1.196780600 6.582224740 C27 -1.036533131 -3.266645349 10.441852959 C28 0.410373449 -3.614678126 10.725666656 C29 4.898076275 -12.594289333 0.341005200 C30 5.687967113 -11.296824582 0.241491701 C31 6.184094531 -9.197793272 1.461054191 C32 7.405587517 -9.150290554 2.394901201

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C41	-3.846277016	-1.922134178	-2.403626733
C42	-3.348891081	-3.299389907	-2.886490020
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H147	-6.727010129	-5.487493688	-2.948705234
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H150	-9.026755455	-6.621553417	-1.492148016
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H153	-9.825706223	-2.983878785	1.443693791
H154	-8.570894018	-7.241278060	3.694732286
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	H219	-3.512856251	-1.783142010	-1.365863931
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	H240	-10.128929521	1.035821003	-0.453253405
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	H255	-1.904214582	10.400187768	-0.450792508
	H256	-2.899062392	10.749256856	-3.354643603
	H257	-2.088268950	6.464371332	-4.257419437
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	H264	-8.206912962	0.850661678	-1.738377115
	H265	4.357181534	10.521295125	-0.921460588
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Fe6NH3 to core **S=1, 35** **reactant** Fe(139) -2.370 Fe(140) -2.202 Fe(141) -2.276 Fe(142) 2.758 Fe(143) 2.960 Fe(144) 2.268 Fe(145) 0.890	9651826nh3d35tb.car_4 C1 -8.030443159 -4.997428818 -0.547480714 C2 -8.393293582 -5.779550208 -1.814805208 C3 -8.863113413 -3.473724241 1.194904603 C4 -8.346529619 -4.165146964 2.452863645 C5 -8.106799801 -6.252969690 3.706127174 C6 -6.583574203 -6.420393055 3.705951176 C7 -4.514253334 -6.392639562 2.405881971 C8 -3.925818601 -5.058741579 2.877193170 C9 -4.201057368 -2.626896187 2.914057574 C10 -4.266110620 -2.497012369 4.441580777 C11 -5.469954789 -2.923013532 6.495735580 C12 -4.509803829 -3.817861223 7.294179505 C13 -3.684887397 -6.098399373 7.662056792 C14 -2.212633136 -6.354709761 7.307883731 C15 -0.541811784 -6.514695679 5.503760728 C16 0.250915065 -5.255360062 5.139262497 C17 0.163751922 -2.830557197 4.719845554 C18 0.317709164 -1.975872170 5.994802436 C19 -0.473360777 -2.101629594 3.518788295 C20 0.189169896 -0.740186548 3.283249645 C21 -0.401462632 -2.988597775 2.271335624 C22 -0.758296151 -0.628284812 7.735848098 C23 -0.485448958 -1.415311493 9.030337030 C24 -2.019944275 0.264183907 7.814804810

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	C30	5.695224280	-11.297323760	0.240675911
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	C32	7.406076581	-9.156079597	2.394017064
	C33	5.088804713	-8.239635469	1.963397864
	C34	5.548265990	-6.786754800	1.928421309
	C35	4.432749465	-5.798553299	2.246724835
	C36	4.973535140	-3.439201054	2.895581665
	C37	9.665855237	-8.267282763	2.707321046
	C38	9.897577302	-6.828408551	3.112561855
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	C40	-5.726573030	-0.492537333	-1.615453230
	C41	-3.832348251	-1.931484884	-2.407249562
	C42	-3.334702757	-3.313159964	-2.878686925
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	C45	-7.043165738	2.241636298	-0.821057065
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	C47	-9.296461518	1.633412296	-0.079149928
	C48	-8.995057144	1.184348789	1.355946297
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	C53	-3.840659815	3.294865293	1.994149221
	C54	-3.226220913	2.399739047	0.972375202
	C55	-2.966340314	1.045249747	0.938091501
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	C59	-8.057863071	5.661244512	4.183860365
	C60	-8.599420553	7.034933820	4.449490103
	C61	-8.541179582	7.827845941	5.579186409
	C62	-9.696202404	8.843037987	3.984186556
	C63	9.253629972	0.161340468	3.943898805
	C64	10.252499607	-0.887203211	3.489299302
	C65	7.857795980	-0.381401028	3.557578364
	C66	6.718156033	0.514842589	3.984734377
	C67	6.101440187	0.367917401	5.240261717
	C68	6.226336647	1.513311851	3.123971328
	C69	5.028934778	1.181286063	5.625035458
	C70	5.167436877	2.340642029	3.498107153
	C71	4.566817624	2.172022965	4.749230677
	C72	5.786016990	6.613174445	0.788189461
	C73	4.818990434	7.803025199	0.909118934
	C74	4.996085570	5.311979368	0.659371539
	C75	3.941937146	9.831408935	-0.199656714
	C76	2.474613185	9.595325288	-0.568454197
	C77	0.772911249	7.875916251	-1.160659100
	C78	0.163138926	7.172434582	0.077257764
	C79	0.816441823	6.962075164	-2.405145064
	C80	-0.460186448	6.230167589	-2.836947466
	C81	-1.545441414	7.074812604	-3.521895439
	C82	-2.968207087	8.869131368	-2.536934277
	C83	0.408744702	5.563714307	1.895643758
	C84	0.342877320	6.450828273	3.149462349
	C85	1.202751442	4.295072764	2.248378312
	C86	1.550797407	8.097457841	4.504149145
	C87	1.059001349	9.534559754	4.608257618
	C88	-0.149230350	11.364134483	3.529354920
	C89	-1.403114807	11.783868685	4.331410783
	C90	-0.240284805	11.857662280	2.080497533
	C91	-1.423888144	11.286510329	1.306063722
	C92	-3.470428077	11.065986331	5.425080524
	C93	-3.370661284	11.825274280	6.738672545
	C94	-4.242145568	9.732248088	5.634724471
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	C102	2.849383224	-1.306922122	-9.153716155
	C103	1.434793118	-0.123132078	-7.484726517
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H173	-2.051252130	0.466397663	10.005214195
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	H188	3.143180236	2.754969937	5.928895157
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	H190	6.658992532	1.628320279	2.127480782
	H191	6.450969564	-0.406770461	5.928172284
	H192	-1.485282365	-4.163188131	5.045196007
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	H199	-1.446371058	-2.701560878	11.355432412
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	H207	-3.006827238	-1.901551644	-8.276011372
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	H257	-2.082769340	6.459068788	-4.260066037
	H258	-6.709744926	9.025733096	1.709504718
	H259	-2.722712864	7.768436013	4.401586556
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	H263	-0.899624158	5.663992522	-2.000567716
	H264	-8.203584968	0.838420491	-1.747352820

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	H266	-5.822193193	0.432241803	-3.373696837
	H267	1.187416231	7.572065708	-3.245511743
	H268	-3.008741634	6.844421249	2.134105902
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	H271	-4.357424510	10.060165257	-1.630921437
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	H278	-0.140696169	5.476753950	-3.571384496
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	H286	4.724080402	-2.249626564	-8.960521358
	H287	7.831249449	-4.117979409	-6.244350596
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	H293	4.377989760	5.152394854	1.553304760
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	H328	2.948370416	-4.805509570	-8.558712766
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N402	2.136122539	8.333428576	-0.900271571
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O424	-2.936282457	-4.998596116	3.629844427

	O425	-3.370078534	-1.920478844	5.076257234
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	O427	-1.406784163	-6.651147312	8.202067912
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	O431	0.833630096	-3.825972475	11.878399655
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	O434	10.988634035	-6.386444240	3.437727035
	O435	-5.831338110	-0.520420787	-0.374927346
	O436	-3.771893491	-2.887570914	-5.242796918
	O437	-6.896355006	3.047910159	0.113395350
	O438	-5.881733212	4.307868549	-2.522046636
	O439	-9.768839294	1.517504275	2.266126685
	O440	-5.844668467	0.551318984	4.584221462
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	O442	-6.257862084	6.016135321	6.925001531
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	O445	4.110682816	7.981590949	1.915620659
	O446	1.684515941	10.561323732	-0.549453833
	O447	-0.986105774	7.457301363	0.451147901
	O448	-0.501900505	6.232391635	4.026653434
	O449	2.456361464	4.638236342	2.847171646
	O450	1.408870609	10.253973177	5.552076532
	O451	-1.665262349	12.984591564	4.497277060
	O452	-2.559619311	11.232258053	1.800924672
	O453	-4.311489229	12.432334905	7.227118407
	O454	-5.002068618	7.350094180	0.498958112
	O455	1.911203701	-1.996690522	-9.623929654
	O456	0.160593685	1.719164130	-8.434648003
	O457	2.696180439	5.724301604	-7.083039030
	O458	6.405906206	6.405027782	-7.376471883
	O459	-4.630946117	0.406885902	-9.492895889
	O460	-1.551224763	-4.540087931	-7.732970209
	O461	0.450147386	-3.637768373	-8.136890638
	O462	-3.299507136	4.916691209	-7.582024135
	O463	9.807562919	-4.853107707	-4.918764017
	O464	12.308041248	-6.923197867	-3.647335123
	O465	0.060898358	-5.469535832	-2.963719723
	O466	-0.659517638	-7.022458392	-1.503603132
	O467	4.603361410	-9.826977815	-6.106413726
	O468	2.348096254	-9.671095457	-6.160118122
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	O470	4.598750669	-7.517909466	-1.861867832
	O471	2.374215718	-5.329001834	-3.626412632
	O472	8.487202365	-7.210547167	-0.625038832
	O473	6.711147430	-4.956530512	-0.751810741
	O474	-3.908552976	5.577878972	-1.107397046
	O475	7.190478433	-9.818080336	-5.155475438
	O476	6.979837222	-8.765769486	-2.340986210
	S477	3.876121906	5.314431518	-0.815674200
	S478	2.272214548	2.709315875	-2.917909555
	S479	1.957673197	-2.233324431	-4.001538089
	S480	3.308550632	1.624060623	0.340747940
	S481	0.568722798	-0.362111229	-1.630217212
	S482	4.310657984	0.630212223	-5.432394036
	S483	3.631994594	-3.466927672	-1.131645910
	S484	5.810444372	2.294650482	-2.188403110
	S485	5.698484921	-2.365073800	-3.877318329
	S486	6.271318184	-0.941001512	-0.318915207
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Fe6NH3 to core **S=1, 35** **TS** Fe(139) -2.353 Fe(140) -2.337 Fe(141) -2.434 Fe(142) 2.758 Fe(143) 2.984 Fe(144) 2.239 Fe(145) 1.179	9651826nh3d35td_1_53010.00			
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	C3	-8.856194088	-3.465385806	1.194316303
	C4	-8.337858946	-4.156742563	2.451218460
	C5	-8.098747413	-6.242449599	3.707509657
	C6	-6.575575360	-6.410700496	3.704113437
	C7	-4.508688028	-6.387115580	2.400706663
	C8	-3.919576888	-5.053902481	2.873703898
	C9	-4.196872710	-2.619803448	2.902864121
	C10	-4.261588891	-2.484557047	4.430122458
	C11	-5.457083345	-2.910220266	6.487516391
	C12	-4.494660585	-3.802247175	7.286289155
	C13	-3.664670651	-6.081142668	7.654201395
	C14	-2.193705358	-6.344124742	7.299214891
	C15	-0.526559694	-6.534943151	5.495899334
	C16	0.268335323	-5.274925314	5.137193075

