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The activating capture of N2 at the active site of Mo-nitrogenase.

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Supplementary Information

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1. Protein model

The quantum computed protein model is an extract from crystal 3U7Q, shown in Figure 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 Figure 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 Figure S1.

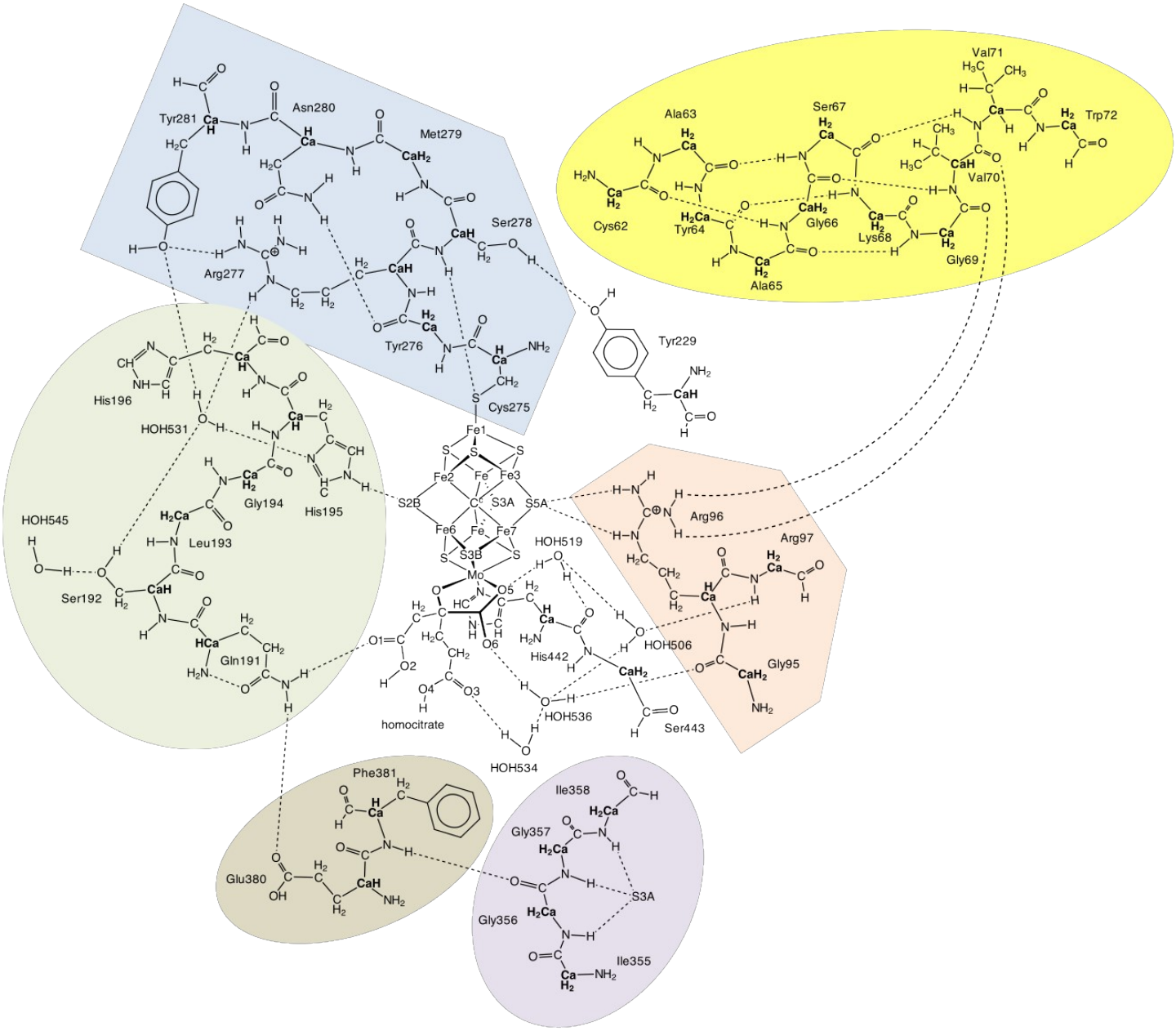


Figure S1. The quantum computed model, with residues and water molecules labelled according to *Azotobacter vinelandii* protein, crystal structure 3U7Q. Cα are labelled as Ca, and hydrogen bonds are broken lines. Non-influential sidechains are truncated to gly. In the 'front' chain (yellow highlight) 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 Figure S1.

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 Figure 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 (Figure 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 about 1Å away from FeMo-co. This is consistent with experimental data on mutation of amino acid 70 with smaller and larger side chains.[10-12] Accordingly the Cα(Val70) -- C^c distance was constrained to 8.2Å and the Cα(Val70) -- CZ(Arg96) distance to 4.7Å, longer than the crystal distances by 1Å and 0.7Å respectively.

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 for 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 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 S2, 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.

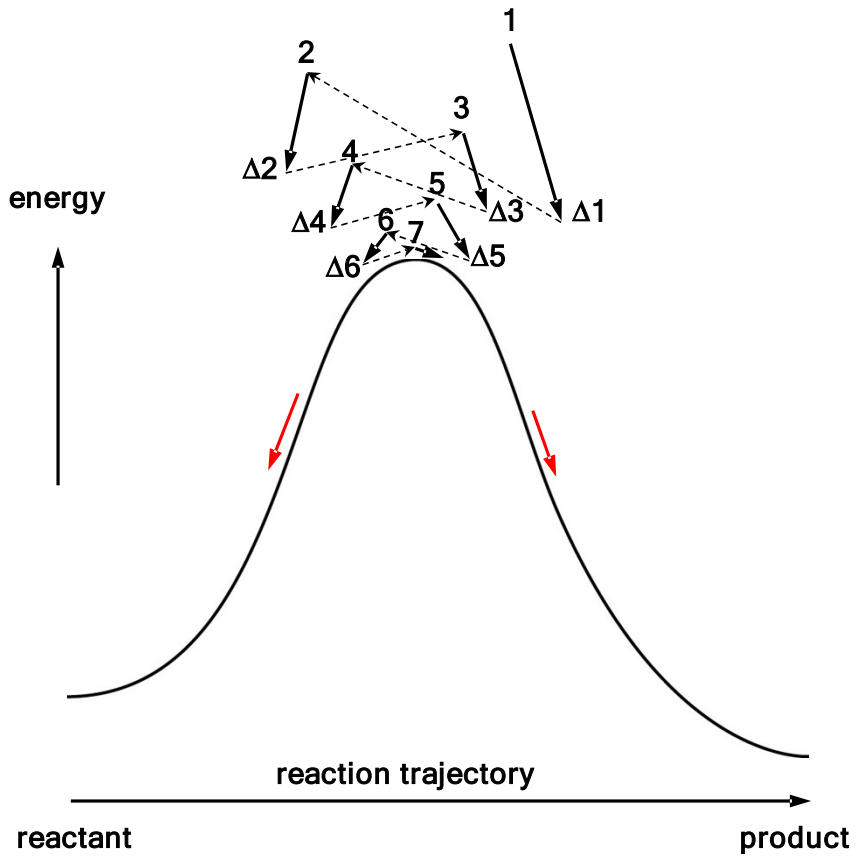
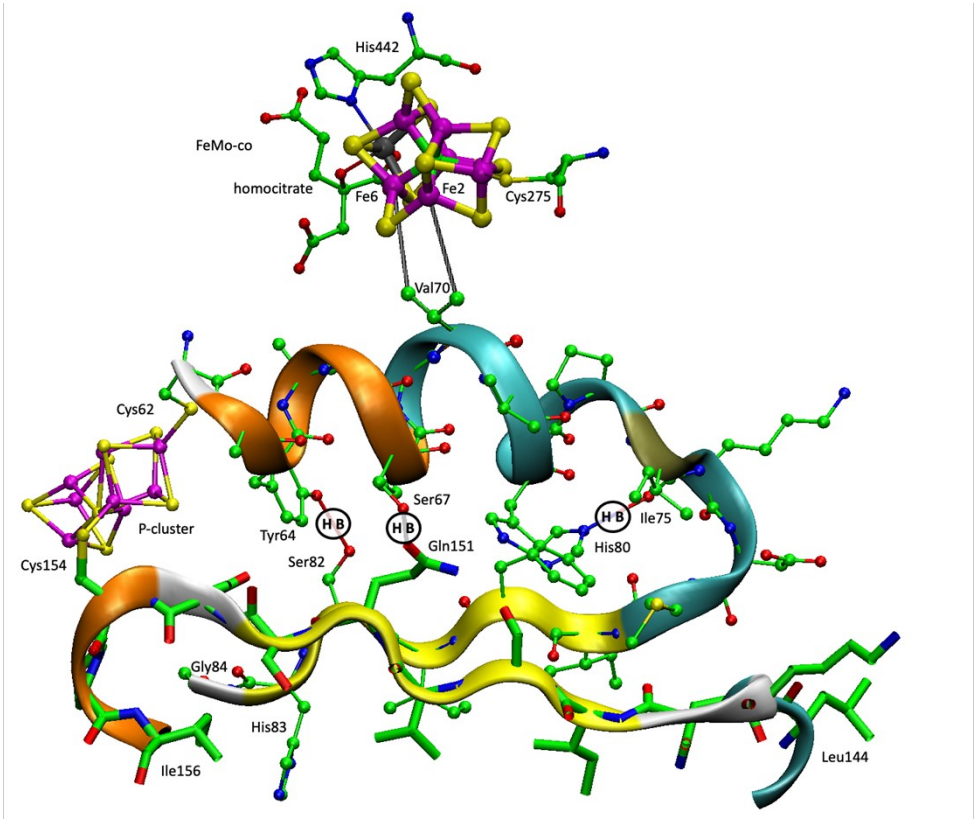


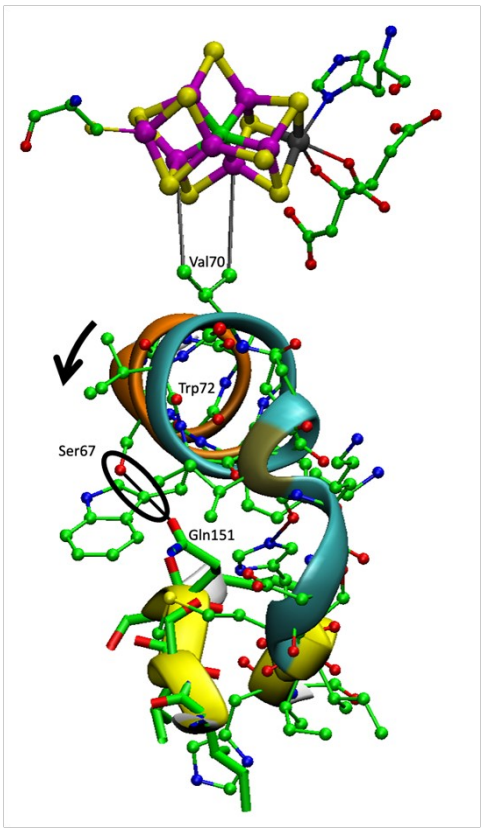
Figure S2. Generalised diagram of the procedure for locating a reaction transition state. The solid arrows represent the course of limited small-step energy reductions from the numbered positions, which are generated (broken arrows) from Δ positions partway along the previous energy reduction, chosen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

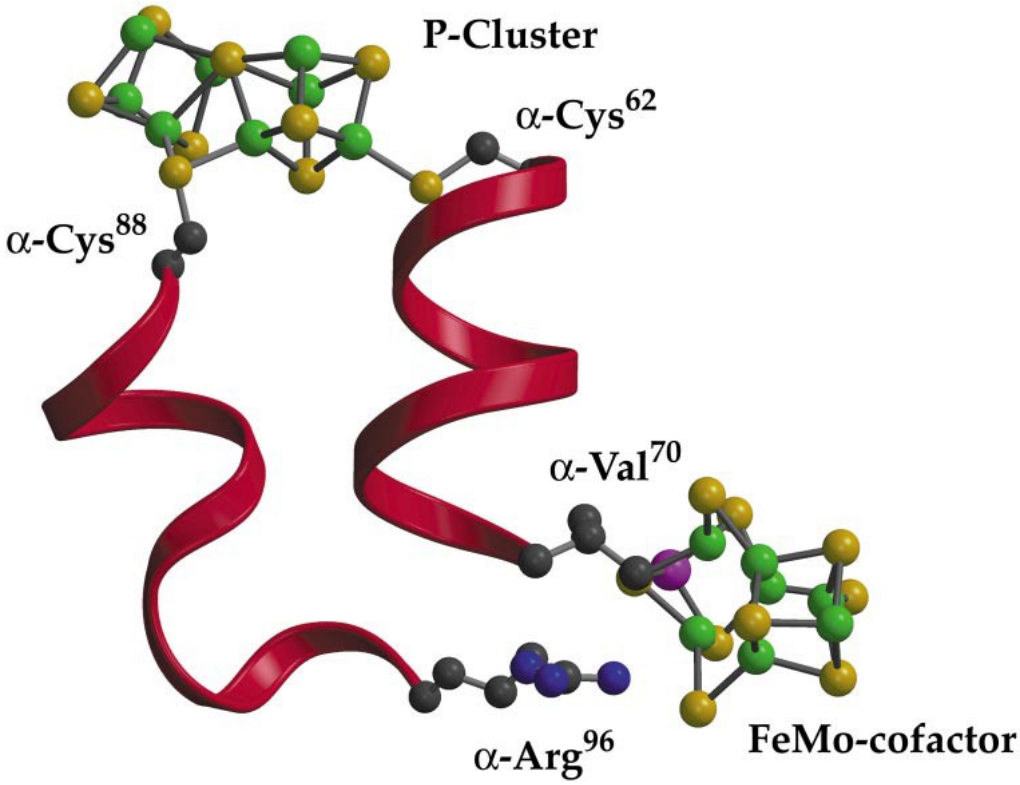
Previous calculations have revealed some steric interference between diffusing N_2 in the Fe2--Fe6 reaction zone and the immediately contiguous protein (mainly the side chain of Val70) in its resting position.[9, 36] This is consistent with experimental data on mutation of residue 70 to larger side chains.[11, 12] Therefore I postulated that the protein dynamics can accommodate and incorporate movement of Val70 and adjacent residues away from FeMo-co.[9] Figure S3 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 (Figure S3 (a)), of which Ser67 → Gln151 is most relevant because it is almost opposite Val70. Figure S3 (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)

Figure 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 β-sheet (yellow ribbons). The α-helical section of the closest chain (residues 63-68, orange ribbon) changes to π-turn (cyan ribbon) through Val70, before looping back to the β-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].

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Coordinates

Translation of Fe numbering

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

N2-ready-b to Fe2-NH-NH-b

Figure 8, scheme A

structure, S **spin densities**	**filename** **coordinates**
reactant **N2-ready-b** (S=3/2) Fe(139) -2.160 Fe(140) -0.780 Fe(141) -2.516 Fe(142) 2.833 Fe(143) 2.642	bm52exp335fe2captgfcc_3_53279.75 C1 -7.743059129 -5.371461377 1.284427864 C2 -8.133275354 -6.516148670 0.341551306 C3 -8.558870076 -3.443578655 2.569954210 C4 -7.921118997 -3.704146315 3.930900564 C5 -7.490425080 -5.295633855 5.738135417 C6 -5.965589326 -5.415346506 5.670442014 C7 -3.991998645 -5.721476590 4.275258441 C8 -3.474336594 -4.281928472 4.314199205

Fe(144) 1.302
Fe(145) 1.630

C9	-3.887657664	-1.959217976	3.622666474
C10	-3.904029576	-1.331800140	5.025457137
C11	-4.926689473	-1.171643357	7.203993622
C12	-3.861563285	-1.724985405	8.162293119
C13	-2.858435722	-3.741857868	9.137476902
C14	-1.389974937	-4.054659511	8.815113152
C15	0.243455989	-4.790410687	7.124784822
C16	0.983385936	-3.646537888	6.421643713
C17	0.652725362	-1.402989197	5.396346367
C18	0.781020264	-0.187061587	6.329758838
C19	-0.251387846	-1.194058385	4.164411842
C20	0.011494495	0.148584187	3.470942003
C21	-0.139087266	-2.405957125	3.230137207
C22	-0.360154154	1.560090019	7.623554997
C23	0.003514966	1.232421140	9.083103656
C24	-1.690218736	2.339174693	7.486656056
C25	-1.758917572	3.505562199	8.478134594
C26	-1.868703291	2.849813796	6.050047427
C27	-0.409005622	-0.092354400	11.069799295
C28	1.055793641	-0.363047230	11.350500077
C29	5.897340558	-11.606417796	3.746233093
C30	6.516226970	-10.327569929	3.191238644
C31	6.791423123	-7.902624677	3.682768739
C32	8.014172886	-7.509569494	4.531631968
C33	5.614226420	-6.943658293	3.923619263
C34	5.949508455	-5.502360497	3.549593513
C35	4.704893734	-4.620189086	3.493436662
C36	4.893408390	-2.117065688	3.499847812
C37	10.270470882	-6.554698756	4.479339838
C38	10.487611284	-5.058678544	4.467684203
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C40	-5.701337621	-1.244891435	-1.132130336
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C46	-6.358198335	1.604980237	-3.435069927
C47	-9.424992457	0.935927543	-0.008886384
C48	-9.027107060	0.953684046	1.470247728
C49	-7.322210635	0.436324756	3.152041921
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C51	-4.606179651	3.048138071	2.434073319
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C53	-4.020417954	3.483157920	1.082104493
C54	-3.401268860	2.421814514	0.236365816
C55	-2.971297243	1.141311222	0.474311656
C56	-2.540236273	1.610800761	-1.661784929
C57	-6.850909480	6.035022238	3.245721958
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C63	9.234547806	1.627989661	3.419779108
C64	10.270888893	0.531642154	3.251766518
C65	7.841592930	0.979868527	3.239819574
C66	6.709041871	1.956272211	3.456067913
C67	6.136716762	2.149915613	4.725666926
C68	6.198496428	2.709596058	2.383264854
C69	5.088102297	3.057220999	4.921261191
C70	5.168578614	3.632047573	2.565793935
C71	4.605781227	3.796983024	3.833857879
C72	5.368696636	6.853342375	-1.399966903
C73	4.314437161	7.954809708	-1.608109763
C74	4.694983684	5.516176409	-1.105111146
C75	3.308191387	9.543603090	-3.209590214
C76	1.833636366	9.163928019	-3.371181264
C77	0.214709633	7.267757544	-3.331339237
C78	-0.249383864	6.926449323	-1.891732171
C79	0.243975352	6.022710609	-4.245678087
C80	-1.010152722	5.146988382	-4.351142575
C81	-2.154870759	5.683624476	-5.227092864
C82	-3.676662619	7.603244130	-4.745461611
C83	0.274851485	5.979050174	0.303311882
C84	0.117703569	7.197763216	1.224159479
C85	1.276218142	5.013930311	0.971160641
C86	1.199117861	9.261864708	1.969342814
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	C91	-2.157196674	11.016004652	-1.899289261
	C92	-4.070911895	11.948129190	2.224413582
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	C94	-4.729642817	10.681527425	2.838452724
	C95	-4.971213890	9.608138743	1.801951123
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	C97	-4.006996996	8.625065895	1.526551929
	C98	-6.357045018	8.671609174	0.028021857
	C99	-4.183047466	7.696268326	0.496092216
	C100	-5.358627232	7.736889681	-0.247716159
	C101	4.088445247	-3.984904423	-9.001253520
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	C103	1.208061528	-2.193632983	-7.246404500
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	H187	2.674206675	5.322847925	2.326013532
	H188	3.216863371	4.681787014	4.863341741
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	H260	-4.695861549	7.772170080	-2.962384389
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	H266	-6.098301797	-0.957242464	-3.064791517
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	H288	5.048202671	-5.096979122	-10.413912906
	H289	3.511675745	-5.583549057	-10.123754292
	H290	5.483728369	4.767425154	-0.960716399
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	H293	4.095223869	5.592812343	-0.187465235
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transition state (S=3/2) Fe(139) -2.287 Fe(140) -0.369 Fe(141) -2.543 Fe(142) 2.576 Fe(143) 2.508 Fe(144) 1.648 Fe(145) 1.562	bm52exp335fe2captgfe.car_1 C1 -7.731913308 -5.366053776 1.276023179 C2 -8.137645330 -6.510085396 0.338259933 C3 -8.534035593 -3.433208156 2.564460021 C4 -7.894562426 -3.692703616 3.924567204 C5 -7.461431207 -5.279736448 5.734650468 C6 -5.936623155 -5.400134129 5.667394522 C7 -3.962264294 -5.707229341 4.273955256 C8 -3.451681999 -4.264672851 4.303877819 C9 -3.877000776 -1.948259323 3.599945203 C10 -3.891173613 -1.315308427 5.000793486 C11 -4.911763368 -1.151308630 7.181795075 C12 -3.854230444 -1.702751655 8.148991602 C13 -2.848886774 -3.718291689 9.127171996 C14 -1.382155039 -4.038379789 8.803068839 C15 0.238514962 -4.809097053 7.117576133 C16 0.974803902 -3.656468351 6.425173494 C17 0.636318355 -1.426342302 5.382583833 C18 0.768375198 -0.210575245 6.315013015 C19 -0.243272851 -1.219512512 4.131488347 C20 0.017278201 0.122618059 3.427640441 C21 -0.090788687 -2.410084897 3.175601262 C22 -0.356105535 1.543433725 7.610953293 C23 0.013363769 1.220183868 9.070979942 C24 -1.683296251 2.327419102 7.477766960 C25 -1.746518145 3.494171562 8.468945891 C26 -1.863728860 2.837435480 6.041115252 C27 -0.401173140 -0.089554644 11.069111503 C28 1.064569246 -0.355416666 11.349443516 C29 5.896472676 -11.596603222 3.752955298 C30 6.516233454 -10.321251666 3.193763436 C31 6.786307735 -7.894740459 3.681092115 C32 8.007058375 -7.498609120 4.531363803 C33 5.605586588 -6.941144653 3.922102862 C34 5.939799079 -5.499759427 3.551819054 C35 4.698634559 -4.613838113 3.505639260 C36 4.902122156 -2.114451473 3.533413111 C37 10.268169690 -6.557518976 4.483857235 C38 10.496157601 -5.063351139 4.471677094 C39 -5.328150199 -2.676785056 -1.559147082 C40 -5.691877232 -1.243482004 -1.124263758 C41 -3.790503658 -2.823001728 -1.503129818 C42 -3.244471464 -4.261040386 -1.621129895 C43 -2.977948156 -4.747635748 -3.046404285 C44 -6.183521003 0.995951941 -2.029680502 C45 -7.274170878 1.450500133 -1.049308064 C46 -6.361750712 1.604290952 -3.426387939 C47 -9.428106953 0.926123949 -0.003564137 C48 -9.031041994 0.947300344 1.475706128 C49 -7.325131576 0.437977144 3.158894813 C50 -6.154756261 1.400063633 3.369814227 C51 -4.604386654 3.043324085 2.435136653 C52 -5.046473048 4.351803337 3.132539393 C53 -4.021214193 3.477316011 1.081706618 C54 -3.403533195 2.414894774 0.235724602 C55 -2.976732657 1.132884547 0.472329203 C56 -2.545103460 1.602883032 -1.663283261 C57 -6.849746888 6.031619081 3.240219900 C58 -6.756860543 6.187062302 4.757008685 C59 -8.321904386 6.086161499 2.770025297 C60 -8.945202182 7.446525575 2.656377597 C61 -8.870396521 8.549985317 3.483956990 C62 -10.199635638 8.966527105 1.760585349 C63 9.238103587 1.624707088 3.434018187 C64 10.267406561 0.521211676 3.266402840 C65 7.843771076 0.980771576 3.252985684 C66 6.711350031 1.957853662 3.466366346 C67 6.140922360 2.156137536 4.736246713 C68 6.195397568 2.703129989 2.390796790 C69 5.089202657 3.060164392 4.929338927 C70 5.161697466 3.622287129 2.570704518 C71 4.601016656 3.792018501 3.839091990 C72 5.370967457 6.864111350 -1.392886733 C73 4.314855580 7.962136242 -1.602033823 C74 4.700400547 5.521840931 -1.098318844 C75 3.307609288 9.545057958 -3.207832773 C76 1.832658710 9.167001565 -3.367692373

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	O453	2.422499537	5.700533174	1.459530922
	O454	0.858468085	11.624937482	2.300232196
	O455	-2.508215256	13.587383032	0.577347736
	O456	-3.268842968	10.989380369	-1.342644149
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	O458	-5.509749618	6.834196724	-1.325338684
	O459	1.757884888	-4.571170617	-8.767032065
	O460	-0.271107092	-0.738026190	-8.510913153
	O461	2.109033378	3.598410313	-8.531567901
	O462	5.885667991	4.311432381	-9.108681389
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	O464	-1.456028884	-6.607792905	-6.012172225
	O465	0.463075311	-5.773764416	-6.787467714
	O466	-3.996278081	2.320553500	-8.406579950
	O467	9.938892733	-5.405871987	-3.701458232
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	O469	0.282303158	-6.301372878	-1.318725454
	O470	-0.258200886	-7.408011626	0.560379780
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	O473	5.076809001	-5.852874389	-1.284009367
	O474	5.011159869	-7.575430919	0.156895328
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	O477 6.979205532 -4.569441683 0.371304195 O478 -4.379482878 4.744665723 -2.453724378 O479 7.709013140 -10.434405696 -2.511207372 O480 7.509579758 -8.633067344 -0.090678846 S481 3.582139296 4.970207173 -2.471213214 S482 2.102699325 1.944562848 -3.409106267 S483 2.069453183 -3.405584884 -3.632098442 S484 3.879790164 1.952111535 -0.330969943 S485 0.550067183 -0.850856507 -1.858533628 S486 4.034173270 -0.801685954 -5.534808940 S487 3.400445400 -3.518513976 -0.214545707 S488 5.670060770 1.680665719 -3.342862266 S489 5.677217169 -3.073335577 -3.019959856 S490 6.326410791 -0.859230339 -0.337435455 end
product **Fe2-NH-NH-b** (S=3/2) Fe(139) -2.282 Fe(140) 0.074 Fe(141) -2.537 Fe(142) 2.756 Fe(143) 3.159 Fe(144) 2.189 Fe(145) -0.927	bm52exp335fe2captgfe.car_8 C1 -7.721286179 -5.351656198 1.294045201 C2 -8.053320278 -6.513299232 0.350157161 C3 -8.635875864 -3.469374434 2.582681114 C4 -8.008588737 -3.736869922 3.949195159 C5 -7.605778978 -5.343513669 5.750267501 C6 -6.079685160 -5.461699389 5.698405679 C7 -4.094232931 -5.774215002 4.314961404 C8 -3.546571124 -4.345525146 4.361707261 C9 -3.926863885 -2.002983512 3.737134439 C10 -3.935909396 -1.403955260 5.150872361 C11 -4.968584772 -1.265560226 7.325015418 C12 -3.886755345 -1.839931921 8.252696268 C13 -2.872780683 -3.875181926 9.170777017 C14 -1.393325273 -4.118893290 8.838682264 C15 0.267175951 -4.686369269 7.109023352 C16 0.991652211 -3.554932203 6.375611290 C17 0.657214195 -1.288207590 5.387156022 C18 0.782241900 -0.071067978 6.320210671 C19 -0.253732230 -1.076278961 4.160663409 C20 0.090334839 0.238133199 3.454070200 C21 -0.191412789 -2.312151222 3.253057880 C22 -0.394119044 1.627230762 7.657048406 C23 -0.040335923 1.262423192 9.110648510 C24 -1.734324009 2.389527084 7.528432548 C25 -1.813121977 3.547495413 8.528855521 C26 -1.925107602 2.906179723 6.095876687 C27 -0.445269058 -0.142533316 11.043197823 C28 1.020280501 -0.415120319 11.318163252 C29 5.879318168 -11.628841620 3.689099989 C30 6.515077154 -10.348804289 3.159863923 C31 6.817947874 -7.937261288 3.686218218 C32 8.044127952 -7.547193923 4.531009404 C33 5.640052943 -6.980379686 3.934111808 C34 5.965222295 -5.537304060 3.556052388 C35 4.710066025 -4.669382396 3.484387944 C36 4.862365752 -2.166121060 3.480334291 C37 10.285111035 -6.552104744 4.464972968 C38 10.461136168 -5.049989334 4.467827612 C39 -5.325222460 -2.664471069 -1.587692197 C40 -5.689042833 -1.230058729 -1.159000238 C41 -3.789073148 -2.811156891 -1.525209253 C42 -3.241375412 -4.248520625 -1.639606060 C43 -2.981664822 -4.747746878 -3.061546938 C44 -6.161004023 1.008997080 -2.071734693 C45 -7.246821375 1.474266418 -1.090785521 C46 -6.337013770 1.614023068 -3.470068185 C47 -9.406021856 0.973299292 -0.045547027 C48 -9.009490648 0.971587843 1.433972795 C49 -7.310301961 0.412874523 3.109066438 C50 -6.122740074 1.351062757 3.327818142 C51 -4.599628367 3.035453219 2.417424302 C52 -5.029731095 4.350407224 3.113472754 C53 -4.002895357 3.458799637 1.066465139 C54 -3.359200668 2.397409796 0.235469661 C55 -2.877289147 1.137456892 0.487390368 C56 -2.456191099 1.598983790 -1.649198411 C57 -6.826875793 6.033932880 3.255958916 C58 -6.703249143 6.204504820 4.769010644 C59 -8.310824446 6.095625505 2.821839605 C60 -8.919957582 7.461549811 2.694370370 C61 -8.859968713 8.562082087 3.527288171 C62 -10.136665690 8.995458376 1.768960462 C63 9.253105661 1.653097393 3.401354840 C64 10.296444550 0.565344697 3.223702158

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C67	6.125677960	2.129308521	4.689513687
C68	6.243102637	2.744563438	2.363068683
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C70	5.221100556	3.674871467	2.547029251
C71	4.634848394	3.817858576	3.807213744
C72	5.384762976	6.866615681	-1.438811240
C73	4.328391475	7.968703716	-1.635605895
C74	4.708112052	5.529557157	-1.154652085
C75	3.302121960	9.549404500	-3.233379027
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C78	-0.246927656	6.921978951	-1.911296362
C79	0.241868265	6.020178731	-4.265381932
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C138	3.595899919	-0.692890739	-2.244994686
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Fe141	4.986187569	0.509146219	-1.490631859
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	Fe145	2.221732583	-2.268300353	-1.826147770
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	H148	-9.717042738	-4.845338354	1.357505053
	H149	-8.766664883	-6.158354188	-0.411234431
	H150	-8.599790677	-7.260274982	0.952137850
	H151	-7.998036004	-2.723180094	2.086564900
	H152	-8.774289160	-5.637551141	3.967754457
	H153	-9.624575571	-3.016748852	2.739311095
	H154	-8.026299187	-6.307542804	6.064725268
	H155	-6.130010034	-5.861467410	3.677982228
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	H159	-3.856578784	-6.229241050	3.343886135
	H160	-4.821246208	-0.177679289	7.301783128
	H161	-5.720406123	-2.339912698	5.606681958
	H162	-3.586470025	-6.346314186	5.100445732
	H163	-4.645566513	-1.461521676	3.106582796
	H164	-4.275233506	-3.742433903	7.558709484
	H165	-5.954185723	-1.479774680	7.761351934
	H166	-0.591721846	-3.197632156	3.765612204
	H167	-0.800788102	-2.155962629	2.347063934
	H168	0.837000424	-2.521790838	2.929922345
	H169	-1.283138029	-0.986953364	4.534628474
	H170	-3.331282136	-4.856793029	9.363416117
	H171	-1.938860619	2.091956982	5.358779425
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	H175	-0.092917204	1.101431582	4.107204031
	H176	9.322478758	2.008942963	4.446981708
	H177	-2.879725903	3.444325567	6.007752855
	H178	-2.758307428	4.091665312	8.388902328
	H179	-1.115169579	3.604870753	5.828768873
	H180	-0.985292233	4.256570461	8.369506972
	H181	-2.549571441	1.678178804	7.754925474
	H182	0.425031100	2.286688626	7.332703303
	H183	-1.279497507	0.098001677	6.434656080
	H184	-0.535016663	0.366972917	2.559662130
	H185	1.591243216	4.229727920	0.184241196
	H186	0.774832894	4.484823296	1.751561660
	H187	2.693239709	5.316585416	2.280501759
	H188	3.235082929	4.693909424	4.827919903
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	H190	6.661019857	2.608817356	1.362998966
	H191	6.473012488	1.531960645	5.537640921
	H192	-0.730079887	-2.502157705	6.457519631
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	H206	-0.798733236	-5.362626291	-8.952788572
	H207	-3.107900626	-4.346705395	-7.195886085
	H208	-3.092851019	1.050548176	-9.788274153
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	H221	-2.311855168	-4.324267545	-1.057364906
	H222	-3.834721842	2.585718485	3.066210548
	H223	-2.885180324	0.542024692	1.390962302
	H224	-8.117543760	0.758875066	3.769286838

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	H257	-2.658169033	4.844430046	-5.757133068
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	H263	-1.387812218	4.869757505	-3.371032737
	H264	-8.354003372	-0.189020109	-1.513729662
	H265	3.632392436	10.017067545	-4.170633710
	H266	-6.075653627	-0.945694396	-3.094465144
	H267	0.531426658	6.358235554	-5.273833282
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	H273	-5.757977978	-3.322616266	-0.810783285
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	H276	-0.491918679	8.020046586	-3.720085877
	H277	-1.750313867	6.340243552	-6.009260142
	H278	-0.677841877	4.199132629	-4.831675463
	H279	-3.589325047	5.870184029	-3.667749038
	H280	0.788097306	8.881731084	2.935912380
	H281	-0.457508320	9.755526621	0.100412016
	H282	-0.068712991	12.616560607	0.406169274
	H283	2.265640811	9.404847922	2.091719279
	H284	-2.439607191	10.644077911	1.730540638
	H285	4.599789178	-3.048429078	-9.173668581
	H286	4.572197764	-4.490426764	-8.140145827
	H287	7.925734037	-5.248518702	-5.169372304
	H288	5.026945442	-5.140000334	-10.398214728
	H289	3.490142831	-5.616780256	-10.094226009
	H290	5.492867317	4.773416570	-1.026118686
	H291	5.731684406	7.414488603	0.497206883
	H292	4.814603228	8.094869690	-3.630360684
	H293	4.118781855	5.599904259	-0.230139993
	H294	6.828867582	8.027061363	-0.549436738
	H295	5.404635858	2.764999078	-6.857034940
	H296	5.987922644	6.772220813	-2.354857670
	H297	5.337284370	-7.048631467	4.992156485
	H298	7.079944923	-7.915581285	2.620526734
	H299	3.615069841	1.352984307	-6.880835680
	H300	5.148856114	-0.144827543	3.239280235
	H301	0.545206189	1.561509579	-8.708838394
	H302	-1.169874553	-2.178004386	-4.359243769
	H303	0.429427713	2.094862129	-7.026122430
	H304	4.266242922	-4.539911291	4.478334523

H305	2.064340485	0.069399358	-6.584295844
H306	3.948489727	-5.151250407	2.850429775
H307	4.798590786	-7.343082038	3.322067260
H308	6.450718193	-5.519472241	2.569486245
H309	6.671201229	-5.090562347	4.273681645
H310	-5.195876438	-0.790230493	-6.454107633
H311	5.949871562	-9.508821416	4.885061004
H312	4.977750806	-11.792222479	3.079754013
H313	0.189948163	-0.097473900	-4.126679109
H314	6.264353096	-11.888946499	5.696262093
H315	4.700535641	-12.159153957	5.291544960
H316	5.518683855	-3.392557782	2.008400411
H317	-0.710896507	2.062084259	-4.875697066
H318	-3.394013748	-2.082663034	-5.466022967
H319	7.669893639	-9.927669234	-1.678065599
H320	6.640127891	-7.636963602	-3.737336975
H321	6.645081604	-8.156383176	-0.124433535
H322	6.801510831	-10.526620268	-2.817934311
H323	4.888561651	2.585192674	-9.578484882
H324	6.359174235	-5.009918498	-0.214637721
H325	2.316769249	-7.676606013	0.827369096
H326	3.275974333	-1.993144510	-7.670037371
H327	3.078669241	-9.150430255	-0.818423205
H328	3.121164029	-7.036946753	-7.049934359
H329	2.257514083	-5.542869658	-5.196067219
H330	6.574447843	-12.452283814	3.450195170
H331	5.737061662	-1.115766252	1.909682391
H332	8.349512699	-5.802630944	0.813752480
H333	7.258076798	-3.755826402	-0.073078353
H334	8.978484715	-6.867502243	2.792705267
H335	3.650675166	-2.743826969	5.083598153
H336	3.799593476	-8.271266119	-3.662927400
H337	5.002667456	-8.572538718	-2.404684086
H338	1.939601581	-8.653447838	-2.080344840
H339	1.344581850	-2.122501727	-6.178384759
H340	-2.958744265	2.178044480	-5.999461867
H341	-5.112919941	0.985644090	-6.599892361
H342	2.347962828	-5.915126480	0.597135531
H343	8.512397382	-7.333444796	0.580394683
H344	7.399804898	-9.253100446	0.661951037
H345	4.127999629	-1.092239490	5.046331141
H346	5.582892975	-7.677932633	-6.707794478
H347	6.565928795	-5.973563866	-3.178708144
H348	0.456891312	-2.929471557	-7.503664767
H349	4.283096346	4.137511947	-7.006840908
H350	7.791050694	0.158083388	3.929594817
H351	7.815762723	0.569919157	2.199211724
H352	9.017072637	-6.904430366	-6.444324137
H353	8.257269061	-8.133748916	-5.676359835
H354	10.312682412	-8.557305608	-1.657038438
H355	8.599236494	-8.267867857	-3.128753008
H356	11.724387122	-7.564929781	-3.812692458
H357	10.173326095	-6.832585784	-1.264494071
H358	10.561007620	0.353189642	2.159165518
H359	-2.972576619	13.210165568	3.713918148
H360	10.247657506	-6.873847538	5.520838597
H361	9.513655599	-4.461431058	4.404572804
H362	-4.700108258	12.313952138	1.400633378
H363	-4.087177051	10.303594027	3.654399579
H364	-5.676299266	11.001433853	3.291730806
H365	1.157642116	-3.203845474	-1.322981563
H366	3.492129047	-0.414786300	0.809992769
H367	-6.435020150	6.814682221	-1.569853452
H368	0.846726090	-1.156592753	0.907622262
H369	-1.774342517	-0.189184058	-0.817820766
Mo370	3.837939754	-4.369352734	-2.494697919
N371	-6.931772420	-7.161810157	-0.303637173
N372	-8.799374580	-4.651656707	1.751426836
N373	-8.214976961	-4.963899224	4.485565417
N374	-5.537088944	-5.821290653	4.508143918
N375	-4.273702700	-3.415219945	3.691933074
N376	-4.930859654	-1.804679208	5.976349752
N377	-3.685564522	-3.182030782	8.180093350
N378	-1.089575749	-4.380892461	7.533588307
N379	0.242296026	-2.452789751	6.158543987
N380	-0.386378256	0.450140959	6.787293535
N381	-0.695746212	0.206898603	9.657955882
N382	5.500189025	-11.552029193	5.106442652
N383	6.411427885	-9.296689805	3.994235667
N384	5.026799911	-3.361495811	2.906176544