	C17	0.170768198	-2.849500153	4.707945184
	C18	0.327130935	-1.995313842	5.983484740
	C19	-0.491885168	-2.128439794	3.517943558
	C20	0.132568816	-0.746892760	3.297848620
	C21	-0.419570241	-3.011412836	2.266907939
	C22	-0.742235188	-0.637083121	7.720860126
	C23	-0.466538137	-1.418810631	9.017316065
	C24	-2.003333670	0.256844440	7.801781039
	C25	-2.020077765	1.086476568	9.090238561
	C26	-2.079368957	1.174226014	6.574365170
	C27	-1.040204460	-3.255524983	10.486938885
	C28	0.404854798	-3.629348469	10.751476401
	C29	4.919798493	-12.594538133	0.350954265
	C30	5.694956189	-11.287202734	0.248332324
	C31	6.171614767	-9.178137551	1.462296780
	C32	7.391575390	-9.141033255	2.398747676
	C33	5.074593208	-8.226271071	1.968981288
	C34	5.528755805	-6.771572609	1.931049774
	C35	4.414284610	-5.791677487	2.279860579
	C36	4.990720879	-3.434172018	2.902780597
	C37	9.653793388	-8.261639721	2.711926516
	C38	9.895591450	-6.824210758	3.115438239
	C39	-5.368508406	-1.726472983	-2.461993690
	C40	-5.734667330	-0.493372381	-1.616621302
	C41	-3.840892722	-1.934593978	-2.408364193
	C42	-3.346786003	-3.315827865	-2.884717288
	C43	-3.086007967	-3.465047340	-4.383192018
	C44	-5.923406282	1.975185115	-1.818846744
	C45	-7.057641520	2.237984377	-0.821229541
	C46	-5.967473465	2.951518019	-3.003042429
	C47	-9.308313890	1.621294451	-0.077648208
	C48	-9.003636913	1.175465640	1.357870419
	C49	-7.450756817	0.051192111	2.880044953
	C50	-6.249724764	0.818149015	3.441610201
	C51	-4.539295069	2.546113859	3.125475461
	C52	-4.958723033	3.612700016	4.148405787
	C53	-3.845505311	3.295000294	1.976719521
	C54	-3.232429935	2.402986311	0.951092728
	C55	-2.971781487	1.048632046	0.910231418
	C56	-2.279880338	1.822354554	-0.971767376
	C57	-6.592712199	5.385698912	4.587133991
	C58	-6.506971445	5.135672769	6.090812691
	C59	-8.060841825	5.653426275	4.171444946
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	C61	-8.537559584	7.823438665	5.563949253
	C62	-9.708815333	8.830035894	3.975292221
	C63	9.232551480	0.131230821	3.944591205
	C64	10.224968042	-0.924373021	3.488890639
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	C66	6.698521376	0.505819828	3.993251522
	C67	6.081274460	0.356300341	5.248482527
	C68	6.218842076	1.517876234	3.141514633
	C69	5.020653435	1.181348753	5.641889462
	C70	5.173223644	2.357116104	3.525261447
	C71	4.571650631	2.186232495	4.775684497
	C72	5.793925144	6.603758261	0.780540442
	C73	4.830646040	7.795846063	0.904070067
	C74	4.999940993	5.303993959	0.650262350
	C75	3.956388592	9.825763794	-0.203907324
	C76	2.486812439	9.592440271	-0.566623741
	C77	0.779932740	7.875912892	-1.150517892
	C78	0.173467115	7.173848706	0.090113401
	C79	0.818764298	6.959356255	-2.393665155
	C80	-0.460913012	6.232310229	-2.824752265
	C81	-1.541175290	7.079260825	-3.515123218
	C82	-2.969267186	8.872386998	-2.533339428
	C83	0.425271225	5.567660072	1.910526287
	C84	0.358975311	6.457431119	3.162336526
	C85	1.224194508	4.302240508	2.265063961
	C86	1.565054968	8.109432258	4.511747047
	C87	1.063437909	9.543592678	4.609858384
	C88	-0.152669675	11.361286959	3.520420382
	C89	-1.410125420	11.780266647	4.316749709
	C90	-0.239754675	11.848386447	2.069388393
	C91	-1.420467463	11.274754272	1.292559542
	C92	-3.473534976	11.062354457	5.418420410
	C93	-3.374665160	11.823086375	6.730905867
	C94	-4.243431282	9.727372896	5.628446590
	C95	-4.498565642	9.017648582	4.319220556
	C96	-5.626995659	9.336743984	3.549770171

	C97	-3.586505923	8.083553937	3.802183125
	C98	-5.827544362	8.765880972	2.292253243
	C99	-3.757782029	7.521407523	2.534758320
	C100	-4.878090600	7.876043791	1.788351756
	C101	4.271161155	-1.505862885	-9.660740131
	C102	2.847965951	-1.305310660	-9.169678403
	C103	1.432660952	-0.116978803	-7.506632253
	C104	1.038005632	1.358545422	-7.643897510
	C105	1.547440794	3.645460234	-6.905517955
	C106	2.791220586	4.525999782	-6.807413620
	C107	5.097527333	4.834137843	-6.103620329
	C108	5.659680817	5.447666498	-7.369947529
	C109	-2.454136813	-0.538041231	-9.889216248
	C110	-3.425630157	0.499698320	-9.315599175
	C111	-2.104815591	-1.593133297	-8.814286265
	C112	-1.448316106	-2.831274369	-9.451853994
	C113	-0.877010860	-3.748483670	-8.393224891
	C114	-3.714389839	2.556958181	-8.027463949
	C115	-3.094788787	3.920755939	-8.255382212
	C116	-4.191954276	2.294637886	-6.579847308
	C117	-3.032879945	1.929156079	-5.695243819
	C118	-2.224223113	2.922131430	-5.119077265
	C119	-2.656648272	0.581274320	-5.563219725
	C120	-1.034891642	2.573423384	-4.472992923
	C121	-1.467753894	0.235592165	-4.916770867
	C122	-0.640953066	1.234177094	-4.394651252
	C123	7.769775593	-5.208285106	-6.183467518
	C124	8.903672361	-5.638472542	-5.237943989
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	C132	1.729477190	-6.715421116	-1.777490121
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	C137	4.137152189	-6.549742609	-2.509931967
	C138	3.673461372	-0.276792521	-2.245637887
	Fe139	3.896945708	-1.079354692	-4.071547979
	Fe140	2.282035416	0.891708659	-1.564357340
	Fe141	4.867889181	0.661258941	-0.985761775
	Fe142	4.074199359	1.370025977	-3.375061762
	Fe143	3.816316713	3.067384650	-1.295600920
	Fe144	4.900199785	-1.820106422	-1.815409694
	Fe145	2.329688227	-1.701700073	-2.002915634
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	H147	-6.745001579	-5.502275379	-2.963279808
	H148	-9.972924238	-4.303994445	-0.418178192
	H149	-9.056614858	-5.139999296	-2.445864909
	H150	-9.043588226	-6.621189887	-1.492632939
	H151	-8.128418411	-2.678867280	0.945998794
	H152	-9.156281401	-5.936787362	1.859049925
	H153	-9.808415612	-2.976587420	1.440963770
	H154	-8.564127523	-7.236617631	3.694202533
	H155	-6.501269678	-6.176289347	1.657818168
	H156	-8.359514519	-5.758844299	4.658431440
	H157	-3.175414209	-2.366793382	2.596771824
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	H161	-6.128037454	-3.368016180	4.490494963
	H162	-4.071579181	-7.179897708	3.019167436
	H163	-4.876678060	-1.894969046	2.435743383
	H164	-4.941214368	-5.410495371	6.071815299
	H165	-6.486375312	-3.171711992	6.770125685
	H166	-0.949058595	-3.961619522	2.419749682
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	H168	0.622831869	-3.255298078	2.012302277
	H169	-1.549003066	-1.972777625	3.778665268
	H170	-4.198556266	-7.040534541	7.568531235
	H171	-2.115080572	0.607830653	5.634094727
	H172	-1.997139994	-2.782584755	8.639852421
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	H184	-0.319471667	-0.264227314	2.418462504
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	O473	6.697547010	-4.958468797	-0.752414047
	O474	-3.915414519	5.576227514	-1.117090369
	O475	7.193491025	-9.819951060	-5.156637187
	O476	6.979330448	-8.765227685	-2.344623741
	S477	3.875389969	5.320565216	-0.822287446
	S478	2.239468884	2.675627454	-2.910654097
	S479	1.982858522	-2.236894311	-4.152870373
	S480	3.302716296	1.651640790	0.344624689
	S481	0.556314636	-0.448083207	-1.575937789
	S482	4.318464357	0.616111482	-5.441654467
	S483	3.479797436	-3.419517393	-1.161750940
	S484	5.784358176	2.297269833	-2.187357009
	S485	5.703247629	-2.390645337	-3.825647005
	S486	6.262994103	-0.946641702	-0.326538360
	end			
Fe6NH3 to core **S=1, 35** **product** Fe(139) -2.427 Fe(140) -2.397 Fe(141) -2.442	9651826nh3d35ta.car_5			
	C1	-8.023712003	-4.998468265	-0.548953040
	C2	-8.377521294	-5.780760063	-1.818330844
	C3	-8.867818547	-3.480010380	1.191691116
	C4	-8.354096530	-4.171526771	2.450727535
	C5	-8.112335892	-6.261063322	3.701313618
	C6	-6.588917838	-6.427638439	3.704966251
	C7	-4.515573021	-6.394101304	2.410534894
	C8	-3.930388931	-5.059054712	2.882371348

Fe(142) 2.825	C9	-4.209229559	-2.628566856	2.923102915
Fe(143) 2.942	C10	-4.279629176	-2.499567665	4.450481695
Fe(144) 1.808	C11	-5.484216712	-2.934964855	6.501889552
Fe(145) 1.636	C12	-4.521238001	-3.829670472	7.297344885
	C13	-3.690297727	-6.108467652	7.659326796
	C14	-2.215376991	-6.355113146	7.307301217
	C15	-0.536788821	-6.486261137	5.505382144
	C16	0.255778858	-5.229744375	5.127423581
	C17	0.165076550	-2.804031954	4.688667272
	C18	0.322711424	-1.958147663	5.968972330
	C19	-0.509355436	-2.069292332	3.513344053
	C20	0.097999071	-0.675651961	3.307650899
	C21	-0.454911512	-2.935778944	2.247091034
	C22	-0.755564033	-0.619787486	7.718823092
	C23	-0.479955434	-1.414328020	9.007141908
	C24	-2.022719477	0.265283194	7.805625508
	C25	-2.040808328	1.089242306	9.097801164
	C26	-2.108791233	1.187756152	6.582803802
	C27	-1.050916078	-3.273703164	10.447571024
	C28	0.395567413	-3.623910091	10.730569488
	C29	4.891658365	-12.589245145	0.320414428
	C30	5.688184570	-11.296166818	0.225919298
	C31	6.190988985	-9.201557017	1.450698157
	C32	7.413374178	-9.157545135	2.383852456
	C33	5.091209615	-8.252319345	1.955462526
	C34	5.548519741	-6.800178023	1.920405285
	C35	4.427237433	-5.808613999	2.204817818
	C36	4.973365470	-3.464440193	2.878519770
	C37	9.665213514	-8.243830139	2.691475059
	C38	9.889507008	-6.806280225	3.103192621
	C39	-5.362039449	-1.727041378	-2.457917647
	C40	-5.723496708	-0.490497620	-1.615705941
	C41	-3.835254220	-1.932186641	-2.406187155
	C42	-3.333416405	-3.311054962	-2.878944190
	C43	-3.080262956	-3.465146059	-4.378527940
	C44	-5.901226512	1.977481207	-1.822488938
	C45	-7.033147682	2.244935634	-0.823657442
	C46	-5.944054820	2.952593424	-3.007430037
	C47	-9.288077475	1.642193306	-0.082260296
	C48	-8.989343081	1.190861156	1.352636091
	C49	-7.448853651	0.047347792	2.873277831
	C50	-6.249864871	0.810452901	3.444680132
	C51	-4.536537675	2.538738523	3.144511046
	C52	-4.956059077	3.606215065	4.164480332
	C53	-3.834129305	3.287286685	2.001161583
	C54	-3.211979883	2.393607396	0.983530609
	C55	-2.933206400	1.042735553	0.955725664
	C56	-2.257005966	1.806565660	-0.934978937
	C57	-6.569901838	5.398040051	4.583757207
	C58	-6.470957316	5.163458410	6.089245861
	C59	-8.044024317	5.664713071	4.183440456
	C60	-8.586099162	7.038066711	4.451260148
	C61	-8.535810214	7.826264839	5.584652299
	C62	-9.681296563	8.847809569	3.986777095
	C63	9.250037501	0.175983770	3.904572237
	C64	10.263770075	-0.863479934	3.460081998
	C65	7.859213616	-0.371599512	3.528032781
	C66	6.712959696	0.515229685	3.959491952
	C67	6.106706382	0.373922604	5.221300623
	C68	6.219470844	1.516961116	3.103577588
	C69	5.031376564	1.182352614	5.607466849
	C70	5.156168914	2.336961891	3.479916700
	C71	4.556780497	2.164670070	4.730414581
	C72	5.774207601	6.606330514	0.786707794
	C73	4.804027038	7.792720275	0.902297223
	C74	4.986128908	5.296970294	0.668821708
	C75	3.931990509	9.830145150	-0.199558218
	C76	2.464560151	9.596001107	-0.571914172
	C77	0.762553659	7.876110848	-1.169488608
	C78	0.153548627	7.169999435	0.067791020
	C79	0.809704200	6.964607957	-2.416025018
	C80	-0.466372234	6.232298050	-2.848373021
	C81	-1.553896522	7.078119100	-3.528735360
	C82	-2.975135657	8.874099627	-2.541186344
	C83	0.393160123	5.559440730	1.886378347
	C84	0.330291012	6.444077878	3.141815460
	C85	1.184232245	4.287065121	2.235712860
	C86	1.545658012	8.081719510	4.499529435
	C87	1.061346819	9.520693838	4.603312057
	C88	-0.140652692	11.355833383	3.527794314

	C89	-1.390476825	11.772871410	4.337081336
	C90	-0.238013259	11.856727083	2.081611861
	C91	-1.425884665	11.291326420	1.309610978
	C92	-3.459293653	11.056300174	5.422517096
	C93	-3.358731614	11.819046173	6.734023584
	C94	-4.236806502	9.727045770	5.635774179
	C95	-4.494266016	9.018284852	4.326986168
	C96	-5.618933603	9.344526371	3.555050776
	C97	-3.584769139	8.081388759	3.810853729
	C98	-5.818328506	8.777423599	2.295837122
	C99	-3.755006643	7.523430839	2.541429429
	C100	-4.871605676	7.884408765	1.792681515
	C101	4.273199246	-1.503891712	-9.686624141
	C102	2.857939941	-1.301411934	-9.174391511
	C103	1.458443506	-0.115038329	-7.500647017
	C104	1.053890792	1.357118023	-7.634645766
	C105	1.541778980	3.646559570	-6.878688419
	C106	2.782044754	4.532580104	-6.790548286
	C107	5.104100423	4.835110023	-6.141268809
	C108	5.649309803	5.462641053	-7.406738736
	C109	-2.447561565	-0.536325943	-9.916615636
	C110	-3.419071554	0.507083595	-9.351084842
	C111	-2.106638546	-1.587654001	-8.833963480
	C112	-1.449371483	-2.831354837	-9.459961989
	C113	-0.882439957	-3.742093543	-8.392666212
	C114	-3.702391808	2.568612087	-8.061453069
	C115	-3.071210266	3.929442714	-8.281538921
	C116	-4.167185539	2.300539104	-6.610431107
	C117	-3.016267547	1.910715335	-5.723375327
	C118	-2.209258219	2.886351263	-5.115537050
	C119	-2.665754815	0.557038488	-5.583477165
	C120	-1.054902377	2.516491763	-4.420349510
	C121	-1.510732322	0.188226124	-4.889292485
	C122	-0.689473867	1.168963377	-4.326124858
	C123	7.770631687	-5.228044368	-6.196063363
	C124	8.904886298	-5.650669955	-5.249037121
	C125	6.404820290	-5.621330475	-5.612765930
	C126	5.203473121	-5.119570708	-6.346542351
	C127	4.856915846	-5.354530844	-7.662171848
	C128	3.180097044	-4.342451028	-6.630682713
	C129	9.947191275	-7.358428777	-3.880775797
	C130	11.336148432	-7.039478901	-4.386340646
	C131	0.247646833	-6.417568317	-2.070279205
	C132	1.718904056	-6.677422145	-1.758916832
	C133	2.669518411	-6.542364926	-2.988096436
	C134	2.510972452	-7.780634338	-3.914971870
	C135	3.573555110	-7.923385294	-5.008040820
	C136	3.495988812	-9.245522610	-5.803353035
	C137	4.121124154	-6.495081260	-2.484450372
	C138	3.679008210	-0.267359099	-2.272480629
	Fe139	3.997205577	-1.042103353	-4.171255024
	Fe140	2.281118966	0.829342008	-1.477956166
	Fe141	4.881297134	0.619325689	-0.977373133
	Fe142	4.063622370	1.398570270	-3.351871985
	Fe143	3.810823993	3.007069135	-1.180075968
	Fe144	4.819505796	-1.814649080	-1.855461501
	Fe145	2.298101858	-1.633184498	-2.333708731
	H146	-6.633307785	-6.820343995	-2.005219692
	H147	-6.702160087	-5.492723212	-2.951588955
	H148	-9.964099886	-4.322313973	-0.433860191
	H149	-9.022063841	-5.151672799	-2.453649294
	H150	-9.003133886	-6.632695058	-1.500216322
	H151	-8.144057408	-2.687048158	0.951876461
	H152	-9.156502710	-5.953981445	1.845841943
	H153	-9.825620544	-2.999180390	1.431665410
	H154	-8.576796934	-7.255637585	3.683869742
	H155	-6.504380000	-6.179903593	1.660891252
	H156	-8.378586356	-5.779557171	4.651907694
	H157	-3.185137539	-2.379677770	2.622662749
	H158	-5.349089110	-4.047775089	1.787885518
	H159	-4.226818609	-6.573006371	1.365518481
	H160	-5.291148986	-1.900734674	6.816242609
	H161	-6.147321229	-3.381099068	4.499925253
	H162	-4.078866332	-7.184194178	3.032655101
	H163	-4.883908307	-1.899216915	2.455312645
	H164	-4.978030911	-5.438758031	6.086081977
	H165	-6.514014534	-3.200635975	6.778844882
	H166	-1.004106641	-3.877724983	2.391297538
	H167	-0.896015856	-2.401270102	1.391284027
	H168	0.578965772	-3.195967594	1.972473765