	N385	4.279358786	-2.032509241	4.691116810
	N386	5.314454152	-1.067908296	2.848988159
	N387	9.058522496	-6.984716974	3.827005355
	N388	-5.852931945	-2.939046411	-2.930173806
	N389	-1.935597942	-5.580742630	-3.210735823
	N390	-6.069177675	-0.435423428	-2.195017286
	N391	-8.336381578	0.679939488	-0.984216413
	N392	-7.840225813	0.353071105	1.760127021
	N393	-5.693429154	2.086833665	2.256682880
	N394	-3.085255552	2.650042823	-1.104050259
	N395	-2.334260963	0.668215125	-0.694583280
	N396	-6.313496088	4.722759235	2.876995585
	N397	-9.720499196	7.745933219	1.598939753
	N398	-9.636415563	9.526110213	2.920696487
	N399	9.481640654	2.691249218	2.393257758
	N400	6.295242718	7.182092443	-0.327096572
	N401	4.213274475	8.469178528	-2.901030760
	N402	1.552184553	7.845543002	-3.368998771
	N403	-3.173315153	6.395571055	-4.458082886
	N404	-3.390993935	8.222070858	-5.905935584
	N405	-4.449521237	8.235247352	-3.843890100
	N406	0.665478336	6.323450711	-1.093060406
	N407	0.971128480	8.204018877	0.968338852
	N408	-0.363633553	10.602447172	0.660544076
	N409	-1.883590648	10.374311807	-3.057848598
	N410	-2.742133819	11.614800016	1.708827927
	N411	4.079651112	-4.791532696	-10.235312990
	N412	2.458462928	-2.563502271	-7.900212668
	N413	1.388590050	0.246186300	-7.345452193
	N414	3.478556679	2.217003285	-7.413250866
	N415	-1.705257853	-3.010982315	-10.095129277
	N416	-3.263450304	-1.173171194	-8.522161093
	N417	8.141707626	-7.161577031	-5.979394199
	N418	4.263162204	-5.692701817	-4.407705996
	N419	3.700077514	-6.697859817	-6.286440117
	N420	9.249735275	-7.478639997	-3.072930009
	N421	0.133227907	2.199539932	0.021455328
	N422	2.513442558	-0.481917196	0.479953803
	N423	0.910139567	1.517919248	-0.420657494
	N424	1.800587393	-1.065409715	1.325809931
	O425	-6.565711206	-5.087799678	1.673292927
	O426	-7.346302277	-2.854745432	4.522772967
	O427	-5.398657697	-5.248718677	6.714972881
	O428	-2.512907574	-4.056931977	4.984391089
	O429	-3.067623888	-0.595183923	5.513464844
	O430	-3.278812418	-1.104840779	9.050740162
	O431	-0.553685349	-4.114953288	9.747971042
	O432	2.175667017	-3.699008389	6.013440266
	O433	1.895491990	0.378367023	6.632066880
	O434	0.809679804	1.904206075	9.749665905
	O435	1.516389746	-0.337661151	12.432228296
	O436	7.047496820	-10.339999453	2.031137072
	O437	8.062786209	-7.733315991	5.760469738
	O438	11.546992081	-4.499142085	4.554006874
	O439	-5.622116877	-0.830209680	0.019639204
	O440	-3.717322702	-4.424678556	-4.022752185
	O441	-7.098944728	2.516744782	-0.428087311
	O442	-6.324707086	3.051821917	-3.375366623
	O443	-9.757336191	1.512455922	2.259523879
	O444	-5.594766991	1.422230970	4.441748614
	O445	-4.224483152	5.042221865	3.743688886
	O446	-6.517561534	7.268638720	5.332712677
	O447	10.810256968	-0.051401310	4.145172676
	O448	3.600436546	4.727112103	3.924589127
	O449	3.624877753	8.388513099	-0.699969545
	O450	0.982379927	10.068459522	-3.549905567
	O451	-1.402282941	7.186906865	-1.544344119
	O452	-0.689916120	7.137850936	2.140234460
	O453	2.454832521	5.678497049	1.403002147
	O454	0.853233289	11.581591455	2.336778454
	O455	-2.491542841	13.586460953	0.591748848
	O456	-3.250126402	11.030768822	-1.347042812
	O457	-4.949440223	13.709872373	3.615770901
	O458	-5.491070591	6.837563513	-1.319451294
	O459	1.744884872	-4.577585276	-8.740854969
	O460	-0.248202900	-0.745621779	-8.608625572
	O461	2.103232930	3.620935048	-8.554616508
	O462	5.725395238	4.404032972	-9.179969750
	O463	-4.983800346	-2.623898282	-8.884484510
	O464	-1.483730472	-6.631991138	-6.024608864

	O465	0.434802751	-5.760891740	-6.758001296
	O466	-3.959932271	2.329299132	-8.458803236
	O467	9.924106138	-5.407448035	-3.699250196
	O468	12.670720644	-6.990590282	-2.097591323
	O469	0.312083499	-6.208850162	-1.346455847
	O470	-0.227622587	-7.291098903	0.548031426
	O471	5.161088240	-10.881689763	-3.316236634
	O472	2.900162193	-10.921939129	-3.284228301
	O473	5.088101825	-5.768026551	-1.376715010
	O474	5.049470257	-7.435199995	0.125154150
	O475	2.614110268	-6.075080689	-2.125584985
	O476	8.946709607	-6.558376604	1.034183758
	O477	6.964755915	-4.546263583	0.418692053
	O478	-4.375936315	4.741274628	-2.450357380
	O479	7.755894748	-10.416651125	-2.526645618
	O480	7.516462479	-8.631897021	-0.101756814
	S481	3.577099106	5.013903075	-2.526989699
	S482	1.897009587	1.755483749	-3.222009581
	S483	2.078781826	-3.350790193	-3.734420484
	S484	3.813893794	1.934461842	-0.254559756
	S485	0.454511953	-1.070140461	-1.616229677
	S486	4.031811001	-0.691356012	-5.587215438
	S487	3.418738547	-3.423975275	-0.344498471
	S488	5.629205281	1.718700298	-3.255960625
	S489	5.688023503	-3.082186669	-3.221131548
	S490	6.280932553	-0.886992320	-0.344622033
	end			

N2-ready-b to Fe2-NH-N-b

Figure 8, scheme B

reactant **N2-ready-b** (S=3/2)	bm52capexp347tf.car_6			
Fe(139) 2.323	C1	-7.734132254	-5.365012870	1.276604324
Fe(140) 0.829	C2	-8.135095861	-6.509447875	0.337697222
Fe(141) 1.454	C3	-8.542266679	-3.434833417	2.564909518
Fe(142) -2.433	C4	-7.904586471	-3.695017532	3.925772290
Fe(143) 2.902	C5	-7.472554345	-5.284144170	5.734509489
Fe(144) -0.986	C6	-5.947916775	-5.405031596	5.666779587
Fe(145) -1.531	C7	-3.974526188	-5.711226394	4.272326340
	C8	-3.463373429	-4.269210762	4.307144548
	C9	-3.885620162	-1.950437432	3.606634116
	C10	-3.901796370	-1.318888201	5.007921171
	C11	-4.919983835	-1.157099533	7.188735644
	C12	-3.858294284	-1.708688511	8.151596358
	C13	-2.853486602	-3.724262863	9.129149260
	C14	-1.385905188	-4.041750987	8.806375371
	C15	0.241012621	-4.801885830	7.120788103
	C16	0.982416258	-3.653212613	6.426467315
	C17	0.644416790	-1.415925815	5.389442684
	C18	0.775525275	-0.201278523	6.324885437
	C19	-0.264658075	-1.208764723	4.160292876
	C20	-0.036905604	0.146219692	3.472912911
	C21	-0.136328042	-2.410321624	3.213774049
	C22	-0.357769944	1.551163263	7.617731148
	C23	0.008562942	1.227270525	9.077618505
	C24	-1.686391070	2.332687168	7.481501753
	C25	-1.751986824	3.500047822	8.471891701
	C26	-1.865845570	2.842350687	6.044621656
	C27	-0.404814848	-0.087708881	11.070366157
	C28	1.060151879	-0.355847498	11.351400638
	C29	5.897438758	-11.599477165	3.752826448
	C30	6.515109272	-10.322149756	3.194306265
	C31	6.786739860	-7.895604748	3.681069787
	C32	8.007947931	-7.501893869	4.531792055
	C33	5.607863757	-6.938593258	3.920726303
	C34	5.942207087	-5.497114713	3.547990804
	C35	4.698287110	-4.614084078	3.497846122
	C36	4.896158159	-2.113339938	3.511592423
	C37	10.268917503	-6.559342420	4.484984470
	C38	10.493878240	-5.064815543	4.471899230
	C39	-5.329820364	-2.675253566	-1.562613377
	C40	-5.692860319	-1.241572292	-1.128322278
	C41	-3.791583510	-2.821571234	-1.504547471
	C42	-3.244071881	-4.259171157	-1.621370396
	C43	-2.976988784	-4.746658587	-3.046282312
	C44	-6.183862568	0.997988729	-2.033538777
	C45	-7.273827425	1.452982777	-1.052564252

	C46	-6.361075868	1.606883985	-3.430021444
	C47	-9.427898140	0.930348014	-0.006368156
	C48	-9.030699668	0.950428247	1.472806420
	C49	-7.325362296	0.439000544	3.155712533
	C50	-6.155049882	1.401097318	3.366966910
	C51	-4.605098204	3.045594005	2.433939223
	C52	-5.046854949	4.354197080	3.130952169
	C53	-4.020209484	3.480098665	1.081377156
	C54	-3.402965453	2.417824599	0.234845671
	C55	-2.981172767	1.133960065	0.469933970
	C56	-2.547690903	1.605324815	-1.665338245
	C57	-6.849273214	6.033666756	3.239678770
	C58	-6.755909664	6.189682711	4.756428035
	C59	-8.322537089	6.088922064	2.772004571
	C60	-8.945267436	7.449626443	2.657513575
	C61	-8.871846814	8.553007491	3.485323793
	C62	-10.198693907	8.969697737	1.760179309
	C63	9.237686775	1.628910296	3.433849452
	C64	10.269303793	0.527581377	3.265961846
	C65	7.845389819	0.982658597	3.250750780
	C66	6.709668151	1.956636238	3.461767442
	C67	6.139784088	2.155645915	4.731869500
	C68	6.191397600	2.699411147	2.385384554
	C69	5.087851758	3.059368520	4.924798834
	C70	5.156803308	3.617619937	2.564950327
	C71	4.598311884	3.789521948	3.834032190
	C72	5.383191279	6.858685926	-1.385085721
	C73	4.324989542	7.959208293	-1.597045966
	C74	4.698852697	5.531125550	-1.098262093
	C75	3.314160314	9.544044228	-3.201954322
	C76	1.839594791	9.161968384	-3.365236751
	C77	0.216065770	7.270657545	-3.328513642
	C78	-0.253169829	6.927332490	-1.890722879
	C79	0.245003373	6.024673038	-4.242902343
	C80	-1.008079362	5.147104815	-4.349479383
	C81	-2.152316458	5.682633518	-5.226592316
	C82	-3.673260666	7.602827886	-4.743899390
	C83	0.268942385	5.982485670	0.306372589
	C84	0.115119622	7.202671269	1.225957410
	C85	1.265350621	5.013469963	0.975877320
	C86	1.199353237	9.267336187	1.966153954
	C87	0.555887218	10.610767544	1.657731085
	C88	-0.855685449	11.875464793	0.127184267
	C89	-2.130072045	12.430592283	0.810150004
	C90	-1.016197506	11.883580059	-1.395343550
	C91	-2.159569859	11.012427401	-1.899336108
	C92	-4.073956176	11.948219387	2.222095369
	C93	-3.987108932	13.049918640	3.270989674
	C94	-4.731361174	10.680565451	2.835046187
	C95	-4.972190027	9.607000122	1.798443365
	C96	-6.154531881	9.602678048	1.042679860
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	C98	-6.360069336	8.666298447	0.028020718
	C99	-4.182222166	7.697152038	0.490687385
	C100	-5.359638504	7.734431240	-0.250435150
	C101	4.086761212	-3.979197898	-8.998739705
	C102	2.660105600	-3.726271740	-8.544102819
	C103	1.204285542	-2.191311682	-7.242924338
	C104	0.707097328	-0.834022967	-7.754558396
	C105	1.122611543	1.587715882	-7.711900278
	C106	2.296165926	2.542446861	-7.913440391
	C107	4.575760538	3.213399525	-7.404814295
	C108	5.169628498	3.373799853	-8.789356960
	C109	-2.761123087	-3.492841836	-9.150223984
	C110	-3.787153112	-2.402996715	-8.816533210
	C111	-2.270604897	-4.170100407	-7.849189053
	C112	-1.538112897	-5.490303357	-8.150473374
	C113	-0.860099292	-6.019182701	-6.906957997
	C114	-4.191700907	-0.084983649	-8.157008905
	C115	-3.713913388	1.199562033	-8.804585987
	C116	-4.569408299	0.045820740	-6.660166883
	C117	-3.334177572	0.058411715	-5.805593412
	C118	-2.607642526	1.245799583	-5.610187954
	C119	-2.798045732	-1.153073672	-5.339158204
	C120	-1.328521151	1.199621888	-5.046967464
	C121	-1.520808387	-1.197900945	-4.774076507
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	C123	7.914975220	-6.235921298	-4.770929301
	C124	9.096912089	-6.322801127	-3.794110912
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	C132	2.092256707	-6.968840807	0.121029270
	C133	3.011757127	-7.093483184	-1.132748949
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	C137	4.467741997	-6.827072245	-0.710496413
	C138	3.588716262	-0.695288962	-2.229729898
	Fe139	3.876336923	-2.025436924	-3.720688680
	Fe140	2.222662579	0.818331092	-1.518946186
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	Fe145	2.163085956	-2.417726232	-1.752547046
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	H148	-9.705256833	-4.783381044	1.389267487
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	H152	-8.655826823	-5.599457795	3.964906408
	H153	-9.506458834	-2.935170931	2.727607164
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	H159	-3.732824791	-6.171849720	3.305123593
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	H162	-3.452931733	-6.263996653	5.062238776
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	H175	0.224455283	0.942382578	4.184321632
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	H178	-2.693760729	4.050239947	8.330755294
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	H181	-2.510642858	1.633416672	7.712312273
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	H194	0.833322036	-5.100194341	7.994946250
	H195	-1.855537935	-4.538997676	6.840400642
	H196	-2.836696628	-3.093945609	10.026206782
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	H199	-0.750692759	0.717122935	11.739474441
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transition state (S=3/2) Fe(139) 2.294 Fe(140) 0.312 Fe(141) 2.662 Fe(142) -2.179 Fe(143) 2.218 Fe(144) -1.656 Fe(145) -1.368	bm52exp347fe2captc.car_1 C1 -7.726107802 -5.362056808 1.269789384 C2 -8.143236077 -6.505349136 0.336393130 C3 -8.517556493 -3.424937404 2.559853486 C4 -7.873679835 -3.684015788 3.917598677 C5 -7.440176386 -5.265656629 5.731886879 C6 -5.915418146 -5.384901146 5.665334464 C7 -3.940342178 -5.695603168 4.274368235 C8 -3.434744913 -4.251244696 4.297053611 C9 -3.868623639 -1.938796336 3.582953512 C10 -3.883517792 -1.301065710 4.982085476 C11 -4.899961952 -1.135679752 7.165105438 C12 -3.848424273 -1.685817322 8.139357415 C13 -2.841452443 -3.701342695 9.118878483 C14 -1.375893485 -4.026000358 8.792613153 C15 0.234116757 -4.824506046 7.110512170 C16 0.969563986 -3.666575484 6.425330127 C17 0.625354985 -1.443142225 5.373706147 C18 0.762079973 -0.227605900 6.304748802 C19 -0.258546582 -1.238926717 4.123997054 C20 -0.029481323 0.119340754 3.432667185 C21 -0.083432406 -2.422900404 3.161697552 C22 -0.352329401 1.531453487 7.601027393 C23 0.021356447 1.212770871 9.061564870 C24 -1.678030134 2.318349594 7.469911216 C25 -1.737988637 3.485306941 8.461008216 C26 -1.860722091 2.828037281 6.033441924 C27 -0.397320419 -0.087783401 11.068440003 C28 1.069522768 -0.350129592 11.346572381 C29 5.898749184 -11.590525922 3.760432675 C30 6.516793777 -10.316365146 3.195974266 C31 6.781953327 -7.887470314 3.678151937 C32 8.001495472 -7.489711483 4.529997008 C33 5.598010032 -6.938012543 3.918533158

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product **Fe2-NH-N-b** (=3/2) Fe(139) 2.314 Fe(140) 0.042 Fe(141) 2.653 Fe(142) -2.372 Fe(143) 2.260 Fe(144) -2.021 Fe(145) -0.659	bm52capexp347tb.car_5 C1 -7.724180018 -5.349614055 1.284866943 C2 -8.061496756 -6.512273481 0.344053157 C3 -8.634050408 -3.468731807 2.579142324 C4 -8.002458282 -3.737334638 3.943437791 C5 -7.587767472 -5.344068582 5.741653737 C6 -6.060825446 -5.452271775 5.687893874 C7 -4.074204184 -5.762964302 4.304618258 C8 -3.535691684 -4.330069349 4.343083075 C9 -3.937312198 -1.992126992 3.717018757 C10 -3.951898394 -1.382600844 5.126807943 C11 -4.974174016 -1.255980752 7.306403565 C12 -3.884444920 -1.820852897 8.230578943 C13 -2.868836363 -3.849831165 9.161581496 C14 -1.393323641 -4.107588242 8.826931540 C15 0.260509713 -4.694100355 7.098397003 C16 0.978366115 -3.559959133 6.363433512 C17 0.632691007 -1.295493495 5.371935641 C18 0.765290541 -0.087369627 6.315248101 C19 -0.290225475 -1.078599381 4.153697696 C20 -0.032350895 0.283503882 3.501638103 C21 -0.160632649 -2.257508526 3.179847263

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	C34	5.962487472	-5.542229945	3.557167043
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	C36	4.879137557	-2.178439242	3.561364969
	C37	10.287352239	-6.554612949	4.464515963
	C38	10.464455155	-5.052720967	4.465193604
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	C40	-5.686908388	-1.232852814	-1.153953357
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	C42	-3.237508423	-4.250926121	-1.632937418
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	C44	-6.163081392	1.005203858	-2.066446631
	C45	-7.248351554	1.469485294	-1.084574951
	C46	-6.342429635	1.610038194	-3.464555483
	C47	-9.406602355	0.966487876	-0.037684665
	C48	-9.010920785	0.969079433	1.442094187
	C49	-7.315133196	0.419386030	3.122190302
	C50	-6.137679100	1.370945040	3.344069943
	C51	-4.598050910	3.036534683	2.428498151
	C52	-5.031103164	4.347412679	3.125565911
	C53	-4.010747075	3.470115711	1.077806370
	C54	-3.372319424	2.413683173	0.238706809
	C55	-2.886901179	1.153815722	0.484156099
	C56	-2.470484968	1.630212896	-1.651489384
	C57	-6.822892407	6.033229638	3.246034207
	C58	-6.703577589	6.202986006	4.759989505
	C59	-8.306513989	6.093053895	2.808050020
	C60	-8.920363294	7.457397202	2.684536313
	C61	-8.859565792	8.557045734	3.518434636
	C62	-10.148151266	8.987952115	1.768045432
	C63	9.251864290	1.659019264	3.394567439
	C64	10.291484072	0.567319136	3.219214232
	C65	7.862778823	0.996675284	3.220134494
	C66	6.721621873	1.961442135	3.437853147
	C67	6.136290533	2.135399815	4.704207250
	C68	6.221051190	2.730684709	2.371465162
	C69	5.086738916	3.041026477	4.903608565
	C70	5.192659533	3.653570240	2.559195817
	C71	4.619923535	3.802948942	3.824656500
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	C73	4.321453820	7.953736912	-1.623547039
	C74	4.719082063	5.519924247	-1.095943640
	C75	3.302632048	9.536537814	-3.223142492
	C76	1.827839516	9.159254050	-3.386293970
	C77	0.207777970	7.259540437	-3.338041765
	C78	-0.257130194	6.914603914	-1.898878536
	C79	0.243251972	6.014214887	-4.253589271
	C80	-1.006942260	5.132578666	-4.366741801
	C81	-2.153626873	5.674893345	-5.236375669
	C82	-3.681480430	7.585569226	-4.753064205
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	C84	0.114969882	7.173591922	1.225198760
	C85	1.300345581	5.004530151	0.948876346
	C86	1.188419680	9.237833715	1.985246472
	C87	0.555837989	10.587469640	1.680129337
	C88	-0.837761297	11.866720232	0.142595447
	C89	-2.116067090	12.420397084	0.816600969
	C90	-0.980962444	11.875849507	-1.381735122
	C91	-2.139513476	11.034744314	-1.904286084
	C92	-4.062818817	11.937505782	2.220944595
	C93	-3.980866519	13.046887021	3.262488119
	C94	-4.723523466	10.674793170	2.837776480
	C95	-4.964822393	9.600849753	1.802349543
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	C99	-4.180920563	7.678143370	0.511302189
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	C104	0.677607016	-0.825394553	-7.816066798
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	C121	-1.571979223	-1.259985726	-4.684666029
	C122	-0.803104237	-0.101879176	-4.533643607
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	H150	-8.609377935	-7.255572150	0.948892518
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	H172	-1.461989723	-0.254996014	9.179598577
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	H265	3.635533914	10.004019094	-4.159369495
	H266	-6.077296708	-0.949255157	-3.089163081
	H267	0.536641683	6.354484347	-5.260174442
	H268	-3.396445395	6.954170810	0.287728945
	H269	3.335405310	10.302569203	-2.434693821
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	H292	4.823592723	8.089087086	-3.615218173
	H293	4.139492568	5.607618688	-0.167650761
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	H295	5.383793674	2.771984881	-6.844625471
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	H297	5.337157755	-7.056065895	4.990971532
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	H303	0.409410479	2.091166448	-7.044033384
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	H309	6.670396196	-5.097062415	4.273885459
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	H322	6.795594483	-10.536421437	-2.814085557
	H323	4.885736085	2.581162378	-9.577146634
	H324	6.362745695	-5.024956919	-0.209225831
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	H333	7.242612923	-3.755313857	-0.088579911
	H334	8.980178487	-6.870913764	2.792316458
	H335	3.607103369	-2.769147716	5.114602434
	H336	3.786943860	-8.279439717	-3.663208972
	H337	5.003016486	-8.581686238	-2.416911047
	H338	1.944052033	-8.665951589	-2.068667862
	H339	1.326123288	-2.136843761	-6.201818374
	H340	-2.921887967	2.153997205	-5.985186238
	H341	-5.092865615	0.985933056	-6.573208504

H342	2.361290584	-5.916491521	0.587747509
H343	8.507461281	-7.342970681	0.581302931
H344	7.404657585	-9.262363080	0.661097831
H345	4.159028171	-1.140336380	5.155840959
H346	5.566112312	-7.713081506	-6.696808232
H347	6.560076601	-5.997450146	-3.176527137
H348	0.435535688	-2.934604180	-7.533665777
H349	4.262164214	4.141886197	-7.019192889
H350	7.796292915	0.163340190	3.934643940
H351	7.808755497	0.573498330	2.204361609
H352	9.028661713	-6.874325185	-6.441712741
H353	8.268553939	-8.116777636	-5.694492406
H354	10.310853466	-8.570227538	-1.663495051
H355	8.590512492	-8.268535506	-3.129077085
H356	11.714887988	-7.567598063	-3.821081095
H357	10.173897770	-6.846761202	-1.265117223
H358	10.559628052	0.356757813	2.155153230
H359	-2.971684747	13.205216793	3.710429911
H360	10.249216968	-6.874307013	5.520459557
H361	9.517894604	-4.462399638	4.406429132
H362	-4.698684764	12.306214110	1.398528573
H363	-4.084998349	10.295742139	3.650915337
H364	-5.673594230	10.994038617	3.289752418
H365	1.299281625	-3.239025157	-1.106444776
H366	3.773686898	-0.598893807	0.495073182
H367	-6.435478551	6.807671506	-1.573477627
H368	0.365651290	-1.158637666	-0.127454644
H369	-1.815261666	-0.172757543	-0.841833789
Mo370	3.850926407	-4.380930141	-2.482142583
N371	-6.943616468	-7.166131613	-0.310304455
N372	-8.800559828	-4.649778739	1.746900754
N373	-8.200777469	-4.966296524	4.478170587
N374	-5.516509684	-5.818111462	4.500574411
N375	-4.277232797	-3.406017900	3.680306087
N376	-4.936280375	-1.797013489	5.958770408
N377	-3.681408547	-3.163455626	8.166173096
N378	-1.096377198	-4.392096584	7.524846090
N379	0.222573869	-2.466059035	6.135274816
N380	-0.397424457	0.438455515	6.791722742
N381	-0.681937072	0.202758358	9.656955698
N382	5.500478551	-11.549938806	5.116306637
N383	6.415495072	-9.298836300	3.998495129
N384	5.023518368	-3.356354167	2.948128196
N385	4.275903470	-2.070832753	4.763402429
N386	5.388952305	-1.072988465	2.984982055
N387	9.060836130	-6.988004669	3.826775017
N388	-5.849448021	-2.941456678	-2.925237362
N389	-1.929109411	-5.580158157	-3.204372459
N390	-6.068419298	-0.438760181	-2.189932400
N391	-8.336336780	0.673709421	-0.975890214
N392	-7.841417960	0.352778700	1.771854887
N393	-5.689413194	2.085093419	2.265432184
N394	-3.095632993	2.677628459	-1.097425062
N395	-2.344706647	0.695610437	-0.701739800
N396	-6.308896416	4.724211581	2.867955079
N397	-9.728323703	7.740099369	1.594110799
N398	-9.643011049	9.519124874	2.917538905
N399	9.474791654	2.691832810	2.379575717
N400	6.311598994	7.197468824	-0.333983955
N401	4.205804124	8.448553106	-2.891969866
N402	1.547599846	7.839623501	-3.351464301
N403	-3.168662625	6.392112833	-4.457865327
N404	-3.380757094	8.221108397	-5.902930867
N405	-4.444913757	8.231686867	-3.843411530
N406	0.655830846	6.329657089	-1.071777927
N407	0.966932275	8.210710920	0.984365196
N408	-0.359971028	10.600405338	0.664805780
N409	-1.882909791	10.366157848	-3.061922733
N410	-2.740652626	11.608100422	1.705938990
N411	4.078200350	-4.791553155	-10.244813946
N412	2.436099074	-2.561409130	-7.929734185
N413	1.370874522	0.241392603	-7.362210044
N414	3.466264632	2.216424665	-7.417667564
N415	-1.716625289	-3.008056922	-10.095884112
N416	-3.274146969	-1.174546137	-8.518748639
N417	8.150871389	-7.141526233	-5.986803798
N418	4.271291072	-5.681739974	-4.419914081
N419	3.699224663	-6.694493456	-6.293282906
N420	9.246139271	-7.483845358	-3.073751726
N421	0.218474460	2.184143009	0.177677161

	N422	2.733142212	-0.379292825	0.522615683
	N423	1.032800296	1.620117177	-0.358424097
	N424	2.058649676	-0.657245216	1.463815490
	O425	-6.567030268	-5.084925561	1.657354801
	O426	-7.342743336	-2.853310116	4.516972386
	O427	-5.379737119	-5.224538179	6.701282280
	O428	-2.497255621	-4.034382878	4.954034484
	O429	-3.096861543	-0.556982579	5.480673588
	O430	-3.272868325	-1.078220344	9.018336893
	O431	-0.548918363	-4.096306180	9.731890886
	O432	2.165813989	-3.700956646	6.010562409
	O433	1.882633948	0.350993582	6.628635727
	O434	0.818125569	1.905081172	9.744624649
	O435	1.534259718	-0.330987371	12.429988426
	O436	7.050965270	-10.348913496	2.038362361
	O437	8.061720314	-7.727453712	5.762039392
	O438	11.551909547	-4.503739376	4.546019357
	O439	-5.618347883	-0.832280543	0.024242270
	O440	-3.710804784	-4.422567871	-4.015993673
	O441	-7.100492471	2.513463393	-0.424452851
	O442	-6.325895956	3.048112473	-3.370966887
	O443	-9.760143582	1.511910228	2.265053353
	O444	-5.629292314	1.466426210	4.464750119
	O445	-4.234528197	5.036009595	3.769415907
	O446	-6.519854543	7.267893182	5.323405390
	O447	10.796472087	-0.055483437	4.141707183
	O448	3.580758449	4.706361775	3.945751078
	O449	3.616174171	8.374829226	-0.690282668
	O450	0.985006125	10.062629429	-3.545684464
	O451	-1.417890957	7.167090021	-1.542194579
	O452	-0.699035622	7.151864865	2.157363509
	O453	2.444351594	5.705379249	1.443234165
	O454	0.857953289	11.594185552	2.331877680
	O455	-2.494249289	13.576982275	0.582594055
	O456	-3.246625661	11.016451289	-1.347434895
	O457	-4.949285546	13.701117432	3.613348598
	O458	-5.491354534	6.831178839	-1.323892038
	O459	1.737068738	-4.588252579	-8.754495484
	O460	-0.284053713	-0.739947655	-8.608470763
	O461	2.089574637	3.623851847	-8.552732856
	O462	5.771364838	4.373488049	-9.161039166
	O463	-4.994164902	-2.625923417	-8.880747417
	O464	-1.498658122	-6.610423176	-6.020998736
	O465	0.434499741	-5.785800971	-6.770802646
	O466	-3.956454065	2.328740417	-8.438635196
	O467	9.923773794	-5.411329456	-3.692189231
	O468	12.671192204	-7.007670743	-2.106950982
	O469	0.331746040	-6.215678518	-1.361075970
	O470	-0.227099785	-7.281838662	0.537281710
	O471	5.156746848	-10.895990785	-3.317721155
	O472	2.896069285	-10.929773155	-3.292709188
	O473	5.113158779	-5.794138943	-1.356313237
	O474	5.057466649	-7.466757168	0.140673580
	O475	2.638049908	-6.094365837	-2.123467153
	O476	8.943818592	-6.568012538	1.033892105
	O477	6.974183493	-4.549412060	0.411043032
	O478	-4.372405353	4.735710897	-2.452549282
	O479	7.749233425	-10.428240193	-2.519463893
	O480	7.514633981	-8.640228947	-0.102410906
	S481	3.559655387	4.953450117	-2.419070619
	S482	1.956683026	1.740094192	-3.314387900
	S483	2.030819032	-3.364581749	-3.653779136
	S484	3.888700340	2.089514499	-0.418613056
	S485	0.532818410	-0.942405114	-1.478012819
	S486	3.955720914	-0.712691873	-5.594986109
	S487	3.485449418	-3.439312660	-0.299348299
	S488	5.581733402	1.739680080	-3.358019839
	S489	5.677364627	-3.070909278	-3.242103465
	S490	6.208138356	-0.863012177	-0.292984338
	end			

Fe2-NH-N-b to Fe2-NH-NH-b

Figure 8, scheme B

reactant **Fe2-NH-N-b** (S=3/2) Fe(139) 2.314	bm52capexp347tb.car_5			
	C1	-7.724180018	-5.349614055	1.284866943
	C2	-8.061496756	-6.512273481	0.344053157

Fe(140) 0.042 Fe(141) 2.653 Fe(142) -2.372 Fe(143) 2.260 Fe(144) -2.021 Fe(145) -0.659	C3	-8.634050408	-3.468731807	2.579142324
	C4	-8.002458282	-3.737334638	3.943437791
	C5	-7.587767472	-5.344068582	5.741653737
	C6	-6.060825446	-5.452271775	5.687893874
	C7	-4.074204184	-5.762964302	4.304618258
	C8	-3.535691684	-4.330069349	4.343083075
	C9	-3.937312198	-1.992126992	3.717018757
	C10	-3.951898394	-1.382600844	5.126807943
	C11	-4.974174016	-1.255980752	7.306403565
	C12	-3.884444920	-1.820852897	8.230578943
	C13	-2.868836363	-3.849831165	9.161581496
	C14	-1.393323641	-4.107588242	8.826931540
	C15	0.260509713	-4.694100355	7.098397003
	C16	0.978366115	-3.559959133	6.363433512
	C17	0.632691007	-1.295493495	5.371935641
	C18	0.765290541	-0.087369627	6.315248101
	C19	-0.290225475	-1.078599381	4.153697696
	C20	-0.032350895	0.283503882	3.501638103
	C21	-0.160632649	-2.257508526	3.179847263
	C22	-0.390399132	1.620197875	7.654730609
	C23	-0.030896397	1.259588126	9.107672701
	C24	-1.727980871	2.387856579	7.528695986
	C25	-1.805230421	3.546991079	8.527795325
	C26	-1.919499736	2.902552610	6.095646913
	C27	-0.428556040	-0.145120423	11.042528553
	C28	1.038077392	-0.414279161	11.316704697
	C29	5.877269858	-11.629380356	3.698582984
	C30	6.517035774	-10.352806735	3.166334420
	C31	6.819988458	-7.939753753	3.686471575
	C32	8.044919616	-7.546481806	4.531594386
	C33	5.639862978	-6.985905087	3.932910217
	C34	5.962487472	-5.542229945	3.557167043
	C35	4.706201681	-4.676835921	3.495305263
	C36	4.879137557	-2.178439242	3.561364969
	C37	10.287352239	-6.554612949	4.464515963
	C38	10.464455155	-5.052720967	4.465193604
	C39	-5.323174963	-2.667134607	-1.582470885
	C40	-5.686908388	-1.232852814	-1.153953357
	C41	-3.786851704	-2.813882132	-1.518334165
	C42	-3.237508423	-4.250926121	-1.632937418
	C43	-2.974998797	-4.747770235	-3.055103102
	C44	-6.163081392	1.005203858	-2.066446631
	C45	-7.248351554	1.469485294	-1.084574951
	C46	-6.342429635	1.610038194	-3.464555483
	C47	-9.406602355	0.966487876	-0.037684665
	C48	-9.010920785	0.969079433	1.442094187
	C49	-7.315133196	0.419386030	3.122190302
	C50	-6.137679100	1.370945040	3.344069943
	C51	-4.598050910	3.036534683	2.428498151
	C52	-5.031103164	4.347412679	3.125565911
	C53	-4.010747075	3.470115711	1.077806370
	C54	-3.372319424	2.413683173	0.238706809
	C55	-2.886901179	1.153815722	0.484156099
	C56	-2.470484968	1.630212896	-1.651489384
	C57	-6.822892407	6.033229638	3.246034207
	C58	-6.703577589	6.202986006	4.759989505
	C59	-8.306513989	6.093053895	2.808050020
	C60	-8.920363294	7.457397202	2.684536313
	C61	-8.859565792	8.557045734	3.518434636
	C62	-10.148151266	8.987952115	1.768045432
	C63	9.251864290	1.659019264	3.394567439
	C64	10.291484072	0.567319136	3.219214232
	C65	7.862778823	0.996675284	3.220134494
	C66	6.721621873	1.961442135	3.437853147
	C67	6.136290533	2.135399815	4.704207250
	C68	6.221051190	2.730684709	2.371465162
	C69	5.086738916	3.041026477	4.903608565
	C70	5.192659533	3.653570240	2.559195817
	C71	4.619923535	3.802948942	3.824656500
	C72	5.381458306	6.858237216	-1.422226678
	C73	4.321453820	7.953736912	-1.623547039
	C74	4.719082063	5.519924247	-1.095943640
	C75	3.302632048	9.536537814	-3.223142492
	C76	1.827839516	9.159254050	-3.386293970
	C77	0.207777970	7.259540437	-3.338041765
	C78	-0.257130194	6.914603914	-1.898878536
	C79	0.243251972	6.014214887	-4.253589271
	C80	-1.006942260	5.132578666	-4.366741801
	C81	-2.153626873	5.674893345	-5.236375669
	C82	-3.681480430	7.585569226	-4.753064205