	H169	-1.565116614	-1.920253450	3.785819356
	H170	-4.216311418	-7.070540583	7.564527091
	H171	-2.148053593	0.626496910	5.639604024
	H172	-1.999529867	-2.783964491	8.603293664
	H173	-2.051403659	0.456332838	9.997079227
	H174	1.184687525	-0.715753074	3.149608954
	H175	-0.091044431	-0.020594337	4.170689814
	H176	9.304928484	0.239910923	5.011343174
	H177	-3.011523006	1.812774525	6.631009148
	H178	-2.935674768	1.728682461	9.119172379
	H179	-1.234739814	1.859103591	6.548996136
	H180	-1.155741938	1.743339393	9.153365469
	H181	-2.902077470	-0.403936507	7.806367576
	H182	0.123791504	0.033022066	7.608962755
	H183	-1.721387613	-1.651934244	6.096135735
	H184	-0.341860789	-0.202034333	2.417291266
	H185	1.337374806	3.691116406	1.318722227
	H186	0.565856855	3.701665039	2.932924641
	H187	2.621795888	3.999631131	3.560445383
	H188	3.123011852	2.735899020	5.907586831
	H189	4.764644813	3.087752341	2.794643112
	H190	6.647856186	1.638423878	2.105575333
	H191	6.462013470	-0.396701654	5.910477100
	H192	-1.480400870	-4.141355080	5.021120368
	H193	-0.559633536	-7.142473804	4.621791821
	H194	0.033063562	-6.998880594	6.290546660
	H195	-2.596715515	-6.012100115	5.297440850
	H196	-3.707311233	-5.807208973	8.713790858
	H197	4.555674698	1.035644789	6.580242677
	H198	1.197905124	-3.047638343	4.409167455
	H199	-1.456274909	-2.726934395	11.314415359
	H200	-1.601367067	-4.223264531	10.354650148
	H201	1.033368259	-3.763054579	9.827028173
	H202	10.558591338	-8.613597967	2.165387808
	H203	-1.884315443	-4.450267044	-5.714043504
	H204	1.038868463	-5.225247213	-3.377912523
	H205	-2.206046171	-3.396056114	-10.024209692
	H206	-0.654323533	-2.526979905	-10.155884949
	H207	-3.019913484	-1.895262990	-8.301685331
	H208	-2.395646085	3.982167769	-9.168148824
	H209	-3.041394360	-1.044705299	-10.693393308
	H210	-3.353978981	-1.133836970	-2.991341845
	H211	-4.055796958	-4.097521474	-2.594770026
	H212	-1.855437184	1.560213611	-8.480411157
	H213	-4.613071568	2.591854622	-8.696145164
	H214	-0.637136854	0.481918328	-9.916259584
	H215	-1.460118453	-4.733863661	-4.027090702
	H216	-1.444636741	-1.129894901	-8.081896382
	H217	-0.814713203	-0.584606505	-11.157815982
	H218	-6.768326764	-1.940567601	-3.959480954
	H219	-3.502041248	-1.786226218	-1.369358016
	H220	0.882491044	-2.957368618	-8.749064841
	H221	-2.407465755	-3.555265167	-2.338476296
	H222	-3.835658863	1.870204170	3.662468474
	H223	-3.143105527	0.307561144	1.727979427
	H224	-8.287721986	0.219146011	3.561556004
	H225	-7.277504962	0.171058418	0.746826234
	H226	-6.707159368	3.844788275	3.119483424
	H227	-8.058548813	7.688874128	6.548424561
	H228	-6.725623709	4.119615537	6.394524823
	H229	-8.682037593	4.893200212	4.649992269
	H230	-5.940792853	6.261576912	4.313806181
	H231	-10.270945686	9.617353805	3.494059350
	H232	-3.073138671	3.936885452	2.466192942
	H233	-4.566369678	3.953829578	1.514008059
	H234	-9.382932524	9.767148292	5.885040878
	H235	-8.120070476	5.511462626	3.095643965
	H236	-6.034801591	1.948331535	1.720373061
	H237	-7.216919063	-1.027314226	2.917876632
	H238	-9.642745121	2.679133674	-0.006090170
	H239	-1.836683367	1.904593162	-1.932923866
	H240	-10.118663493	1.034563263	-0.465941759
	H241	10.345762174	1.885140996	3.635417750
	H242	8.749101562	2.085573012	3.358860967
	H243	1.828467667	5.936683293	0.312176124
	H244	-0.645663264	5.267213618	1.673849595
	H245	2.054418492	7.399860649	2.563154079
	H246	-2.901240199	3.834547205	-0.573528221
	H247	-4.621468155	5.097685231	-1.594788252
	H248	-6.100557375	4.885976070	-3.276767682

	H249	-4.341340064	6.026533223	-0.346114751
	H250	-5.089324059	2.731265366	-3.668065913
	H251	-6.879628849	2.804333012	-3.570657640
	H252	0.713789800	11.672556490	1.564163154
	H253	-0.382545670	12.947579981	2.128565884
	H254	-0.186064729	10.755873739	-0.267532487
	H255	-1.904027906	10.394835475	-0.435220836
	H256	-2.900484320	10.754140599	-3.363544955
	H257	-2.094311547	6.462679163	-4.265030767
	H258	-6.704336770	9.032894303	1.709340157
	H259	-2.723696459	7.758629042	4.402887953
	H260	-3.992123445	8.614133019	-0.771089287
	H261	1.578599230	6.197519362	-2.233754359
	H262	2.860748664	7.618252034	-0.905498527
	H263	-0.902415907	5.664860755	-2.011120027
	H264	-8.197322349	0.844743422	-1.750635998
	H265	4.348955310	10.545978932	-0.920626179
	H266	-5.821504834	0.430052860	-3.375935389
	H267	1.180871608	7.575868903	-3.255665641
	H268	-3.009162458	6.842315436	2.131948571
	H269	3.924167912	10.316996693	0.786471094
	H270	-2.257249951	9.497295528	-4.372627469
	H271	-4.361146776	10.065864221	-1.631456162
	H272	-5.183047274	-2.033469340	-4.484690722
	H273	-5.841925955	-2.581856639	-1.942872589
	H274	-6.356117041	10.051466731	3.941831009
	H275	-4.972377458	2.141598008	-1.254921425
	H276	0.136621421	8.755938428	-1.346745456
	H277	-1.080348328	7.899786593	-4.081967647
	H278	-0.148153424	5.480566524	-3.585288937
	H279	-2.998411419	6.921098260	-1.961750483
	H280	1.062194545	7.513206975	5.307789913
	H281	0.061214847	9.324919094	2.826386080
	H282	0.675802143	11.913202895	4.012065641
	H283	2.627513814	8.092331151	4.691365880
	H284	-1.937603633	9.831241766	4.559578896
	H285	4.846211841	-0.572715861	-9.573083425
	H286	4.731055434	-2.244727543	-8.999190199
	H287	7.835749815	-4.131178956	-6.253495951
	H288	5.180501455	-2.298027451	-11.327414570
	H289	3.594596857	-2.686937326	-11.192839695
	H290	5.708584715	4.477689508	0.565469649
	H291	6.110809026	6.531103118	2.803369349
	H292	5.368376566	8.451479840	-0.962732797
	H293	4.374891682	5.136548993	1.566060949
	H294	7.257004734	7.364845086	1.986950276
	H295	5.901417568	4.209623280	-5.709744282
	H296	6.400015459	6.721697695	-0.113122851
	H297	4.793320197	-8.549325475	2.975185863
	H298	6.485111671	-8.897814836	0.437799788
	H299	4.026227548	2.994253713	-6.119214342
	H300	5.400533174	-1.498721478	3.142481250
	H301	1.022329851	3.895553647	-7.811812869
	H302	-1.243951328	-0.866459017	-4.789626104
	H303	0.881202594	3.955040598	-6.050865187
	H304	4.067023023	-5.919533079	3.234661401
	H305	2.385048388	1.790622921	-6.155774910
	H306	3.566524377	-5.979745192	1.539704649
	H307	4.218061416	-8.384837090	1.296796017
	H308	5.955608666	-6.576973814	0.923894076
	H309	6.360306002	-6.624438394	2.643570433
	H310	-4.916612397	1.496909425	-6.640658880
	H311	5.141601004	-10.964151415	2.123217938
	H312	3.992502265	-12.434379043	-0.294389780
	H313	0.216397400	0.888036411	-3.789289381
	H314	5.206033291	-13.503003759	2.139192165
	H315	3.635944638	-13.492896662	1.677074606
	H316	5.346681242	-4.284599394	1.065229668
	H317	-0.421646580	3.271003264	-3.947569851
	H318	-3.302928915	-0.213815778	-6.022602343
	H319	7.106184527	-9.572420805	-4.208840552
	H320	6.337782743	-6.722536613	-5.575783553
	H321	6.130030761	-8.230331174	-2.257417149
	H322	6.244838755	-9.762720991	-5.486078306
	H323	5.338102859	4.962860670	-8.354397366
	H324	6.067388300	-5.147184691	-1.450768762
	H325	1.823300999	-7.663892112	-1.292809585
	H326	3.550768686	0.038105498	-7.785384126
	H327	2.548241705	-8.668564762	-3.264033974
	H328	3.012924011	-4.908868037	-8.655598520

H329	2.198013133	-3.915344312	-6.473688774
H330	5.489734111	-13.368344691	-0.182474160
H331	5.779266278	-2.086458420	1.581393966
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H333	7.063644074	-4.071225797	-0.943805191
H334	8.421576023	-8.012385305	0.956893808
H335	3.736444465	-4.310170019	4.304913979
H336	3.461670173	-7.100885894	-5.730961226
H337	4.581289511	-7.837074401	-4.578091703
H338	1.508489200	-7.759813483	-4.370883767
H339	1.550655962	-0.399977906	-6.441174931
H340	-2.483239811	3.940244685	-5.212966861
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H342	2.005446750	-5.922654586	-1.007958200
H343	8.014183338	-7.786552999	-1.295742721
H344	6.764727259	-9.570365814	-1.807348935
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H346	5.397645501	-5.844740253	-8.462121734
H347	6.348812132	-5.282148558	-4.570916130
H348	0.680657999	-0.723039927	-7.967963080
H349	4.875431362	5.629609670	-5.413840580
H350	7.761735991	-1.363805458	3.993911336
H351	7.828528928	-0.519576755	2.436231570
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H353	7.984571368	-6.777157003	-7.541845609
H354	9.880311447	-8.453456544	-3.780545305
H355	8.196827579	-7.618387816	-5.073211000
H356	11.429753639	-6.981365958	-5.497090348
H357	9.805451947	-6.923330702	-2.878936162
H358	10.509788096	-0.822151408	2.362399005
H359	-2.371058282	11.759095471	7.248089151
H360	9.555807492	-8.831652162	3.619848478
H361	8.976213241	-6.163559542	3.110834607
H362	-4.027017543	11.688060064	4.718732964
H363	-3.667202098	9.084547859	6.324976997
H364	-5.186259063	9.982277850	6.127903469
H365	3.301192804	-0.866904510	1.537705465
H366	-5.921343493	7.492359082	0.200645076
H367	2.454789215	-2.027888660	2.328913224
H368	1.970967169	-1.482337560	0.839091968
Mo369	3.701666919	-3.656919477	-3.522420046
N370	2.791041112	-1.745556551	1.404451985
N371	-7.260222068	-6.276135604	-2.603209530
N372	-9.071318882	-4.361881344	0.052111795
N373	-8.628037836	-5.491759371	2.581610822
N374	-5.970385287	-6.423990537	2.498114315
N375	-4.576104988	-3.952776403	2.444164580
N376	-5.355353776	-3.053189985	5.059157019
N377	-4.406870402	-5.115346671	6.872298630
N378	-1.888022648	-6.267608602	5.990343344
N379	-0.465029336	-4.089811970	4.980149820
N380	-0.816455385	-1.490556763	6.545820209
N381	-1.208276147	-2.542484303	9.204358115
N382	4.487253124	-12.929391241	1.691618504
N383	5.669430652	-10.551215901	1.347968109
N384	4.919989117	-4.449103449	1.983586837
N385	4.456083743	-3.613827530	4.121483079
N386	5.612586836	-2.317665883	2.575481996
N387	8.462800261	-8.440320270	1.908326719
N388	-5.832161124	-1.546430046	-3.840052381
N389	-2.080294624	-4.300723360	-4.719591970
N390	-5.913135786	0.627873689	-2.366732833
N391	-8.181168287	1.550136982	-1.017392560
N392	-7.883332632	0.421104292	1.540408989
N393	-5.671932481	1.760947763	2.657810506
N394	-2.767202646	2.872961348	-0.236862776
N395	-2.346521435	0.684833898	-0.236606462
N396	-6.146982827	4.195244026	3.892930205
N397	-9.306412943	7.688472220	3.460562545
N398	-9.233851148	8.972775696	5.268614919
N399	9.528496916	1.437153812	3.214536694
N400	6.675446523	6.522416973	1.947532464
N401	4.781925162	8.654504509	-0.157203620
N402	2.124586944	8.335320627	-0.907855905
N403	-2.533048466	7.619774354	-2.580091646
N404	-2.639809728	9.780287302	-3.477990237
N405	-3.716428806	9.292931383	-1.486154595
N406	0.926527309	6.252035597	0.712307743
N407	1.283399754	7.417040956	3.235543599
N408	0.214319186	9.948853755	3.618359376