C83	0.282167338	5.963309822	0.295858212
C84	0.114969882	7.173591922	1.225198760
C85	1.300345581	5.004530151	0.948876346
C86	1.188419680	9.237833715	1.985246472
C87	0.555837989	10.587469640	1.680129337
C88	-0.837761297	11.866720232	0.142595447
C89	-2.116067090	12.420397084	0.816600969
C90	-0.980962444	11.875849507	-1.381735122
C91	-2.139513476	11.034744314	-1.904286084
C92	-4.062818817	11.937505782	2.220944595
C93	-3.980866519	13.046887021	3.262488119
C94	-4.723523466	10.674793170	2.837776480
C95	-4.964822393	9.600849753	1.802349543
C96	-6.135581971	9.610969907	1.029511188
C97	-4.007223022	8.608090678	1.540999408
C98	-6.337626839	8.676329179	0.012849187
C99	-4.180920563	7.678143370	0.511302189
C100	-5.346592094	7.729637904	-0.247205124
C101	4.064598023	-3.999528122	-9.013637072
C102	2.637675622	-3.734931841	-8.566118081
C103	1.182093774	-2.174972073	-7.293639176
C104	0.677607016	-0.825394553	-7.816066798
C105	1.079023427	1.603120161	-7.773262192
C106	2.265892214	2.548100555	-7.957019451
C107	4.559677664	3.175396369	-7.454468398
C108	5.104927909	3.400557608	-8.850927775
C109	-2.749343897	-3.495595513	-9.173289906
C110	-3.773181293	-2.399052346	-8.854466631
C111	-2.260076139	-4.159554014	-7.866109747
C112	-1.545927379	-5.492421772	-8.157216112
C113	-0.884351508	-6.027256522	-6.908010361
C114	-4.168746896	-0.078779703	-8.193522481
C115	-3.688554197	1.204830978	-8.841018895
C116	-4.527901067	0.048769567	-6.691986167
C117	-3.297572370	0.029494798	-5.826768044
C118	-2.545332203	1.197987829	-5.612858666
C119	-2.811372977	-1.190441147	-5.327730794
C120	-1.302226462	1.127171008	-4.975290614
C121	-1.571979223	-1.259985726	-4.684666029
C122	-0.803104237	-0.101879176	-4.533643607
C123	7.941604575	-6.284139638	-4.806600085
C124	9.108697681	-6.347370610	-3.808669603
C125	6.620939152	-6.602068810	-4.088768346
C126	5.367395311	-6.412033227	-4.879362352
C127	5.010603575	-7.041252097	-6.054447354
C128	3.282863167	-5.885918892	-5.290574056
C129	10.315296647	-7.557204079	-2.094985337
C130	11.672617218	-7.340719274	-2.728106847
C131	0.638048850	-6.838003399	-0.216319131
C132	2.128479128	-6.881116225	0.104937526
C133	3.048848505	-7.047228724	-1.141314458
C134	2.959990542	-8.498952227	-1.679388121
C135	3.993474275	-8.858138255	-2.749658999
C136	4.009136574	-10.351599389	-3.140978666
C137	4.506202295	-6.767546090	-0.731646740
C138	3.598246602	-0.700290494	-2.249825070
Fe139	3.800698734	-1.995141653	-3.804567280
Fe140	2.270308319	0.588063551	-1.205745125
Fe141	5.014529702	0.502319861	-1.556712290
Fe142	3.742100480	0.527610513	-3.792508263
Fe143	3.770709808	2.736796542	-2.526360073
Fe144	4.797827885	-2.066564927	-1.469364188
Fe145	2.284667965	-2.298559609	-1.749772693
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H165	-5.956254605	-1.477848443	7.746724644
H166	-0.472219919	-3.197453172	3.657464322
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H174	0.997016148	0.365191348	3.136282399
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H178	-2.751051372	4.090624778	8.387754656
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H184	-0.688798599	0.416684967	2.628065248
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H188	3.230626090	4.685725598	4.855391755
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	H246	-3.439564936	3.529428591	-1.611839287
	H247	-5.106438605	4.156833749	-2.795381765
	H248	-6.683907439	3.393078766	-4.208395565
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	H253	-1.186274750	12.916133514	-1.679348939
	H254	-0.910301584	10.209482730	-3.354601201
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	H256	-3.764795143	9.144535071	-6.078943800
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	H259	-3.101493980	8.537862871	2.148710481
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	H261	1.065266710	5.372464270	-3.897971100
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	H264	-8.352345930	-0.196250265	-1.503742145
	H265	3.635533914	10.004019094	-4.159369495
	H266	-6.077296708	-0.949255157	-3.089163081
	H267	0.536641683	6.354484347	-5.260174442
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	H269	3.335405310	10.302569203	-2.434693821
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	H276	-0.495144620	8.011355893	-3.710731065
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	H278	-0.673684292	4.195522412	-4.835734731
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	O450	0.985006125	10.062629429	-3.545684464
	O451	-1.417890957	7.167090021	-1.542194579
	O452	-0.699035622	7.151864865	2.157363509
	O453	2.444351594	5.705379249	1.443234165
	O454	0.857953289	11.594185552	2.331877680
	O455	-2.494249289	13.576982275	0.582594055
	O456	-3.246625661	11.016451289	-1.347434895
	O457	-4.949285546	13.701117432	3.613348598
	O458	-5.491354534	6.831178839	-1.323892038
	O459	1.737068738	-4.588252579	-8.754495484
	O460	-0.284053713	-0.739947655	-8.608470763
	O461	2.089574637	3.623851847	-8.552732856
	O462	5.771364838	4.373488049	-9.161039166
	O463	-4.994164902	-2.625923417	-8.880747417
	O464	-1.498658122	-6.610423176	-6.020998736
	O465	0.434499741	-5.785800971	-6.770802646
	O466	-3.956454065	2.328740417	-8.438635196
	O467	9.923773794	-5.411329456	-3.692189231
	O468	12.671192204	-7.007670743	-2.106950982
	O469	0.331746040	-6.215678518	-1.361075970
	O470	-0.227099785	-7.281838662	0.537281710
	O471	5.156746848	-10.895990785	-3.317721155
	O472	2.896069285	-10.929773155	-3.292709188
	O473	5.113158779	-5.794138943	-1.356313237
	O474	5.057466649	-7.466757168	0.140673580
	O475	2.638049908	-6.094365837	-2.123467153
	O476	8.943818592	-6.568012538	1.033892105
	O477	6.974183493	-4.549412060	0.411043032
	O478	-4.372405353	4.735710897	-2.452549282
	O479	7.749233425	-10.428240193	-2.519463893
	O480	7.514633981	-8.640228947	-0.102410906
	S481	3.559655387	4.953450117	-2.419070619
	S482	1.956683026	1.740094192	-3.314387900

	S483	2.030819032	-3.364581749	-3.653779136
	S484	3.888700340	2.089514499	-0.418613056
	S485	0.532818410	-0.942405114	-1.478012819
	S486	3.955720914	-0.712691873	-5.594986109
	S487	3.485449418	-3.439312660	-0.299348299
	S488	5.581733402	1.739680080	-3.358019839
	S489	5.677364627	-3.070909278	-3.242103465
	S490	6.208138356	-0.863012177	-0.292984338
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	C1	-7.722453428	-5.348611426	1.286579128
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	C3	-8.638537529	-3.470284755	2.579761157
	C4	-8.008342463	-3.738509538	3.944716018
	C5	-7.596452165	-5.346240200	5.742817008
	C6	-6.069682163	-5.457518546	5.690893966
	C7	-4.081910161	-5.765460127	4.309076021
	C8	-3.541855302	-4.333336914	4.350042685
	C9	-3.940150004	-1.994903075	3.725464414
	C10	-3.953535390	-1.389391285	5.136965253
	C11	-4.976415043	-1.261471019	7.316891588
	C12	-3.888161217	-1.829987391	8.240813530
	C13	-2.872843213	-3.861644801	9.165366068
	C14	-1.395966156	-4.112114941	8.829166601
	C15	0.257900675	-4.686751250	7.095902213
	C16	0.977748286	-3.555153446	6.358170720
	C17	0.635925071	-1.286564638	5.369273602
	C18	0.765081043	-0.078923569	6.314517097
	C19	-0.282475641	-1.071242803	4.148699392
	C20	-0.007116868	0.280039590	3.480547271
	C21	-0.164636544	-2.259352248	3.186249755
	C22	-0.396611997	1.624140089	7.654542223
	C23	-0.037450284	1.260787729	9.106438370
	C24	-1.734345895	2.391742930	7.531559796
	C25	-1.808666363	3.550105775	8.532304678
	C26	-1.928576132	2.909669170	6.100019543
	C27	-0.432937511	-0.149647296	11.036641522
	C28	1.033619399	-0.416510402	11.311334428
	C29	5.876786247	-11.631946851	3.693545882
	C30	6.517408109	-10.354588769	3.163069149
	C31	6.820903263	-7.941878168	3.685188151
	C32	8.046284432	-7.548558844	4.529716280
	C33	5.640963094	-6.987912108	3.932629247
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	C35	4.706801776	-4.678595323	3.498324263
	C36	4.878640226	-2.180369271	3.555304919
	C37	10.287335139	-6.553687994	4.463633332
	C38	10.462649597	-5.051625362	4.465536602
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	C40	-5.686704468	-1.230828883	-1.156413733
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	C42	-3.236950221	-4.248648825	-1.633443731
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	C44	-6.160845713	1.007029605	-2.069886623
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	C48	-9.010069357	0.971088952	1.437777945
	C49	-7.314136556	0.417952769	3.117224268
	C50	-6.133434749	1.364466459	3.339136934
	C51	-4.597086961	3.034642476	2.427114312
	C52	-5.029744363	4.345226143	3.124725786
	C53	-4.008129308	3.469500943	1.077390420
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	C56	-2.462376857	1.629153407	-1.647530815
	C57	-6.819088422	6.033006101	3.244923021
	C58	-6.699011205	6.203950534	4.758426583
	C59	-8.303602667	6.094781692	2.811142103
	C60	-8.916274347	7.459502253	2.687341383
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	C64	10.294414927	0.571894512	3.215196281
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	C66	6.721587053	1.962640103	3.434541103
	C67	6.135580349	2.136070316	4.700759067
	C68	6.222186235	2.733524996	2.368821939
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C78	-0.257025470	6.913331499	-1.900356792
C79	0.243447826	6.012755125	-4.255647703
C80	-1.006610361	5.131350209	-4.369056682
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C91	-2.139522593	11.036964739	-1.905719328
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C94	-4.722688498	10.674480106	2.837860375
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C96	-6.134823027	9.611553582	1.029368120
C97	-4.006908243	8.607657135	1.541717762
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C118	-2.535981335	1.191388193	-5.612698299
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C121	-1.578102564	-1.267225887	-4.675503284
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C124	9.108485009	-6.349753898	-3.810180704
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	H161	-5.725230295	-2.345555462	5.603323119
	H162	-3.571260476	-6.332011564	5.096667772
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	H164	-4.278259087	-3.735267273	7.555440602
	H165	-5.958958176	-1.482113735	7.756874662
	H166	-0.483322327	-3.193990225	3.667957410
	H167	-0.807620698	-2.100924921	2.305860013
	H168	0.861262664	-2.368474839	2.814467177
	H169	-1.313315679	-1.038672487	4.527897151
	H170	-3.332849699	-4.840800283	9.366039553
	H171	-1.953268884	2.095203466	5.363893652
	H172	-1.468431864	-0.255160146	9.177175433
	H173	-1.762303010	3.207624169	9.575767813
	H174	1.026943250	0.354490314	3.121479348
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	H176	9.325638175	2.021595998	4.434020220
	H177	-2.879017726	3.455676121	6.016443157
	H178	-2.754098756	4.095039167	8.394450288
	H179	-1.114108609	3.600892401	5.827133525
	H180	-0.980833030	4.258918179	8.370745084
	H181	-2.550889607	1.682650848	7.760542882
	H182	0.423880204	2.279502736	7.325361792
	H183	-1.294179553	0.106562846	6.426524095
	H184	-0.662077977	0.408498465	2.606538550
	H185	1.612503942	4.259556347	0.199575787
	H186	0.782478826	4.485275775	1.763538817
	H187	2.687451138	5.332024109	2.310075527
	H188	3.228362406	4.683407805	4.851738739
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	H191	6.495140719	1.546406945	5.549104237
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	H195	-1.838738060	-4.427118570	6.816589531
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	H235	-8.373393515	5.636655688	1.811721720
	H236	-6.170807434	2.022847792	1.361636179
	H237	-7.017269893	-0.580223990	3.471423632
	H238	-9.832846507	1.962060590	-0.243834715
	H239	-2.116152062	1.535571772	-2.673680618
	H240	-10.201630741	0.228241801	-0.185876358
	H241	10.288689282	3.256706050	2.635857078
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	H243	1.555020170	5.982630530	-1.443323208
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	H246	-3.438004757	3.525958074	-1.613214124
	H247	-5.102729518	4.156781371	-2.795560547
	H248	-6.681034955	3.395210927	-4.211265148
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	H250	-5.513101807	1.255289906	-4.104837801
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	H253	-1.184200866	12.917039460	-1.677455179
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	H256	-3.771500550	9.140459875	-6.081485430
	H257	-2.651576073	4.845610127	-5.763635517
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product **Fe2-NH-NH-b** (S=3/2) Fe(139) 2.157 Fe(140) 0.124 Fe(141) 1.808 Fe(142) -2.496 Fe(143) 3.118 Fe(144) -2.272 Fe(145) 0.158	bm526hxexpfe2n2h347.car_3 C1 -7.846386180 -5.297110566 0.398072742 C2 -8.143862136 -6.352244558 -0.675333493 C3 -8.797508797 -3.498651014 1.776362652 C4 -8.271010379 -3.877213859 3.157412469 C5 -8.007457509 -5.626235196 4.849072337 C6 -6.481185230 -5.747832790 4.897267034 C7 -4.412273148 -5.994425769 3.623270520 C8 -3.860366921 -4.577761349 3.801890397 C9 -4.185736500 -2.193524672 3.311325510 C10 -4.272594391 -1.704330724 4.764641932 C11 -5.440435737 -1.698901828 6.873599794 C12 -4.419917761 -2.340612982 7.824831506 C13 -3.481069492 -4.442831771 8.669621769 C14 -1.988970219 -4.697546478 8.411446999 C15 -0.241614601 -5.220797354 6.755151109 C16 0.529946007 -4.058667669 6.122192942 C17 0.284427339 -1.724014033 5.283499082 C18 0.380951656 -0.585851720 6.315121778 C19 -0.537003911 -1.402468305 4.020095745 C20 -0.134423011 -0.041848949 3.442171273 C21 -0.412199084 -2.551331362 3.010778261 C22 -0.833606404 1.050706222 7.695314256 C23 -0.565534940 0.574750755 9.135652032 C24 -2.153852717 1.844931912 7.555279727 C25 -2.269624081 2.924315523 8.637593562 C26 -2.264047154 2.470639201 6.158706725 C27 -1.123928605 -0.930480835 10.951011849 C28 0.321130291 -1.237083673 11.288562452 C29 5.472897801 -11.957133437 3.178450646 C30 6.177526783 -10.663930507 2.784294686 C31 6.473652847 -8.295627668 3.489752800 C32 7.649598059 -7.991802656 4.435545150 C33 5.298462860 -7.335067566 3.737540077 C34 5.660691799 -5.878095522 3.460735803 C35 4.423094307 -4.985708628 3.405480986 C36 4.616142654 -2.498238242 3.632188446 C37 9.899397028 -7.032501278 4.592140981 C38 10.100693437 -5.538833260 4.722657248 C39 -5.238174062 -2.454104457 -2.098808599 C40 -5.622088392 -1.055187532 -1.579463524 C41 -3.711285820 -2.627632841 -1.953137161 C42 -3.181873391 -4.064208825 -2.148267001 C43 -2.826052490 -4.446522770 -3.584703010 C44 -6.011759001 1.255640934 -2.352339192 C45 -7.153351141 1.661330018 -1.410244465 C46 -6.106998149 1.956086966 -3.714440818 C47 -9.380411717 1.116011820 -0.544240205 C48 -9.072823992 1.032084977 0.955060973 C49 -7.499660442 0.329044603 2.697445501 C50 -6.305731309 1.219029067 3.043227439 C51 -4.702309514 2.925191969 2.333040196 C52 -5.161388010 4.191009317 3.099031988 C53 -4.033183254 3.434956487 1.048146715 C54 -3.333578372 2.429673453 0.195847517 C55 -2.851842519 1.160994363 0.400885865 C56 -2.305486525 1.753686696 -1.671642020 C57 -6.947617251 5.884176741 3.257814495 C58 -6.927315099 5.923152809 4.784557019

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	C92	-4.042814700	11.819308720	2.855152930
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	C97	-3.972158213	8.561046157	1.913657592
	C98	-6.223251166	8.740479703	0.278809927
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	C102	3.130968841	-3.135946991	-8.634086669
	C103	1.617447309	-1.656874794	-7.335144762
	C104	1.166416318	-0.260645287	-7.779757725
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	C106	2.816738575	3.078809819	-7.600676063
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	C109	-2.218536341	-2.763910840	-9.547225359
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	C112	-1.103390431	-4.859249600	-8.624870147
	C113	-0.516101408	-5.487132586	-7.381134254
	C114	-3.648003044	0.599315119	-8.413607221
	C115	-3.113959874	1.918588187	-8.934099561
	C116	-4.098372128	0.627629936	-6.932943586
	C117	-2.922029256	0.531576819	-6.001556023
	C118	-2.170989921	1.670164568	-5.665639577
	C119	-2.474745606	-0.728240790	-5.567018021
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	C121	-1.274806387	-0.857182316	-4.862733310
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	C123	8.125070186	-6.044682408	-4.745156801
	C124	9.232631154	-6.203338993	-3.694070285
	C125	6.760940638	-6.426024991	-4.152066999
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	C133	3.001271627	-6.991329557	-1.462178114
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N393	-5.791903627	2.001221164	2.046000915
N394	-2.979214302	2.765713136	-1.105865979
N395	-2.230672696	0.767488632	-0.769774919
N396	-6.419318705	4.605888999	2.801030157
N397	-9.754987169	7.758124678	1.596879470
N398	-9.676541169	9.440635226	3.041437363
N399	9.336108179	2.339180174	3.175291935
N400	6.400561027	7.087448356	0.599511064
N401	4.485143953	8.606594672	-1.970887412
N402	1.851329187	8.049552562	-2.656892207
N403	-2.810080534	6.763550629	-4.171192969
N404	-2.890208619	8.715817401	-5.461756615
N405	-4.075672293	8.582906409	-3.475369011
N406	0.809205060	6.385195748	-0.570282315
N407	0.995495287	8.093599901	1.639119799
N408	-0.272000612	10.534869489	1.430052492
N409	-1.565483526	10.588225718	-2.376875011
N410	-2.698740227	11.504054928	2.389089088
N411	4.654415144	-4.070050992	-10.311031105
N412	2.906544085	-2.019030930	-7.910783513
N413	1.862021021	0.754553537	-7.223026668
N414	3.972091460	2.700144980	-6.997383230
N415	-1.120572754	-2.220932076	-10.358049772
N416	-2.750657551	-0.485707650	-8.763806669
N417	8.410970329	-6.792183906	-5.983600920
N418	4.450297918	-5.450915736	-4.560237321
N419	3.997249032	-6.287010560	-6.548898154
N420	9.306315024	-7.388290883	-3.030142732
N421	0.189981776	2.247857207	0.234479748
N422	2.626967922	-0.444215367	0.651267782
N423	1.029324844	1.633526644	-0.197928072
N424	1.896949787	-1.158134124	1.368922039
O425	-6.710459247	-5.096794982	0.862726923
O426	-7.656096676	-3.042961440	3.844988554
O427	-5.870232509	-5.598138524	5.968439296
O428	-2.876925306	-4.344304690	4.520893230
O429	-3.413110159	-0.946363634	5.240167103
O430	-3.858713369	-1.662666073	8.703138859
O431	-1.199341359	-4.730558477	9.364160131
O432	1.727603863	-4.199589850	5.808413330
O433	1.485220586	-0.204832744	6.732260158
O434	0.272339547	1.140777781	9.858418476
O435	0.756685005	-1.223935361	12.430505878
O436	6.799448055	-10.596533192	1.703814989
O437	7.586129558	-8.270627416	5.645367757
O438	11.188688958	-5.020382141	4.916203182
O439	-5.640505734	-0.754798982	-0.370276981
O440	-3.473385378	-4.013901653	-4.566197595
O441	-7.040982395	2.654578615	-0.669645052
O442	-6.066462131	3.383943048	-3.525170441
O443	-9.851781041	1.555898639	1.761639650
O444	-5.850262613	1.218380636	4.191755755
O445	-4.393521497	4.818014472	3.834056597
O446	-6.766139211	6.933375989	5.447522686
O447	10.511326408	-0.587004433	4.749595925
O448	3.394902325	4.353001877	4.488913145
O449	3.752059744	8.326120986	0.170234957
O450	1.318134584	10.286848373	-2.734742782
O451	-1.241760503	7.229197542	-1.123850979
O452	-0.759518301	6.976953685	2.610713735
O453	2.425278254	5.533809196	1.989592417
O454	0.870708195	11.364742558	3.237680086
O455	-2.338608153	13.558138428	1.464290492
O456	-3.023437724	11.151056185	-0.708790565
O457	-4.971232096	13.482111020	4.340561110
O458	-5.293081959	7.007699872	-1.154206633

	O459 2.230466886 -3.948150862 -8.956421510 O460 0.241564234 -0.097447834 -8.601980979 O461 2.697617057 4.185168420 -8.151694400 O462 6.366648244 4.956096546 -8.464395075 O463 -4.466562679 -1.893489919 -9.286901905 O464 -1.177917397 -6.131344632 -6.573679531 O465 0.793206367 -5.262454750 -7.152648741 O466 -3.407804987 3.011918905 -8.470368237 O467 10.065956632 -5.300568513 -3.482268640 O468 12.657227955 -6.962430161 -1.830769302 O469 0.303516046 -6.141496972 -1.780073328 O470 -0.365621160 -7.337723628 0.003981412 O471 5.192860272 -10.718064304 -3.778367489 O472 2.935959117 -10.690449521 -3.917199909 O473 5.070961219 -5.737719226 -1.452568357 O474 4.917216849 -7.509288052 -0.079085360 O475 2.653721519 -5.975645128 -2.404016501 O476 8.775392348 -6.774786813 1.082984071 O477 6.868255098 -4.689262663 0.489068794 O478 -4.154925685 4.977191889 -2.378354446 O479 7.734272134 -10.345134698 -2.801211421 O480 7.371787970 -8.734232838 -0.273063930 S481 3.784373062 5.147340958 -1.908701636 S482 2.162347857 1.887478926 -3.021408065 S483 2.248567551 -3.130428248 -3.863073925 S484 4.019263671 1.938931859 0.044158523 S485 0.578367390 -0.874903236 -1.480144246 S486 4.310774204 -0.388760107 -5.376025267 S487 3.279188928 -3.455651485 -0.438282656 S488 5.770977988 1.914505324 -2.822272868 S489 5.815655106 -2.945431139 -3.047939101 S490 6.198229007 -0.924558668 0.030322854 end

N2-ready-b to **Fe2-brNH-NH-Fe6**

Figure 8, scheme C

reactant **N2-ready-b** (S=3/2)	bm52capexp347tf.car_6			
Fe(139) 2.323	C1	-7.734132254	-5.365012870	1.276604324
Fe(140) 0.829	C2	-8.135095861	-6.509447875	0.337697222
Fe(141) 1.454	C3	-8.542266679	-3.434833417	2.564909518
Fe(142) -2.433	C4	-7.904586471	-3.695017532	3.925772290
Fe(143) 2.902	C5	-7.472554345	-5.284144170	5.734509489
Fe(144) -0.986	C6	-5.947916775	-5.405031596	5.666779587
Fe(145) -1.531	C7	-3.974526188	-5.711226394	4.272326340
	C8	-3.463373429	-4.269210762	4.307144548
	C9	-3.885620162	-1.950437432	3.606634116
	C10	-3.901796370	-1.318888201	5.007921171
	C11	-4.919983835	-1.157099533	7.188735644
	C12	-3.858294284	-1.708688511	8.151596358
	C13	-2.853486602	-3.724262863	9.129149260
	C14	-1.385905188	-4.041750987	8.806375371
	C15	0.241012621	-4.801885830	7.120788103
	C16	0.982416258	-3.653212613	6.426467315
	C17	0.644416790	-1.415925815	5.389442684
	C18	0.775525275	-0.201278523	6.324885437
	C19	-0.264658075	-1.208764723	4.160292876
	C20	-0.036905604	0.146219692	3.472912911
	C21	-0.136328042	-2.410321624	3.213774049
	C22	-0.357769944	1.551163263	7.617731148
	C23	0.008562942	1.227270525	9.077618505
	C24	-1.686391070	2.332687168	7.481501753
	C25	-1.751986824	3.500047822	8.471891701
	C26	-1.865845570	2.842350687	6.044621656
	C27	-0.404814848	-0.087708881	11.070366157
	C28	1.060151879	-0.355847498	11.351400638
	C29	5.897438758	-11.599477165	3.752826448
	C30	6.515109272	-10.322149756	3.194306265
	C31	6.786739860	-7.895604748	3.681069787
	C32	8.007947931	-7.501893869	4.531792055
	C33	5.607863757	-6.938593258	3.920726303
	C34	5.942207087	-5.497114713	3.547990804
	C35	4.698287110	-4.614084078	3.497846122
	C36	4.896158159	-2.113339938	3.511592423
	C37	10.268917503	-6.559342420	4.484984470
	C38	10.493878240	-5.064815543	4.471899230
	C39	-5.329820364	-2.675253566	-1.562613377

C40	-5.692860319	-1.241572292	-1.128322278
C41	-3.791583510	-2.821571234	-1.504547471
C42	-3.244071881	-4.259171157	-1.621370396
C43	-2.976988784	-4.746658587	-3.046282312
C44	-6.183862568	0.997988729	-2.033538777
C45	-7.273827425	1.452982777	-1.052564252
C46	-6.361075868	1.606883985	-3.430021444
C47	-9.427898140	0.930348014	-0.006368156
C48	-9.030699668	0.950428247	1.472806420
C49	-7.325362296	0.439000544	3.155712533
C50	-6.155049882	1.401097318	3.366966910
C51	-4.605098204	3.045594005	2.433939223
C52	-5.046854949	4.354197080	3.130952169
C53	-4.020209484	3.480098665	1.081377156
C54	-3.402965453	2.417824599	0.234845671
C55	-2.981172767	1.133960065	0.469933970
C56	-2.547690903	1.605324815	-1.665338245
C57	-6.849273214	6.033666756	3.239678770
C58	-6.755909664	6.189682711	4.756428035
C59	-8.322537089	6.088922064	2.772004571
C60	-8.945267436	7.449626443	2.657513575
C61	-8.871846814	8.553007491	3.485323793
C62	-10.198693907	8.969697737	1.760179309
C63	9.237686775	1.628910296	3.433849452
C64	10.269303793	0.527581377	3.265961846
C65	7.845389819	0.982658597	3.250750780
C66	6.709668151	1.956636238	3.461767442
C67	6.139784088	2.155645915	4.731869500
C68	6.191397600	2.699411147	2.385384554
C69	5.087851758	3.059368520	4.924798834
C70	5.156803308	3.617619937	2.564950327
C71	4.598311884	3.789521948	3.834032190
C72	5.383191279	6.858685926	-1.385085721
C73	4.324989542	7.959208293	-1.597045966
C74	4.698852697	5.531125550	-1.098262093
C75	3.314160314	9.544044228	-3.201954322
C76	1.839594791	9.161968384	-3.365236751
C77	0.216065770	7.270657545	-3.328513642
C78	-0.253169829	6.927332490	-1.890722879
C79	0.245003373	6.024673038	-4.242902343
C80	-1.008079362	5.147104815	-4.349479383
C81	-2.152316458	5.682633518	-5.226592316
C82	-3.673260666	7.602827886	-4.743899390
C83	0.268942385	5.982485670	0.306372589
C84	0.115119622	7.202671269	1.225957410
C85	1.265350621	5.013469963	0.975877320
C86	1.199353237	9.267336187	1.966153954
C87	0.555887218	10.610767544	1.657731085
C88	-0.855685449	11.875464793	0.127184267
C89	-2.130072045	12.430592283	0.810150004
C90	-1.016197506	11.883580059	-1.395343550
C91	-2.159569859	11.012427401	-1.899336108
C92	-4.073956176	11.948219387	2.222095369
C93	-3.987108932	13.049918640	3.270989674
C94	-4.731361174	10.680565451	2.835046187
C95	-4.972190027	9.607000122	1.798443365
C96	-6.154531881	9.602678048	1.042679860
C97	-4.006061335	8.626393081	1.520663033
C98	-6.360069336	8.666298447	0.028020718
C99	-4.182222166	7.697152038	0.490687385
C100	-5.359638504	7.734431240	-0.250435150
C101	4.086761212	-3.979197898	-8.998739705
C102	2.660105600	-3.726271740	-8.544102819
C103	1.204285542	-2.191311682	-7.242924338
C104	0.707097328	-0.834022967	-7.754558396
C105	1.122611543	1.587715882	-7.711900278
C106	2.296165926	2.542446861	-7.913440391
C107	4.575760538	3.213399525	-7.404814295
C108	5.169628498	3.373799853	-8.789356960
C109	-2.761123087	-3.492841836	-9.150223984
C110	-3.787153112	-2.402996715	-8.816533210
C111	-2.270604897	-4.170100407	-7.849189053
C112	-1.538112897	-5.490303357	-8.150473374
C113	-0.860099292	-6.019182701	-6.906957997
C114	-4.191700907	-0.084983649	-8.157008905
C115	-3.713913388	1.199562033	-8.804585987
C116	-4.569408299	0.045820740	-6.660166883
C117	-3.334177572	0.058411715	-5.805593412
C118	-2.607642526	1.245799583	-5.610187954
C119	-2.798045732	-1.153073672	-5.339158204

	C120	-1.328521151	1.199621888	-5.046967464
	C121	-1.520808387	-1.197900945	-4.774076507
	C122	-0.769255634	-0.024008926	-4.667636959
	C123	7.914975220	-6.235921298	-4.770929301
	C124	9.096912089	-6.322801127	-3.794110912
	C125	6.602924794	-6.605129414	-4.066380631
	C126	5.351455459	-6.397397417	-4.853830250
	C127	4.996199944	-6.986501931	-6.050137220
	C128	3.261911801	-5.876922584	-5.238666527
	C129	10.307927783	-7.550477505	-2.093392706
	C130	11.658760312	-7.321966256	-2.734924833
	C131	0.601453562	-6.925198813	-0.196784370
	C132	2.092256707	-6.968840807	0.121029270
	C133	3.011757127	-7.093483184	-1.132748949
	C134	2.921335994	-8.534682529	-1.700373720
	C135	3.954494311	-8.875327210	-2.776732727
	C136	3.978834253	-10.365132834	-3.179894983
	C137	4.467741997	-6.827072245	-0.710496413
	C138	3.588716262	-0.695288962	-2.229729898
	Fe139	3.876336923	-2.025436924	-3.720688680
	Fe140	2.222662579	0.818331092	-1.518946186
	Fe141	5.015746138	0.430307490	-1.635596709
	Fe142	3.798116639	0.516151440	-3.838420559
	Fe143	3.791597206	2.786236903	-2.488509547
	Fe144	4.680500200	-2.055097214	-1.277713957
	Fe145	2.163085956	-2.417726232	-1.752547046
	H146	-6.370108375	-7.533002531	0.332357210
	H147	-6.548548847	-6.539547393	-0.950245677
	H148	-9.705256833	-4.783381044	1.389267487
	H149	-8.851849077	-6.119634962	-0.403014371
	H150	-8.695405760	-7.239201765	0.947302023
	H151	-7.881923365	-2.727636826	2.041847003
	H152	-8.655826823	-5.599457795	3.964906408
	H153	-9.506458834	-2.935170931	2.727607164
	H154	-7.891098246	-6.243308434	6.065691684
	H155	-6.014987045	-5.841236180	3.651954463
	H156	-7.691449498	-4.531291041	6.502798451
	H157	-2.889721536	-1.761117121	3.185100487
	H158	-4.977665544	-3.701489760	3.034493242
	H159	-3.732824791	-6.171849720	3.305123593
	H160	-4.768889694	-0.071044817	7.136447001
	H161	-5.653834117	-2.290225737	5.503390768
	H162	-3.452931733	-6.263996653	5.062238776
	H163	-4.624725731	-1.445961449	2.968197441
	H164	-4.207383828	-3.622517121	7.474281657
	H165	-5.911867954	-1.354459356	7.619088368
	H166	-0.522110707	-3.325640622	3.681474709
	H167	-0.699470669	-2.247238147	2.281522634
	H168	0.909218729	-2.589797995	2.927849769
	H169	-1.292923914	-1.189789340	4.542104244
	H170	-3.352018340	-4.672259716	9.380852146
	H171	-1.870748782	2.025428246	5.311075858
	H172	-1.449541786	-0.255165337	9.215969032
	H173	-1.706970700	3.166176932	9.518264033
	H174	0.757817255	0.110285263	2.728176054
	H175	0.224455283	0.942382578	4.184321632
	H176	9.311671102	1.987601663	4.478578296
	H177	-2.821048703	3.378057612	5.946362357
	H178	-2.693760729	4.050239947	8.330755294
	H179	-1.055180928	3.542575121	5.783228559
	H180	-0.919389346	4.201465116	8.303423709
	H181	-2.510642858	1.633416672	7.712312273
	H182	0.469708383	2.186661609	7.267026039
	H183	-1.279100378	0.037068529	6.403079767
	H184	-0.957201232	0.466111569	2.960423220
	H185	1.557794621	4.248956254	0.242217907
	H186	0.730054169	4.519308174	1.799920918
	H187	2.665700649	5.321491900	2.329383862
	H188	3.214132007	4.680580239	4.864476315
	H189	4.759762351	4.177736904	1.718232975
	H190	6.589183005	2.540220866	1.380413537
	H191	6.514606125	1.588784688	5.588798281
	H192	-0.789782738	-2.680707952	6.314305877
	H193	0.220010076	-5.650388128	6.421877116
	H194	0.833322036	-5.100194341	7.994946250
	H195	-1.855537935	-4.538997676	6.840400642
	H196	-2.836696628	-3.093945609	10.026206782
	H197	4.645178428	3.188928772	5.916405760
	H198	1.670165437	-1.623686683	5.061824106
	H199	-0.750692759	0.717122935	11.739474441

	H200	-0.957585835	-1.003529806	11.330958664
	H201	1.649398263	-0.728841654	10.481865329
	H202	11.143243622	-7.060119971	4.042069202
	H203	-1.753528603	-5.984933742	-4.123916350
	H204	1.241612940	-6.065216176	-1.805170829
	H205	-2.268888078	-6.240824620	-8.485128197
	H206	-0.802366869	-5.342199866	-8.953983117
	H207	-3.121986586	-4.377215219	-7.182292988
	H208	-3.109453652	1.047398843	-9.729863709
	H209	-3.348899848	-4.237815876	-9.708160442
	H210	-3.349752386	-2.193930269	-2.297161902
	H211	-3.950740254	-4.971949038	-1.162695010
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transition state (S=3/2) Fe(139) 2.318 Fe(140) -0.328 Fe(141) 2.595 Fe(142) -2.214 Fe(143) 2.184 Fe(144) -1.858 Fe(145) -0.101	bm52capexp347tg_1_53249.10 C1 -7.721612170 -5.357528774 1.267310014 C2 -8.143776791 -6.501647436 0.336778067 C3 -8.513860167 -3.421330352 2.559347949 C4 -7.868652602 -3.680697863 3.916300973 C5 -7.435804518 -5.260737729 5.732036158 C6 -5.910978401 -5.378881529 5.665935805 C7 -3.935406106 -5.691247981 4.275886762 C8 -3.430509898 -4.246574557 4.296123878 C9 -3.867251474 -1.935395820 3.579414012 C10 -3.881934789 -1.296582140 4.978059046 C11 -4.897487833 -1.130485039 7.161674075 C12 -3.847680652 -1.680522237 8.137733270 C13 -2.840662688 -3.696284704 9.117662159 C14 -1.375358103 -4.022097226 8.791080296 C15 0.232176680 -4.825838668 7.108936665 C16 0.967487577 -3.667196094 6.424002184 C17 0.623186168 -1.445274949 5.367362985 C18 0.760057649 -0.230040454 6.299783914 C19 -0.259789394 -1.241348589 4.117031540 C20 -0.032097030 0.114249054 3.420534406 C21 -0.078445511 -2.417550315 3.150654129 C22 -0.351717429 1.530174025 7.597391383 C23 0.023577950 1.212045583 9.057416163 C24 -1.677492529 2.317337850 7.468120311 C25 -1.736784137 3.484076473 8.459605129 C26 -1.861086659 2.826996316 6.031850730 C27 -0.395963445 -0.087353290 11.064691618

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C35	4.685235442	-4.606709721	3.511639487
C36	4.907266252	-2.107271520	3.551207749
C37	10.265479095	-6.558264204	4.487224367
C38	10.502178956	-5.065125947	4.475024518
C39	-5.314906902	-2.671359069	-1.555552625
C40	-5.685669005	-1.240977756	-1.117338113
C41	-3.778704394	-2.819131377	-1.504746915
C42	-3.243033974	-4.261100867	-1.620956205
C43	-2.978321813	-4.748544243	-3.046068153
C44	-6.186878865	0.997613911	-2.021979407
C45	-7.279639458	1.449825169	-1.043165962
C46	-6.367287690	1.604239949	-3.419181967
C47	-9.433571657	0.920514435	0.000258916
C48	-9.037200870	0.944941032	1.479797222
C49	-7.328641647	0.441772875	3.163192968
C50	-6.155191389	1.400327992	3.372217152
C51	-4.603206516	3.041048612	2.435063578
C52	-5.047211813	4.347330797	3.134152835
C53	-4.025464207	3.477962156	1.080408407
C54	-3.407054077	2.416473780	0.234108434
C55	-2.987677312	1.131917103	0.470077371
C56	-2.553961206	1.601082547	-1.665314914
C57	-6.847785337	6.028765214	3.232950693
C58	-6.759701911	6.184481386	4.749944001
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C60	-8.945414657	7.443079255	2.650331731
C61	-8.869160231	8.546793093	3.477536167
C62	-10.205220442	8.961327444	1.758878199
C63	9.239262761	1.622978043	3.446448339
C64	10.259520619	0.511884685	3.276144875
C65	7.842522210	0.982124250	3.262086840
C66	6.709183012	1.958956737	3.473335381
C67	6.140575019	2.161076973	4.743484231
C68	6.187327909	2.696175947	2.394972048
C69	5.087517309	3.063941093	4.934827043
C70	5.152098157	3.614063849	2.572854758
C71	4.595683795	3.789918954	3.842319585
C72	5.378032217	6.872830267	-1.382869730
C73	4.319300720	7.967891178	-1.595631100
C74	4.711007177	5.532013208	-1.082404533
C75	3.308366112	9.545211711	-3.206036941
C76	1.833578493	9.167242853	-3.365700598
C77	0.210884270	7.275300149	-3.323832009
C78	-0.256899309	6.928161178	-1.886629287
C79	0.243165355	6.027572241	-4.236575790
C80	-1.009629174	5.149380419	-4.344760798
C81	-2.152816741	5.683819942	-5.224448654
C82	-3.672663897	7.605768178	-4.740563793
C83	0.262810629	5.987135553	0.312414194
C84	0.111199815	7.211289537	1.227924167
C85	1.254936546	5.017582473	0.986837788
C86	1.203524524	9.274605961	1.963076359
C87	0.559061749	10.617667744	1.653104027
C88	-0.858240713	11.880686768	0.123480901
C89	-2.131197227	12.433028872	0.809499680
C90	-1.025342599	11.883493940	-1.398857810
C91	-2.164762670	11.003251161	-1.896313877
C92	-4.075806821	11.948797747	2.221379969
C93	-3.983271787	13.047865183	3.271132674
C94	-4.729838803	10.677947753	2.833630703
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C98	-6.368085170	8.657758190	0.033720314
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C101	4.086649253	-3.977198268	-9.000441316
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C103	1.207630691	-2.196830753	-7.232201734
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C106	2.295026358	2.546218855	-7.901745690
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C121	-1.514368322	-1.203165578	-4.779877750
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H152	-8.626786387	-5.582242899	3.968141412
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H162	-3.412298186	-6.232086946	5.072935539
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H169	-1.295436221	-1.245753566	4.477396205
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H173	-1.679312607	3.148937676	9.504981080
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H182	0.476804524	2.159671976	7.238190546
H183	-1.290889826	0.021480284	6.387970300
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	H188	3.209729332	4.680913604	4.870348207
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	H190	6.580697812	2.530416160	1.389400736
	H191	6.515900405	1.596111992	5.601367843
	H192	-0.822330255	-2.733388919	6.235751025
	H193	0.205278403	-5.666267923	6.400478428
	H194	0.832649407	-5.134179849	7.974146992
	H195	-1.866370334	-4.571687654	6.846500843
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	H198	1.652251881	-1.653525406	5.049359018
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	H206	-0.802894987	-5.340405084	-8.954639755
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	H208	-3.121055470	1.048218693	-9.724073060
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	H213	-5.132899116	-0.319519964	-8.688001493
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	H239	-2.213560973	1.500466561	-2.693468915
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	H263	-1.396916543	4.887130652	-3.347779753
	H264	-8.364733896	-0.227772530	-1.466965647
	H265	3.641732894	10.003074457	-4.146932994
	H266	-6.087300092	-0.954263662	-3.048177668
	H267	0.537586023	6.363737378	-5.244273741

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	H272	-5.168258158	-3.513844356	-3.430419228
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	H279	-3.606773035	5.869503880	-3.680279001
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	H290	5.497766077	4.782211951	-0.938055939
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	H293	4.111102666	5.611415408	-0.165341535
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	H312	4.981480044	-11.764009746	3.177248386
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	H324	6.364580545	-5.072432446	-0.236836271
	H325	2.283557718	-7.802342643	0.838099643
	H326	3.282164609	-2.024168938	-7.604660116
	H327	3.018004502	-9.233544789	-0.870564044
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	H339	1.346128472	-2.171258062	-6.139372447
	H340	-3.031444679	2.191928026	-5.935959676
	H341	-5.152121370	0.972601345	-6.541528797
	H342	2.304794711	-6.036762778	0.649773711
	H343	8.503913260	-7.337845172	0.581439844
	H344	7.409167820	-9.253808870	0.675110352
	H345	4.154095329	-1.040527861	5.127783575
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	H347	6.535266529	-6.055292611	-3.099427517

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H350	7.759365174	0.148270427	3.974400036
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H353	8.259993933	-8.002231598	-5.737038421
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H356	11.697169596	-7.545197498	-3.826947644
H357	10.169943469	-6.873235341	-1.239044349
H358	10.540771153	0.305343165	2.214819714
H359	-2.973247513	13.185460654	3.724415628
H360	10.192764165	-6.865073445	5.545558860
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N392	-7.856315265	0.352634701	1.814609874
N393	-5.686439144	2.078012044	2.278632416
N394	-3.125502597	2.673719204	-1.101596167
N395	-2.474036254	0.655684091	-0.720963943
N396	-6.320174384	4.725062221	2.852949549
N397	-9.783466744	7.714835109	1.580666806
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N401	4.212541014	8.461025989	-2.865250821
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N403	-3.176443043	6.401335248	-4.458235833
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N406	0.649234828	6.334601501	-1.057597029
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N415	-1.724678661	-2.980964532	-10.047899748
N416	-3.294305200	-1.177698604	-8.467410341
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O426	-7.203342397	-2.788502866	4.470635113
O427	-5.220546305	-5.142147647	6.670874678

	O428	-2.437027241	-3.910472593	4.957382907
	O429	-3.040438021	-0.441105389	5.292253272
	O430	-3.292776277	-0.922046824	8.952098883
	O431	-0.499292371	-3.878137374	9.652682200
	O432	2.186833269	-3.744324165	6.182687317
	O433	1.886285828	0.193391886	6.608110500
	O434	0.896430431	1.865077667	9.654043749
	O435	1.574030265	-0.213345098	12.448672106
	O436	7.058010812	-10.324238299	2.072400030
	O437	7.995434501	-7.647734521	5.763364803
	O438	11.608915034	-4.559147528	4.573250677
	O439	-5.615588314	-0.847361907	0.063481645
	O440	-3.687058108	-4.383479587	-4.012618126
	O441	-7.145537000	2.496381630	-0.383958437
	O442	-6.335848412	3.041951160	-3.325718970
	O443	-9.795673240	1.481742926	2.297633070
	O444	-5.663731819	1.531755926	4.496578571
	O445	-4.263509474	5.031682672	3.797203711
	O446	-6.595632689	7.246113259	5.326076106
	O447	10.731164781	-0.133775854	4.201061049
	O448	3.547598151	4.683563897	3.955872133
	O449	3.604436438	8.389872310	-0.669796704
	O450	0.987939561	10.069496891	-3.520351278
	O451	-1.417429661	7.186920712	-1.532171335
	O452	-0.704472060	7.210341106	2.159303645
	O453	2.413041158	5.703899894	1.467698830
	O454	0.860454965	11.630980295	2.295035432
	O455	-2.509273424	13.590284263	0.578500286
	O456	-3.273737180	10.983697457	-1.343407196
	O457	-4.942840501	13.714559721	3.622555762
	O458	-5.513851408	6.831370813	-1.328301182
	O459	1.756240854	-4.568411207	-8.772741747
	O460	-0.275504729	-0.736409379	-8.497804735
	O461	2.097240138	3.602549612	-8.524585072
	O462	5.911840465	4.302171154	-9.100997222
	O463	-5.008295156	-2.639784462	-8.815736351
	O464	-1.448414364	-6.607371525	-6.011916011
	O465	0.466406745	-5.765025444	-6.789755860
	O466	-3.995308136	2.322393186	-8.394887517
	O467	9.938116049	-5.406010590	-3.699854706
	O468	12.648232150	-6.966757352	-2.115654441
	O469	0.274313885	-6.298307206	-1.310736010
	O470	-0.262785711	-7.420685602	0.560607738
	O471	5.118791986	-10.903636149	-3.344829798
	O472	2.857115378	-10.944649274	-3.351072902
	O473	5.089819423	-5.890685644	-1.330348817
	O474	5.001770847	-7.573731330	0.154015748
	O475	2.598236534	-6.106452309	-2.062502210
	O476	8.947967421	-6.563271118	1.027095725
	O477	6.985023699	-4.575186960	0.354607211
	O478	-4.374566306	4.743523938	-2.450720375
	O479	7.701806536	-10.433619585	-2.510056051
	O480	7.503065329	-8.632630685	-0.091318901
	S481	3.590891810	4.967593669	-2.440282977
	S482	2.092967845	1.856262860	-3.478295715
	S483	2.017473812	-3.364916884	-3.447070375
	S484	3.839382163	2.014716913	-0.425159243
	S485	0.540773344	-0.874014624	-1.842964160
	S486	3.993957626	-0.813354200	-5.518672734
	S487	3.530728484	-3.629756307	-0.182417230
	S488	5.652384041	1.684026968	-3.293870947
	S489	5.673676060	-3.065962293	-3.046884809
	S490	6.380703249	-0.865037346	-0.335834794
	end			
product **Fe2-brNH-NH-Fe6** (S=3/2) Fe(139) 2.416 Fe(140) 0.020 Fe(141) 2.627 Fe(142) -2.342 Fe(143) 2.373 Fe(144) -2.287 Fe(145) -0.161	bm52capexp347tg.car_6			
	C1	-7.718196511	-5.352898645	1.290072937
	C2	-8.055309545	-6.509440248	0.341622422
	C3	-8.618108083	-3.462385737	2.576097494
	C4	-7.988527564	-3.730318018	3.941305396
	C5	-7.584772214	-5.336284121	5.743091369
	C6	-6.058787113	-5.454981761	5.688530758
	C7	-4.076041724	-5.775869210	4.303546090
	C8	-3.525144431	-4.348686083	4.347349185
	C9	-3.889564906	-2.009653104	3.704947089
	C10	-3.892450980	-1.407962363	5.117339591
	C11	-4.947735751	-1.237231246	7.281716398
	C12	-3.885133107	-1.812513504	8.229522525
	C13	-2.891932090	-3.846464297	9.173569206
	C14	-1.415589991	-4.104940764	8.843842827
	C15	0.237185520	-4.699170018	7.117812770

	C16	0.962792251	-3.564102574	6.390909710
	C17	0.669537458	-1.313802553	5.392615873
	C18	0.787021688	-0.086593742	6.310664676
	C19	-0.158142990	-1.094191192	4.108168663
	C20	0.332118036	0.146923945	3.351437850
	C21	-0.123197806	-2.345782293	3.227201847
	C22	-0.386802056	1.618567093	7.634458425
	C23	-0.032748760	1.263275716	9.090789835
	C24	-1.724875528	2.382738639	7.499829442
	C25	-1.807972421	3.539244752	8.501590988
	C26	-1.904092372	2.900579520	6.066013213
	C27	-0.447471745	-0.110500916	11.044731593
	C28	1.014957994	-0.397395460	11.322018738
	C29	5.881751941	-11.626740449	3.689987025
	C30	6.519423088	-10.347941135	3.159693324
	C31	6.823601965	-7.937319293	3.684101215
	C32	8.051440643	-7.551473685	4.527995772
	C33	5.652203709	-6.974105137	3.935198272
	C34	5.994838500	-5.533511418	3.568166483
	C35	4.757595756	-4.641728777	3.520820935
	C36	4.898534991	-2.137225183	3.514435238
	C37	10.290092677	-6.551949614	4.464320033
	C38	10.467726825	-5.050257679	4.465200272
	C39	-5.320830990	-2.666286783	-1.588800276
	C40	-5.692644145	-1.235148768	-1.156479792
	C41	-3.784909960	-2.806670642	-1.520875733
	C42	-3.231182397	-4.241496488	-1.628126769
	C43	-2.967934607	-4.745724734	-3.047226302
	C44	-6.163179402	1.006279653	-2.066420365
	C45	-7.251014580	1.468881404	-1.086957043
	C46	-6.340383643	1.610911847	-3.464957991
	C47	-9.409244446	0.959859395	-0.042005422
	C48	-9.015426993	0.959999729	1.438458250
	C49	-7.317204393	0.407803055	3.116516499
	C50	-6.130475966	1.348847339	3.331114211
	C51	-4.601071741	3.020274195	2.404301491
	C52	-5.027953427	4.348116678	3.082019680
	C53	-3.992866398	3.419818736	1.050658081
	C54	-3.329391814	2.360871485	0.225105749
	C55	-2.781157468	1.124366178	0.470158061
	C56	-2.426515903	1.590243755	-1.672298118
	C57	-6.836885123	6.025236574	3.250658657
	C58	-6.713036520	6.186229560	4.764289084
	C59	-8.318891100	6.086921092	2.811890257
	C60	-8.928610250	7.453298108	2.687906825
	C61	-8.863318953	8.553937125	3.520326904
	C62	-10.150198898	8.987477457	1.769388441
	C63	9.251943088	1.658552181	3.409912883
	C64	10.298367969	0.573896804	3.234572200
	C65	7.865014573	0.993716806	3.222962078
	C66	6.722427388	1.958340539	3.435547477
	C67	6.136785432	2.136709230	4.701327322
	C68	6.221576086	2.723467637	2.366423583
	C69	5.087506271	3.042975967	4.897828258
	C70	5.191777077	3.645743219	2.550693486
	C71	4.619477159	3.799547124	3.815738633
	C72	5.386529335	6.867462314	-1.399558518
	C73	4.320044182	7.955784367	-1.608513956
	C74	4.732683069	5.539844061	-1.026408840
	C75	3.309217292	9.540915185	-3.209272354
	C76	1.832878242	9.168804253	-3.373841739
	C77	0.210227678	7.271568869	-3.330102763
	C78	-0.260546744	6.925734929	-1.892709401
	C79	0.245784458	6.028952443	-4.247742202
	C80	-1.003957941	5.147497026	-4.359557890
	C81	-2.151987338	5.684757743	-5.230526148
	C82	-3.683688702	7.592587005	-4.749430831
	C83	0.264362883	5.967970876	0.302375192
	C84	0.104217290	7.178543086	1.231127570
	C85	1.273877091	5.002932776	0.959595452
	C86	1.182048787	9.241857790	1.984311118
	C87	0.550837802	10.592882735	1.679083363
	C88	-0.845032249	11.876505877	0.146039599
	C89	-2.122569771	12.428855015	0.821394835
	C90	-0.989474333	11.889160036	-1.378228410
	C91	-2.145221092	11.045489241	-1.902995066
	C92	-4.070985581	11.945692609	2.224059947
	C93	-3.989739524	13.053181289	3.266522933
	C94	-4.731150630	10.681030105	2.839676081
	C95	-4.968748225	9.606493480	1.803816795