	N409 -1.157637231 10.906722965 0.033831603 N410 -2.137244367 10.777202597 4.876605763 N411 4.261639315 -1.915988587 -11.091716987 N412 2.713123788 -0.388716052 -8.190551142 N413 1.751357005 2.209708655 -6.852713443 N414 3.953204591 3.982181175 -6.386094156 N415 -1.312982099 0.106025800 -10.592394211 N416 -2.867427996 1.529485340 -8.638242155 N417 7.956014213 -5.752842215 -7.561996948 N418 4.142255469 -4.471368195 -5.717231869 N419 3.582425628 -4.855636188 -7.815701717 N420 8.917859778 -6.939673127 -4.815458898 O421 -6.881923846 -4.982648424 -0.055322764 O422 -7.718963042 -3.526287611 3.302355333 O423 -5.981505382 -6.580034012 4.778624911 O424 -2.940364018 -4.997004434 3.634295523 O425 -3.389398073 -1.918869260 5.089341623 O426 -3.931160321 -3.391259917 8.300498400 O427 -1.415613604 -6.668812346 8.201421824 O428 1.485872660 -5.308318605 4.958192240 O429 1.450156121 -1.725747656 6.432798365 O430 0.371390751 -1.043268632 9.833329530 O431 0.828385937 -3.823357450 11.856729335 O432 6.265930004 -10.996712795 -0.839373871 O433 7.391905233 -9.712201430 3.496556384 O434 10.979500203 -6.361786866 3.428939542 O435 -5.822724315 -0.515134550 -0.374816908 O436 -3.775053374 -2.881363841 -5.242192925 O437 -6.884400204 3.050871180 0.110694204 O438 -5.874841260 4.307954190 -2.526397922 O439 -9.762615427 1.525741888 2.262515037 O440 -5.849484472 0.546429390 4.585892988 O441 -4.225728644 3.967211221 5.094607812 O442 -6.228397209 6.030812521 6.912766310 O443 10.745838694 -1.713734100 4.195259633 O444 3.495092679 2.989351356 5.042581254 O445 4.088080141 7.963775545 1.904535970 O446 1.676238673 10.562990695 -0.553966962 O447 -0.995347310 7.455961377 0.441471518 O448 -0.515931109 6.227503145 4.018010991 O449 2.440293330 4.625094373 2.831223616 O450 1.411519062 10.237775445 5.548708244 O451 -1.648735567 12.972843202 4.513891847 O452 -2.560900068 11.242975579 1.806805579 O453 -4.298675445 12.427974968 7.221661788 O454 -5.000826119 7.355784042 0.497325054 O455 1.911116386 -1.986425054 -9.631888121 O456 0.162854983 1.720836930 -8.430541009 O457 2.677953622 5.744151815 -7.048578253 O458 6.406687473 6.420250973 -7.406752334 O459 -4.645735699 0.408252145 -9.521824681 O460 -1.564848337 -4.522481187 -7.737484508 O461 0.439504392 -3.629805643 -8.145952345 O462 -3.297637004 4.918751185 -7.599128458 O463 9.810935194 -4.859592059 -4.919222805 O464 12.313751248 -6.928328006 -3.658626753 O465 0.038072410 -5.462045892 -2.978699266 O466 -0.673214997 -6.999002346 -1.497638234 O467 4.604552761 -9.818488882 -6.094192835 O468 2.349057866 -9.656117993 -6.139183666 O469 4.800233084 -5.417090154 -2.766421342 O470 4.592765266 -7.462363022 -1.852843372 O471 2.355299853 -5.320228081 -3.665224126 O472 8.477663743 -7.201254445 -0.634768352 O473 6.682667667 -4.935848814 -0.698905971 O474 -3.907464625 5.581509192 -1.106859958 O475 7.190588721 -9.822023952 -5.155809237 O476 6.966238429 -8.763294007 -2.345359138 S477 3.850103565 5.269582098 -0.790694225 S478 2.210151909 2.629175961 -2.796058507 S479 2.091208436 -2.173420737 -4.477432646 S480 3.335486296 1.532757364 0.423130493 S481 0.666495693 -0.631809150 -1.337258977 S482 4.430343862 0.718365359 -5.447702360 S483 3.267448728 -3.260978691 -1.216960580 S484 5.776249914 2.294141467 -2.123345222 S485 5.723216546 -2.425461146 -3.794548747 S486 6.249260461 -1.011437669 -0.395629128 end
Core-S2BH to resting	bm502bhtohiso.car_1

S=3/2, 35 reactant

C1	-3.225899167	3.305625220	-8.414186250
C2	-2.621339857	4.493432903	-9.171877346
C3	-5.296000955	2.264274398	-7.601390574
C4	-5.081429226	0.813004772	-8.024906182
C5	-4.450592096	-0.757687306	-9.783750855
C6	-3.227699635	-1.387916978	-9.107308593
C7	-1.089135652	-1.025368344	-7.987007728
C8	-1.439023542	-1.448039897	-6.558566824
C9	-2.800785479	-1.030289441	-4.573029634
C10	-3.534686388	-2.380074997	-4.540516566
C11	-5.152588841	-3.860990327	-5.596988359
C12	-4.343900075	-5.101077451	-5.997227668
C13	-2.801339096	-6.088972461	-7.628100764
C14	-1.399516337	-6.359412000	-7.064349887
C15	0.683942849	-5.352962736	-6.218439474
C16	0.918093187	-5.208181453	-4.710429898
C17	0.189406728	-4.183701546	-2.579618254
C18	-0.549507335	-5.315562751	-1.829175703
C19	-0.260508528	-2.778664852	-2.139335683
C20	-0.208096260	-2.657462116	-0.612396964
C21	0.611667735	-1.706986040	-2.803849770
C22	-2.701660010	-6.454713904	-1.417067965
C23	-2.661420485	-7.822951819	-2.131285686
C24	-4.146505560	-5.943314459	-1.203631832
C25	-5.040211688	-7.039137935	-0.607964534
C26	-4.153345275	-4.699702522	-0.308193590
C27	-3.069442283	-9.143659006	-4.128337028
C28	-1.834757420	-9.994196591	-3.906431552
C29	9.935329806	-4.457917532	-8.140571810
C30	9.804148063	-4.346945792	-6.622800439
C31	8.458505174	-5.167044920	-4.685861888
C32	8.903419615	-6.549960573	-4.173614904
C33	6.950766904	-4.937748806	-4.481778662
C34	6.523282855	-5.010713628	-3.014228881
C35	5.084985401	-4.529694779	-2.828808108
C36	3.629662379	-5.057845785	-0.846695091
C37	10.172656065	-7.740018410	-2.446645245
C38	9.503166167	-8.093046134	-1.138264707
C39	-2.056187266	4.256802784	-4.064321333
C40	-3.288017866	3.816498728	-3.252825075
C41	-0.830550420	3.498717390	-3.500442245
C42	0.448367127	3.554125939	-4.362621940
C43	1.380114872	4.740112720	-4.105151621
C44	-4.579383215	4.421806779	-1.222194645
C45	-5.991887967	4.076742336	-1.715725065
C46	-4.581691798	5.622458498	-0.261999806
C47	-7.641343022	4.328626721	-3.510268147
C48	-7.842137630	2.853177145	-3.881010550
C49	-6.814073059	0.650722005	-4.199989834
C50	-6.521363445	-0.251952432	-3.001393588
C51	-6.082623167	-0.476146224	-0.608922366
C52	-7.403469231	-1.041735187	-0.069964791
C53	-5.468734093	0.325986076	0.548688351
C54	-4.035234396	0.678217871	0.375734810
C55	-3.016593855	0.124570016	-0.368093700
C56	-2.113023085	1.724667903	0.758342555
C57	-9.726858095	-0.490113117	0.447989099
C58	-10.219680962	-1.862378249	-0.007790770
C59	-10.736946403	0.600362071	0.009782968
C60	-11.960742127	0.771409845	0.864307798
C61	-12.789147085	-0.160521340	1.460929579
C62	-13.512825461	1.892138633	1.877314875
C63	4.944901399	-7.657961182	3.952714561
C64	6.413385146	-7.792052570	3.595126444
C65	4.308596981	-6.706653056	2.910686577
C66	2.830397165	-6.485541904	3.129999496
C67	1.870402669	-7.351530676	2.578084377
C68	2.371029666	-5.391347007	3.884776420
C69	0.500091503	-7.127863804	2.753645603
C70	1.008843597	-5.159728242	4.075421763
C71	0.073272855	-6.023410831	3.499623226
C72	0.498181858	-2.432395354	8.366381002
C73	-0.859892144	-1.938057402	8.889523521
C74	0.573009169	-2.220588481	6.855522220
C75	-2.022830620	-0.291377526	10.311891607
C76	-2.866240998	0.606863198	9.404115646
C77	-3.011739797	1.662258140	7.149203730
C78	-3.668072404	0.736860052	6.094451188
C79	-1.967952628	2.614411869	6.522268926
C80	-2.378572353	3.448074415	5.304141304