C96	-6.139137933	9.613597449	1.030342050
C97	-4.009376269	8.614955708	1.543767025
C98	-6.338704785	8.677724361	0.014128816
C99	-4.180803376	7.684069353	0.514593107
C100	-5.345647626	7.732689514	-0.245331598
C101	4.081554416	-3.990439210	-9.002013102
C102	2.656964000	-3.730995739	-8.544195681
C103	1.205612322	-2.177607116	-7.262872985
C104	0.703810067	-0.831434303	-7.803377221
C105	1.106503283	1.599254774	-7.774182458
C106	2.291439457	2.541187220	-7.956045345
C107	4.580747101	3.174266182	-7.450965968
C108	5.105520210	3.398997610	-8.855624630
C109	-2.743649357	-3.503529976	-9.160291562
C110	-3.764326617	-2.403671950	-8.844151916
C111	-2.251558060	-4.165000725	-7.853969183
C112	-1.536733705	-5.498007819	-8.143584508
C113	-0.869190605	-6.026022976	-6.894551369
C114	-4.155972512	-0.081504733	-8.200946327
C115	-3.656866308	1.200094110	-8.837594478
C116	-4.578239354	0.059435323	-6.717539637
C117	-3.355651620	0.088915251	-5.849479221
C118	-2.635931791	1.281961247	-5.669094531
C119	-2.813579518	-1.117974547	-5.377178618
C120	-1.352678248	1.246008142	-5.114322097
C121	-1.537429676	-1.148456010	-4.814055532
C122	-0.787974055	0.028568537	-4.726700371
C123	7.892327830	-6.271405536	-4.792876872
C124	9.079766629	-6.343490540	-3.817145702
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C126	5.312143937	-6.343981334	-4.807821359
C127	4.932188652	-6.918572094	-6.003427854
C128	3.207317702	-5.830390139	-5.141441416
C129	10.308070869	-7.554355757	-2.117037410
C130	11.663332011	-7.336092324	-2.753353155
C131	0.613962156	-6.899657256	-0.111503008
C132	2.111248512	-6.933994381	0.185633312
C133	3.008565049	-7.052209041	-1.080731988
C134	2.912447332	-8.487401136	-1.667108650
C135	3.951524296	-8.833735531	-2.737376440
C136	3.979012861	-10.325874516	-3.137676122
C137	4.476376901	-6.798566669	-0.700919197
C138	3.599357723	-0.688650324	-2.240557868
Fe139	3.750849165	-1.984855322	-3.702257375
Fe140	2.130825397	0.607584794	-1.336987583
Fe141	4.983395718	0.495229954	-1.464999086
Fe142	3.770543098	0.535027618	-3.729127445
Fe143	3.740571091	2.743114442	-2.404623116
Fe144	4.874420084	-2.044459274	-1.421271281
Fe145	2.152406763	-2.247033145	-1.294476489
H146	-6.256438398	-7.471901563	0.384439190
H147	-6.435079300	-6.487025746	-0.904556118
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O452    -0.705238115    7.159673642    2.167148089
O453     2.424842258    5.697839475    1.445287742
O454     0.855501679   11.598813632    2.331020367
O455    -2.500139172   13.586000047    0.588906391
O456    -3.254199272   11.027653035   -1.349738341
O457    -4.958347920   13.707298241    3.616710048
O458    -5.486440380    6.832928742   -1.321344702
O459     1.755275991   -4.581006724   -8.740534306
O460    -0.252090905   -0.752736088   -8.602029337
O461     2.119639597    3.613489675   -8.558889215
O462     5.751552296    4.380867758   -9.182823476
O463    -4.986244680   -2.623226808   -8.888771089
O464    -1.472366441   -6.623616723   -6.010042018
O465     0.447738246   -5.764550548   -6.757096193
O466    -3.996343817    2.321133984   -8.486159915
O467     9.896337915   -5.407616076   -3.712337327
O468    12.660277548   -6.998868349   -2.131832377
O469     0.276921062   -6.248502707   -1.233812243
O470    -0.231454786   -7.375763172    0.642606518
O471     5.132116836  -10.853654861   -3.326361790
O472     2.871078410  -10.914592819   -3.284384423
O473     5.088374044   -5.841603171   -1.353521330
O474     5.040120058   -7.501111448    0.157866136
O475     2.579920725   -6.054887759   -2.008718214
O476     8.957485052   -6.552725891    1.029180579
O477     6.984586223   -4.551690179    0.388139743
O478    -4.378921905    4.735588984   -2.457772944
O479     7.739766316  -10.420505788   -2.531085487
O480     7.524858289   -8.626602786   -0.102461482
S481     3.541678154    4.962744070   -2.314961544
S482     1.988153895    1.826228151   -3.374687429
S483     1.947539784   -3.301143615   -3.305460146
S484     3.751890978    1.980358591   -0.310920343
S485     0.440210451   -0.883791164   -1.973319365
S486     3.930743344   -0.722382121   -5.521432807
S487     3.680184643   -3.492713183   -0.177789970
S488     5.564884826    1.772681081   -3.235954901
S489     5.635753885   -3.097712091   -3.225858844
S490     6.339261496   -0.830383982   -0.340563649
end
```

Fe2-NH-NH-b to Fe2-brNH-NH-Fe6

Figure 8, scheme C

transition state **(S=3/2)**

Fe(139)	-2.358
Fe(140)	0.099
Fe(141)	-2.512
Fe(142)	2.559
Fe(143)	2.553
Fe(144)	2.275
Fe(145)	-0.074

bm52exp335fe2fe2fe6tg_1_53285.62

C1	-7.753016861	-5.460934552	-0.117222561
C2	-8.000481435	-6.488563657	-1.227917650
C3	-8.771352435	-3.727968237	1.294942905
C4	-8.272833524	-4.148434100	2.674641962
C5	-8.020704886	-5.944760863	4.314572645
C6	-6.495410678	-6.050711423	4.399583148
C7	-4.385730071	-6.201725809	3.180724081
C8	-3.873040364	-4.784029742	3.446252283
C9	-4.206099248	-2.388624656	3.022956106
C10	-4.365926294	-1.953475790	4.486968054
C11	-5.629962721	-2.033988174	6.537705343
C12	-4.653027249	-2.698123490	7.519112884
C13	-3.724231320	-4.822298621	8.328105989
C14	-2.216064795	-5.032603507	8.129428475
C15	-0.399156595	-5.514934528	6.538020047
C16	0.380139539	-4.298185933	6.028626718
C17	0.132326353	-1.960528858	5.236741089
C18	0.163151279	-0.844234860	6.294681715
C19	-0.603644968	-1.605511448	3.928409954
C20	-0.123697214	-0.256492993	3.383428999
C21	-0.439141096	-2.737778285	2.908409744
C22	-1.136918304	0.713552256	7.685713912
C23	-0.920616218	0.198628273	9.122845935
C24	-2.460434381	1.495743287	7.511283489
C25	-2.630543034	2.546103019	8.613788082
C26	-2.518668876	2.155683088	6.126372113
C27	-1.521642883	-1.375338864	10.870904467
C28	-0.079614996	-1.664142371	11.240719304
C29	5.597254610	-11.976912255	2.926589202
C30	6.278975697	-10.652522758	2.602541722
C31	6.506242856	-8.309137126	3.410555232
C32	7.633589570	-8.023181801	4.418711100
C33	5.305996280	-7.376822082	3.646450925
C34	5.670650160	-5.905468093	3.474185968
C35	4.441719492	-5.001759005	3.446095135
C36	4.541979760	-2.507986853	3.705321029
C37	9.851431994	-7.024708637	4.716548137
C38	10.029501019	-5.530393596	4.870725504
C39	-5.106729935	-2.470283688	-2.395581694
C40	-5.536953447	-1.098221778	-1.842332550
C41	-3.580059797	-2.611854455	-2.201447732
C42	-3.006297630	-4.026755994	-2.415301403
C43	-2.597892799	-4.366488808	-3.848438083
C44	-5.944891007	1.232144348	-2.537143617
C45	-7.127139769	1.570352859	-1.619462516
C46	-6.011461946	1.991322091	-3.868936697
C47	-9.371124916	0.938215944	-0.864026462
C48	-9.128124776	0.785693232	0.641406550
C49	-7.601514129	0.062764411	2.418504812
C50	-6.450848582	0.973890541	2.848519574
C51	-4.850030261	2.728548426	2.259174054
C52	-5.356412528	3.967953534	3.043437373
C53	-4.129930028	3.282632984	1.020006001
C54	-3.376835080	2.327259318	0.148128135
C55	-2.848820807	1.068926116	0.306452813
C56	-2.268719203	1.780288554	-1.717587341
C57	-7.191366300	5.619360443	3.210687191
C58	-7.221318539	5.613060249	4.736721091
C59	-8.620215588	5.728584330	2.629888853
C60	-9.234777514	7.097448721	2.609903240
C61	-9.241380746	8.106430332	3.554143286
C62	-10.393698232	8.718366769	1.762806950
C63	8.857436883	1.230321011	4.485247155
C64	9.906871921	0.157133192	4.264983960
C65	7.490735117	0.612750764	4.093196013
C66	6.332675008	1.559575454	4.301769912
C67	5.627015054	1.600944086	5.518687752
C68	5.930097832	2.438505870	3.280236300
C69	4.551693594	2.477780313	5.709665045
C70	4.873415363	3.330996591	3.461729246
C71	4.174830910	3.341384272	4.672792116
C72	5.409677498	6.982996378	-0.077334750
C73	4.361441072	8.092637889	-0.265284747
C74	4.729002495	5.618609860	0.036933710
C75	3.495154411	9.844772042	-1.774985929

C76	2.049110343	9.490035801	-2.128410845
C77	0.455461959	7.597150801	-2.456355224
C78	-0.149136503	7.073547585	-1.128940386
C79	0.597821094	6.476713206	-3.512621266
C80	-0.618576580	5.608941845	-3.854271234
C81	-1.687767997	6.238749389	-4.760994742
C82	-3.271507009	8.084559121	-4.206249887
C83	0.178237567	5.895668976	0.994744433
C84	-0.095319287	6.995283699	2.030837500
C85	1.129346927	4.866647163	1.640730300
C86	0.874528992	8.959837044	3.123736480
C87	0.254860812	10.332139707	2.911959671
C88	-0.984118228	11.784495822	1.392564243
C89	-2.323866191	12.260908475	2.003890676
C90	-0.989137409	11.966121837	-0.127714435
C91	-2.074432879	11.173088253	-0.845617016
C92	-4.396392144	11.617653122	3.146858152
C93	-4.432924177	12.592547354	4.315901464
C94	-5.087836827	10.282648766	3.544362008
C95	-5.213772331	9.335282777	2.372739389
C96	-6.316302139	9.417624607	1.508328837
C97	-4.215737267	8.389510473	2.083689425
C98	-6.407160747	8.607564538	0.374537906
C99	-4.276042991	7.589593284	0.939251754
C100	-5.374958388	7.712315344	0.092829534
C101	5.003190687	-2.934226170	-8.943399438
C102	3.536216220	-2.738370854	-8.606173946
C103	1.934799192	-1.346363824	-7.311602848
C104	1.479469951	0.056405680	-7.731977725
C105	1.854461145	2.462482011	-7.389476855
C106	3.033566288	3.429645847	-7.333162966
C107	5.265064117	3.991700621	-6.549715906
C108	5.928926955	4.375738701	-7.857025836
C109	-1.789381390	-2.437456687	-9.718403110
C110	-2.852115358	-1.388387127	-9.368777769
C111	-1.428323949	-3.261647082	-8.463234370
C112	-0.660517154	-4.543690147	-8.835829542
C113	-0.110676971	-5.206963280	-7.593124438
C114	-3.338160225	0.845278204	-8.509323775
C115	-2.808013858	2.191699005	-8.959289090
C116	-3.879703206	0.811198519	-7.059227675
C117	-2.737502690	0.752805736	-6.088065432
C118	-2.065758764	1.924459893	-5.703708208
C119	-2.205352022	-0.493565412	-5.711181649
C120	-0.840052727	1.845049607	-5.034685929
C121	-0.985233740	-0.569488198	-5.039618957
C122	-0.279450155	0.599701568	-4.737088719
C123	8.388723737	-5.676273923	-4.642094279
C124	9.475626754	-5.873551463	-3.573599954
C125	7.014473999	-6.086520848	-4.089978672
C126	5.826663980	-5.769550376	-4.944466899
C127	5.575827900	-6.196905681	-6.232420753
C128	3.767996056	-5.201904934	-5.431719858
C129	10.538558232	-7.283030539	-1.916034397
C130	11.944058406	-6.964496690	-2.376086847
C131	0.693380206	-6.847918391	-0.822406876
C132	2.155034542	-6.915268794	-0.390692271
C133	3.174292530	-6.888915298	-1.568148245
C134	3.146892512	-8.246208346	-2.323871915
C135	4.290923525	-8.471089217	-3.316995300
C136	4.366692410	-9.904863170	-3.888372561
C137	4.587426894	-6.679445494	-1.002413348
C138	3.811906069	-0.433801343	-1.930531497
Fe139	4.117701957	-1.563144109	-3.518174412
Fe140	2.246091589	0.767753421	-1.031123783
Fe141	5.130624733	0.664048591	-0.913094684
Fe142	4.083568878	0.952530110	-3.260998097
Fe143	4.083463402	2.979785883	-1.537938535
Fe144	4.967598392	-1.861762578	-1.141636901
Fe145	2.289798425	-2.079364582	-1.488499606
H146	-6.229220713	-7.496280937	-1.109617837
H147	-6.257774332	-6.366788710	-2.288313579
H148	-9.744139613	-4.939646090	-0.168804149
H149	-8.615274212	-6.012905829	-2.009362690
H150	-8.629761807	-7.283971265	-0.792736388
H151	-8.085649295	-2.945315554	0.940100304
H152	-8.999998556	-6.041860738	2.401145749
H153	-9.766617530	-3.278131062	1.412844436
H154	-8.455988098	-6.939953188	4.475747831
H155	-6.351048253	-6.237334678	2.352296341

H156	-8.338629686	-5.296420367	5.141896101
H157	-3.169162952	-2.172154865	2.737362607
H158	-5.251683986	-4.025912607	2.116466700
H159	-4.053567502	-6.538179068	2.189523789
H160	-5.494396477	-0.949046423	6.635001689
H161	-6.182670130	-2.924784110	4.647715899
H162	-3.937118078	-6.855892910	3.938061463
H163	-4.867090043	-1.784513220	2.386414777
H164	-4.930077558	-4.514828340	6.586525529
H165	-6.655261555	-2.290587922	6.837521769
H166	-0.841072100	-3.684587221	3.292144109
H167	-0.984020286	-2.503517252	1.980048015
H168	0.615182724	-2.875868754	2.632126298
H169	-1.670396489	-1.504635711	4.173627268
H170	-4.196286887	-5.815303879	8.363015423
H171	-2.461557219	1.420838799	5.311603302
H172	-2.383544184	-1.277069213	8.919252204
H173	-2.654940701	2.094768587	9.616042549
H174	0.919691173	-0.307589625	3.043268846
H175	-0.204021610	0.544203957	4.133460601
H176	8.833388939	1.452220222	5.569569828
H177	-3.461475613	2.707748366	6.003668888
H178	-3.572144739	3.093864832	8.462759476
H179	-1.688827693	2.871719039	6.005795253
H180	-1.804046583	3.273667394	8.591303945
H181	-3.291877912	0.771738066	7.591693644
H182	-0.292704938	1.397367381	7.511237479
H183	-1.898231586	-0.675250830	6.232578087
H184	-0.741148295	0.046546325	2.523851813
H185	1.506936295	4.195453458	0.855802818
H186	0.529386327	4.274031431	2.346607093
H187	2.381200879	5.031070117	3.153639702
H188	2.673122451	4.098778981	5.644246955
H189	4.559034048	3.992265990	2.654401624
H190	6.434662483	2.407638922	2.311539994
H191	5.916088612	0.931933093	6.334031670
H192	-1.376996897	-3.293913674	5.936133628
H193	-0.326707516	-6.296460792	5.768202547
H194	0.107646865	-5.878631269	7.441274635
H195	-2.460821654	-5.251397346	6.071303012
H196	-3.843041809	-4.347088191	9.309550577
H197	4.004007217	2.479958116	6.656078196
H198	1.186876467	-2.146686468	4.999917007
H199	-1.956341386	-0.690711730	11.616758951
H200	-2.062887779	-2.333146393	10.928432941
H201	0.581698806	-1.928989652	10.382736419
H202	10.783601120	-7.467114698	4.331769253
H203	-1.270027128	-5.502246896	-4.916467193
H204	1.435738922	-5.799770027	-2.257672916
H205	-1.347002350	-5.249538291	-9.325173308
H206	0.154681408	-4.311589353	-9.536787436
H207	-2.342070253	-3.540428344	-7.916428765
H208	-2.079360214	2.142732385	-9.802382965
H209	-2.313475321	-3.110008379	-10.414601197
H210	-3.071428077	-1.896374558	-2.868284131
H211	-3.744306834	-4.785267848	-2.100235230
H212	-1.399762162	-0.063273154	-8.694173333
H213	-4.209069304	0.675550766	-9.176062507
H214	-0.047154405	-1.310338050	-9.845047214
H215	-1.021589622	-5.552733125	-3.173783365
H216	-0.832958625	-2.635097624	-7.780815930
H217	-0.116689961	-2.573370501	-10.901960796
H218	-6.369852656	-3.112133442	-3.898361393
H219	-3.354439102	-2.310961155	-1.167759327
H220	1.629426213	-4.394043061	-8.001098998
H221	-2.138139736	-4.166660411	-1.754649913
H222	-4.145371095	2.219593947	2.931788699
H223	-2.900717952	0.378219067	1.138583520
H224	-8.473497361	0.343956638	3.025559870
H225	-7.327176595	-0.202339519	0.318815943
H226	-7.178769598	3.772996167	2.124082952
H227	-8.785043343	8.195279271	4.533680017
H228	-7.400889512	4.605300086	5.183095186
H229	-9.273813621	5.006989027	3.151635443
H230	-6.577406326	6.470926443	2.876397972
H231	-10.998029871	9.341476597	1.109442174
H232	-3.421204297	4.045703614	1.382578982
H233	-4.869807395	3.806939023	0.393922642
H234	-10.173607222	10.027711157	3.427204487
H235	-8.575470141	5.399608761	1.579815510

	H236	-6.309325141	1.835338293	0.956459923
	H237	-7.339002634	-0.968915395	2.697550612
	H238	-9.799600838	1.940569000	-1.004049223
	H239	-1.820005912	1.814527144	-2.707696997
	H240	-10.131121515	0.206508320	-1.167090264
	H241	9.965699461	2.893558491	4.033230266
	H242	8.384558698	3.036260709	3.648079299
	H243	1.624201497	6.114124329	-0.587580608
	H244	-0.786823822	5.401290704	0.813489331
	H245	1.596582893	7.968182326	1.401531717
	H246	-3.310138250	3.636568934	-1.569931632
	H247	-4.851169932	4.452460659	-2.808894852
	H248	-6.294493159	3.850760563	-4.428765928
	H249	-4.641442262	5.570104411	-1.695799313
	H250	-5.141170978	1.698505635	-4.479144898
	H251	-6.931365863	1.718583414	-4.408208783
	H252	0.009860475	11.751904633	-0.532809807
	H253	-1.200091908	13.029755677	-0.320368601
	H254	-0.695651642	10.507096074	-2.244688074
	H255	-2.368963256	9.981330426	-2.445743196
	H256	-3.192695862	9.813165720	-5.309717671
	H257	-2.124575700	5.469940208	-5.416556871
	H258	-7.279525835	8.670280193	-0.281615335
	H259	-3.366728616	8.252042678	2.758883162
	H260	-4.415603815	8.064555474	-2.493305212
	H261	1.391720225	5.796975875	-3.163650671
	H262	2.563650418	7.521816628	-2.150956046
	H263	-1.088049682	5.206701727	-2.942575739
	H264	-8.154122913	-0.043492558	-2.336880071
	H265	3.917846299	10.412968353	-2.613745344
	H266	-5.724453996	-0.592092024	-3.761647992
	H267	0.979795814	6.943054211	-4.435701494
	H268	-3.460739676	6.903887539	0.704392764
	H269	3.443382397	10.517228316	-0.905977048
	H270	-2.408108375	8.450690118	-6.045119392
	H271	-4.762460046	9.347550359	-3.602112735
	H272	-4.752798110	-3.096905027	-4.325193149
	H273	-5.597192614	-3.218542586	-1.745501718
	H274	-7.122573735	10.124142343	1.720345124
	H275	-5.062548404	1.577433314	-1.980163915
	H276	-0.216579587	8.388883442	-2.801331477
	H277	-1.215267632	6.985340704	-5.412400566
	H278	-0.220936905	4.742782082	-4.399721985
	H279	-3.264185543	6.248665706	-3.327195581
	H280	0.390229647	8.506538420	4.001612622
	H281	-0.564007220	9.684035369	1.154479094
	H282	-0.250234571	12.495401821	1.803175679
	H283	1.933852426	9.119191587	3.368553855
	H284	-2.716983953	10.385160239	2.665666854
	H285	5.517912663	-1.962007778	-8.957624365
	H286	5.427999721	-3.511247003	-8.095495910
	H287	8.385761386	-4.595268725	-4.847856036
	H288	6.106478847	-3.913638532	-10.350387407
	H289	4.552450087	-4.422466884	-10.256270270
	H290	5.513762089	4.863662418	0.173152601
	H291	5.580408908	7.358717016	1.921666978
	H292	5.064389884	8.449335146	-2.164417421
	H293	4.056414456	5.605985181	0.906041392
	H294	6.757762098	8.065171617	1.031787817
	H295	6.030188150	3.520712132	-5.912889834
	H296	6.090340836	6.970792802	-0.942686542
	H297	4.898636867	-7.562503893	4.654328193
	H298	6.875087991	-8.168009583	2.386956993
	H299	4.276837501	2.119163834	-6.284283115
	H300	4.767723871	-0.463801130	3.672970623
	H301	1.416119525	2.529341666	-8.392621556
	H302	-0.571554785	-1.537047443	-4.747097631
	H303	1.098772425	2.854516554	-6.687461377
	H304	3.947799802	-4.990063133	4.424716459
	H305	2.726090218	0.800673299	-6.306846829
	H306	3.706409321	-5.366965621	2.710614329
	H307	4.530738583	-7.658282770	2.916249474
	H308	6.215615398	-5.771508282	2.528215785
	H309	6.338161177	-5.569242904	4.282967214
	H310	-4.527092716	-0.072964200	-6.965995024
	H311	5.530551814	-9.995544031	4.337353400
	H312	4.743488099	-12.053095379	2.235588055
	H313	0.680651140	0.536847579	-4.226514763
	H314	5.828733783	-12.434219221	4.922275083
	H315	4.311603650	-12.696754798	4.363977950

H316	5.392784532	-3.576925978	2.210967975
H317	-0.301219589	2.751878378	-4.755509664
H318	-2.741092992	-1.410268172	-5.967916197
H319	7.873253590	-9.688694020	-2.013017924
H320	7.013765051	-7.175847466	-3.911740405
H321	6.697543985	-8.111599942	-0.371500000
H322	7.119333090	-10.150739522	-3.290747118
H323	5.772139499	3.656769744	-8.696473347
H324	6.408493882	-4.978207634	-0.155320575
H325	2.305814123	-7.799481220	0.239427034
H326	4.034226521	-1.115279599	-7.470240764
H327	3.176763348	-9.036992340	-1.558122397
H328	3.762145061	-6.047380768	-7.363204950
H329	2.748122038	-4.844474409	-5.379413651
H330	6.303424573	-12.777357738	2.647316338
H331	5.524878259	-1.288651544	2.331125211
H332	8.304647128	-5.861918195	0.963786573
H333	7.283918293	-3.738075085	0.170507624
H334	8.741530080	-7.147641599	2.882508363
H335	3.210632373	-3.280551070	5.115971128
H336	4.175640776	-7.783634976	-4.168740858
H337	5.257350350	-8.241859689	-2.847563932
H338	2.178354227	-8.335651621	-2.840201625
H339	1.954353138	-1.430683753	-6.213239169
H340	-2.485949332	2.893850892	-5.982104843
H341	-4.499010959	1.710052269	-6.919835944
H342	2.322724398	-6.024825832	0.238777210
H343	8.492984120	-7.360773011	0.592903420
H344	7.405088868	-9.281423029	0.345435698
H345	3.582214774	-1.609404207	5.267194283
H346	6.196255901	-6.745269981	-6.930679623
H347	6.872285306	-5.623156971	-3.106112648
H348	1.226031688	-2.070297001	-7.717852009
H349	4.923645338	4.907111937	-6.042283374
H350	7.348517859	-0.295832947	4.696666114
H351	7.538936562	0.310130258	3.034778375
H352	9.612073841	-6.035390691	-6.247351284
H353	8.814986683	-7.369994312	-5.739908108
H354	10.521830763	-8.346880950	-1.630909494
H355	8.906876717	-7.855745780	-3.162386221
H356	12.115413463	-7.069487554	-3.474558857
H357	10.303420976	-6.694924825	-1.014798590
H358	10.264516986	0.074526405	3.209973247
H359	-3.472348065	12.705082709	4.872053819
H360	9.676722321	-7.436173416	5.726656466
H361	9.096318803	-4.927395473	4.747849961
H362	-4.959063990	12.080343859	2.318919515
H363	-4.513536408	9.811262025	4.357217456
H364	-6.080376798	10.532892592	3.944782770
H365	1.215352158	-3.092162902	-1.209333101
H366	3.217009228	-0.663546992	0.908010813
H367	-6.321020801	6.949305056	-1.428584498
H368	0.608444311	-1.279282733	0.271464146
H369	-1.515349325	-0.035004207	-1.027241635
Mo370	4.076141976	-4.069595685	-2.437038356
N371	-6.824769051	-7.086141420	-1.833388920
N372	-8.867666655	-4.812829212	0.330932245
N373	-8.508080985	-5.428716111	3.046789910
N374	-5.838550796	-6.279655342	3.234158871
N375	-4.520167353	-3.789629039	2.784760316
N376	-5.440054377	-2.435115262	5.153408981
N377	-4.425292622	-4.024603799	7.330006525
N378	-1.797055085	-5.268638124	6.852123623
N379	-0.370627603	-3.194062697	5.818093779
N380	-1.043818385	-0.367147816	6.703387323
N381	-1.649619576	-0.879061574	9.511068672
N382	5.104008135	-12.054957657	4.308581017
N383	6.076822936	-9.691506590	3.524558163
N384	4.839616328	-3.643805109	3.069425586
N385	3.826909422	-2.504661306	4.851701324
N386	4.981693161	-1.339655851	3.205533544
N387	8.711802191	-7.384245105	3.898719068
N388	-5.494753213	-2.592554047	-3.806100937
N389	-1.567847672	-5.224461279	-3.975660357
N390	-5.817048313	-0.188769816	-2.813831983
N391	-8.206133690	0.760028390	-1.714243809
N392	-7.990170906	0.139861737	1.022903281
N393	-5.912951065	1.800070099	1.899610607
N394	-2.998237712	2.737914942	-1.125641938
N395	-2.180093272	0.754425844	-0.863169639

	N396	-6.617215364	4.364878217	2.731000462
	N397	-9.959322458	7.492465305	1.495636270
	N398	-9.980350870	9.127675226	2.995608066
	N399	9.172563557	2.382774939	3.637374600
	N400	6.216283899	7.202140431	1.132804349
	N401	4.370702098	8.725841862	-1.474648001
	N402	1.781364564	8.174116866	-2.264647782
	N403	-2.781009904	6.862268082	-4.008433151
	N404	-2.888465625	8.847203539	-5.245781961
	N405	-4.118285219	8.622555232	-3.297510456
	N406	0.686730145	6.412700885	-0.277329362
	N407	0.768136970	8.049690798	1.997874785
	N408	-0.543968301	10.464713494	1.809975243
	N409	-1.694056537	10.621006918	-2.029952069
	N410	-3.027228899	11.351965070	2.724891172
	N411	5.143512503	-3.586020785	-10.247738683
	N412	3.254115211	-1.659047427	-7.846595563
	N413	2.129727893	1.065080397	-7.109183855
	N414	4.182209575	3.038146387	-6.724958751
	N415	-0.674722284	-1.838502703	-10.462641313
	N416	-2.401981136	-0.210761029	-8.846415386
	N417	8.704273446	-6.365084045	-5.907067490
	N418	4.681366529	-5.135828710	-4.463146092
	N419	4.279446755	-5.827054944	-6.516547292
	N420	9.560153274	-7.090924187	-2.971219816
	N421	0.079176712	2.301171754	0.249296603
	N422	2.312958952	-0.570464064	0.413594558
	N423	0.916502484	1.728374269	-0.245561252
	N424	1.477080013	-1.423617221	0.841348822
	O425	-6.634596596	-5.252305070	0.384849984
	O426	-7.686294861	-3.329632246	3.404531711
	O427	-5.916213292	-5.941081205	5.492637955
	O428	-2.941978907	-4.561720179	4.235523221
	O429	-3.544933441	-1.194510544	5.025818768
	O430	-4.155452701	-2.048534440	8.455258920
	O431	-1.454331792	-5.036013387	9.104793647
	O432	1.605918498	-4.376847301	5.821448135
	O433	1.244074418	-0.434390079	6.745127845
	O434	-0.114847219	0.750722891	9.891070478
	O435	0.324314507	-1.685483131	12.394090933
	O436	6.927777805	-10.525392603	1.543628154
	O437	7.520075111	-8.348228850	5.613502789
	O438	11.099573587	-5.001115699	5.127757716
	O439	-5.601625223	-0.841593155	-0.624513083
	O440	-3.199968430	-3.898773670	-4.842183136
	O441	-7.068870571	2.531107514	-0.831291995
	O442	-5.998801810	3.409356833	-3.612660148
	O443	-9.966769247	1.235349481	1.432962468
	O444	-6.045857821	0.946768797	4.015279083
	O445	-4.618803737	4.587358431	3.815109793
	O446	-7.107227469	6.609064025	5.430778296
	O447	10.327498586	-0.584394703	5.140888385
	O448	3.111024044	4.216148374	4.781067274
	O449	3.559420553	8.404213284	0.632299517
	O450	1.216812074	10.405127880	-2.276751280
	O451	-1.349456371	7.262017472	-0.877281420
	O452	-1.005074756	6.870251931	2.859989978
	O453	2.220221543	5.502161808	2.310908559
	O454	0.460529811	11.252510088	3.712329590
	O455	-2.681669674	13.440457992	1.874241144
	O456	-3.230142942	11.092462401	-0.405974225
	O457	-5.443136890	13.193577747	4.645039835
	O458	-5.406438127	6.938850291	-1.085378567
	O459	2.674016100	-3.564766563	-8.989827486
	O460	0.596061912	0.232607489	-8.595537421
	O461	2.896208227	4.572389947	-7.800585369
	O462	6.619444744	5.373573153	-7.987801295
	O463	-4.062285561	-1.613714286	-9.536857654
	O464	-0.788424235	-5.897430912	-6.839737990
	O465	1.183267110	-4.962527802	-7.300398882
	O466	-3.170463304	3.265653770	-8.500013532
	O467	10.281806167	-4.966212481	-3.288057216
	O468	12.859292623	-6.680021627	-1.615825839
	O469	0.460051420	-6.092444129	-1.904495235
	O470	-0.215630595	-7.391727714	-0.199559562
	O471	5.533193553	-10.424692150	-3.999710250
	O472	3.283165318	-10.454298728	-4.234070293
	O473	5.240792112	-5.635072740	-1.445738731
	O474	5.069115642	-7.487341091	-0.187003585
	O475	2.829971133	-5.793352007	-2.415434527

	O476	8.877238459	-6.641436610	1.167172853
	O477	6.965720277	-4.574584564	0.559502772
	O478	-4.160275628	4.988693163	-2.334724966
	O479	8.039914689	-10.083925376	-2.897717776
	O480	7.577018265	-8.572629041	-0.325690711
	S481	3.729366062	5.204586802	-1.468911124
	S482	2.344839412	2.305791118	-2.810033086
	S483	2.319900444	-2.931581914	-3.538464864
	S484	3.822405680	1.924653546	0.372797703
	S485	0.631944644	-0.655170236	-1.929390696
	S486	4.476223323	-0.112678252	-5.153095654
	S487	3.596771167	-3.402959957	-0.231276140
	S488	5.892332619	2.054859031	-2.509412057
	S489	5.950406270	-2.710101801	-2.942524363
	S490	6.359755183	-0.792463911	0.188190450
	end			
	end			

N2-ready-a to Fe6-NH-NH-a

Figure 8, scheme D

reactant N2-ready-a S=3/2)	bm52rda6nhntg_5_53281.86			
Fe(139) -2.232	C1	-7.743908671	-5.366496598	1.289343050
Fe(140) -0.890	C2	-8.109923312	-6.516787929	0.343849330
Fe(141) -2.522	C3	-8.593674907	-3.454551021	2.576368922
Fe(142) 2.828	C4	-7.957456065	-3.717331140	3.938438242
Fe(143) 2.695	C5	-7.530248928	-5.315721974	5.740738566
Fe(144) 1.293	C6	-6.004547693	-5.430806126	5.674659184
Fe(145) 1.819	C7	-4.028317301	-5.741492819	4.279060702
	C8	-3.492889419	-4.307675899	4.311615426
	C9	-3.905456278	-1.977557040	3.656115659
	C10	-3.916349136	-1.358497929	5.062465437
	C11	-4.943287942	-1.202271107	7.239799684
	C12	-3.869685128	-1.761197075	8.185545895
	C13	-2.865917363	-3.782522129	9.147316754
	C14	-1.394693876	-4.076258942	8.821406718
	C15	0.251767760	-4.755272327	7.118271143
	C16	0.988591476	-3.620938880	6.397711959
	C17	0.665720413	-1.360218838	5.402949405
	C18	0.786445251	-0.150579123	6.344483889
	C19	-0.238358593	-1.137345884	4.166224141
	C20	-0.018700417	0.232157852	3.509679176
	C21	-0.084850183	-2.304479965	3.179729517
	C22	-0.370920419	1.583805796	7.640863837
	C23	-0.011848791	1.248261131	9.098755639
	C24	-1.704601329	2.355836835	7.502706545
	C25	-1.779303786	3.520572359	8.495580290
	C26	-1.884258816	2.867580781	6.066844714
	C27	-0.418423396	-0.104717007	11.064889193
	C28	1.045208006	-0.378697442	11.347148859
	C29	5.893725472	-11.618333859	3.731195325
	C30	6.516580380	-10.336746149	3.186208508
	C31	6.800639962	-7.916093661	3.688900808
	C32	8.026486841	-7.527513982	4.535276804
	C33	5.627891142	-6.952056653	3.933645463
	C34	5.968141055	-5.511197886	3.561017117
	C35	4.728178949	-4.621705146	3.512338992
	C36	4.887348827	-2.114567088	3.479719683
	C37	10.275630659	-6.553850620	4.476783474
	C38	10.476079520	-5.055358377	4.467714460
	C39	-5.343615888	-2.677180648	-1.574140897
	C40	-5.703446917	-1.241847857	-1.143005628
	C41	-3.804978356	-2.820453688	-1.509937840
	C42	-3.247777229	-4.254219064	-1.625222865
	C43	-2.977693312	-4.742737749	-3.049025285
	C44	-6.180400266	0.999079385	-2.049930061
	C45	-7.265922049	1.460787904	-1.067065924
	C46	-6.354195036	1.609946081	-3.446141789
	C47	-9.420734638	0.949961647	-0.016769795
	C48	-9.021288868	0.963578962	1.461870940
	C49	-7.316727036	0.436439063	3.140719846
	C50	-6.142159970	1.392386903	3.355913727
	C51	-4.602355226	3.053305000	2.434635212
	C52	-5.040708733	4.361821479	3.132651614
	C53	-4.011665658	3.489161697	1.085113314
	C54	-3.408665285	2.422105200	0.235409509
	C55	-3.003288748	1.132664201	0.468974095

	C56	-2.580382246	1.596017138	-1.670159488
	C57	-6.841079849	6.040455957	3.249317120
	C58	-6.738615035	6.201928604	4.764951921
	C59	-8.319038682	6.096825398	2.795108223
	C60	-8.937865932	7.458995418	2.674540787
	C61	-8.871540400	8.561585539	3.504082073
	C62	-10.180151194	8.982079990	1.766100149
	C63	9.237130889	1.641874393	3.408112128
	C64	10.280704238	0.552445744	3.241746258
	C65	7.848964966	0.985722302	3.221210269
	C66	6.711559379	1.956090454	3.435093326
	C67	6.137873443	2.146106801	4.704509704
	C68	6.199370896	2.708572299	2.362595675
	C69	5.088011088	3.051363020	4.901049679
	C70	5.167189598	3.628859344	2.545818670
	C71	4.605729027	3.792782153	3.814711873
	C72	5.369117848	6.849377470	-1.402408145
	C73	4.315197754	7.951842996	-1.606789360
	C74	4.697893727	5.513721483	-1.093107071
	C75	3.310604052	9.544264681	-3.206408251
	C76	1.836598775	9.164467158	-3.373541169
	C77	0.219989217	7.265820873	-3.332681267
	C78	-0.245014442	6.923136225	-1.893855333
	C79	0.249301429	6.023757613	-4.250041583
	C80	-1.004443430	5.147302246	-4.352941852
	C81	-2.150848408	5.682934765	-5.227244397
	C82	-3.673728408	7.601375905	-4.747274719
	C83	0.273507127	5.964049025	0.295860746
	C84	0.117052043	7.180060482	1.220823741
	C85	1.271663943	4.993485829	0.960139627
	C86	1.193776684	9.245088475	1.970870746
	C87	0.553390434	10.591120558	1.667000622
	C88	-0.847762176	11.868007860	0.137377507
	C89	-2.122738409	12.423874011	0.816755166
	C90	-0.999994415	11.883976064	-1.385755914
	C91	-2.150562996	11.029289346	-1.901947182
	C92	-4.067414206	11.944550987	2.225789963
	C93	-3.985442664	13.051603051	3.269370815
	C94	-4.729905585	10.681856305	2.841764631
	C95	-4.971355640	9.608583542	1.805758224
	C96	-6.147322477	9.613269112	1.040488541
	C97	-4.009551452	8.621917511	1.536117243
	C98	-6.350585889	8.678726720	0.023884119
	C99	-4.183916145	7.693616817	0.505013871
	C100	-5.354976712	7.739239830	-0.245453080
	C101	4.085418064	-3.989996376	-9.003291193
	C102	2.660005919	-3.735784831	-8.544751256
	C103	1.209531806	-2.196299297	-7.239720122
	C104	0.709939193	-0.842040210	-7.756394194
	C105	1.126345158	1.581547171	-7.714118707
	C106	2.307501576	2.527126938	-7.920495129
	C107	4.591279911	3.184845302	-7.417622059
	C108	5.142531754	3.384472053	-8.815629148
	C109	-2.760583692	-3.497785280	-9.168599855
	C110	-3.785000873	-2.404061350	-8.842072836
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	C112	-1.538749290	-5.488783837	-8.152699547
	C113	-0.867282199	-6.013641931	-6.903510181
	C114	-4.187603838	-0.086357822	-8.181052726
	C115	-3.705394956	1.199036798	-8.824461000
	C116	-4.565133190	0.046301551	-6.683629315
	C117	-3.331492419	0.065546169	-5.825607375
	C118	-2.612546113	1.256720812	-5.624579002
	C119	-2.793733039	-1.141825887	-5.349737955
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	C121	-1.525682771	-1.177573852	-4.762967400
	C122	-0.783900734	0.001882817	-4.642075990
	C123	7.926898326	-6.261788902	-4.800287485
	C124	9.105173908	-6.336487589	-3.816457761
	C125	6.613363518	-6.607172534	-4.084871994
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	C127	4.984828272	-6.981027533	-6.055114294
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	C131	0.625206938	-6.905053068	-0.187645552
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	C133	3.029298433	-7.090164862	-1.133439378
	C134	2.929512712	-8.531618059	-1.702824841
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H149	-8.823238585	-6.141516904	-0.407819428
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H162	-3.511561619	-6.305513118	5.064437337
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H164	-4.245499058	-3.673693478	7.513985428
H165	-5.931453993	-1.409271364	7.674170635
H166	-0.421834816	-3.249698500	3.627031639
H167	-0.690419821	-2.130406883	2.275611874
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H184	-0.830660439	0.432601343	2.793061600
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H187	2.670241714	5.305043687	2.315177683
H188	3.221208739	4.679223120	4.848422131
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H206	-0.799387932	-5.346793635	-8.953897002
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	H221	-2.320306803	-4.326337684	-1.039150613
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	H238	-9.858077333	1.937064230	-0.222750523
	H239	-2.244175263	1.492450406	-2.699617993
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	H245	1.733127077	8.056414926	0.307834606
	H246	-3.443744095	3.544447407	-1.610286855
	H247	-5.112766552	4.165047579	-2.787675352
	H248	-6.700596124	3.396952631	-4.178237428
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	H254	-0.907797925	10.194499386	-3.334757269
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	H259	-3.099192518	8.555298239	2.137227853
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	H263	-1.386767640	4.885266271	-3.354005014
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	H265	3.646395632	10.010730877	-4.142264557
	H266	-6.098104082	-0.954167999	-3.076528571
	H267	0.536465626	6.365293324	-5.257972344
	H268	-3.395114197	6.977059077	0.272595089
	H269	3.340737548	10.310122005	-2.417824978
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	H272	-5.180748072	-3.523846689	-3.444015820
	H273	-5.774934536	-3.336835731	-0.798532152
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	H276	-0.481451942	8.020692614	-3.701637276
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	H278	-0.673769906	4.204202153	-4.809458842
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	H281	-0.460670582	9.750016482	0.101722398
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	H291	5.728321466	7.420242955	0.525114526
	H292	4.824242497	8.088491799	-3.596058735
	H293	4.111559771	5.596952474	-0.167874485
	H294	6.808357073	8.034535193	-0.537858724
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	H328	3.073263169	-6.946231173	-7.023460337
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	H348	0.459676885	-2.951793050	-7.481349350
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	H350	7.771847155	0.151948089	3.934442087
	H351	7.798395167	0.564303828	2.204790933
	H352	9.002100871	-6.802299254	-6.460886287
	H353	8.264305464	-8.069872654	-5.733257578
	H354	10.307570474	-8.559701769	-1.671703946
	H355	8.572621627	-8.245419485	-3.116992046
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	H357	10.175690925	-6.836405897	-1.270060502
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	H360	10.225013499	-6.867023469	5.534540187
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	H366	4.506039744	-1.411294461	-0.031829729
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	H368	0.097947662	-0.937443456	-0.499905885
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transition state S=3/2) Fe(139) -2.250 Fe(140) -0.979 Fe(141) -2.580 Fe(142) 2.740 Fe(143) 2.749 Fe(144) 1.876 Fe(145) 1.460	bm52rda6nhntg_2_53254.76 C1 -7.735209417 -5.363591469 1.283768508 C2 -8.114105303 -6.512166683 0.340776568 C3 -8.573825814 -3.447217573 2.573017553 C4 -7.941208775 -3.709666275 3.936575240 C5 -7.511264870 -5.307493029 5.738595469 C6 -5.985882046 -5.426143075 5.671450232 C7 -4.012390414 -5.732804300 4.272687359 C8 -3.483981502 -4.296278707 4.306026837 C9 -3.901227747 -1.968895292 3.639536970 C10 -3.913003414 -1.345933411 5.044344417 C11 -4.937788471 -1.187080394 7.222396357 C12 -3.866778996 -1.742608898 8.172827845 C13 -2.863467645 -3.760753209 9.142221408 C14 -1.393639505 -4.064012156 8.818125354 C15 0.248747231 -4.769902457 7.122591983 C16 0.987456068 -3.632898042 6.407117349 C17 0.660180992 -1.379773309 5.396755113 C18 0.782872534 -0.169715720 6.337674395 C19 -0.237589982 -1.161010577 4.158819856 C20 -0.005015529 0.202088349 3.492951813 C21 -0.078428630 -2.328009801 3.173862063 C22 -0.366030732 1.571118655 7.631133625 C23 -0.004229201 1.240159665 9.089643132 C24 -1.697485654 2.347576830 7.494653468 C25 -1.768219705 3.512864431 8.487331432 C26 -1.876712331 2.859842279 6.058802837 C27 -0.411987766 -0.098104102 11.066009495 C28 1.052046369 -0.370230304 11.349140976 C29 5.890915249 -11.610900439 3.735041661 C30 6.512863477 -10.330453052 3.187047191 C31 6.796255774 -7.908886699 3.688084328 C32 8.020808884 -7.518694755 4.535930942 C33 5.621958758 -6.947130569 3.932375250 C34 5.962454181 -5.506419446 3.562301017 C35 4.724313616 -4.615355334 3.513764972 C36 4.892923366 -2.108408733 3.488095129 C37 10.274026058 -6.553964378 4.480969170 C38 10.481655935 -5.056357761 4.468272705 C39 -5.333575909 -2.674264791 -1.569961982 C40 -5.694980874 -1.239565141 -1.138126351 C41 -3.795988912 -2.820034867 -1.507708261 C42 -3.243955915 -4.255697202 -1.623863312 C43 -2.976712902 -4.744146900 -3.048223419