C81	-3.271356585	4.668469724	5.585411335
C82	-5.682776289	4.704276969	6.236951465
C83	-3.497075995	-1.204769462	4.625270239
C84	-4.536633972	-2.171267796	5.214324175
C85	-2.431828071	-2.039026398	3.893373732
C86	-5.034790731	-3.659449779	7.098045995
C87	-6.195906197	-3.323349953	8.023889487
C88	-7.533731050	-1.558918041	9.061442073
C89	-9.026977392	-1.639099002	8.667751504
C90	-7.204683603	-0.164580545	9.608832569
C91	-7.419856873	0.956777532	8.597724991
C92	-10.675909177	-1.843361853	6.879176145
C93	-11.558974015	-2.963042134	7.411022085
C94	-10.668758680	-1.872417422	5.325836745
C95	-9.914579122	-0.696216361	4.751005694
C96	-10.568891015	0.520322590	4.504547655
C97	-8.530981523	-0.765899854	4.511651436
C98	-9.860910060	1.644546681	4.072959348
C99	-7.801765734	0.356437223	4.111079778
C100	-8.478177731	1.556593457	3.901548716
C101	8.103362700	6.451792308	2.145463019
C102	6.734836094	6.666529156	1.522330363
C103	4.367469402	5.907246371	1.557219367
C104	3.390895698	6.424388674	2.618843031
C105	2.261095893	5.857973628	4.732433690
C106	2.661550338	5.314131812	6.100217626
C107	3.834355077	3.668459057	7.445128384
C108	4.566026887	4.576894036	8.411378660
C109	2.782548635	9.771633673	-0.523072962
C110	1.279526734	9.818516534	-0.227918269
C111	3.113643336	8.514223028	-1.359699929
C112	4.505675657	8.633327996	-2.007556166
C113	4.949922159	7.307308183	-2.587137745
C114	-0.571170153	9.076789459	1.185144489
C115	-0.741874803	9.195906287	2.687394956
C116	-1.410759905	7.963234297	0.513766233
C117	-0.752370101	6.624828614	0.686822029
C118	-0.904088461	5.913648714	1.888663058
C119	0.149893263	6.150650050	-0.279444767
C120	-0.103664454	4.800633847	2.150136910
C121	0.947092790	5.033508161	-0.018005709
C122	0.848838358	4.385503302	1.216321730
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C126	9.136774349	2.606463258	-0.886517313
C127	9.580886896	3.900069724	-1.065571561
C128	7.377866318	3.845738695	-1.268225494
C129	12.754494553	-1.905811477	-0.677901985
C130	13.847664491	-2.025424242	0.361667460
C131	4.336964331	0.947989960	-5.198901439
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C134	7.539983444	1.388717104	-4.945613680
C135	8.857402069	1.878167238	-4.339389422
C136	9.866684552	2.434148915	-5.365333940
C137	7.417708222	-0.456783872	-3.252764480
C138	3.750814817	0.303843606	1.814321641
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	O423	-4.484004797	-6.177153480	-5.389013828
	O424	-0.957805540	-7.517579590	-7.047593348
	O425	1.866448166	-5.822833293	-4.190239863
	O426	0.053579163	-6.059973618	-1.030836702
	O427	-2.358411514	-8.859287456	-1.515144593
	O428	-1.849284151	-11.215232052	-3.973197564
	O429	10.591332582	-3.613953220	-5.988370171
	O430	8.583399609	-7.588901666	-4.777563992
	O431	10.002189500	-8.828885051	-0.301570489
	O432	-3.876051303	2.732569193	-3.433164405
	O433	0.944150518	5.882686561	-3.826749385
	O434	-6.721164433	3.294533610	-1.081551162
	O435	-5.477405842	5.368525627	0.837423576
	O436	-8.990693933	2.437039774	-4.093077503
	O437	-6.547689812	-1.481463814	-3.147052573
	O438	-7.461846534	-2.114587996	0.542982574
	O439	-10.913413541	-2.612975136	0.656758489
	O440	6.890912320	-8.736452508	2.982270423
	O441	-1.262508115	-5.723332746	3.689928714
	O442	-1.928443677	-2.500966326	8.591764546
	O443	-3.969382496	1.017391945	9.817509052
	O444	-4.826355205	0.963539866	5.709053273
	O445	-5.450455805	-2.621824349	4.510578071
	O446	-1.937898728	-3.074595476	4.746843462
	O447	-6.737395118	-4.207483531	8.699138349
	O448	-9.905264202	-1.459022955	9.523025297
	O449	-8.430889909	1.008846979	7.882737714
	O450	-12.777057120	-2.887351391	7.447129119
	O451	-7.730737902	2.693572296	3.540506221
	O452	6.581781683	7.452266691	0.555721970
	O453	2.906739822	7.573202302	2.567543405
	O454	2.102756133	5.763876803	7.115733161
	O455	4.576899400	4.408221330	9.620022311
	O456	0.502778304	10.475804616	-0.940442209
	O457	4.591923511	6.892690006	-3.683882704
	O458	5.747433820	6.546331072	-1.808182311
	O459	-1.726169053	8.820286639	3.307820433
	O460	11.748716686	-0.671511599	1.533558350
	O461	14.240806340	-3.095187013	0.805402290
	O462	4.130921347	1.956602292	-4.369819914
	O463	3.668663244	0.756740497	-6.221931601
	O464	11.100362748	2.141071414	-5.181082766
	O465	9.416104776	3.162980120	-6.293818547
	O466	7.485256473	-0.377294305	-1.950003223
	O467	7.999361893	-1.338168868	-3.913404573
	O468	6.027787674	1.512203484	-2.987559129
	O469	10.238146447	-4.093829940	-1.701798281
	O470	7.894563918	-2.863497112	-0.653512229
	O471	-5.326973464	3.434151093	2.772150123
	O472	12.568969731	0.110927241	-4.028565413
	O473	10.625648768	-2.146066913	-3.637897992
	S474	0.368285563	-0.438271154	6.396144313
	S475	1.485483294	1.823767876	3.709712012
	S476	4.581812185	2.695482370	-0.313423425
	S477	1.303912595	-1.601004808	2.693143696
	S478	1.311276088	1.379791183	-0.092729990
	S479	5.248269297	2.840147189	3.486575594
	S480	4.459101949	-0.862148871	-1.217165489

	S481	3.887989606	-0.550925172	5.016983332
	S482	7.022779163	0.362534880	1.216057331
	S483	5.099648382	-2.679265651	2.132831692
	end			
Core-S2BH to resting **S=3/2, 35** **TS** Fe(139) -2.422 Fe(140) -2.524 Fe(141) -2.515 Fe(142) 2.784 Fe(143) 2.969 Fe(144) 2.216 Fe(145) 2.314	bm502bhtohism.car_1			
	C1	-3.853259908	3.453061647	-8.095702903
	C2	-3.426746992	4.754338257	-8.783917049
	C3	-5.751205201	2.125513960	-7.276587992
	C4	-5.392620608	0.736261012	-7.793114075
	C5	-4.659170440	-0.641666014	-9.671769973
	C6	-3.353085047	-1.179645871	-9.078842465
	C7	-1.239210714	-0.677783422	-7.967618362
	C8	-1.512828410	-1.230629266	-6.567617784
	C9	-2.872793343	-1.077128008	-4.540134611
	C10	-3.438353151	-2.503493352	-4.592144747
	C11	-4.903043468	-4.082428880	-5.710640329
	C12	-3.944243179	-5.182317131	-6.184146228
	C13	-2.367445748	-5.910212390	-7.908006208
	C14	-0.928922131	-6.065779057	-7.397960024
	C15	1.067625005	-4.900246599	-6.553035040
	C16	1.342696573	-4.791830031	-5.050076212
	C17	0.547805352	-3.985233446	-2.843848996
	C18	-0.022463742	-5.239057068	-2.140009670
	C19	-0.080087415	-2.669029494	-2.340086603
	C20	-0.028929198	-2.592796183	-0.810612894
	C21	0.621045134	-1.464298739	-2.979977744
	C22	-2.013688077	-6.647093093	-1.739532419
	C23	-1.849364023	-7.957225835	-2.538079109
	C24	-3.499497080	-6.311708538	-1.458210729
	C25	-4.254740049	-7.535427953	-0.923889917
	C26	-3.614697009	-5.140056104	-0.475972103
	C27	-2.187539517	-9.184809583	-4.607654898
	C28	-0.882309995	-9.940300587	-4.474906688
	C29	10.093261676	-2.805443531	-8.684466735
	C30	10.006457883	-2.807142661	-7.158393374
	C31	8.812207622	-3.877064591	-5.242511163
	C32	9.413951512	-5.236149060	-4.834335826
	C33	7.296540354	-3.826369537	-4.984327909
	C34	6.921807003	-4.042582956	-3.515468389
	C35	5.449838621	-3.713293933	-3.261323467
	C36	4.133268228	-4.528622946	-1.278063229
	C37	10.858106464	-6.402372151	-3.238014365
	C38	10.322402303	-6.913663750	-1.919373127
	C39	-2.649435070	4.250059308	-3.722095488
	C40	-3.807885038	3.623929385	-2.923028283
	C41	-1.333737325	3.592709362	-3.243591903
	C42	-0.096305195	3.844680148	-4.129285691
	C43	0.707134716	5.106145932	-3.815459572
	C44	-5.111276332	3.957105881	-0.840166484
	C45	-6.490758627	3.489993842	-1.319294030
	C46	-5.210559707	5.081615720	0.200915733
	C47	-8.209032390	3.648909342	-3.060130875
	C48	-8.245937511	2.185724967	-3.517771810
	C49	-6.974461543	0.138189131	-3.976601865
	C50	-6.561867854	-0.787285940	-2.830976891
	C51	-5.984886041	-1.058921775	-0.469030426
	C52	-7.212077547	-1.816634451	0.075258613
	C53	-5.427965515	-0.230692489	0.696715128
	C54	-4.069849551	0.355401112	0.480788299
	C55	-3.027299102	0.060056170	-0.371905948
	C56	-2.299200481	1.617157338	0.953755689
	C57	-9.594713595	-1.591818653	0.639539025
	C58	-9.947279358	-2.978674222	0.107702357
	C59	-10.714798772	-0.575907780	0.309353851
	C60	-11.923429966	-0.597779283	1.199253902
	C61	-12.611573116	-1.653320048	1.767349363
	C62	-13.540174580	0.274218358	2.343159019
	C63	5.879391334	-7.296031272	3.298371096
	C64	7.338148566	-7.269462300	2.882795022
	C65	5.109271117	-6.354689623	2.336246719
	C66	3.624703670	-6.326123726	2.611923296
	C67	2.753260201	-7.258361717	2.020359161
	C68	3.070982485	-5.361036861	3.471645440
	C69	1.375552834	-7.221823030	2.261758548
	C70	1.700896664	-5.320598429	3.732477172
	C71	0.851757357	-6.248641119	3.120939328
	C72	1.060065036	-2.873723284	8.173223969
	C73	-0.327477772	-2.568847306	8.765220607
	C74	1.064667985	-2.571326488	6.678939910
	C75	-1.604268110	-1.154280087	10.339301425