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product **Fe6-NH-NH-a** (S=3/2) Fe(139) -2.371 Fe(140) 0.216 Fe(141) -2.561 Fe(142) 2.573 Fe(143) 2.407 Fe(144) 2.299 Fe(145) 0.193	bm52rda6nhnth.car_7 C1 -7.723366809 -5.351388498 1.295039836 C2 -8.051085073 -6.511917488 0.348151966 C3 -8.638362588 -3.470155115 2.583278561 C4 -8.007117606 -3.737085653 3.948065768 C5 -7.599464881 -5.343741126 5.748139253 C6 -6.073111385 -5.460888688 5.694628280 C7 -4.087526858 -5.775009200 4.310516449 C8 -3.535330320 -4.347436656 4.348775438 C9 -3.918930632 -2.005396075 3.732093719 C10 -3.924627892 -1.408153230 5.147084834 C11 -4.960266937 -1.266771312 7.320886818 C12 -3.881886639 -1.844877809 8.250072595 C13 -2.871000870 -3.883136266 9.163988956 C14 -1.391517338 -4.124228607 8.831633812 C15 0.270865031 -4.680643518 7.099502185 C16 0.995044378 -3.545873023 6.370388067 C17 0.667149284 -1.273414558 5.397173867 C18 0.781468195 -0.062656055 6.339998718 C19 -0.224768730 -1.050961483 4.159327969 C20 0.077978770 0.304015711 3.511010212 C21 -0.096217380 -2.248230006 3.209965440 C22 -0.402388202 1.632153952 7.668512358 C23 -0.048307747 1.269361875 9.121802772 C24 -1.743103110 2.392615532 7.538156900 C25 -1.822513644 3.552535640 8.536736166 C26 -1.934957097 2.907754472 6.105239062 C27 -0.445940840 -0.146407314 11.047987575 C28 1.020184469 -0.414819941 11.321744920 C29 5.885037605 -11.633752218 3.686489151 C30 6.523077790 -10.353371136 3.159172721 C31 6.827153510 -7.943524115 3.687367051

C32	8.056376400	-7.559117207	4.529905221
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C35	4.761853778	-4.645436522	3.530428930
C36	4.867125740	-2.138891136	3.473337001
C37	10.291750470	-6.552735699	4.464563445
C38	10.462970042	-5.050143471	4.468484598
C39	-5.326243438	-2.664900376	-1.593133014
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C41	-3.789368002	-2.807451712	-1.523226842
C42	-3.236065410	-4.243466738	-1.629573484
C43	-2.965265915	-4.743548762	-3.048810873
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C48	-9.010288532	0.973425210	1.436821043
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C51	-4.599224827	3.039115508	2.422711085
C52	-5.026239170	4.355122652	3.117546607
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C54	-3.382219640	2.389389729	0.233491816
C55	-2.902578218	1.127263718	0.483272462
C56	-2.529762382	1.571586275	-1.664789160
C57	-6.822541009	6.040426318	3.258568592
C58	-6.698357278	6.211757386	4.771367295
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C65	7.869033336	0.987967840	3.199100374
C66	6.720463064	1.946336112	3.407115313
C67	6.134370383	2.123987932	4.672834083
C68	6.219920248	2.711870546	2.337584247
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C81	-2.150941767	5.681207682	-5.236356021
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C85	1.282701160	4.985129501	0.947312013
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C124	9.102998107	-6.360074421	-3.843340395
C125	6.611892874	-6.594987308	-4.092614521
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C131	0.650173392	-6.868329912	-0.160589229
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C133	3.048350055	-7.060678844	-1.119713722
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C136	4.000968753	-10.354813646	-3.148197395
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Fe139	3.772765866	-2.002555383	-3.725741109
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Fe142	3.844777242	0.512158228	-3.749487300
Fe143	3.892832635	2.708106319	-2.236557895
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H150	-8.597017946	-7.261863706	0.946595794
H151	-8.002431909	-2.723491862	2.085350499
H152	-8.771255231	-5.637971757	3.967673972
H153	-9.627134106	-3.018504902	2.742193483
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H156	-7.829378011	-4.602906411	6.524917157
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H184	-0.553389586	0.452083266	2.622560420
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H186	0.754213299	4.483376050	1.770894561
H187	2.681687925	5.306235273	2.300138356
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	H274	-6.909095216	10.360923021	1.224997669
	H275	-5.239658925	1.392919510	-1.641175777
	H276	-0.490797953	8.020328663	-3.705508127
	H277	-1.742044429	6.345205435	-6.008464523
	H278	-0.665180960	4.207846512	-4.837867672
	H279	-3.582495572	5.871225152	-3.668638187
	H280	0.783860332	8.877320015	2.941500767
	H281	-0.458630576	9.753029188	0.103512502
	H282	-0.067962474	12.614852193	0.412346909
	H283	2.260123333	9.396372562	2.091700302
	H284	-2.440041472	10.642406640	1.731868011
	H285	4.594035739	-3.043264848	-9.169150118
	H286	4.574051062	-4.486819561	-8.137086751
	H287	7.909975674	-5.258884904	-5.189974491
	H288	5.036548017	-5.136621454	-10.392016244
	H289	3.499937643	-5.616754102	-10.093914869
	H290	5.509763780	4.788637143	-0.937289845
	H291	5.759069396	7.448510980	0.500660681
	H292	4.822858439	8.092715652	-3.611437548
	H293	4.133313953	5.623101767	-0.150761283
	H294	6.832031397	8.049099648	-0.579673332
	H295	5.428114989	2.738976483	-6.882395280
	H296	5.963956729	6.748556128	-2.341062791
	H297	5.355695968	-7.047475897	4.999028325
	H298	7.086552511	-7.921153988	2.620975592
	H299	3.627571420	1.343610121	-6.854069281
	H300	5.086941061	-0.114959638	3.174526027
	H301	0.546835698	1.547135732	-8.684003935
	H302	-1.120060317	-2.110113273	-4.390030914
	H303	0.449773191	2.080225505	-7.002442147
	H304	4.348094340	-4.510985867	4.536545704
	H305	2.079504455	0.041860028	-6.576526983
	H306	3.975239924	-5.105780369	2.910627660
	H307	4.811438443	-7.331972607	3.328607463
	H308	6.461584769	-5.524718583	2.569124045
	H309	6.729673548	-5.110421613	4.269031166
	H310	-5.197839410	-0.798984651	-6.456730814
	H311	5.949457290	-9.513111805	4.882158959
	H312	4.985632146	-11.797075640	3.073881935
	H313	0.208795034	-0.016089662	-4.193366901
	H314	6.263930482	-11.893569715	5.694743613
	H315	4.701699754	-12.164371854	5.285137015
	H316	5.587052895	-3.386622056	2.049490077
	H317	-0.761381086	2.144540885	-4.915189525
	H318	-3.365108604	-2.056330970	-5.459323588
	H319	7.666006751	-9.928734237	-1.686166746
	H320	6.619102211	-7.647797746	-3.761471336
	H321	6.661444960	-8.159955839	-0.121327978
	H322	6.794329121	-10.531381293	-2.822989501
	H323	4.875394644	2.579956890	-9.593682750
	H324	6.400043217	-5.041663236	-0.244993714
	H325	2.337651365	-7.730261249	0.858005058
	H326	3.267297362	-2.005899950	-7.662013356
	H327	3.070571534	-9.184642500	-0.828713847
	H328	3.049720849	-6.936909925	-7.004390659
	H329	2.240511840	-5.469825024	-5.100734015
	H330	6.581013537	-12.456722736	3.449556401
	H331	5.743885893	-1.098765637	1.890095995
	H332	8.367945716	-5.793463020	0.805528320
	H333	7.266679072	-3.761288911	-0.111230685
	H334	8.984727667	-6.866753694	2.792356744
	H335	3.655619140	-2.716103747	5.080347549
	H336	3.776996241	-8.282894110	-3.671323794
	H337	4.989796192	-8.584676168	-2.423015482
	H338	1.930643193	-8.659196311	-2.078901079
	H339	1.333369638	-2.151626776	-6.167014329
	H340	-3.022213957	2.209947330	-5.995574044
	H341	-5.141199930	0.977022637	-6.613265827
	H342	2.385492931	-5.965728325	0.643045648
	H343	8.527498072	-7.325541377	0.578485921
	H344	7.430939585	-9.250297834	0.653899293
	H345	4.072501746	-1.046892115	5.001132863
	H346	5.513543779	-7.609159862	-6.727429980
	H347	6.580106367	-5.994063536	-3.176783668
	H348	0.448244402	-2.946880669	-7.501841477
	H349	4.303602013	4.112660577	-6.999585653
	H350	7.795578441	0.149705452	3.908057407
	H351	7.834810691	0.570950275	2.179889162

H352	8.985224362	-6.917435427	-6.470560607
H353	8.216643576	-8.143628057	-5.704183570
H354	10.308422540	-8.565183715	-1.682782474
H355	8.587091321	-8.276378539	-3.145945973
H356	11.724172242	-7.577839872	-3.835848065
H357	10.166125737	-6.840005901	-1.292805698
H358	10.577264329	0.374190554	2.166918445
H359	-2.973907628	13.208544466	3.716203042
H360	10.254415060	-6.874626405	5.520230024
H361	9.513932358	-4.464693843	4.396609235
H362	-4.700044486	12.312665933	1.401309108
H363	-4.089373514	10.302707534	3.656217817
H364	-5.678044574	10.999519338	3.290542851
H365	1.237099843	-3.157985468	-0.844007787
H366	3.247819186	-1.145748815	0.787553172
H367	-6.427177856	6.811828406	-1.571446998
H368	0.540377224	-0.961326928	0.489644104
H369	-1.806100950	-0.195470894	-0.838458608
Mo370	3.860927226	-4.380276605	-2.416672034
N371	-6.926257917	-7.156194143	-0.304476767
N372	-8.802203541	-4.652658871	1.752184491
N373	-8.211060605	-4.964373247	4.484566791
N374	-5.530544764	-5.817999120	4.503607394
N375	-4.269310056	-3.416296087	3.687539777
N376	-4.922053823	-1.805174470	5.971810870
N377	-3.682875600	-3.187121406	8.174791665
N378	-1.086874396	-4.378476844	7.525090447
N379	0.243369315	-2.446573440	6.149100841
N380	-0.390880125	0.451962809	6.803895432
N381	-0.697076004	0.207438918	9.664465782
N382	5.501525499	-11.556799728	5.102584311
N383	6.414085684	-9.301000497	3.993026281
N384	5.105584673	-3.345055314	2.952164068
N385	4.250640514	-1.989162431	4.664726670
N386	5.259196500	-1.043036084	2.798771005
N387	9.066845915	-6.989004367	3.826097398
N388	-5.845396894	-2.940324628	-2.938374873
N389	-1.919713329	-5.578805056	-3.189131644
N390	-6.079776361	-0.437991827	-2.199923742
N391	-8.344733988	0.679006548	-0.983213542
N392	-7.839726388	0.355902792	1.760486985
N393	-5.695270415	2.093276897	2.260922236
N394	-3.139037075	2.630152568	-1.112979995
N395	-2.390237395	0.645857148	-0.708362151
N396	-6.309506645	4.728820240	2.880833739
N397	-9.717879155	7.749324462	1.601632564
N398	-9.636666810	9.529450467	2.923735529
N399	9.481154582	2.705545143	2.405954010
N400	6.307782193	7.205849139	-0.330398798
N401	4.207807769	8.456648757	-2.888241214
N402	1.552551508	7.847782142	-3.352051774
N403	-3.165062731	6.398868344	-4.457020392
N404	-3.383498004	8.225201005	-5.904676206
N405	-4.443044847	8.237028828	-3.842959947
N406	0.657639889	6.313545219	-1.080047926
N407	0.959400064	8.199005879	0.973120820
N408	-0.364748682	10.600038291	0.663662555
N409	-1.877772540	10.380039628	-3.057825290
N410	-2.742634582	11.613167573	1.710444842
N411	4.087821574	-4.789850152	-10.232796989
N412	2.451110229	-2.577693942	-7.892456052
N413	1.397052095	0.225543317	-7.330404984
N414	3.494873688	2.193036897	-7.410002685
N415	-1.701792680	-3.012938194	-10.090700330
N416	-3.260340553	-1.178028400	-8.510433130
N417	8.109275116	-7.169628744	-6.004100486
N418	4.255337578	-5.675679342	-4.351862281
N419	3.648448019	-6.619492248	-6.246873223
N420	9.243435830	-7.491209700	-3.100666480
N421	0.042211590	2.366221822	-0.336118172
N422	2.331728854	-1.276168670	0.330331700
N423	0.806801400	1.728804302	-0.866126189
N424	1.414651542	-0.839640811	1.057559959
O425	-6.568516531	-5.085260326	1.675178260
O426	-7.344362699	-2.854267325	4.520025703
O427	-5.391896783	-5.249983390	6.711618114
O428	-2.493751849	-4.059710413	4.958461452
O429	-3.051644375	-0.605167110	5.511023622
O430	-3.274417810	-1.112674090	9.051102774
O431	-0.551997150	-4.124476887	9.741127529

O432	2.181855620	-3.686175003	6.015427281
O433	1.891559151	0.391922379	6.656021026
O434	0.796374543	1.915320793	9.763642631
O435	1.515835960	-0.339003427	12.435907696
O436	7.061463660	-10.343464435	2.033484876
O437	8.079343174	-7.751452350	5.758316693
O438	11.545853677	-4.495497781	4.564352150
O439	-5.629196479	-0.831806516	0.014163368
O440	-3.692864088	-4.418243967	-4.015551179
O441	-7.105095474	2.515746761	-0.431653337
O442	-6.329139018	3.051657806	-3.378180338
O443	-9.756222634	1.514495745	2.264007236
O444	-5.591243611	1.418265637	4.442804202
O445	-4.219604932	5.046410508	3.746403887
O446	-6.512324022	7.276763240	5.334154621
O447	10.817730498	-0.034848879	4.153366330
O448	3.579948955	4.691362104	3.909685085
O449	3.611511020	8.383452339	-0.688643757
O450	0.987381976	10.070750970	-3.544636290
O451	-1.405567330	7.184344216	-1.537592331
O452	-0.704094232	7.139235932	2.147453510
O453	2.432997474	5.682649939	1.431218742
O454	0.849957466	11.575910014	2.343435248
O455	-2.489162566	13.585681211	0.594955135
O456	-3.247291805	11.034085954	-1.348630983
O457	-4.950810963	13.707511008	3.616585470
O458	-5.483443502	6.834926499	-1.320185391
O459	1.748134214	-4.591546466	-8.744683926
O460	-0.255718504	-0.749080738	-8.584240346
O461	2.119591648	3.591359853	-8.557317708
O462	5.691669526	4.408949830	-9.198497210
O463	-4.981502927	-2.623538203	-8.890231786
O464	-1.484801614	-6.609011384	-6.007232195
O465	0.444251403	-5.775927321	-6.760275921
O466	-3.988962118	2.325668858	-8.473966581
O467	9.921137788	-5.425307728	-3.740237184
O468	12.661887357	-6.990132623	-2.120601055
O469	0.327004681	-6.228389742	-1.291757253
O470	-0.202817539	-7.323724137	0.598974311
O471	5.152625345	-10.890017092	-3.325959980
O472	2.891345158	-10.939394437	-3.298835795
O473	5.134643343	-5.856032063	-1.384796584
O474	5.069324421	-7.503572331	0.137591580
O475	2.628981094	-6.077732831	-2.068317981
O476	8.960056961	-6.550574771	1.034959221
O477	6.988130474	-4.553545608	0.386155709
O478	-4.375760165	4.738892267	-2.458859400
O479	7.748858737	-10.421353959	-2.532997347
O480	7.540684755	-8.624506011	-0.106386669
S481	3.563062525	4.943063617	-2.413532439
S482	2.162972002	1.986981150	-3.483963890
S483	1.988229351	-3.323623104	-3.390135314
S484	3.626955117	1.758307962	-0.258895647
S485	0.527947336	-0.909931217	-1.869919939
S486	4.008763583	-0.759876692	-5.541756965
S487	3.711457259	-3.546266553	-0.240765355
S488	5.688271833	1.719583493	-3.180593991
S489	5.670086389	-3.088237299	-3.250980065
S490	6.388340431	-0.847089720	-0.354380719
end			

N2-ready-a to Fe2-N-NH-a

Figure 8, scheme E

transition state (S=3/2)	bm52rda2nnhtrk_1_53266.24		
Fe(139) -2.227	C1	-7.748113706	-5.373374575	1.284556779
Fe(140) -0.001	C2	-8.148092803	-6.514982935	0.342272984
Fe(141) -2.472	C3	-8.545282873	-3.437010543	2.567838341
Fe(142) 2.446	C4	-7.903738065	-3.694760806	3.927374876
Fe(143) 2.623	C5	-7.467280893	-5.281069314	5.737644466
Fe(144) 1.535	C6	-5.942293172	-5.399694844	5.668090656
Fe(145) 1.187	C7	-3.968774214	-5.708534098	4.273258607
	C8	-3.451363420	-4.268109754	4.296792333
	C9	-3.879050953	-1.950097142	3.603812409
	C10	-3.887659587	-1.320371731	5.006030854
	C11	-4.913239187	-1.153202870	7.185493726
	C12	-3.856011473	-1.706138178	8.151931197

	C13	-2.853761301	-3.722397122	9.130480798
	C14	-1.387211880	-4.042389469	8.806740253
	C15	0.234804237	-4.809875531	7.121079742
	C16	0.971467935	-3.659904663	6.426461051
	C17	0.645792885	-1.425539903	5.398831400
	C18	0.767954788	-0.208190670	6.329220032
	C19	-0.216952931	-1.209372833	4.129616394
	C20	0.032066805	0.143527914	3.441026709
	C21	-0.034808156	-2.370748302	3.141849803
	C22	-0.361073496	1.546431927	7.617262535
	C23	0.007784084	1.224792484	9.077959056
	C24	-1.687618983	2.331203067	7.482346052
	C25	-1.750814760	3.498873805	8.472636253
	C26	-1.866004284	2.840917046	6.045323553
	C27	-0.405789069	-0.086073227	11.077215087
	C28	1.060220949	-0.354254637	11.355142086
	C29	5.900926515	-11.602181719	3.759760337
	C30	6.516207737	-10.324143280	3.198805013
	C31	6.784545530	-7.895877117	3.682417546
	C32	8.006100451	-7.500499998	4.532247498
	C33	5.604870009	-6.940035471	3.922365103
	C34	5.937028219	-5.498138040	3.549780547
	C35	4.692096513	-4.616122892	3.500584044
	C36	4.903070546	-2.116713628	3.531248065
	C37	10.266818215	-6.557113942	4.484524643
	C38	10.492548013	-5.062229198	4.471766575
	C39	-5.345762281	-2.681194813	-1.559460765
	C40	-5.705312805	-1.246537194	-1.125522046
	C41	-3.806945314	-2.824937148	-1.500120846
	C42	-3.252934718	-4.259698205	-1.618864082
	C43	-2.983759070	-4.744033193	-3.044447691
	C44	-6.186778883	0.994926365	-2.031683783
	C45	-7.275531382	1.452152800	-1.050613772
	C46	-6.363440937	1.603981297	-3.428331763
	C47	-9.429451966	0.930879415	-0.003151876
	C48	-9.031542845	0.951097523	1.475891188
	C49	-7.326053018	0.439205967	3.158478876
	C50	-6.155421937	1.400932463	3.369601630
	C51	-4.608195214	3.047501712	2.435175396
	C52	-5.049344410	4.357209673	3.132077403
	C53	-4.024028164	3.479161952	1.081375960
	C54	-3.408858339	2.415634278	0.234514528
	C55	-2.971688160	1.137093602	0.472595007
	C56	-2.557996614	1.602998770	-1.667077863
	C57	-6.855759197	6.036041774	3.245731537
	C58	-6.761033097	6.190807305	4.762132894
	C59	-8.327202859	6.089731536	2.775236817
	C60	-8.949053674	7.450455787	2.659930223
	C61	-8.873686955	8.554297794	3.486935071
	C62	-10.200275207	8.971538235	1.761718804
	C63	9.232936426	1.625039517	3.424290197
	C64	10.264123548	0.523700882	3.257365897
	C65	7.838807067	0.981457844	3.246000868
	C66	6.708470552	1.960039912	3.462644273
	C67	6.138681282	2.156261870	4.732982550
	C68	6.193983868	2.708689566	2.389047907
	C69	5.088905429	3.062022115	4.928247799
	C70	5.162462827	3.629652337	2.571019878
	C71	4.602240841	3.797166902	3.839591301
	C72	5.364034248	6.852248331	-1.395485000
	C73	4.310935052	7.953365438	-1.605155521
	C74	4.690584974	5.512946064	-1.097447166
	C75	3.308107369	9.541916399	-3.207590594
	C76	1.833143805	9.164056613	-3.367887511
	C77	0.214160403	7.267265732	-3.327011116
	C78	-0.250295148	6.925445798	-1.887314987
	C79	0.243836564	6.022296588	-4.241526230
	C80	-1.010562244	5.146839634	-4.348310543
	C81	-2.154149563	5.684169878	-5.225590961
	C82	-3.675058440	7.605063275	-4.743264316
	C83	0.274416673	5.982160924	0.310350161
	C84	0.117534325	7.203648339	1.227825189
	C85	1.275173315	5.018899500	0.982337731
	C86	1.201536673	9.267912125	1.968951660
	C87	0.557348339	10.610590715	1.659433819
	C88	-0.854520586	11.872876241	0.127867311
	C89	-2.128175376	12.428379028	0.810926763
	C90	-1.015920531	11.880166005	-1.394568028
	C91	-2.160184770	11.009907351	-1.898043911
	C92	-4.072683567	11.949758916	2.224144996

C93	-3.984394931	13.050799495	3.272282967
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C96	-6.155071795	9.603982797	1.046320035
C97	-4.006417694	8.627006774	1.522100815
C98	-6.361645089	8.668100715	0.031429589
C99	-4.183523103	7.698248797	0.491784395
C100	-5.361519236	7.736340768	-0.248417996
C101	4.088678571	-3.980531108	-8.998051976
C102	2.662701545	-3.726897265	-8.542935599
C103	1.209769988	-2.192452560	-7.237829890
C104	0.709759686	-0.836727257	-7.749128674
C105	1.125746026	1.585919760	-7.705830533
C106	2.299543465	2.541707280	-7.906206008
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C112	-1.541549787	-5.489182421	-8.153998914
C113	-0.864083380	-6.015259866	-6.908668764
C114	-4.200898957	-0.086251704	-8.161199955
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C116	-4.565980485	0.045807801	-6.661029593
C117	-3.325841193	0.059682907	-5.811860065
C118	-2.600310065	1.247449642	-5.614009341
C119	-2.787050923	-1.150854914	-5.345478677
C120	-1.322735794	1.203796033	-5.045378524
C121	-1.511015460	-1.193964535	-4.777223476
C122	-0.761664350	-0.018688587	-4.663676184
C123	7.918825290	-6.236506029	-4.772870038
C124	9.098054641	-6.321158066	-3.792611320
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Fe139	3.844256703	-2.001955776	-3.707068886
Fe140	2.155037359	0.694361762	-1.322490833
Fe141	5.012336852	0.457671598	-1.509684973
Fe142	3.772341332	0.506877925	-3.766072730
Fe143	3.906521758	2.726579132	-2.335425123
Fe144	4.665532363	-2.064332496	-1.259247359
Fe145	2.153995207	-2.423139708	-1.768853778
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H148	-9.716546309	-4.781062360	1.394959280
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	H181	-2.513037501	1.633516720	7.713552109
	H182	0.467404322	2.179509110	7.264297746
	H183	-1.286676232	0.033142770	6.401557273
	H184	-0.893627102	0.479609007	2.946618035
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	H186	0.739017677	4.523175437	1.804914361
	H187	2.675154815	5.327716874	2.335194189
	H188	3.212325559	4.680934506	4.868960354
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	H191	6.510284367	1.583977083	5.587728065
	H192	-0.806424725	-2.692683959	6.292045684
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	H194	0.829693854	-5.105085167	7.994648277
	H195	-1.861179854	-4.546463109	6.843857542
	H196	-2.835974627	-3.091134171	10.026857520
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	H198	1.678043680	-1.634421637	5.094067062
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	H200	-0.957215693	-1.003076562	11.336092530
	H201	1.648786584	-0.728480118	10.485369432
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	H204	1.229368397	-6.070914904	-1.813723537
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	H206	-0.804844323	-5.340075252	-8.956423647
	H207	-3.129120012	-4.378886445	-7.187817461
	H208	-3.118251719	1.045978776	-9.734768450
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	H210	-3.367029133	-2.194414910	-2.291496716
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	H213	-5.143314341	-0.320213966	-8.698211298
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	H248	-6.714532231	3.389077835	-4.162477708
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	H256	-3.680201630	9.207941379	-6.025651934
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N405	-4.455543536	8.238219512	-3.837970746
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product **Fe2-N-NH-a** (S=3/2)	bm52rda2nnhtrk.car_6

Fe(139) -2.304	C1	-7.771779709	-5.379421248	1.305127670
Fe(140) -0.246	C2	-8.125275932	-6.534562450	0.361550957
Fe(141) -2.498	C3	-8.635928848	-3.472155776	2.588637083
Fe(142) 2.392	C4	-7.986043448	-3.731880749	3.945158193
Fe(143) 3.004	C5	-7.560537609	-5.323535352	5.753995518
Fe(144) 2.037	C6	-6.035191857	-5.437293469	5.683092106
Fe(145) 0.864	C7	-4.060084988	-5.767195622	4.288307455
	C8	-3.497160168	-4.343768992	4.315305041
	C9	-3.868420749	-2.004454672	3.684110251
	C10	-3.871134801	-1.401190964	5.096703096
	C11	-4.932517041	-1.225697982	7.258927351
	C12	-3.876949541	-1.801968557	8.213558888
	C13	-2.892482455	-3.837352519	9.163375658
	C14	-1.420322485	-4.119810672	8.834427032
	C15	0.227069385	-4.740730194	7.110973868
	C16	0.966713165	-3.608499380	6.396548287
	C17	0.698825994	-1.328935039	5.454341438
	C18	0.786811565	-0.110859073	6.389642135
	C19	-0.106666239	-1.097218630	4.150907151
	C20	0.279536575	0.225195247	3.477113427
	C21	0.066236280	-2.277470765	3.186856738
	C22	-0.400701017	1.610163040	7.670494262
	C23	-0.049975552	1.270177185	9.130631003
	C24	-1.736837373	2.374751400	7.521963390
	C25	-1.820285243	3.542354559	8.510805047
	C26	-1.905783236	2.880708854	6.082425180
	C27	-0.453656717	-0.100443141	11.087890492
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	C29	5.892977657	-11.636612005	3.715940363
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	C32	8.030945439	-7.540949256	4.538188177
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	C34	5.945394624	-5.547276464	3.562186899
	C35	4.690156434	-4.682009107	3.488749327
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	C38	10.462596658	-5.056150761	4.469815773
	C39	-5.374771880	-2.681927923	-1.581732923
	C40	-5.732966663	-1.245975707	-1.152983810
	C41	-3.837026945	-2.822576134	-1.513907855
	C42	-3.273577875	-4.253547206	-1.632819122
	C43	-3.005995373	-4.740182480	-3.057932598
	C44	-6.192078284	0.996198977	-2.064940749
	C45	-7.273840899	1.468559984	-1.083247446
	C46	-6.361238535	1.603451899	-3.463095010
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	C48	-9.022272941	0.975763457	1.451190770
	C49	-7.315335019	0.418058478	3.119679867
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	C51	-4.624408155	3.061312288	2.425925674
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	C53	-4.032592796	3.496166356	1.076907455
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	C55	-2.921436874	1.175883363	0.474534689
	C56	-2.558905791	1.634624978	-1.674971036
	C57	-6.865745338	6.043557895	3.276447303
	C58	-6.754629417	6.209920164	4.790566003
	C59	-8.345061924	6.104022364	2.827158426
	C60	-8.952225606	7.470448230	2.696232295
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	C65	7.861081706	1.011523552	3.205926197
	C66	6.725788356	1.981783540	3.430922310
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	C68	6.228111817	2.757194535	2.367919736
	C69	5.095075549	3.061142173	4.900914374
	C70	5.202578969	3.682236569	2.558638987
	C71	4.629555776	3.826878728	3.824288544
	C72	5.379113955	6.844259089	-1.440675563
	C73	4.324616576	7.946345317	-1.639565387
	C74	4.705747721	5.495755610	-1.202160075
	C75	3.311905336	9.542750823	-3.227698055
	C76	1.836523517	9.164988425	-3.386201452
	C77	0.216856513	7.269224281	-3.344506443
	C78	-0.231473131	6.924370606	-1.900947198
	C79	0.237808770	6.022534097	-4.258386362
	C80	-1.018325887	5.148220729	-4.358476938

	C81	-2.163302574	5.687944886	-5.232481238
	C82	-3.690874740	7.600299398	-4.752683034
	C83	0.317470095	5.968973696	0.286625707
	C84	0.136260915	7.180969313	1.212119189
	C85	1.341523115	5.022588593	0.949029016
	C86	1.189863280	9.252677819	1.977531088
	C87	0.547478858	10.598810587	1.677052379
	C88	-0.852062720	11.877761989	0.144418165
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	C90	-0.995074972	11.885878239	-1.380276077
	C91	-2.149023665	11.039406381	-1.903970028
	C92	-4.075640821	11.962583715	2.228887807
	C93	-3.991616078	13.067611802	3.273709768
	C94	-4.736183554	10.697120019	2.842845336
	C95	-4.974660918	9.622737226	1.806627901
	C96	-6.146892444	9.629388417	1.035788253
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	C101	4.082438479	-3.989861553	-8.977411636
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	C103	1.186872386	-2.176744609	-7.270354235
	C104	0.686685849	-0.824953397	-7.792257825
	C105	1.103645003	1.600583935	-7.749251976
	C106	2.292283223	2.543613458	-7.925731289
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	C112	-1.545535105	-5.485927796	-8.163584393
	C113	-0.883139186	-6.013797769	-6.911401855
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	C115	-3.713777275	1.203627691	-8.852403687
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	C117	-3.303889926	0.051096881	-5.837157407
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	C121	-1.546139110	-1.217645354	-4.722221833
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	C132	2.107898076	-6.918802257	0.070260346
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	C134	2.972601898	-8.522721044	-1.700516542
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	C136	4.028895609	-10.369344490	-3.160614493
	C137	4.488204047	-6.772158667	-0.743313468
	C138	3.548178906	-0.709047747	-2.209662547
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	Fe140	2.097778998	0.614668135	-1.095687773
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	Fe142	3.775228632	0.519129418	-3.719211856
	Fe143	3.870033461	2.719117983	-2.433773797
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	Fe145	2.197388291	-2.356816404	-1.827507433
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	H149	-8.840819034	-6.170147085	-0.393217045
	H150	-8.674129493	-7.278414225	0.964358165
	H151	-7.998397431	-2.739917056	2.071957352
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	H153	-9.615420634	-3.004933294	2.758419189
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	H176	9.330354485	2.028490287	4.419151641
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	H213	-5.130647177	-0.315248219	-8.727440591
	H214	-1.035992782	-2.404404293	-9.605921049
	H215	-1.316464620	-5.807126174	-2.446445380
	H216	-1.607898802	-3.458700953	-7.337472350
	H217	-1.201470102	-3.785417681	-10.488093153
	H218	-6.782613656	-3.459627547	-2.877174775
	H219	-3.519112248	-2.417580737	-0.541650488
	H220	0.818670453	-5.301267155	-7.579464848
	H221	-2.343289454	-4.320238027	-1.050047540
	H222	-3.855632051	2.613458861	3.070854205
	H223	-2.904562797	0.579837881	1.378513609
	H224	-8.120525915	0.760095940	3.784666072
	H225	-7.270084937	-0.067199375	1.042860675
	H226	-6.963910828	4.077242523	2.429202655
	H227	-8.356465278	8.760389817	4.451200626
	H228	-6.901810848	5.257794519	5.357362688
	H229	-8.950140313	5.466147308	3.495917152
	H230	-6.283639849	6.841267729	2.788715844
	H231	-10.820882726	9.558868994	1.101207578
	H232	-3.276772041	4.268089916	1.294067063
	H233	-4.823707577	3.983414310	0.484897450
	H234	-9.821219371	10.479808884	3.263872820
	H235	-8.402445692	5.644975481	1.827267225
	H236	-6.206024347	2.051052224	1.369008630
	H237	-7.019300743	-0.582302842	3.468899005
	H238	-9.855296998	1.963988092	-0.227485259
	H239	-2.227018866	1.537814990	-2.706064658
	H240	-10.225922151	0.230897793	-0.163328016

	H241	10.298867902	3.254813043	2.617978864
	H242	8.689605016	3.346539413	2.354280644
	H243	1.578405755	5.986989164	-1.466943158
	H244	-0.656452005	5.458194253	0.262175067
	H245	1.745943441	8.076640693	0.310774396
	H246	-3.502743468	3.545736731	-1.623750514
	H247	-5.137458220	4.171431151	-2.802990913
	H248	-6.705113453	3.384667985	-4.206964190
	H249	-4.817515981	5.414434021	-1.855766664
	H250	-5.531998842	1.246264987	-4.095710802
	H251	-7.313769473	1.270562154	-3.902999727
	H252	-0.040447291	11.598057304	-1.842586260
	H253	-1.205370222	12.925477779	-1.677299609
	H254	-0.911461209	10.206064695	-3.341699883
	H255	-2.600283934	9.699210087	-3.342385041
	H256	-3.760014200	9.165955893	-6.073267919
	H257	-2.659571737	4.858179646	-5.758458902
	H258	-7.271985422	8.703645491	-0.564507449
	H259	-3.108300573	8.563189976	2.149721464
	H260	-4.674906268	7.793494394	-2.952979029
	H261	1.058477812	5.376966359	-3.906480773
	H262	2.347394742	7.195338323	-3.276730938
	H263	-1.401085499	4.888301315	-3.358932623
	H264	-8.382892736	-0.196076517	-1.493727748
	H265	3.642820796	10.012894177	-4.163309230
	H266	-6.119958397	-0.960475224	-3.087850218
	H267	0.525591896	6.358506956	-5.268184511
	H268	-3.402619327	6.978656553	0.289733857
	H269	3.345392760	10.305211130	-2.435818318
	H270	-3.048871944	7.722503215	-6.705700859
	H271	-5.118080498	8.945481697	-4.168448853
	H272	-5.212689387	-3.533953794	-3.448960088
	H273	-5.808863431	-3.340412383	-0.806487732
	H274	-6.921615541	10.374635942	1.230904912
	H275	-5.257003062	1.374192416	-1.627962287
	H276	-0.487800935	8.023741161	-3.707052933
	H277	-1.748684752	6.353713431	-5.999945476
	H278	-0.691329633	4.203712727	-4.815358212
	H279	-3.602865362	5.878141243	-3.672230624
	H280	0.791272424	8.903719064	2.942005799
	H281	-0.465583171	9.759819285	0.111063735
	H282	-0.082777424	12.622214080	0.402266995
	H283	2.266253437	9.433719469	2.098510238
	H284	-2.444645827	10.661919561	1.748348592
	H285	4.604225388	-3.035298257	-9.138091629
	H286	4.573956109	-4.481581971	-8.110956847
	H287	7.923290515	-5.228685033	-5.151030714
	H288	5.050677632	-5.126976103	-10.366434248
	H289	3.506345713	-5.598613321	-10.084089911
	H290	5.492426433	4.746404893	-1.052338077
	H291	5.672606028	7.370464941	0.509846557
	H292	4.827381192	8.091365903	-3.629507845
	H293	4.082447960	5.548052352	-0.298700122
	H294	6.800537560	7.988238781	-0.499435432
	H295	5.401430686	2.767036350	-6.787122819
	H296	6.008033737	6.771823364	-2.341121188
	H297	5.319189911	-7.058247776	4.997513602
	H298	7.067293220	-7.918807539	2.627943484
	H299	3.614090723	1.357495727	-6.818927495
	H300	5.169880373	-0.184401735	3.285491215
	H301	0.562516082	1.568729946	-8.702819814
	H302	-1.150353561	-2.170735213	-4.363711426
	H303	0.434214721	2.084370934	-7.016947139
	H304	4.235484954	-4.564321776	4.479297102
	H305	2.091023786	0.046750740	-6.605391784
	H306	3.936546481	-5.151748723	2.837506483
	H307	4.784286777	-7.355648173	3.326150289
	H308	6.432499149	-5.527712064	2.576391475
	H309	6.649042322	-5.099000840	4.281239222
	H310	-5.191747104	-0.792807947	-6.432125460
	H311	5.946901588	-9.509993015	4.898067615
	H312	4.990784606	-11.806659459	3.109147731
	H313	0.203754081	-0.076608185	-4.135959511
	H314	6.285909303	-11.875544154	5.724097451
	H315	4.724686605	-12.169412356	5.324709869
	H316	5.556725862	-3.395878944	2.061302876
	H317	-0.719459970	2.079813592	-4.865204930
	H318	-3.376213567	-2.080911899	-5.462142802
	H319	7.660942841	-9.924485366	-1.673249709
	H320	6.654951436	-7.640480013	-3.742579107

H321	6.633820267	-8.163128397	-0.115785622
H322	6.807219148	-10.530386157	-2.822541908
H323	4.906790597	2.566465183	-9.516378326
H324	6.328619325	-5.021821337	-0.195229297
H325	2.299675917	-7.718983335	0.795765150
H326	3.265614107	-2.005582133	-7.628117675
H327	3.114642361	-9.182729810	-0.830222383
H328	3.161417183	-7.077493389	-7.080949059
H329	2.278650269	-5.551887312	-5.253452703
H330	6.592224909	-12.456770953	3.479293906
H331	5.883063908	-1.152740615	2.059823845
H332	8.332061112	-5.805777408	0.820905894
H333	7.218356686	-3.760698176	-0.064238878
H334	8.967681812	-6.866145171	2.798616229
H335	3.607089658	-2.765851799	5.093703372
H336	3.798316748	-8.299169873	-3.683848360
H337	5.016046913	-8.595340156	-2.435633462
H338	1.957689099	-8.706968844	-2.084005706
H339	1.319495630	-2.140751654	-6.177389586
H340	-2.960008464	2.179979576	-5.996408906
H341	-5.114928076	0.982808784	-6.579390987
H342	2.323855712	-5.957472237	0.567067495
H343	8.500091770	-7.335438758	0.587847054
H344	7.394156942	-9.255904662	0.670437779
H345	4.205712690	-1.140398252	5.154698741
H346	5.618864724	-7.713285233	-6.701136763
H347	6.557997427	-5.981518075	-3.176243530
H348	0.442848144	-2.936130372	-7.517665120
H349	4.286135326	4.140933892	-6.964102827
H350	7.791751617	0.176191353	3.917650849
H351	7.799331869	0.592819158	2.188666759
H352	9.039718729	-6.855829989	-6.435260722
H353	8.294107799	-8.103765567	-5.684009233
H354	10.308356239	-8.526940572	-1.630847376
H355	8.589574993	-8.235549295	-3.098158486
H356	11.721409502	-7.555100764	-3.791411349
H357	10.174392799	-6.800647318	-1.245060509
H358	10.552634594	0.351080400	2.141053426
H359	-2.982627347	13.221440467	3.723227218
H360	10.236693335	-6.876043973	5.527726112
H361	9.519487713	-4.460583514	4.410496111
H362	-4.710262513	12.333058192	1.406610727
H363	-4.098590408	10.317753445	3.656796153
H364	-5.687557038	11.014286980	3.293760589
H365	1.172272822	-3.313994858	-1.279853496
H366	3.718527150	-1.503277465	0.766724255
H367	-6.446487466	6.829265979	-1.567960364
H368	0.103031894	-1.367841631	-0.286115461
H369	-1.894278966	-0.164515965	-0.874283410
Mo370	3.830443141	-4.391144736	-2.524691527
N371	-7.013807855	-7.190017846	-0.302911588
N372	-8.832521092	-4.660917992	1.773225988
N373	-8.189346931	-4.952195466	4.496510045
N374	-5.502174197	-5.797819133	4.489876697
N375	-4.225708850	-3.413422289	3.646142990
N376	-4.879868673	-1.778442763	5.916279921
N377	-3.686617568	-3.146577768	8.156335437
N378	-1.126774760	-4.423197719	7.535402826
N379	0.228764686	-2.499380723	6.175465850
N380	-0.390305237	0.419149120	6.820237010
N381	-0.702394447	0.221918620	9.695167915
N382	5.515946520	-11.553162525	5.133545360
N383	6.408782096	-9.299770210	4.007120730
N384	5.019856207	-3.366874975	2.933301075
N385	4.243574161	-2.054961435	4.714433314
N386	5.515323000	-1.104086100	3.020970975
N387	9.047192288	-6.983035040	3.833481843
N388	-5.895764357	-2.954171505	-2.926343701
N389	-1.958295795	-5.569574441	-3.210317261
N390	-6.109948378	-0.449534882	-2.188515539
N391	-8.363607300	0.676105168	-0.969625804
N392	-7.851134171	0.358780835	1.772970827
N393	-5.712580430	2.106251768	2.264878905
N394	-3.165501999	2.687861839	-1.112936901
N395	-2.418346702	0.704147840	-0.723403861
N396	-6.345628915	4.734547166	2.898834682
N397	-9.757446219	7.751321559	1.603490812
N398	-9.660638186	9.538527629	2.914996591
N399	9.480719416	2.696949338	2.361306566
N400	6.258164526	7.142982702	-0.300261963

N401	4.219190536	8.457217109	-2.901515424
N402	1.558190727	7.844358127	-3.371664428
N403	-3.180519588	6.405683211	-4.457619894
N404	-3.390146068	8.236410796	-5.900907443
N405	-4.456070999	8.245851795	-3.843887694
N406	0.687673675	6.333786474	-1.083487988
N407	0.979606946	8.225387444	0.973942306
N408	-0.374677293	10.609850661	0.667050741
N409	-1.886430240	10.367803748	-3.059274217
N410	-2.753747738	11.630141756	1.711987519
N411	4.102596527	-4.775979781	-10.212953676
N412	2.448612559	-2.564515708	-7.889012187
N413	1.394200089	0.235924130	-7.346436361
N414	3.482238871	2.217278834	-7.361762402
N415	-1.718360222	-2.997062331	-10.093576765
N416	-3.287604457	-1.172787910	-8.522643903
N417	8.165985637	-7.130073892	-5.977070777
N418	4.273739424	-5.695934678	-4.441996997
N419	3.729615381	-6.728027958	-6.313631955
N420	9.246359337	-7.451142557	-3.049912002
N421	-0.013016557	2.517935592	-0.232315467
N422	2.325231198	-0.195205174	0.561684226
N423	0.801063989	1.802630428	-0.525480872
N424	2.963182552	-0.916066417	1.263392104
O425	-6.608449524	-5.129801775	1.669269750
O426	-7.310125273	-2.847306764	4.499438458
O427	-5.344061385	-5.219103972	6.692141413
O428	-2.451906247	-4.058076112	4.919505724
O429	-2.986732841	-0.609407447	5.458879632
O430	-3.280879994	-1.064490154	9.018241548
O431	-0.575201029	-4.107589931	9.738482237
O432	2.156897308	-3.753317870	6.055099221
O433	1.891579481	0.342301189	6.726178781
O434	0.794897572	1.928042919	9.760362918
O435	1.506873661	-0.299865649	12.477494627
O436	7.053807791	-10.347477132	2.050133404
O437	8.047109981	-7.720748044	5.768820302
O438	11.553354360	-4.513230433	4.548017361
O439	-5.657728500	-0.845457110	0.025141993
O440	-3.738956127	-4.408915442	-4.018858765
O441	-7.121123626	2.514218569	-0.426613413
O442	-6.343072353	3.041619721	-3.370516929
O443	-9.764990796	1.520060122	2.279200587
O444	-5.597166268	1.430381260	4.446598750
O445	-4.249111361	5.071771947	3.742831355
O446	-6.572675815	7.272543482	5.358529794
O447	10.801596988	-0.043116817	4.128901771
O448	3.589496411	4.728745299	3.948668448
O449	3.615430254	8.360099381	-0.705791620
O450	0.990463604	10.068801304	-3.527930304
O451	-1.386705669	7.182312903	-1.529833081
O452	-0.682292479	7.153470490	2.140409873
O453	2.478813322	5.733175614	1.442623774
O454	0.847674876	11.606109931	2.328928984
O455	-2.506954752	13.591421354	0.576151749
O456	-3.257841219	11.020768687	-1.350777141
O457	-4.958626159	13.723084700	3.626023991
O458	-5.502389505	6.849267631	-1.317738852
O459	1.750098977	-4.575189304	-8.754711403
O460	-0.283460907	-0.732703512	-8.573400583
O461	2.124913624	3.613757995	-8.534930158
O462	5.769096195	4.373064042	-9.120072288
O463	-5.003361298	-2.629553635	-8.886733682
O464	-1.498637986	-6.587011271	-6.018572394
O465	0.437721660	-5.781048503	-6.780786429
O466	-3.977464481	2.327786448	-8.448002782
O467	9.937166710	-5.392344786	-3.701101145
O468	12.670009505	-6.968312566	-2.081218349
O469	0.311254109	-6.275909303	-1.409755194
O470	-0.243416661	-7.339634495	0.491704577
O471	5.178559487	-10.909494003	-3.335931545
O472	2.919273055	-10.953444883	-3.312670887
O473	5.087725266	-5.783403711	-1.348313820
O474	5.038513113	-7.473993093	0.128517003
O475	2.627948016	-6.117801304	-2.161998552
O476	8.931741973	-6.559347369	1.042927708
O477	6.942886744	-4.555678772	0.430847832
O478	-4.404198559	4.751562096	-2.462513521
O479	7.758140463	-10.410323128	-2.522541048
O480	7.508838193	-8.635381262	-0.093411880

	S481 3.640103758 4.983644287 -2.630306333 S482 1.944153413 1.756277751 -3.254345761 S483 2.071705234 -3.369966800 -3.765427960 S484 3.865373604 2.018918366 -0.333209570 S485 0.424703713 -0.978130769 -1.553637989 S486 4.016067072 -0.686475611 -5.571065566 S487 3.357900243 -3.491726173 -0.344709899 S488 5.689192745 1.613111130 -3.267552550 S489 5.688648322 -3.067828613 -3.159302279 S490 6.245946290 -0.912951121 -0.310145221 end

Fe2-N-NH-a to Fe2-NH-NH-a

Figure 8, scheme E

reactant Fe2-N-NH-a (S=3/2)	bm522nnhtrha335td.car_3		
Fe(139) -2.255	C1 -7.763288267 -5.376633909 1.313923337		
Fe(140) 0.036	C2 -8.096510588 -6.536688647 0.369043092		
Fe(141) -2.443	C3 -8.659116445 -3.481498644 2.593630301		
Fe(142) 2.380	C4 -8.011985367 -3.742601818 3.951932560		
Fe(143) 2.799	C5 -7.598786118 -5.339182399 5.760107136		
Fe(144) 1.965	C6 -6.073230516 -5.460819901 5.693228227		
Fe(145) 0.517	C7 -4.095950153 -5.791711028 4.302749320		
	C8 -3.520386595 -4.373995858 4.329151063		
	C9 -3.865021962 -2.027523688 3.724493264		
	C10 -3.869871417 -1.435486798 5.141151755		
	C11 -4.941521968 -1.265053199 7.299207340		
	C12 -3.889847035 -1.856293769 8.248866612		
	C13 -2.910184009 -3.904679500 9.173798636		
	C14 -1.433843364 -4.155367891 8.837941857		
	C15 0.217296213 -4.701204380 7.093861874		
	C16 0.950105719 -3.570826363 6.370699023		
	C17 0.695668629 -1.279626032 5.436240421		
	C18 0.775963745 -0.073157608 6.387133087		
	C19 -0.093117947 -1.024272051 4.130203792		
	C20 0.320808553 0.308153358 3.498607903		
	C21 0.092769903 -2.191874670 3.153021437		
	C22 -0.427410014 1.633602713 7.672986073		
	C23 -0.078859897 1.281129008 9.130551226		
	C24 -1.768285642 2.391367097 7.530300801		
	C25 -1.855925796 3.553886368 8.525064109		
	C26 -1.945816369 2.903912689 6.094508243		
	C27 -0.473801726 -0.128800973 11.061488870		
	C28 0.990465492 -0.407195119 11.337327827		
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transition state (S=3/2) Fe(139) -2.183 Fe(140) -0.075 Fe(141) -2.401 Fe(142) 2.249 Fe(143) 2.552 Fe(144) 2.100 Fe(145) 0.586	bm522nnhtrha335te_1_53271.78 C1 -7.765154289 -5.375438049 1.305712183 C2 -8.110567579 -6.533825822 0.362776671 C3 -8.644884664 -3.475699095 2.589977592 C4 -7.997509215 -3.736955696 3.947769104 C5 -7.576431093 -5.332223601 5.754778083 C6 -6.050752932 -5.447782777 5.687817467 C7 -4.073801799 -5.777018673 4.295438868 C8 -3.508644339 -4.354603003 4.323110860 C9 -3.870623351 -2.013554016 3.700162840 C10 -3.875687072 -1.412116716 5.113190998 C11 -4.939190097 -1.240735306 7.274810620 C12 -3.883590798 -1.821439399 8.226716636 C13 -2.899688013 -3.861353809 9.167319896 C14 -1.425548771 -4.130072435 8.834837835 C15 0.222614527 -4.719182201 7.101258278 C16 0.955559311 -3.588049594 6.377989209 C17 0.684972984 -1.308189188 5.426030167 C18 0.776235648 -0.097679425 6.369172665 C19 -0.119497066 -1.067575988 4.125477301 C20 0.265891066 0.264075691 3.474147921 C21 0.067285076 -2.238149687 3.151442262 C22 -0.409339144 1.617262296 7.659989668 C23 -0.056254705 1.270498028 9.117581196 C24 -1.746888154 2.380970457 7.519153437 C25 -1.830405068 3.544007705 8.513404786 C26 -1.922506602 2.892407615 6.082730309 C27 -0.454972340 -0.117724861 11.062872382 C28 1.008413567 -0.397709516 11.341557555 C29 5.880553298 -11.643888768 3.697704297 C30 6.518644737 -10.365260745 3.167635738 C31 6.814191679 -7.952944034 3.691409930 C32 8.038342962 -7.552934049 4.534794894 C33 5.629375038 -7.005546982 3.938598007 C34 5.947931663 -5.561649169 3.562815480 C35 4.689913145 -4.700165649 3.488024153 C36 4.914005976 -2.212089249 3.585311612 C37 10.275151785 -6.548466704 4.465367230 C38 10.451277229 -5.046587935 4.463646557 C39 -5.371875296 -2.679193311 -1.583981080 C40 -5.733354413 -1.243826871 -1.157003250 C41 -3.834667787 -2.819362408 -1.516143955 C42 -3.272848893 -4.250939401 -1.632440605 C43 -3.006297067 -4.742011179 -3.055753742 C44 -6.192092099 0.996731108 -2.071502160 C45 -7.273264903 1.470320999 -1.089835704 C46 -6.362488299 1.602472293 -3.470334761 C47 -9.426629513 0.975891350 -0.030078575 C48 -9.019701440 0.975407587 1.446699121 C49 -7.312123451 0.410973245 3.111777264

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	O450 0.997918621 10.064262238 -3.531120175 O451 -1.404263384 7.173996868 -1.526226979 O452 -0.691364920 7.164061741 2.161530693 O453 2.461345896 5.742404132 1.474212032 O454 0.846553058 11.609815524 2.332940958 O455 -2.502521452 13.579497950 0.573897789 O456 -3.251521935 11.016195690 -1.355893331 O457 -4.954721209 13.712254191 3.618090873 O458 -5.499635285 6.841397596 -1.320486793 O459 1.736090113 -4.581930349 -8.768484594 O460 -0.285370418 -0.737561710 -8.577646488 O461 2.114609014 3.607415596 -8.535240014 O462 5.731770168 4.390629965 -9.151144031 O463 -5.012821158 -2.628384214 -8.905199663 O464 -1.511212780 -6.580321290 -6.021210359 O465 0.428152779 -5.786824540 -6.789577280 O466 -3.964290949 2.326671207 -8.450617700 O467 9.928516894 -5.397074352 -3.695248672 O468 12.670065908 -6.965180212 -2.077020263 O469 0.310357228 -6.290151639 -1.398084511 O470 -0.242712511 -7.350934660 0.505282758 O471 5.186771960 -10.912803985 -3.329895526 O472 2.926293226 -10.963023569 -3.304501822 O473 5.079488004 -5.790088976 -1.356287234 O474 5.043576222 -7.471872242 0.133060329 O475 2.623835993 -6.129350251 -2.148959556 O476 8.929495830 -6.559774604 1.040161692 O477 6.941328720 -4.560003208 0.417199718 O478 -4.402537412 4.742844732 -2.464756038 O479 7.765400456 -10.416547889 -2.519298956 O480 7.510294089 -8.637344330 -0.094827229 S481 3.596199779 4.948418630 -2.488651026 S482 2.045752813 1.776809791 -3.426048369 S483 2.034776296 -3.381873737 -3.724955400 S484 3.858041632 1.982407017 -0.297934333 S485 0.527705657 -0.894522889 -1.462477336 S486 3.980195311 -0.692007103 -5.574509862 S487 3.363452568 -3.479522608 -0.342821683 S488 5.641561212 1.703053228 -3.193392926 S489 5.659516452 -3.071658112 -3.188477662 S490 6.171631309 -0.915646683 -0.236979714 end
product Fe2-NH-NH-a (S=3/2) Fe(139) -2.004 Fe(140) 0.024 Fe(141) -2.485 Fe(142) 2.405 Fe(143) 2.724 Fe(144) 2.231 Fe(145) -0.249	bm522nnhtrha335te.car_4 C1 -7.761119156 -5.375390387 1.312380187 C2 -8.096191682 -6.534516981 0.367152864 C3 -8.654026757 -3.479036455 2.592444040 C4 -8.007667077 -3.740895713 3.950700079 C5 -7.593704421 -5.337569832 5.758329472 C6 -6.068183519 -5.458160229 5.692324713 C7 -4.091501848 -5.789865335 4.300670670 C8 -3.518100687 -4.370549085 4.326551495 C9 -3.866748590 -2.026046583 3.717742478 C10 -3.867721999 -1.433522228 5.134335589 C11 -4.939616936 -1.259408677 7.292733520 C12 -3.888173986 -1.849581333 8.243095214 C13 -2.908298380 -3.896175801 9.171963187 C14 -1.432069889 -4.148499253 8.836146843 C15 0.218165467 -4.699720127 7.092873532 C16 0.950027846 -3.569879939 6.368155912 C17 0.694943055 -1.283742703 5.428558528 C18 0.776024030 -0.074765478 6.375793018 C19 -0.095065503 -1.031701394 4.120705259 C20 0.318956022 0.295083660 3.475060763 C21 0.082851685 -2.205176345 3.148311822 C22 -0.423742893 1.631238279 7.666128689 C23 -0.072794925 1.277772873 9.122931524 C24 -1.764324272 2.389843219 7.526041301 C25 -1.850809068 3.551650685 8.521768793 C26 -1.942533354 2.902713009 6.090447812 C27 -0.467907025 -0.128620735 11.056709682 C28 0.995848003 -0.407013639 11.334809419 C29 5.874790606 -11.651048050 3.679263938 C30 6.516874255 -10.372180489 3.154686327 C31 6.818812242 -7.962437325 3.687811874 C32 8.042698763 -7.563197607 4.531690029 C33 5.632556328 -7.016710250 3.937166335 C34 5.943992056 -5.570659386 3.562203207 C35 4.679510263 -4.717543834 3.485432439 C36 4.915876454 -2.230184222 3.590632147 C37 10.273972654 -6.545836352 4.463833236

C38	10.442607539	-5.043029100	4.465273107
C39	-5.372362327	-2.675205477	-1.589584938
C40	-5.733082244	-1.239373647	-1.164319771
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C54	-3.363636193	2.412179819	0.240173527
C55	-2.824667409	1.176112883	0.503924625
C56	-2.515274877	1.590863301	-1.658727401
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C62	-10.137212316	9.005768919	1.773369952
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C66	6.728290013	1.987088110	3.412121685
C67	6.147418865	2.149760848	4.682035298
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C69	5.099329413	3.054294196	4.893530490
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	C129	10.319346599	-7.520184179	-2.067265460
	C130	11.680722549	-7.304157177	-2.691867717
	C131	0.613738505	-6.892613839	-0.244330220
	C132	2.102697611	-6.915095381	0.086293495
	C133	3.031110200	-7.065384978	-1.156757143
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	C136	4.043588116	-10.369552103	-3.142849239
	C137	4.477116173	-6.757494944	-0.734562533
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	Fe140	2.096583163	0.546854160	-1.235619189
	Fe141	4.947159520	0.468508847	-1.472386985
	Fe142	3.784783197	0.491366207	-3.771750617
	Fe143	3.889544163	2.710153125	-2.334712431
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	H147	-6.478417217	-6.508826396	-0.882605704
	H148	-9.752130799	-4.851321605	1.376839197
	H149	-8.811132445	-6.178682508	-0.392239008
	H150	-8.640160678	-7.283688205	0.968244798
	H151	-8.021236219	-2.737820054	2.082638746
	H152	-8.786854139	-5.635457716	3.993362949
	H153	-9.639540497	-3.023282464	2.759848006
	H154	-8.011018457	-6.300934587	6.079309948
	H155	-6.133249190	-5.853348403	3.670382782
	H156	-7.816106019	-4.594298864	6.534952091
	H157	-2.856627496	-1.885137821	3.313086555
	H158	-5.087741510	-3.701942190	3.171024219
	H159	-3.859198014	-6.260699038	3.335880075
	H160	-4.776641177	-0.173658318	7.272108743
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	H165	-5.937113688	-1.457169682	7.709645713
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	H171	-1.944317768	2.087117718	5.354678399
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	H177	-2.897632487	3.438114115	5.990639210
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	H183	-1.289706532	0.091310515	6.434174799
	H184	-0.269211631	0.462545027	2.558433703
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	H186	0.815908802	4.493721631	1.773037768
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	H188	3.236703912	4.690145012	4.865414292
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	H191	6.509763778	1.553655215	5.524803235
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H277	-1.749532180	6.353648468	-5.993388195

	H278	-0.693639208	4.200459228	-4.812373509
	H279	-3.606645690	5.872413769	-3.668718349
	H280	0.783076796	8.904330986	2.958818558
	H281	-0.455021462	9.751603109	0.118655506
	H282	-0.077417837	12.615556443	0.404638497
	H283	2.263336781	9.429538235	2.120460330
	H284	-2.442603701	10.649290545	1.739741516
	H285	4.589580447	-3.055213784	-9.168625676
	H286	4.555554000	-4.491445672	-8.127698880
	H287	7.930026609	-5.256125492	-5.170351001
	H288	5.033635649	-5.160683422	-10.372651500
	H289	3.489724422	-5.627806715	-10.089061451
	H290	5.484246563	4.756514104	-0.969514653
	H291	5.738599531	7.416102679	0.492912333
	H292	4.822437647	8.075368889	-3.627469060
	H293	4.107428585	5.596568152	-0.191579839
	H294	6.830082278	8.004243248	-0.575242768
	H295	5.414662051	2.737952669	-6.853851841
	H296	5.968526129	6.724799522	-2.349806792
	H297	5.330366004	-7.089221821	4.995147140
	H298	7.079675612	-7.937676416	2.621961361
	H299	3.617290619	1.337111864	-6.856170660
	H300	5.217248142	-0.229392823	3.376483140
	H301	0.549339890	1.556793399	-8.698843800
	H302	-1.201882115	-2.189899560	-4.347517055
	H303	0.432676928	2.079813952	-7.014404025
	H304	4.218628875	-4.608915270	4.474338495
	H305	2.065467287	0.045381297	-6.586754315
	H306	3.933106296	-5.191182020	2.829026710
	H307	4.794214699	-7.385366780	3.324488847
	H308	6.435537439	-5.544298926	2.578678158
	H309	6.639000097	-5.116263335	4.286077841
	H310	-5.208728430	-0.782443116	-6.462729512
	H311	5.953201968	-9.537576630	4.882420673
	H312	4.974271494	-11.809690516	3.067196624
	H313	0.176054753	-0.129861532	-4.119462283
	H314	6.254281539	-11.918686228	5.686403158
	H315	4.690042665	-12.180057332	5.277552949
	H316	5.501880323	-3.405366937	2.051077870
	H317	-0.711717502	2.048262741	-4.884225261
	H318	-3.416071020	-2.084855901	-5.467477731
	H319	7.680520893	-9.921797067	-1.674137978
	H320	6.652392472	-7.639969280	-3.723241708
	H321	6.638739822	-8.162157344	-0.120119443
	H322	6.825557274	-10.530236627	-2.819894260
	H323	4.871907958	2.587609849	-9.566591833
	H324	6.322609227	-5.011971593	-0.193235043
	H325	2.299571283	-7.707528667	0.818100328
	H326	3.258451066	-2.009903026	-7.666155724
	H327	3.113748112	-9.182088963	-0.810860850
	H328	3.150384152	-7.066760388	-7.058361278
	H329	2.272216257	-5.558327433	-5.220115816
	H330	6.567548051	-12.476102979	3.440163232
	H331	5.885514621	-1.183234075	2.111106381
	H332	8.329097872	-5.802259863	0.819896895
	H333	7.218120328	-3.754292144	-0.062646296
	H334	8.966165292	-6.865960139	2.793872755
	H335	3.590788877	-2.798246652	5.115542054
	H336	3.816609348	-8.298242595	-3.659452899
	H337	5.023503054	-8.596864087	-2.403835877
	H338	1.962777153	-8.717018389	-2.073071689
	H339	1.313500903	-2.150775799	-6.186375165
	H340	-2.946206226	2.169535860	-6.019451504
	H341	-5.115252911	0.992505347	-6.606105711
	H342	2.314309673	-5.946727313	0.570444565
	H343	8.500656607	-7.331884660	0.585179509
	H344	7.397168700	-9.259733787	0.662167519
	H345	4.263205784	-1.206293977	5.225178839
	H346	5.610135257	-7.701085281	-6.694649778
	H347	6.570046715	-5.973030298	-3.172820161
	H348	0.435635169	-2.941151902	-7.528866492
	H349	4.293339212	4.114432442	-6.970668006
	H350	7.807412641	0.186550902	3.889830850
	H351	7.798518960	0.602981769	2.161284479
	H352	9.035531502	-6.919250298	-6.425071844
	H353	8.268430070	-8.143929728	-5.657028318
	H354	10.317212749	-8.529130552	-1.626201571
	H355	8.609705046	-8.257219734	-3.107485863
	H356	11.736701456	-7.550143955	-3.780174695
	H357	10.168590056	-6.802837951	-1.245108424

	H358	10.559926648	0.372550024	2.101047955
	H359	-2.977495295	13.215034640	3.712856664
	H360	10.240406847	-6.867162159	5.519834024
	H361	9.492537238	-4.459234659	4.398234224
	H362	-4.705897474	12.320388898	1.399961728
	H363	-4.096310454	10.310234124	3.654973099
	H364	-5.684276252	11.008492991	3.289708966
	H365	1.000604696	-3.288256992	-1.471853074
	H366	3.888843307	-0.418079684	0.942660687
	H367	-6.440497103	6.820859136	-1.570293084
	H368	1.143132529	-0.633962437	0.799391044
	H369	-1.715643915	-0.143361120	-0.818071854
	Mo370	3.805661387	-4.383969839	-2.488505993
	N371	-6.973946056	-7.179105782	-0.290051605
	N372	-8.832654881	-4.666248183	1.770555392
	N373	-8.217488303	-4.961523086	4.499790590
	N374	-5.534787113	-5.814774756	4.497455023
	N375	-4.243338653	-3.429469624	3.670163155
	N376	-4.886559928	-1.801211925	5.945332064
	N377	-3.710170371	-3.195086923	8.178885029
	N378	-1.133783282	-4.387992908	7.525720173
	N379	0.214643355	-2.459754493	6.138843699
	N380	-0.404971407	0.448825391	6.803764318
	N381	-0.715678436	0.214210805	9.669451277
	N382	5.493046500	-11.576466797	5.095914851
	N383	6.421593633	-9.324396771	3.995398827
	N384	4.994888126	-3.394767561	2.941108148
	N385	4.271762171	-2.112306745	4.766165784
	N386	5.541616239	-1.146971905	3.080809817
	N387	9.048983557	-6.985476007	3.827937330
	N388	-5.894619045	-2.951467018	-2.933409162
	N389	-1.957387748	-5.569505234	-3.207555034
	N390	-6.109054996	-0.445014730	-2.202110309
	N391	-8.363283428	0.687397251	-0.986197209
	N392	-7.846137972	0.355389153	1.752552389
	N393	-5.705225444	2.097304459	2.254180398
	N394	-3.156772606	2.635254525	-1.115216099
	N395	-2.320034739	0.690498323	-0.688312075
	N396	-6.334815964	4.723580561	2.899901552
	N397	-9.728669801	7.752873354	1.609273484
	N398	-9.640513591	9.536139861	2.926876458
	N399	9.476975350	2.714065407	2.324421141
	N400	6.293394912	7.166983870	-0.332411803
	N401	4.210965204	8.441175489	-2.902264636
	N402	1.549355009	7.841343923	-3.359339778
	N403	-3.184892947	6.400934939	-4.454159421
	N404	-3.403029834	8.223586658	-5.906695752
	N405	-4.463387742	8.240048109	-3.845117172
	N406	0.678190289	6.338469630	-1.065929813
	N407	0.977344135	8.221576066	0.994169362
	N408	-0.366886708	10.603957540	0.671275958
	N409	-1.879510239	10.378272350	-3.070887039
	N410	-2.749299003	11.618394103	1.707171306
	N411	4.085723253	-4.806429498	-10.226031942
	N412	2.440604157	-2.576052973	-7.904855416
	N413	1.387735303	0.229577961	-7.343589061
	N414	3.482557602	2.198969692	-7.392271282
	N415	-1.722700543	-3.004124283	-10.110944100
	N416	-3.289236908	-1.171611159	-8.543565752
	N417	8.156281433	-7.173052724	-5.965357657
	N418	4.270992982	-5.703973736	-4.412733023
	N419	3.722599351	-6.719780223	-6.292968335
	N420	9.256710914	-7.464876442	-3.053687781
	N421	0.049990436	2.503559965	-0.387660221
	N422	2.089024023	-0.340030037	0.493958923
	N423	0.836332229	1.749965916	-0.676268105
	N424	2.953424871	-0.675781800	1.336034909
	O425	-6.603533178	-5.117185678	1.689272239
	O426	-7.328889744	-2.860249991	4.507569773
	O427	-5.379329912	-5.252045039	6.705491851
	O428	-2.463984125	-4.094982029	4.920620297
	O429	-2.972405390	-0.658992438	5.507876039
	O430	-3.283136083	-1.122479561	9.050562883
	O431	-0.590260290	-4.168380024	9.743197972
	O432	2.139059585	-3.721926272	6.025228741
	O433	1.878049215	0.378253455	6.720464433
	O434	0.762962741	1.935370560	9.764623921
	O435	1.490023821	-0.331163212	12.449466014
	O436	7.047586281	-10.360234213	2.025162177
	O437	8.066603229	-7.754757496	5.760214458

	O438	11.525727669	-4.486804535	4.554593434
	O439	-5.664509851	-0.837257117	0.013472757
	O440	-3.743499896	-4.419785771	-4.019292092
	O441	-7.113396663	2.518933822	-0.439667667
	O442	-6.350482986	3.042541469	-3.390133711
	O443	-9.754778708	1.520847745	2.270450716
	O444	-5.575507710	1.392607205	4.426042499
	O445	-4.231630632	5.064296609	3.723099417
	O446	-6.536232066	7.271579997	5.353532550
	O447	10.809658675	-0.023753804	4.088469954
	O448	3.591310039	4.729491423	3.958131819
	O449	3.616394984	8.366561497	-0.702847473
	O450	0.992603214	10.067684014	-3.538244019
	O451	-1.399925469	7.175121812	-1.520997664
	O452	-0.685044939	7.152260362	2.161706565
	O453	2.471425045	5.728947845	1.456547196
	O454	0.843878540	11.604621802	2.339455013
	O455	-2.501145892	13.581567762	0.574308324
	O456	-3.247570465	11.018246480	-1.354867183
	O457	-4.954300428	13.714722907	3.616250705
	O458	-5.497057372	6.838965079	-1.317501521
	O459	1.731484084	-4.583703737	-8.765665626
	O460	-0.269000231	-0.738218750	-8.597677118
	O461	2.114921823	3.605786108	-8.538115323
	O462	5.690976824	4.414726321	-9.165609361
	O463	-5.008065702	-2.623009591	-8.912662597
	O464	-1.515373707	-6.583755005	-6.022730690
	O465	0.424655394	-5.785500844	-6.784576105
	O466	-3.934594897	2.331007115	-8.453340726
	O467	9.929597086	-5.398324622	-3.697357146
	O468	12.670178372	-6.954653951	-2.065263077
	O469	0.306003130	-6.284581498	-1.395492068
	O470	-0.247426159	-7.343825820	0.509699842
	O471	5.195854547	-10.902692826	-3.325025057
	O472	2.935438519	-10.956072153	-3.295449309
	O473	5.060828609	-5.755000765	-1.337504361
	O474	5.044324875	-7.454033194	0.128962976
	O475	2.610015637	-6.122835612	-2.146907677
	O476	8.931181366	-6.554727989	1.039106295
	O477	6.938399590	-4.547877555	0.431990239
	O478	-4.407300985	4.738470528	-2.465218312
	O479	7.777358436	-10.408816600	-2.522796356
	O480	7.512812844	-8.633580727	-0.097680685
	S481	3.576958609	4.945226820	-2.483833449
	S482	2.045699929	1.819800263	-3.319483744
	S483	2.046284123	-3.379280858	-3.747525083
	S484	3.796353369	1.935752083	-0.273758951
	S485	0.396076118	-0.965235099	-1.643429704
	S486	4.023022627	-0.755126889	-5.566968114
	S487	3.249375140	-3.418558934	-0.377696468
	S488	5.628241483	1.640855916	-3.297343848
	S489	5.663594274	-3.080122304	-3.151761572
	S490	6.193978708	-0.894810260	-0.259493172
	end			

N2-ready-b to Fe2-N-N

Figure 8, scheme F

reactant **N2-ready-b** (S=3/2)	bm526hx7hnexp2n2ndtb.car_2			
	C1	-7.759126357	-5.375903109	1.294259097
	C2	-8.119554229	-6.528317982	0.348858971
	C3	-8.615376949	-3.464925813	2.579009556
	C4	-7.972609856	-3.726120376	3.938510057
	C5	-7.543135467	-5.321872155	5.742825846
	C6	-6.017490802	-5.435283060	5.674291100
	C7	-4.042117962	-5.752638687	4.277957841
	C8	-3.495931550	-4.322736160	4.307342631
	C9	-3.898270665	-1.988470476	3.663919334
	C10	-3.906362024	-1.375939804	5.072871304
	C11	-4.941777367	-1.215388627	7.245401448
	C12	-3.870477550	-1.779922850	8.190460367
	C13	-2.870353597	-3.806208852	9.144338963
	C14	-1.398383414	-4.094964482	8.817741039
	C15	0.253828601	-4.753538432	7.112188776
	C16	1.002181921	-3.625020387	6.395868426
	C17	0.699657462	-1.349280285	5.426546540
	C18	0.805542169	-0.136072864	6.365958044

	C19	-0.209971226	-1.131537503	4.189379112
	C20	-0.021673815	0.244738568	3.548005816
	C21	-0.040813298	-2.283110459	3.189630265
	C22	-0.374327127	1.591294774	7.652950583
	C23	-0.021110621	1.254651762	9.111931972
	C24	-1.712385684	2.354165093	7.508794801
	C25	-1.793504727	3.520533849	8.498975171
	C26	-1.892793340	2.862228340	6.071959281
	C27	-0.430204966	-0.108229386	11.069283175
	C28	1.032832409	-0.386501167	11.352398015
	C29	5.892594196	-11.624730161	3.726692415
	C30	6.515932814	-10.344927121	3.182879646
	C31	6.796040303	-7.924801906	3.689969653
	C32	8.021135866	-7.528605914	4.534630193
	C33	5.612489998	-6.975258843	3.938811801
	C34	5.930042260	-5.531062927	3.561176003
	C35	4.673869751	-4.664795502	3.497794519
	C36	4.919290386	-2.168681372	3.525676243
	C37	10.271452958	-6.556724049	4.469047061
	C38	10.469485943	-5.057983384	4.465891020
	C39	-5.361264169	-2.683909285	-1.578223600
	C40	-5.720400351	-1.248146394	-1.148383351
	C41	-3.823352000	-2.824073100	-1.511407511
	C42	-3.259735629	-4.255131464	-1.628738287
	C43	-2.992152173	-4.744722581	-3.052773309
	C44	-6.184458216	0.993798375	-2.058964285
	C45	-7.269088620	1.460770732	-1.077335429
	C46	-6.357537234	1.602104687	-3.456453893
	C47	-9.424742523	0.957114153	-0.025409623
	C48	-9.023828743	0.966803533	1.452861561
	C49	-7.320461382	0.426265512	3.129152692
	C50	-6.140574880	1.375387224	3.343537551
	C51	-4.616315032	3.053153921	2.425693082
	C52	-5.051492432	4.362976042	3.124924027
	C53	-4.029397184	3.488922288	1.075162499
	C54	-3.405769355	2.430473328	0.228945303
	C55	-2.954760662	1.156488062	0.464632253
	C56	-2.526665010	1.639050465	-1.668390784
	C57	-6.853557252	6.039125990	3.255824390
	C58	-6.748364546	6.203242665	4.770921703
	C59	-8.332122177	6.098629926	2.803975733
	C60	-8.945736151	7.462499781	2.678563127
	C61	-8.879311443	8.565976116	3.506896568
	C62	-10.177679381	8.988983127	1.761952521
	C63	9.238260047	1.646878488	3.387824104
	C64	10.280745104	0.556338929	3.220085081
	C65	7.849989779	0.988916389	3.212042175
	C66	6.711575851	1.956519736	3.434163781
	C67	6.130164770	2.134634581	4.702107976
	C68	6.213535379	2.728124020	2.368107068
	C69	5.085750313	3.045933056	4.902423103
	C70	5.189792435	3.655349124	2.556276630
	C71	4.619484894	3.807173730	3.822766185
	C72	5.364481075	6.843031111	-1.422733673
	C73	4.311992357	7.947175906	-1.631012935
	C74	4.697342168	5.506561442	-1.126323325
	C75	3.307821419	9.539511666	-3.227573214
	C76	1.832207332	9.162990238	-3.389363363
	C77	0.216633642	7.263512415	-3.346731079
	C78	-0.237586866	6.922355463	-1.903482886
	C79	0.242206179	6.018927764	-4.261973810
	C80	-1.012872303	5.144145395	-4.363176752
	C81	-2.158813879	5.683178368	-5.236038003
	C82	-3.681632342	7.600418251	-4.755470894
	C83	0.304067379	5.970708973	0.285315314
	C84	0.131750130	7.183296465	1.210617469
	C85	1.323553080	5.017713965	0.944157446
	C86	1.193470580	9.250897870	1.970643797
	C87	0.549210708	10.594823442	1.666950267
	C88	-0.851712676	11.868041339	0.133991264
	C89	-2.126864536	12.424448001	0.810692654
	C90	-1.000391481	11.879417126	-1.389521332
	C91	-2.153705185	11.029648849	-1.907605392
	C92	-4.071794615	11.948983840	2.221653198
	C93	-3.989662567	13.055259666	3.265096606
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	C95	-4.974254420	9.611769927	1.800845246
	C96	-6.148464702	9.617620192	1.033053850
	C97	-4.013678223	8.623055117	1.534549058
	C98	-6.350742911	8.682614669	0.016916047

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	C101	4.081900581	-3.992749212	-9.000904805
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	C103	1.196591216	-2.183199834	-7.269724592
	C104	0.695016448	-0.831504002	-7.789939876
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	C106	2.292383886	2.540013508	-7.937184767
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	C108	5.132278517	3.387679939	-8.804935512
	C109	-2.765560282	-3.499041672	-9.178884593
	C110	-3.792138252	-2.405982885	-8.855189261
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	C112	-1.545258400	-5.489080868	-8.161637865
	C113	-0.876836193	-6.014786581	-6.911290684
	C114	-4.193381322	-0.086102421	-8.192645893
	C115	-3.715717597	1.198263353	-8.841683160
	C116	-4.542682741	0.045358437	-6.688224263
	C117	-3.303599787	0.050524843	-5.834878177
	C118	-2.570869811	1.233161981	-5.630754767
	C119	-2.785961208	-1.159903707	-5.344266826
	C120	-1.311331812	1.185120856	-5.023734592
	C121	-1.528680864	-1.207231107	-4.733784867
	C122	-0.774975557	-0.036177651	-4.606510535
	C123	7.943769511	-6.258339297	-4.791919195
	C124	9.116058740	-6.326975969	-3.801883208
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	C128	3.287809170	-5.904951371	-5.282963871
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	C132	2.101925584	-6.913710780	0.096692682
	C133	3.030160880	-7.064622878	-1.147494891
	C134	2.954517486	-8.518362211	-1.682499113
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	C137	4.481510666	-6.778896417	-0.725928991
	C138	3.560156618	-0.712479178	-2.231915849
	Fe139	3.841628696	-1.967925414	-3.749050075
	Fe140	2.155737501	0.848707222	-1.498402134
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	Fe145	2.148389315	-2.387547169	-1.777134125
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	H147	-6.509639157	-6.522901967	-0.911530386
	H148	-9.742325109	-4.823894279	1.377011416
	H149	-8.832839038	-6.156551375	-0.404505035
	H150	-8.672564879	-7.271610603	0.949244376
	H151	-7.970881717	-2.737090374	2.064172961
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	H160	-4.792233744	-0.128317417	7.207864796
	H161	-5.686998613	-2.313395204	5.540994860
	H162	-3.529004412	-6.318622133	5.064356590
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	H165	-5.931246502	-1.420320394	7.677693378
	H166	-0.364901758	-3.236181824	3.629293213
	H167	-0.654731103	-2.110557558	2.290755986
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	H172	-1.461499483	-0.250659169	9.207651252
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	H174	0.966141148	0.371770308	3.096766272
	H175	-0.159206733	1.058459320	4.271212010
	H176	9.309675316	2.006372585	4.432444122
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	H188	3.233461102	4.692580660	4.854931013
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	H191	6.492619434	1.548953728	5.552142330
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	H193	0.238305944	-5.619238049	6.434970032
	H194	0.836891926	-5.029538357	7.999648558
	H195	-1.837917419	-4.471627802	6.813860308
	H196	-2.864824588	-3.199759462	10.058153413
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	H201	1.628832838	-0.738219484	10.478096504
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	H207	-3.124135867	-4.362565308	-7.201182331
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	H216	-1.614195226	-3.459918154	-7.342766336
	H217	-1.209480696	-3.788518278	-10.487328459
	H218	-6.768781424	-3.461857618	-2.877331613
	H219	-3.505001761	-2.416368553	-0.540398595
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	H221	-2.329755817	-4.321525329	-1.045804526
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	H240	-10.217653681	0.210402473	-0.162817500
	H241	10.287282634	3.237001213	2.642338339
	H242	8.679663515	3.333576529	2.373112044
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	H245	1.744344265	8.070671104	0.303923576
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	H248	-6.704953860	3.386551617	-4.193611144
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	H250	-5.530330933	1.244788404	-4.091816956
	H251	-7.311467898	1.270895467	-3.895046153
	H252	-0.047186038	11.596347670	-1.857723283
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	H254	-0.915015854	10.197784892	-3.345501007
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	H256	-3.742054026	9.171708227	-6.068007483
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	H258	-7.275403095	8.691383211	-0.566014006

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	H263	-1.393567323	4.882727520	-3.363412545
	H264	-8.373840413	-0.205725825	-1.493382295
	H265	3.641329359	10.006330446	-4.163882064
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	N396	-6.334071584	4.731366677	2.878179711
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	N407	0.980910206	8.222048356	0.970101910
	N408	-0.371229185	10.601636628	0.655489076
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	O441	-7.120633313	2.505542482	-0.418398937
	O442	-6.337865717	3.040042526	-3.360763038
	O443	-9.771756459	1.510850797	2.276216784
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	O462	5.802692833	4.354209711	-9.126190564
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	O467	9.947345555	-5.403028335	-3.705269483
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	O476	8.933733588	-6.563226989	1.036343907
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	O480	7.505423866	-8.639995693	-0.091483460
	S481	3.547600878	4.979344881	-2.470080130
	S482	2.013410865	2.049980626	-3.401007921
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	C4	-7.947823765	-3.715522904	3.933904428
	C5	-7.515259223	-5.309743282	5.738478977
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Fe(145) 1.304

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C13	-2.869325608	-3.771067942	9.140271188
C14	-1.399849582	-4.075514266	8.816344249
C15	0.242578480	-4.781795388	7.120897015
C16	0.987557271	-3.647388085	6.408163296
C17	0.682270048	-1.384114553	5.419960619
C18	0.790535524	-0.170006202	6.357909410
C19	-0.209458116	-1.163219617	4.170778204
C20	-0.007439912	0.208389914	3.515078388
C21	-0.039136938	-2.316884299	3.171706685
C22	-0.371959346	1.569956318	7.639893608
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C29	5.895681838	-11.613728100	3.738425828
C30	6.513294570	-10.333296243	3.188132909
C31	6.790886529	-7.911193228	3.685304965
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C33	5.612832868	-6.954464641	3.927865943
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C36	4.906057717	-2.142414102	3.503035756
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C43	-2.985661555	-4.746949853	-3.049260871
C44	-6.187312988	0.992428190	-2.050968958
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C47	-9.427270273	0.944745389	-0.017373049
C48	-9.027870681	0.959333396	1.461286853
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C51	-4.614653946	3.053322993	2.429496113
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C53	-4.028521001	3.487889255	1.077823195
C54	-3.413313594	2.426479671	0.228634347
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C56	-2.556590370	1.623140021	-1.673925998
C57	-6.856979476	6.038357508	3.251370732
C58	-6.758115478	6.198152947	4.767327732
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C63	9.239316150	1.638371403	3.412300691
C64	10.277936137	0.544331650	3.243331435
C65	7.848960565	0.985855796	3.233032792
C66	6.713047961	1.957685869	3.450816375
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C74	4.697121145	5.507486871	-1.162089631
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C77	0.216096825	7.268976650	-3.341433955
C78	-0.239832535	6.924880143	-1.900089940
C79	0.242580698	6.022740686	-4.254682921
C80	-1.011685528	5.146512373	-4.357610399
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C85	1.311555945	5.021885869	0.958815873
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C88	-0.856539336	11.874902625	0.131703655
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C91	-2.157887533	11.022486055	-1.903651207
C92	-4.076489623	11.952773032	2.222276706
C93	-3.992287540	13.055945686	3.269330103
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C96	-6.151580446	9.613724341	1.034990527
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C98	-6.354678013	8.677361978	0.019942581
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C104	0.698571751	-0.832683227	-7.774192201
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H149	-8.843189348	-6.141468483	-0.404579782
H150	-8.685251723	-7.258627470	0.947525277
H151	-7.935276811	-2.735741514	2.055355762
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	H170	-3.360067279	-4.725670313	9.381603290
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	H172	-1.459331082	-0.254412137	9.217047318
	H173	-1.741801509	3.180934277	9.534742721
	H174	0.901431285	0.250571202	2.909883557
	H175	0.045993257	1.023573840	4.248125177
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	H181	-2.527250100	1.643700973	7.726324604
	H182	0.453078640	2.212095569	7.296129017
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	H184	-0.857847727	0.428301628	2.852079240
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	H186	0.782006356	4.512929298	1.777169843
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	H188	3.223194375	4.684649113	4.861091378
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	H195	-1.851189273	-4.507491701	6.827854069
	H196	-2.857909729	-3.151064350	10.044755721
	H197	4.636278864	3.169363982	5.905350675
	H198	1.711660263	-1.588070692	5.106130739
	H199	-0.763748507	0.707239035	11.749744190
	H200	-0.980131889	-1.010084341	11.330257157
	H201	1.634379195	-0.731624908	10.484780470
	H202	11.145895046	-7.050791359	4.023506058
	H203	-1.750255433	-5.969914373	-4.128540516
	H204	1.269392783	-6.047265379	-1.839812706
	H205	-2.275742397	-6.238225962	-8.491314235
	H206	-0.803478241	-5.347002265	-8.957421208
	H207	-3.121419208	-4.367590071	-7.191055771
	H208	-3.105618722	1.046894061	-9.747732339
	H209	-3.348793090	-4.243293477	-9.718301756
	H210	-3.367795557	-2.192042951	-2.294638407
	H211	-3.954315951	-4.977301163	-1.164210727
	H212	-2.279856582	-1.028809671	-8.445272522
	H213	-5.134059006	-0.321685530	-8.711155964
	H214	-1.041721408	-2.407046681	-9.583837947
	H215	-1.303647322	-5.821953692	-2.432057988
	H216	-1.610287082	-3.465494540	-7.325707482
	H217	-1.207750992	-3.780828079	-10.476870532
	H218	-6.756025422	-3.463854316	-2.869681268
	H219	-3.492349707	-2.419365235	-0.536371880
	H220	0.825888927	-5.301327549	-7.585644950
	H221	-2.326577369	-4.331376598	-1.039719386
	H222	-3.842812367	2.609649307	3.074155183
	H223	-2.993217095	0.540132720	1.358376402