C76	-2.567807915	-0.294198181	9.516874649
C77	-2.916347457	0.847243133	7.330323220
C78	-3.497216950	-0.093687230	6.243613232
C79	-2.006281800	1.944932175	6.733033831
C80	-2.544296201	2.826748165	5.599467090
C81	-3.562537466	3.910212359	5.993232523
C82	-5.940646540	3.624793104	6.698707091
C83	-3.153876781	-1.927522605	4.668717880
C84	-4.076149056	-3.020542989	5.234127267
C85	-2.030058021	-2.611737546	3.872072451
C86	-4.364726650	-4.654114685	7.035760444
C87	-5.514699808	-4.476131206	8.017303374
C88	-7.002242054	-2.914048923	9.154118366
C89	-8.493444276	-3.146080459	8.806028866
C90	-6.801756055	-1.524297091	9.767037474
C91	-7.169889675	-0.379446021	8.831186087
C92	-10.166931772	-3.439361956	7.037332360
C93	-10.903766444	-4.682817253	7.510859090
C94	-10.181709604	-3.373620046	5.482666256
C95	-9.588485008	-2.083964689	4.960720621
C96	-10.389985728	-0.942217216	4.800660807
C97	-8.215926602	-1.971299569	4.680554757
C98	-9.840598586	0.278757357	4.401045142
C99	-7.643307438	-0.750779721	4.308651675
C100	-8.464096403	0.368119388	4.184783681
C101	7.416666997	7.163347066	2.330613383
C102	6.010204706	7.267571828	1.766155682
C103	3.730157687	6.286569515	1.822905324
C104	2.727116950	6.609089084	2.934923861
C105	1.751502432	5.800472157	5.039289742
C106	2.227247297	5.191961497	6.356041300
C107	3.632620506	3.602912903	7.550306994
C108	4.373518606	4.483989845	8.536059284
C109	1.650288667	10.021834609	0.022452474
C110	0.159673352	9.875547187	0.348866730
C111	2.096970359	8.872221563	-0.910081927
C112	3.454889482	9.183611109	-1.567311444
C113	4.017756222	7.956095913	-2.247490740
C114	-1.547775842	8.843940043	1.763943010
C115	-1.693914466	8.861383945	3.272340683
C116	-2.235917738	7.651015609	1.058319644
C117	-1.406213714	6.397491538	1.139697550
C118	-1.427071959	5.591111063	2.288746410
C119	-0.500951415	6.086304472	0.109244687
C120	-0.527335041	4.530049747	2.422652478
C121	0.396744233	5.024042642	0.244955037
C122	0.399848882	4.257959897	1.412731199
C123	10.779377115	2.525070412	0.143463655
C124	11.591765516	1.222701527	0.112795395
C125	9.748847959	2.562834306	-0.996551141
C126	8.779650040	3.700385215	-0.970336406
C127	9.074658296	5.044122771	-1.070745244
C128	6.882131450	4.767724215	-1.164716868
C129	12.862842433	-0.415310287	-1.135094586
C130	13.985806950	-0.457813615	-0.123238005
C131	4.053678610	1.779327465	-5.244356693
C132	5.264615486	0.907641761	-4.883928484
C133	6.377930547	1.647630773	-4.092620269
C134	7.203590828	2.557171856	-5.037731538
C135	8.486600873	3.141040793	-4.438925133
C136	9.383006252	3.879421779	-5.460003340
C137	7.327818896	0.623324682	-3.452974786
C138	3.753316658	0.601589336	1.718404223
Fe139	5.015672967	2.177650356	1.563268175
Fe140	1.792391824	0.419286833	1.936802590
Fe141	3.822516899	-1.083412606	2.757696092
Fe142	3.602434405	1.397133423	3.551951569
Fe143	1.867857042	-0.468635418	4.416890863
Fe144	5.255299670	-0.269656044	0.751137982
Fe145	3.344453838	1.169471974	-0.151244436
H146	-1.422840325	4.379647875	-8.873608942
H147	-1.851330049	5.323452681	-7.613809944
H148	-5.829041774	3.977148832	-8.331091531
H149	-4.086263312	5.568597619	-8.443542418
H150	-3.633198541	4.628162702	-9.860336770
H151	-5.409860525	2.167116263	-6.231930144
H152	-5.099939919	1.465317582	-9.682849678
H153	-6.845704749	2.216839132	-7.276522460
H154	-4.528374015	-0.511848630	-10.753627186
H155	-2.698240098	0.732696652	-8.648374734

H156	-5.420058137	-1.416647587	-9.509625072
H157	-2.028960294	-1.087696810	-3.841272588
H158	-2.923906637	0.223557999	-6.241803185
H159	-0.561107333	0.183474452	-7.891590343
H160	-5.294861888	-4.394729799	-4.734002118
H161	-4.612476115	-2.009405006	-6.214152286
H162	-0.733827788	-1.468594935	-8.534650307
H163	-3.631911248	-0.387584519	-4.146964418
H164	-3.283823979	-3.979963937	-7.734847334
H165	-5.740525089	-4.018303286	-6.419396134
H166	0.594554706	-1.507482310	-4.078062215
H167	0.142944295	-0.526462067	-2.659217486
H168	1.672586289	-1.408086438	-2.658384493
H169	-1.139498997	-2.678611633	-2.649970502
H170	-2.315516237	-5.693453119	-8.984866467
H171	-3.118684506	-4.234619151	-0.851781561
H172	-2.641609454	-7.132967151	-4.286923915
H173	-4.253315165	-8.374617377	-1.634769786
H174	-0.526741364	-1.679168169	-0.458720869
H175	1.006650013	-2.547132398	-0.445267921
H176	5.506944561	-8.325807565	3.140511657
H177	-4.672450486	-4.892215532	-0.300275603
H178	-5.302467719	-7.265831199	-0.722864641
H179	-3.162868383	-5.404400107	0.494138286
H180	-3.806534693	-7.889513363	0.018627897
H181	-3.963020780	-6.010748150	-2.415583541
H182	-1.502279549	-6.840015089	-0.785949640
H183	-1.889572831	-4.861161064	-2.927587095
H184	-0.521753505	-3.454919866	-0.336708718
H185	-1.283721704	-1.857161507	3.568358464
H186	-2.490825381	-3.030942388	2.964434498
H187	-1.189714731	-4.390668301	4.061879537
H188	-0.987107410	-6.803102488	2.859906001
H189	1.279940015	-4.548984330	4.377157143
H190	3.717038247	-4.601520973	3.918995435
H191	3.152127172	-8.015551271	1.340414350
H192	-0.342586933	-3.654803091	-4.769276238
H193	1.578881683	-4.058166684	-7.045860626
H194	1.541093265	-5.830866311	-6.887761094
H195	-0.831517032	-4.042905434	-6.969187355
H196	-2.850628190	-6.886591842	-7.777176101
H197	0.712828540	-7.939966824	1.771798518
H198	1.617932707	-3.977003442	-2.604472359
H199	-3.019073758	-9.849854787	-4.321086710
H200	-2.306363309	-8.925242921	-5.671748183
H201	0.017759702	-9.307863339	-4.298046407
H202	11.944108127	-6.242592524	-3.155555771
H203	2.607925776	5.847868922	-3.813936914
H204	4.710695439	2.647136741	-3.532892205
H205	3.317365841	9.964936643	-2.328543920
H206	4.163338788	9.554205770	-0.812414855
H207	1.348782449	8.707644236	-1.700724874
H208	-0.909501967	9.451928617	3.801104188
H209	1.696870924	10.955832549	-0.558212594
H210	-1.133553582	3.917433433	-2.209973133
H211	-0.399556307	3.912760609	-5.188344898
H212	0.574179635	8.541109230	1.884280217
H213	-2.076997117	9.762087166	1.437406163
H214	2.582313352	9.348259748	1.752103046
H215	2.520036314	4.133943176	-4.222074754
H216	2.148803049	7.939378338	-0.327874408
H217	3.381314365	10.562282705	0.982749824
H218	-3.131043567	6.177846869	-4.283258433
H219	-1.505391200	2.507261427	-3.205842145
H220	5.125721062	7.653650941	-0.651079509
H221	0.572102588	2.972915936	-4.068793409
H222	-5.267192087	-1.829965572	-0.779692618
H223	-3.016663043	-0.652936038	-1.189414404
H224	-7.971732676	-0.186378455	-4.304447190
H225	-6.169355985	2.049271612	-3.469056054
H226	-8.395052110	-0.247485514	-0.518194159
H227	-12.456928770	-2.726458653	1.734894863
H228	-9.668231943	-3.134527963	-0.962348325
H229	-11.002643567	-0.695485100	-0.750885369
H230	-9.450152876	-1.656770374	1.730019241
H231	-14.231156666	0.967028041	2.815986233
H232	-5.397584505	-0.898735086	1.573497232
H233	-6.147612277	0.568568625	0.937975977
H234	-14.331361221	-1.576610029	3.037479209
H235	-10.280567364	0.432545869	0.401009974

	H236	-6.433906920	0.786182390	-1.477584584
	H237	-6.286066545	-0.039844520	-4.816720865
	H238	-9.052326032	3.776737705	-2.367113834
	H239	-1.674520649	2.364115915	1.438834337
	H240	-8.395793200	4.287706245	-3.932884466
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	S479	4.937184236	3.189164359	3.533740185
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Core-S2BH to resting S=3/2, 35 product Fe(139) -2.438 Fe(140) -2.496 Fe(141) -2.507 Fe(142) 2.830 Fe(143) 3.017 Fe(144) 2.195 Fe(145) 2.211	bm502bhtohism.car_4			
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	C2	-3.400489323	4.733578338	-8.776460454
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	C7	-1.242330359	-0.658505208	-7.989159879
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	C16	1.328596717	-4.789905990	-5.054554259
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	C23	-1.849958565	-7.941373457	-2.542404619
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	C50	-6.552223152	-0.792398097	-2.839925990
	C51	-5.971741499	-1.070975229	-0.483608980
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	C58	-9.928893147	-2.984344513	0.123667038
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	C60	-11.923915879	-0.616674880	1.204833339
	C61	-12.590853159	-1.670799699	1.799168026
	C62	-13.560706404	0.250686917	2.324856880
	C63	5.883211172	-7.294027093	3.304637086
	C64	7.341698996	-7.265887001	2.891073944
	C65	5.115922443	-6.347597450	2.346404911
	C66	3.631795828	-6.313031979	2.623618087
	C67	2.754386423	-7.236541698	2.027167509
	C68	3.082910945	-5.343750767	3.481589210
	C69	1.375385088	-7.187324891	2.261526730
	C70	1.712126175	-5.290366386	3.736653618

C71	0.857551155	-6.207734790	3.117287020
C72	1.037008161	-2.868805561	8.168548712
C73	-0.349215422	-2.567670276	8.760938099
C74	1.040674984	-2.550432870	6.675773073
C75	-1.626659974	-1.148578403	10.327858688
C76	-2.580790651	-0.279853150	9.502234875
C77	-2.925215596	0.862966736	7.316898756
C78	-3.503388346	-0.066161056	6.221417729
C79	-2.013919035	1.967022678	6.731268451
C80	-2.543321052	2.846698295	5.592082604
C81	-3.580031535	3.918978448	5.966697233
C82	-5.951290429	3.621813676	6.673069829
C83	-3.168821611	-1.893212785	4.643149418
C84	-4.093146225	-2.986762896	5.206056506
C85	-2.050961269	-2.577054507	3.837289069
C86	-4.368533850	-4.640848576	6.990714529
C87	-5.510244824	-4.477965113	7.983837694
C88	-6.991960734	-2.934299604	9.153184123
C89	-8.482329536	-3.174434424	8.807553974
C90	-6.797930121	-1.548680592	9.776917400
C91	-7.185328636	-0.396811686	8.857131502
C92	-10.158523854	-3.443234730	7.039142453
C93	-10.902371569	-4.681673665	7.516848117
C94	-10.178077113	-3.380628079	5.484698684
C95	-9.589653106	-2.089048521	4.962267437
C96	-10.393308775	-0.947186207	4.812216858
C97	-8.219243090	-1.974667542	4.675075812
C98	-9.847338382	0.275444117	4.413195264
C99	-7.649573598	-0.752447269	4.305222971
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C101	7.421514374	7.170682930	2.320461733
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C103	3.739100756	6.268830197	1.823243069
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C105	1.751474596	5.775330328	5.032912678
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C108	4.338976525	4.515116311	8.564334472
C109	1.663138470	10.028519492	0.042187570
C110	0.173992734	9.886564290	0.372511451
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C112	3.461116066	9.186773744	-1.551893246
C113	4.007107851	7.959075557	-2.247785219
C114	-1.533833435	8.850954838	1.780070949
C115	-1.675992933	8.869211576	3.288397538
C116	-2.241143656	7.670815934	1.071471022
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C119	-0.516466785	6.108484379	0.101322278
C120	-0.544653870	4.524050022	2.393605561
C121	0.378438010	5.042097249	0.222022769
C122	0.380791571	4.258539554	1.378404038
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C124	11.589183515	1.216102965	0.111006677
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C130	13.981308697	-0.483212828	-0.123120316
C131	4.005967507	1.765803324	-5.247501789
C132	5.229889291	0.898548312	-4.891789954
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C134	7.181313185	2.538282680	-5.058284551
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C136	9.366489042	3.859944641	-5.464147525
C137	7.304528334	0.601368711	-3.474558008
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	H154	-4.558919546	-0.536391801	-10.753324406
	H155	-2.719783879	0.738032084	-8.657233892
	H156	-5.432195605	-1.427391940	-9.488898294
	H157	-1.979770305	-1.095133933	-3.872597257
	H158	-2.936140827	0.219884963	-6.258584645
	H159	-0.571553348	0.209346766	-7.922655706
	H160	-5.284534694	-4.380080388	-4.735379096
	H161	-4.591386917	-1.995860691	-6.218253711
	H162	-0.735782642	-1.445692295	-8.560635470
	H163	-3.583664750	-0.377681047	-4.131816818
	H164	-3.288439466	-3.970167968	-7.747284951
	H165	-5.735442660	-3.996871556	-6.416837616
	H166	0.639349425	-1.491805332	-4.053846340
	H167	0.235873081	-0.516930749	-2.613143399
	H168	1.738166617	-1.433957767	-2.648031838
	H169	-1.100948846	-2.648589342	-2.607767110
	H170	-2.322771466	-5.683628266	-8.997585657
	H171	-3.102307121	-4.221336882	-0.850427318
	H172	-2.649924032	-7.121549808	-4.289354990
	H173	-4.254803714	-8.353895133	-1.640159594
	H174	-0.363655331	-1.670409408	-0.408244048
	H175	1.097632171	-2.636650429	-0.447677425
	H176	5.507939072	-8.322661282	3.141961872
	H177	-4.666208825	-4.867888197	-0.306088489
	H178	-5.307262946	-7.242357624	-0.736750739
	H179	-3.163405519	-5.395803124	0.491537844
	H180	-3.815738441	-7.865336475	0.013646368
	H181	-3.963298761	-5.986976890	-2.420299760
	H182	-1.503462131	-6.823754472	-0.791840122
	H183	-1.879751574	-4.850864180	-2.945511620
	H184	-0.486515028	-3.445133027	-0.311766272
	H185	-1.306885221	-1.822222957	3.525737730
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	H187	-1.175626641	-4.339483191	4.025373875
	H188	-0.985616918	-6.740294020	2.836989254
	H189	1.294972357	-4.514009554	4.377940888
	H190	3.732127471	-4.589170487	3.931208935
	H191	3.149072755	-7.996404508	1.347448884
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	H193	1.563262961	-4.017253677	-7.037865810
	H194	1.544742106	-5.794454997	-6.909232948
	H195	-0.841255151	-4.026073665	-6.981037407
	H196	-2.849043284	-6.876195743	-7.785329004
	H197	0.707548991	-7.897314174	1.764985009
	H198	1.635611840	-3.987617925	-2.615514743
	H199	-2.994735245	-9.854240957	-4.299568390
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	H201	0.026966276	-9.249647527	-4.339121356
	H202	11.946363457	-6.238962026	-3.149222462
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	H206	4.176684402	9.539935030	-0.794726062
	H207	1.352135930	8.726016758	-1.686746353
	H208	-0.897063008	9.471835657	3.811454967
	H209	1.711983207	10.965293899	-0.534829773
	H210	-1.115157889	3.901975102	-2.219979891
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	H213	-2.052731688	9.777757232	1.458617083
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	H219	-1.493356311	2.500048288	-3.231029742
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	H221	0.579168238	2.976957164	-4.098911235
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	H223	-2.840251224	-0.787853776	-1.018771318
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	H236	-6.441787996	0.778051958	-1.479415828
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	H243	-1.640131514	-0.975925580	5.877296087
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	H245	-2.936805618	-3.087740539	6.903631131
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	H252	-5.765452734	-1.450001364	10.139543613
	H253	-7.464404018	-1.497495535	10.652124506
	H254	-5.358153343	0.521068348	9.206718293
	H255	-6.473096603	1.332134135	8.105473952
	H256	-6.474098814	4.269462476	8.550103479
	H257	-3.427615686	4.816955395	5.348365757
	H258	-10.488174640	1.150108237	4.273992080
	H259	-7.563001624	-2.847766317	4.725829935
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	H264	-6.375665143	4.750142496	-2.890183685
	H265	-1.375816554	-0.592615231	11.240270348
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	H267	-1.698796066	2.609331972	7.570670983
	H268	-6.573113448	-0.674092737	4.154117973
	H269	-2.200350383	-2.038223684	10.623357072
	H270	-4.967705531	4.897600104	7.964290828
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	H276	-3.787941458	1.293193875	7.834093150
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	H278	-1.669577265	3.381997236	5.194321532
	H279	-5.206421497	3.087321814	4.854772300
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	H293	0.307009031	-3.179522383	6.153348260
	H294	1.499233033	-4.469146716	9.372024849
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	H305	3.101295341	4.735067137	3.692688422
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	H316	5.535701722	-3.098081441	-1.221553955
	H317	-0.534645715	3.899281988	3.290367787
	H318	-0.505465830	6.721481642	-0.803265743
	H319	11.813646462	0.930482969	-4.349244260
	H320	10.249719784	2.551070578	-1.961026627
	H321	9.708384601	-0.456897531	-4.018099753
	H322	11.676024967	2.442874481	-4.676754895
	H323	4.765932675	5.458989953	8.146903608
	H324	7.930142642	-1.014213723	-1.473050200
	H325	5.637253125	0.448454341	-5.805741188
	H326	5.434819474	5.689157867	2.946250489
	H327	7.446351489	1.924565361	-5.933768010
	H328	7.729577765	6.671402443	-1.374856746
	H329	5.830748369	4.998269465	-1.307582465
	H330	11.164322073	-2.741009374	-8.933836698
	H331	4.244955366	-3.561650068	0.561280906
	H332	9.769794317	-2.541446810	-1.727124736
	H333	7.948558761	-1.765006695	-0.114218859
	H334	10.322269904	-4.314846485	-3.194019208
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	H344	10.720292489	-1.193746675	-4.932722474
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	H354	13.328324033	-0.481108394	-2.139848497
	H355	11.982166032	1.350311957	-1.947083459
	H356	14.388817570	0.505133581	0.198599778
	H357	12.204796886	-1.288759275	-1.023637093
	H358	7.901908724	-6.371909410	3.255042782
	H359	-10.257276817	-5.534427667	7.832948017
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