	H224	-8.136426136	0.771958674	3.797813842
	H225	-7.266977449	-0.073471453	1.067204721
	H226	-6.943473327	4.081148729	2.385092519
	H227	-8.341503821	8.750238509	4.418750143
	H228	-6.908523609	5.243791919	5.329226002
	H229	-8.939426262	5.446109579	3.447986427
	H230	-6.274509449	6.840425749	2.771506003
	H231	-10.857710167	9.532532506	1.103337428
	H232	-3.264082098	4.252383410	1.290578921
	H233	-4.819874602	3.982278578	0.491957052
	H234	-9.834556601	10.459969491	3.252126783
	H235	-8.378880267	5.646323581	1.786727321
	H236	-6.186342342	2.029044467	1.370275141
	H237	-7.018002312	-0.560136415	3.502264880
	H238	-9.864727730	1.931648690	-0.223932901
	H239	-2.219890293	1.525908590	-2.703550976
	H240	-10.217151166	0.194911557	-0.154538976
	H241	10.292755356	3.225919378	2.665028995
	H242	8.684725221	3.324280286	2.394011788
	H243	1.564287734	5.976785652	-1.458160034
	H244	-0.679379055	5.473280712	0.267834416
	H245	1.741507224	8.076472053	0.304801084
	H246	-3.471000111	3.548812427	-1.619001479

	H247	-5.124718509	4.163132724	-2.798305421
	H248	-6.711935711	3.386968171	-4.182456037
	H249	-4.805688344	5.410592544	-1.858625579
	H250	-5.533513630	1.246127955	-4.083398103
	H251	-7.314587468	1.271076593	-3.886651640
	H252	-0.054923712	11.602845558	-1.860385492
	H253	-1.232316522	12.919002263	-1.686982021
	H254	-0.914507006	10.187566450	-3.335810467
	H255	-2.595212582	9.652723470	-3.317793751
	H256	-3.716533812	9.185951321	-6.055513157
	H257	-2.653873939	4.850322669	-5.753576511
	H258	-7.281959716	8.682950901	-0.558957371
	H259	-3.101144342	8.561316027	2.129841893
	H260	-4.690574379	7.777589022	-2.965877517
	H261	1.063259074	5.378187330	-3.900678748
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	H263	-1.394587642	4.883840779	-3.359093760
	H264	-8.373939888	-0.212470631	-1.488733386
	H265	3.638981910	10.013980138	-4.157536776
	H266	-6.104564880	-0.961727944	-3.076417243
	H267	0.532511656	6.359616305	-5.263435699
	H268	-3.397065526	6.979442769	0.268741756
	H269	3.339361728	10.312977701	-2.431799775
	H270	-2.983499267	7.750387167	-6.687066188
	H271	-5.112428966	8.943876088	-4.174815736
	H272	-5.186663389	-3.530664047	-3.443011173
	H273	-5.782334108	-3.342354972	-0.798952673
	H274	-6.929417824	10.354149155	1.235867460
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	H276	-0.487635405	8.022444767	-3.708003269
	H277	-1.742783116	6.342867547	-6.005216840
	H278	-0.681612652	4.203472317	-4.815241305
	H279	-3.602795686	5.874459584	-3.680274946
	H280	0.799725497	8.916410869	2.935367458
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	H290	5.488610485	4.763743118	-1.006403085
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	H294	6.801651191	7.999293566	-0.490831637
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	H296	5.995084944	6.774700952	-2.322545486
	H297	5.306691606	-7.020370233	4.984995574
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	H303	0.452212463	2.070364337	-6.994880254
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	H324	6.339466447	-5.027524425	-0.199343743
	H325	2.282713609	-7.736971647	0.816681052
	H326	3.277717244	-2.011510136	-7.615841251

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	H333	7.244817946	-3.773528225	-0.100456780
	H334	8.967607823	-6.863117916	2.794764006
	H335	3.673336365	-2.704994812	5.093145023
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	H338	1.924753056	-8.689721705	-2.073046514
	H339	1.327532462	-2.151315161	-6.160590889
	H340	-2.995817004	2.187640822	-5.971390164
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	H357	10.176796032	-6.830292334	-1.251887922
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	H363	-4.096303415	10.306314676	3.648251050
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	N378	-1.114430123	-4.462775508	7.538172899
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	N389	-1.945092096	-5.585789462	-3.197513928
	N390	-6.094301416	-0.451831934	-2.176663759
	N391	-8.356802071	0.654582589	-0.956083653
	N392	-7.852591259	0.354395642	1.792253212
	N393	-5.701807080	2.095905741	2.270132154
	N394	-3.144881464	2.686030851	-1.109438646
	N395	-2.454770313	0.680044433	-0.729857800
	N396	-6.332616140	4.733087426	2.871213457
	N397	-9.771829610	7.733439656	1.588438938
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	N405	-4.455922893	8.240251350	-3.847549853
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O438	11.578511075	-4.537825809	4.544234309
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O450	0.984960663	10.068233905	-3.525044746
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O456	-3.266394551	11.003426053	-1.349583470
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O459	1.753815950	-4.568921707	-8.761104706
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O473	5.072388601	-5.789068631	-1.325632742
O474	5.021819411	-7.487210997	0.141343356
O475	2.604455596	-6.108641255	-2.126144500
O476	8.937227576	-6.564361905	1.034321330
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S482	1.947757544	1.874857818	-3.224130553
S483	2.094864875	-3.356547711	-3.759744832
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	S487	3.322577210	-3.500742059	-0.330810860
	S488	5.601659177	1.652731755	-3.387400189
	S489	5.690464894	-3.047739923	-3.070513875
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product **Fe2-N-N** (S=3/2)

Fe(139) -2.196
Fe(140) 0.085
Fe(141) -2.492
Fe(142) 2.372
Fe(143) 3.016
Fe(144) 1.130
Fe(145) 0.974

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C3	-8.595942619	-3.460010635	2.578410123
C4	-7.955451368	-3.720959898	3.938722564
C5	-7.523618210	-5.315786186	5.743338389
C6	-5.998054864	-5.430262107	5.673780709
C7	-4.024189836	-5.743606093	4.275382903
C8	-3.485390852	-4.310942880	4.304179184
C9	-3.896208327	-1.980824957	3.649343662
C10	-3.903800850	-1.362818760	5.056063430
C11	-4.936962892	-1.201078089	7.231236221
C12	-3.868899387	-1.761762222	8.181778252
C13	-2.870709485	-3.784258099	9.146946894
C14	-1.400828053	-4.085898503	8.822287576
C15	0.242999420	-4.777484238	7.122974283
C16	0.983498463	-3.642371509	6.408536505
C17	0.676577749	-1.375719404	5.431855462
C18	0.785530503	-0.162102468	6.368865672
C19	-0.200584409	-1.153185141	4.173738396
C20	0.039614640	0.209595855	3.513655657
C21	-0.020019454	-2.305140082	3.175750060
C22	-0.376751770	1.575564541	7.653077660
C23	-0.019656344	1.246247045	9.113518525
C24	-1.708697973	2.349324980	7.507992519
C25	-1.783323726	3.517956752	8.496148598
C26	-1.882254687	2.856345056	6.069576807
C27	-0.427987795	-0.097206053	11.087482613
C28	1.036003328	-0.375812002	11.365603074
C29	5.898163267	-11.620369470	3.740698776
C30	6.515414155	-10.338750611	3.191336279
C31	6.793965725	-7.916339326	3.690074311
C32	8.018432496	-7.525427492	4.537762459
C33	5.616286649	-6.958354382	3.932601032
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C35	4.695522645	-4.641963974	3.489177730
C36	4.875099437	-2.139052262	3.462149518
C37	10.273872991	-6.565775138	4.480485070
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C40	-5.712342103	-1.249147042	-1.142114405
C41	-3.813461343	-2.826775565	-1.506066256
C42	-3.255049773	-4.259863648	-1.623015770
C43	-2.986687783	-4.748167617	-3.047269462
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C46	-6.359017368	1.600471463	-3.447998673
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C48	-9.025187033	0.960464213	1.461838525
C49	-7.321552051	0.429570820	3.140325050
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C53	-4.029303189	3.489102285	1.080694380
C54	-3.413450074	2.428344310	0.231323303
C55	-2.966032846	1.152635940	0.466625983
C56	-2.557532600	1.626623577	-1.672341535
C57	-6.859046833	6.039040308	3.259392898
C58	-6.757279204	6.199515632	4.774996941
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C63	9.244021151	1.639612762	3.417883316
C64	10.282778463	0.546431298	3.246365661
C65	7.853007221	0.985760972	3.236290870
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C67	6.135132153	2.139738873	4.719944334
C68	6.217001801	2.723289853	2.384258056
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C70	5.189464121	3.648093794	2.568631832
C71	4.618439669	3.803061905	3.833812316
C72	5.376192798	6.852728344	-1.420007155
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	C76	1.836206434	9.164691548	-3.379527777
	C77	0.219231864	7.267356336	-3.340837102
	C78	-0.235865611	6.923381891	-1.898974604
	C79	0.245018067	6.020723720	-4.254174797
	C80	-1.009372815	5.144469444	-4.355986531
	C81	-2.155331951	5.681162155	-5.230435458
	C82	-3.678022898	7.599742724	-4.750219157
	C83	0.306729275	5.973856018	0.292105455
	C84	0.132395614	7.189819921	1.214218858
	C85	1.323455729	5.022573981	0.958548570
	C86	1.194785707	9.259190210	1.971450841
	C87	0.550167673	10.603594577	1.668988212
	C88	-0.855444227	11.875346402	0.137097861
	C89	-2.131672021	12.431720430	0.813292034
	C90	-1.005485147	11.881687455	-1.386496921
	C91	-2.155275636	11.024342223	-1.900565546
	C92	-4.076651541	11.954674596	2.226391649
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	C95	-4.973412167	9.613002106	1.802700411
	C96	-6.149173545	9.615052795	1.037073787
	C97	-4.011401409	8.625752147	1.534978365
	C98	-6.351750019	8.678479831	0.022157114
	C99	-4.185186154	7.695061088	0.505726412
	C100	-5.355994448	7.738581266	-0.245292913
	C101	4.087128982	-3.987415027	-8.979330431
	C102	2.658089099	-3.728786972	-8.535916302
	C103	1.193443688	-2.185520203	-7.257039987
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	C122	-0.773085383	-0.039948130	-4.616062836
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	H165	-5.927161829	-1.405458639	7.662312560
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	H167	-0.659300292	-2.146619015	2.291922129
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	H186	0.795726118	4.508905241	1.775320413
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	H219	-3.494793769	-2.420786696	-0.534295606
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	H239	-2.219527515	1.530421220	-2.701648101
	H240	-10.216310197	0.198786126	-0.154166044
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	H258	-7.277927712	8.684929148	-0.558521227
	H259	-3.101155936	8.560221407	2.136402556
	H260	-4.685856774	7.778312675	-2.961913350
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	H262	2.349495050	7.193954817	-3.262464616
	H263	-1.391869203	4.882784129	-3.357033253
	H264	-8.372608632	-0.211968621	-1.486110384
	H265	3.641188457	10.015001265	-4.155264325
	H266	-6.105558201	-0.963712103	-3.075983803
	H267	0.534191829	6.357849076	-5.263060229
	H268	-3.396443918	6.977609695	0.275702136
	H269	3.340340219	10.313936474	-2.430183215
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	H272	-5.188954117	-3.534134190	-3.441129985
	H273	-5.784298735	-3.344287835	-0.797923034
	H274	-6.926493346	10.356399497	1.236387291
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	H279	-3.600306196	5.872686984	-3.677149500
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	H282	-0.087461885	12.622466711	0.390163209
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	H284	-2.444775163	10.656327069	1.742018270
	H285	4.610523824	-3.032368632	-9.132927093
	H286	4.579479083	-4.489489377	-8.119603622
	H287	7.902223956	-5.202333449	-5.109781800
	H288	5.052324897	-5.108951015	-10.381215222
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	H290	5.478591914	4.754930596	-1.029758369
	H291	5.671899822	7.384637089	0.529659226
	H292	4.825626112	8.094132825	-3.613182643
	H293	4.070612241	5.560860596	-0.278846991
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	H302	-1.117973556	-2.163284339	-4.396871925
	H303	0.447929409	2.072114765	-6.999375037
	H304	4.261924778	-4.503690576	4.486799977
	H305	2.109576037	0.037243110	-6.604947908
	H306	3.925132466	-5.120744410	2.863857830
	H307	4.776077354	-7.320504931	3.318691158
	H308	6.424538679	-5.501207893	2.563067650
	H309	6.659080662	-5.073272145	4.264835694
	H310	-5.197473962	-0.803563459	-6.412775367
	H311	5.934881541	-9.480709970	4.902712120
	H312	4.992921743	-11.799524979	3.140907684
	H313	0.229642140	-0.061608111	-4.192301304
	H314	6.307634263	-11.836398983	5.746959999

	H315	4.749126054	-12.157582786	5.361410187
	H316	5.524825268	-3.388577048	2.008252885
	H317	-0.728232463	2.093300866	-4.878559242
	H318	-3.365463146	-2.082760935	-5.451628386
	H319	7.639022040	-9.937140098	-1.667826192
	H320	6.646372906	-7.648277163	-3.746250047
	H321	6.626094160	-8.171612840	-0.108211575
	H322	6.776583054	-10.534174634	-2.815449363
	H323	4.924220439	2.549721342	-9.505969518
	H324	6.341822783	-5.025170285	-0.193456297
	H325	2.286004987	-7.726579298	0.815874184
	H326	3.271797054	-2.012080962	-7.605993647
	H327	3.088055512	-9.176782567	-0.820072670
	H328	3.128750700	-7.039962028	-7.048716076
	H329	2.266120166	-5.529557833	-5.206044256
	H330	6.600095479	-12.438604695	3.504814795
	H331	5.809110950	-1.129128362	1.910450295
	H332	8.344759354	-5.810264187	0.815451483
	H333	7.249913413	-3.773698126	-0.092039162
	H334	8.970885944	-6.868687008	2.800462234
	H335	3.656705610	-2.707374622	5.066610921
	H336	3.768505412	-8.275915560	-3.667562405
	H337	4.988105008	-8.580557800	-2.425994395
	H338	1.930344185	-8.688404743	-2.068783052
	H339	1.323061079	-2.151302396	-6.163436753
	H340	-2.988166131	2.183949457	-5.970150154
	H341	-5.129210104	0.973128952	-6.561731794
	H342	2.322371648	-5.963992968	0.612670644
	H343	8.500949767	-7.342484704	0.588993220
	H344	7.390248346	-9.260827863	0.679231446
	H345	4.169113312	-1.052138459	5.046022088
	H346	5.588485444	-7.684323377	-6.697744831
	H347	6.541873879	-5.999248530	-3.149948313
	H348	0.450123154	-2.944758897	-7.507250030
	H349	4.270250307	4.161908136	-6.993612298
	H350	7.776694010	0.150701103	3.948013698
	H351	7.800599655	0.566143792	2.218971933
	H352	9.013991668	-6.795598932	-6.436305296
	H353	8.280101102	-8.063075753	-5.704789920
	H354	10.304487395	-8.550911992	-1.651558334
	H355	8.569956181	-8.234497368	-3.096563168
	H356	11.703721124	-7.564553193	-3.813123729
	H357	10.178737050	-6.827306046	-1.248411373
	H358	10.547306869	0.327160687	2.183316092
	H359	-2.983326383	13.208207926	3.724636376
	H360	10.220879258	-6.878390634	5.538329978
	H361	9.544407953	-4.459287892	4.408886428
	H362	-4.712814163	12.325745278	1.405598117
	H363	-4.095751334	10.307574635	3.651951734
	H364	-5.686309473	11.002321345	3.291484848
	H365	1.133612615	-3.281388603	-1.314466790
	H366	4.580773287	-1.705084195	0.133331047
	H367	-6.448413665	6.813722734	-1.566787445
	H368	0.079295498	-1.300323542	-0.369814444
	H369	-1.955105760	-0.197591359	-0.878648218
	Mo370	3.821772714	-4.368785909	-2.487473343
	N371	-7.025338379	-7.192083458	-0.324037738
	N372	-8.805223356	-4.648389203	1.766361251
	N373	-8.150103983	-4.944927359	4.484384109
	N374	-5.465642985	-5.792192389	4.480397500
	N375	-4.224676873	-3.397059411	3.623876810
	N376	-4.890508394	-1.762271322	5.892023951
	N377	-3.662479823	-3.104608117	8.129783361
	N378	-1.114244118	-4.461349357	7.540885648
	N379	0.230196073	-2.547226650	6.166695808
	N380	-0.383119544	0.375453714	6.814569581
	N381	-0.679113299	0.210619704	9.692118608
	N382	5.528717846	-11.529785306	5.159735731
	N383	6.388216619	-9.274402653	4.006444383
	N384	5.020791124	-3.341639681	2.898689004
	N385	4.230146983	-1.977630586	4.632516286
	N386	5.418992827	-1.062279185	2.858367901
	N387	9.043758843	-6.980815617	3.836179231
	N388	-5.872878296	-2.956515823	-2.917147205
	N389	-1.943526958	-5.583579368	-3.196357317
	N390	-6.094133871	-0.453360886	-2.176444229
	N391	-8.355834447	0.656925623	-0.956408997
	N392	-7.850908477	0.353186470	1.791920120
	N393	-5.703408476	2.097401849	2.272242430
	N394	-3.147818307	2.687859788	-1.107253746

	N395	-2.451868832	0.684192886	-0.727972559
	N396	-6.334537135	4.733194484	2.879282301
	N397	-9.769140285	7.735061285	1.593207766
	N398	-9.669209686	9.521724394	2.905320436
	N399	9.476587178	2.673090827	2.406074349
	N400	6.256477018	7.151409206	-0.279693616
	N401	4.220268113	8.466130244	-2.886023491
	N402	1.560668560	7.843668010	-3.362793973
	N403	-3.173648623	6.401346369	-4.458900946
	N404	-3.362335172	8.245171404	-5.888592693
	N405	-4.453737562	8.238707987	-3.845393739
	N406	0.680289743	6.332213915	-1.078426675
	N407	0.980791041	8.228885656	0.972202640
	N408	-0.372969242	10.610117818	0.659947022
	N409	-1.888140496	10.340242059	-3.046983346
	N410	-2.754861289	11.624265161	1.707781893
	N411	4.103935177	-4.761069187	-10.223116547
	N412	2.456087744	-2.570011755	-7.874727169
	N413	1.408151177	0.227217046	-7.341780619
	N414	3.486967553	2.224887312	-7.357878911
	N415	-1.719171851	-2.997683569	-10.073407080
	N416	-3.285524224	-1.179209397	-8.495054147
	N417	8.144958219	-7.084648825	-5.978236275
	N418	4.265465700	-5.688224231	-4.406445787
	N419	3.706480742	-6.698977342	-6.284977615
	N420	9.234901977	-7.457630104	-3.050657870
	N421	0.031893628	2.399915842	-0.102668217
	N422	2.405733878	-0.232602196	0.516363775
	N423	0.875760730	1.749984017	-0.462899636
	N424	2.583433543	-0.660825819	1.538929364
	O425	-6.585593317	-5.139086452	1.650058370
	O426	-7.291601159	-2.831561526	4.499574393
	O427	-5.306823941	-5.210151051	6.682309027
	O428	-2.453579025	-4.006329319	4.921656498
	O429	-3.039875481	-0.540928438	5.398721043
	O430	-3.278656513	-1.012638313	8.979646461
	O431	-0.548852970	-4.029365822	9.717868766
	O432	2.179043972	-3.771788493	6.082923455
	O433	1.897576276	0.281440344	6.694148344
	O434	0.833873781	1.903718163	9.732195025
	O435	1.534126705	-0.279255865	12.476608778
	O436	7.052949061	-10.339915032	2.065131394
	O437	8.026319888	-7.699599496	5.769404838
	O438	11.576880578	-4.538783644	4.547772308
	O439	-5.635863642	-0.849505919	0.036179369
	O440	-3.716057162	-4.412594933	-4.009514452
	O441	-7.123072168	2.500177054	-0.409159119
	O442	-6.340225497	3.038537947	-3.351652404
	O443	-9.775020887	1.503550090	2.284000831
	O444	-5.634965471	1.487102434	4.473152617
	O445	-4.255217062	5.057044094	3.768513127
	O446	-6.579711121	7.260714378	5.347360958
	O447	10.793029700	-0.067881566	4.171687807
	O448	3.576322195	4.703953864	3.952157228
	O449	3.611313441	8.373224184	-0.692091941
	O450	0.987769978	10.066268272	-3.522860877
	O451	-1.392147721	7.182849305	-1.531613140
	O452	-0.684698066	7.169341871	2.143896134
	O453	2.462320544	5.728586907	1.455464976
	O454	0.849122686	11.613026870	2.318039794
	O455	-2.510441627	13.587001746	0.573766924
	O456	-3.263939654	11.005036016	-1.346934640
	O457	-4.958684515	13.713897200	3.625554115
	O458	-5.503293118	6.838499333	-1.320925157
	O459	1.755231862	-4.572689991	-8.755093753
	O460	-0.284071342	-0.739890942	-8.549280094
	O461	2.120953140	3.605205068	-8.539771385
	O462	5.825640860	4.337418012	-9.111290659
	O463	-5.001456513	-2.634350108	-8.862586943
	O464	-1.477843592	-6.601674880	-6.011566991
	O465	0.451881984	-5.788358061	-6.782824303
	O466	-3.995865107	2.321235484	-8.431627740
	O467	9.943443333	-5.405607573	-3.701721993
	O468	12.667022879	-6.992120850	-2.106449139
	O469	0.305522701	-6.246057026	-1.366154577
	O470	-0.256947154	-7.317074975	0.530841328
	O471	5.145737269	-10.891433865	-3.334864468
	O472	2.884883079	-10.929548517	-3.312834113
	O473	5.065060244	-5.767078916	-1.318523032
	O474	5.027073119	-7.476051890	0.138656550

	O475	2.606843589	-6.103304301	-2.130576234
	O476	8.938889176	-6.567588955	1.039669225
	O477	6.965650944	-4.554879937	0.420205361
	O478	-4.390903500	4.745764330	-2.461078462
	O479	7.728886788	-10.427124867	-2.515401209
	O480	7.501325835	-8.642223148	-0.087140874
	S481	3.628515161	5.006451152	-2.611444324
	S482	1.912644163	1.807785194	-3.191298775
	S483	2.095708072	-3.343611326	-3.768177320
	S484	3.943566505	2.001906435	-0.340829767
	S485	0.452381297	-0.912393366	-1.624327379
	S486	4.011560463	-0.714135405	-5.574356809
	S487	3.300030234	-3.458478684	-0.356631367
	S488	5.611124794	1.633266868	-3.402423906
	S489	5.698071448	-3.045928269	-3.071051722
	S490	6.472332001	-0.811740537	-0.618060532
	end			

Fe2-N-N to Fe2-NH-N-b

Figure 8, scheme F

reactant **Fe2-N-N** (S=3/2)	bm526hx7hnexp2n2n3.car_5			
Fe(139) -2.196	C1	-7.753334463	-5.376553190	1.292458809
Fe(140) 0.085	C2	-8.125229943	-6.525679002	0.348345007
Fe(141) -2.492	C3	-8.595942619	-3.460010635	2.578410123
Fe(142) 2.372	C4	-7.955451368	-3.720959898	3.938722564
Fe(143) 3.016	C5	-7.523618210	-5.315786186	5.743338389
Fe(144) 1.130	C6	-5.998054864	-5.430262107	5.673780709
Fe(145) 0.974	C7	-4.024189836	-5.743606093	4.275382903
	C8	-3.485390852	-4.310942880	4.304179184
	C9	-3.896208327	-1.980824957	3.649343662
	C10	-3.903800850	-1.362818760	5.056063430
	C11	-4.936962892	-1.201078089	7.231236221
	C12	-3.868899387	-1.761762222	8.181778252
	C13	-2.870709485	-3.784258099	9.146946894
	C14	-1.400828053	-4.085898503	8.822287576
	C15	0.242999420	-4.777484238	7.122974283
	C16	0.983498463	-3.642371509	6.408536505
	C17	0.676577749	-1.375719404	5.431855462
	C18	0.785530503	-0.162102468	6.368865672
	C19	-0.200584409	-1.153185141	4.173738396
	C20	0.039614640	0.209595855	3.513655657
	C21	-0.020019454	-2.305140082	3.175750060
	C22	-0.376751770	1.575564541	7.653077660
	C23	-0.019656344	1.246247045	9.113518525
	C24	-1.708697973	2.349324980	7.507992519
	C25	-1.783323726	3.517956752	8.496148598
	C26	-1.882254687	2.856345056	6.069576807
	C27	-0.427987795	-0.097206053	11.087482613
	C28	1.036003328	-0.375812002	11.365603074
	C29	5.898163267	-11.620369470	3.740698776
	C30	6.515414155	-10.338750611	3.191336279
	C31	6.793965725	-7.916339326	3.690074311
	C32	8.018432496	-7.525427492	4.537762459
	C33	5.616286649	-6.958354382	3.932601032
	C34	5.945500639	-5.517033306	3.552824392
	C35	4.695522645	-4.641963974	3.489177730
	C36	4.875099437	-2.139052262	3.462149518
	C37	10.273872991	-6.565775138	4.480485070
	C38	10.479045309	-5.067787063	4.471778732
	C39	-5.351519837	-2.684143097	-1.572730022
	C40	-5.712342103	-1.249147042	-1.142114405
	C41	-3.813461343	-2.826775565	-1.506066256
	C42	-3.255049773	-4.259863648	-1.623015770
	C43	-2.986687783	-4.748167617	-3.047269462
	C44	-6.185823925	0.991102855	-2.051015235
	C45	-7.270565674	1.455551801	-1.068661686
	C46	-6.359017368	1.600471463	-3.447998673
	C47	-9.425333691	0.947507845	-0.016633471
	C48	-9.025187033	0.960464213	1.461838525
	C49	-7.321552051	0.429570820	3.140325050
	C50	-6.147085339	1.385598179	3.354710684
	C51	-4.616080483	3.054339177	2.432072948
	C52	-5.052877383	4.364230356	3.130348760
	C53	-4.029303189	3.489102285	1.080694380
	C54	-3.413450074	2.428344310	0.231323303
	C55	-2.966032846	1.152635940	0.466625983

	C56	-2.557532600	1.626623577	-1.672341535
	C57	-6.859046833	6.039040308	3.259392898
	C58	-6.757279204	6.199515632	4.774996941
	C59	-8.334814769	6.095612681	2.800173713
	C60	-8.950325111	7.458664519	2.676674057
	C61	-8.880210147	8.562740725	3.503916168
	C62	-10.186005420	8.984305828	1.764120900
	C63	9.244021151	1.639612762	3.417883316
	C64	10.282778463	0.546431298	3.246365661
	C65	7.853007221	0.985760972	3.236290870
	C66	6.717097069	1.957602628	3.452991517
	C67	6.135132153	2.139738873	4.719944334
	C68	6.217001801	2.723289853	2.384258056
	C69	5.088291851	3.048651023	4.916857035
	C70	5.189464121	3.648093794	2.568631832
	C71	4.618439669	3.803061905	3.833812316
	C72	5.376192798	6.852728344	-1.420007155
	C73	4.323654021	7.957763777	-1.622925338
	C74	4.695911581	5.508409590	-1.181267558
	C75	3.310174506	9.547597194	-3.218214312
	C76	1.836206434	9.164691548	-3.379527777
	C77	0.219231864	7.267356336	-3.340837102
	C78	-0.235865611	6.923381891	-1.898974604
	C79	0.245018067	6.020723720	-4.254174797
	C80	-1.009372815	5.144469444	-4.355986531
	C81	-2.155331951	5.681162155	-5.230435458
	C82	-3.678022898	7.599742724	-4.750219157
	C83	0.306729275	5.973856018	0.292105455
	C84	0.132395614	7.189819921	1.214218858
	C85	1.323455729	5.022573981	0.958548570
	C86	1.194785707	9.259190210	1.971450841
	C87	0.550167673	10.603594577	1.668988212
	C88	-0.855444227	11.875346402	0.137097861
	C89	-2.131672021	12.431720430	0.813292034
	C90	-1.005485147	11.881687455	-1.386496921
	C91	-2.155275636	11.024342223	-1.900565546
	C92	-4.076651541	11.954674596	2.226391649
	C93	-3.992201009	13.057583146	3.273421765
	C94	-4.734875440	10.687174155	2.839267770
	C95	-4.973412167	9.613002106	1.802700411
	C96	-6.149173545	9.615052795	1.037073787
	C97	-4.011401409	8.625752147	1.534978365
	C98	-6.351750019	8.678479831	0.022157114
	C99	-4.185186154	7.695061088	0.505726412
	C100	-5.355994448	7.738581266	-0.245292913
	C101	4.087128982	-3.987415027	-8.979330431
	C102	2.658089099	-3.728786972	-8.535916302
	C103	1.193443688	-2.185520203	-7.257039987
	C104	0.693381897	-0.832980745	-7.777430939
	C105	1.111236937	1.591656515	-7.739374332
	C106	2.294876834	2.539688022	-7.924396084
	C107	4.578102591	3.185278581	-7.397075251
	C108	5.144547084	3.378070879	-8.790335060
	C109	-2.753932726	-3.495790659	-9.158958039
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	C112	-1.540395329	-5.491651384	-8.151956610
	C113	-0.869733605	-6.022409899	-6.905479776
	C114	-4.183884809	-0.085862283	-8.173994000
	C115	-3.709112408	1.198430270	-8.824083406
	C116	-4.548726358	0.045032004	-6.674011580
	C117	-3.312131757	0.050915209	-5.818951400
	C118	-2.579080856	1.233914381	-5.617732756
	C119	-2.790052822	-1.161393854	-5.338975364
	C120	-1.314346264	1.183689873	-5.021757333
	C121	-1.526212078	-1.210950775	-4.742953418
	C122	-0.773085383	-0.039948130	-4.616062836
	C123	7.933076459	-6.251630768	-4.780776220
	C124	9.108196366	-6.326260746	-3.795278893
	C125	6.616294133	-6.593143963	-4.068561391
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	C127	5.021338154	-7.031841584	-6.046456862
	C128	3.279484014	-5.901425723	-5.278846555
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	C130	11.665357864	-7.326663021	-2.722268454
	C131	0.607511040	-6.869289326	-0.222609292
	C132	2.097526828	-6.915470353	0.102179236
	C133	3.021657454	-7.056168327	-1.145826411
	C134	2.946395058	-8.508913032	-1.684161515
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C138	3.569038087	-0.703968772	-2.211600932
Fe139	3.867273713	-1.966210118	-3.750113721
Fe140	2.156878635	0.609688601	-1.121282523
Fe141	5.013622507	0.488107069	-1.579815092
Fe142	3.687394002	0.534237550	-3.764636735
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Fe144	4.686733098	-2.060708131	-1.317091712
Fe145	2.181576788	-2.323680967	-1.836797881
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H149	-8.839419569	-6.148053044	-0.401310284
H150	-8.680638855	-7.264382516	0.951818526
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H168	1.018543369	-2.373496015	2.820129941
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H174	0.993369849	0.235055980	2.972892136
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H182	0.449119983	2.217569264	7.310870542
H183	-1.274991844	0.047866775	6.435574140
H184	-0.765267873	0.413359185	2.791307792
H185	1.641131300	4.270383192	0.220913346
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	H216	-1.604243694	-3.467222670	-7.319699068
	H217	-1.202749014	-3.783452557	-10.473648502
	H218	-6.758442632	-3.464182271	-2.868483988
	H219	-3.494793769	-2.420786696	-0.534295606
	H220	0.827666911	-5.303241876	-7.581221630
	H221	-2.326631160	-4.331555892	-1.038220102
	H222	-3.844563349	2.609881532	3.076509623
	H223	-2.985203976	0.542588980	1.361020171
	H224	-8.133483027	0.769141417	3.798070515
	H225	-7.265963248	-0.074878439	1.066399095
	H226	-6.946136213	4.080547370	2.394809025
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	H234	-9.831620415	10.461869956	3.256490709
	H235	-8.381565362	5.644542197	1.796263060
	H236	-6.188971871	2.032181764	1.372780092
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	H238	-9.861500650	1.935231010	-0.222321667
	H239	-2.219527515	1.530421220	-2.701648101
	H240	-10.216310197	0.198786126	-0.154166044
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	H244	-0.670476207	5.469512229	0.268115044
	H245	1.745366638	8.077015339	0.307821293
	H246	-3.475058425	3.550584825	-1.616867281
	H247	-5.124528281	4.161992314	-2.796291555
	H248	-6.709281899	3.384943407	-4.183684480
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	H252	-0.051363214	11.600430595	-1.853763219
	H253	-1.226370059	12.919000315	-1.683103023
	H254	-0.912738664	10.190368572	-3.334639272
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	H256	-3.722876839	9.179098557	-6.056723852
	H257	-2.652189883	4.848663271	-5.751446709
	H258	-7.277927712	8.684929148	-0.558521227
	H259	-3.101155936	8.560221407	2.136402556
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	H263	-1.391869203	4.882784129	-3.357033253
	H264	-8.372608632	-0.211968621	-1.486110384
	H265	3.641188457	10.015001265	-4.155264325
	H266	-6.105558201	-0.963712103	-3.075983803
	H267	0.534191829	6.357849076	-5.263060229
	H268	-3.396443918	6.977609695	0.275702136
	H269	3.340340219	10.313936474	-2.430183215
	H270	-2.997422086	7.741457654	-6.689270274
	H271	-5.110446524	8.942161082	-4.172660768
	H272	-5.188954117	-3.534134190	-3.441129985
	H273	-5.784298735	-3.344287835	-0.797923034
	H274	-6.926493346	10.356399497	1.236387291
	H275	-5.253697667	1.376069452	-1.613420568
	H276	-0.485211041	8.020489497	-3.706944025
	H277	-1.741390251	6.341671278	-6.002688509
	H278	-0.680347034	4.200558105	-4.812476607
	H279	-3.600306196	5.872686984	-3.677149500
	H280	0.799326725	8.912991126	2.938036930
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	H282	-0.087461885	12.622466711	0.390163209
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	N424	2.583433543	-0.660825819	1.538929364
	O425	-6.585593317	-5.139086452	1.650058370
	O426	-7.291601159	-2.831561526	4.499574393
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	O428	-2.453579025	-4.006329319	4.921656498
	O429	-3.039875481	-0.540928438	5.398721043
	O430	-3.278656513	-1.012638313	8.979646461
	O431	-0.548852970	-4.029365822	9.717868766
	O432	2.179043972	-3.771788493	6.082923455
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	O446	-6.579711121	7.260714378	5.347360958
	O447	10.793029700	-0.067881566	4.171687807
	O448	3.576322195	4.703953864	3.952157228
	O449	3.611313441	8.373224184	-0.692091941
	O450	0.987769978	10.066268272	-3.522860877
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transition state (S=3/2) Fe(139) -2.237 Fe(140) -0.011 Fe(141) -2.484 Fe(142) 2.368 Fe(143) 2.695 Fe(144) 1.690 Fe(145) 1.168	bm522n2ntoNHN335tc_1_53264.71 C1 -7.735334999 -5.367407626 1.281621284 C2 -8.123726098 -6.514181762 0.340394035 C3 -8.559597072 -3.443564508 2.569466477 C4 -7.924137851 -3.705251158 3.931526784 C5 -7.494617729 -5.298792395 5.737126415 C6 -5.969416611 -5.418021960 5.671103024 C7 -3.994340481 -5.722709708 4.275726599 C8 -3.472952334 -4.283854228 4.312324817 C9 -3.888511602 -1.960340105 3.627369270 C10 -3.906924007 -1.333037570 5.030443080 C11 -4.929302654 -1.176384024 7.209162602 C12 -3.862424335 -1.729425932 8.165716944 C13 -2.857960877 -3.746603682 9.138500852 C14 -1.389199448 -4.057125542 8.815468729 C15 0.245674018 -4.784551306 7.122234715 C16 0.982721260 -3.642561054 6.413038175 C17 0.647457100 -1.397269273 5.388685663 C18 0.777762268 -0.186419232 6.327852506 C19 -0.254306960 -1.180124583 4.154826305 C20 -0.021835429 0.182619081 3.488214641 C21 -0.101391463 -2.353204897 3.175245865 C22 -0.360632474 1.560712098 7.622993833 C23 0.003060668 1.233039363 9.082081559 C24 -1.690530563 2.340176286 7.487120926 C25 -1.759689291 3.506049424 8.479135739 C26 -1.869635465 2.851469489 6.050875905 C27 -0.408564110 -0.095763621 11.065461790 C28 1.056175105 -0.365835166 11.347081628 C29 5.893129612 -11.604161335 3.737971551 C30 6.516576967 -10.326414622 3.187023045 C31 6.794287736 -7.903512001 3.682871654 C32 8.017186266 -7.510035128 4.530949767 C33 5.616601567 -6.946189725 3.924975115 C34 5.951185961 -5.505220542 3.551105466 C35 4.706043712 -4.624601084 3.494280636 C36 4.896464687 -2.125148748 3.516220197 C37 10.272093042 -6.552347260 4.476579556 C38 10.486850256 -5.056065143 4.465936600 C39 -5.334736041 -2.677412481 -1.566337038 C40 -5.695864794 -1.243080561 -1.133511458 C41 -3.796504197 -2.822131833 -1.505789351 C42 -3.245147722 -4.257957055 -1.624150616 C43 -2.978865664 -4.745349782 -3.049156223

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H152	-8.674284509	-5.610440032	3.964464316
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H159	-3.756360521	-6.180794070	3.306305941
H160	-4.780957138	-0.089661403	7.161097309
H161	-5.664552467	-2.301204776	5.518373045
H162	-3.474918222	-6.282021688	5.062579649
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H164	-4.219835457	-3.642928275	7.490097432
H165	-5.919573506	-1.378248111	7.641173816
H166	-0.427778321	-3.297058709	3.634319391
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H173	-1.719104977	3.170964635	9.525349956
H174	0.842736921	0.158759871	2.817981596
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H187	2.671338234	5.323250892	2.324043289
H188	3.215934460	4.680231875	4.861284333
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H208	-3.103322889	1.045044151	-9.738081137
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H220	0.830521238	-5.295833460	-7.587307872
H221	-2.316967868	-4.335181366	-1.039706279
H222	-3.832292321	2.606087596	3.079219827
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product **Fe2-NH-N-b** (S=3/2) Fe(139) -2.303 Fe(140) 0.059 Fe(141) -2.453 Fe(142) 2.333 Fe(143) 2.802 Fe(144) 1.879 Fe(145) 0.987	bm522n2ntoNHN335tc.car_4 C1 -7.744387633 -5.369816252 1.291005632 C2 -8.108727253 -6.522111184 0.347124489 C3 -8.601287862 -3.459654917 2.577013619 C4 -7.964991669 -3.722103157 3.939314710 C5 -7.539074251 -5.319649326 5.742628570 C6 -6.013095132 -5.432903234 5.677943417 C7 -4.034616570 -5.741964993 4.285422501 C8 -3.496843338 -4.308732812 4.319279624 C9 -3.906686639 -1.976827275 3.667506309 C10 -3.923447821 -1.359078593 5.074365524 C11 -4.949398151 -1.212097025 7.251538288 C12 -3.872925594 -1.770670083 8.194504231 C13 -2.866446384 -3.792747195 9.152067069 C14 -1.394967538 -4.083346494 8.824441793 C15 0.251404786 -4.750172123 7.116532019 C16 0.984879451 -3.616419014 6.391339841 C17 0.655050880 -1.353788110 5.400379290 C18 0.779800981 -0.146403801 6.343488240 C19 -0.254912592 -1.130316490 4.166477829 C20 -0.047277707 0.240713255 3.514439848 C21 -0.082930048 -2.277608459 3.160432209 C22 -0.373730341 1.587141535 7.644636296 C23 -0.015875349 1.250009318 9.102147572 C24 -1.707163600 2.360087629 7.506200065 C25 -1.782633306 3.524661180 8.498911353 C26 -1.886902515 2.871697343 6.070212770 C27 -0.422930018 -0.108935577 11.064842130 C28 1.041504065 -0.383840184 11.343902912 C29 5.893129403 -11.617683456 3.723979701 C30 6.519052464 -10.337481890 3.181345349 C31 6.803924547 -7.918066859 3.685768545

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	C69	5.085115096	3.051237174	4.910317307
	C70	5.191796219	3.657677488	2.564644495
	C71	4.618357637	3.810107282	3.829044626
	C72	5.373367409	6.852389835	-1.413895731
	C73	4.315671359	7.950391044	-1.620394701
	C74	4.707005811	5.508943614	-1.119754289
	C75	3.310346562	9.541770502	-3.219135843
	C76	1.834936533	9.165164409	-3.380819866
	C77	0.215233447	7.268138235	-3.340851408
	C78	-0.246356216	6.927759856	-1.900541551
	C79	0.243221873	6.021837786	-4.253724004
	C80	-1.011867509	5.146632979	-4.357136934
	C81	-2.157054601	5.685807012	-5.230863844
	C82	-3.680504640	7.602004574	-4.749735276
	C83	0.284653035	5.973425315	0.291665442
	C84	0.121606469	7.186954973	1.218375713
	C85	1.292482767	5.009070377	0.950124997
	C86	1.194092803	9.252121074	1.974556281
	C87	0.554229295	10.598179848	1.669143221
	C88	-0.848868425	11.872679920	0.137544412
	C89	-2.124440764	12.427842092	0.814739875
	C90	-0.998594775	11.882978258	-1.385960447
	C91	-2.150420733	11.029951000	-1.902551856
	C92	-4.069035289	11.949623471	2.225804574
	C93	-3.985810593	13.055359667	3.269847441
	C94	-4.729526537	10.684882321	2.840602192
	C95	-4.970775992	9.611790858	1.804083900
	C96	-6.146303487	9.617307532	1.038124519
	C97	-4.010625649	8.623120832	1.535740240
	C98	-6.350299755	8.682602786	0.021821485
	C99	-4.185769379	7.694190172	0.505198290
	C100	-5.356052464	7.741441158	-0.246498106
	C101	4.085602104	-3.991537375	-9.000660572
	C102	2.659511195	-3.732131688	-8.548300345
	C103	1.203682159	-2.185005993	-7.260423649
	C104	0.701290291	-0.833367784	-7.780787438
	C105	1.114042474	1.592480940	-7.741128351
	C106	2.296795413	2.539977116	-7.935408095
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	C108	5.139235927	3.384571699	-8.814108890
	C109	-2.759734940	-3.497562893	-9.171843521
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	C111	-2.270540445	-4.165036351	-7.866741159

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C113	-0.874571618	-6.018031208	-6.910469666
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C115	-3.713246572	1.197196701	-8.838438295
C116	-4.542680243	0.045922155	-6.683996772
C117	-3.303507166	0.054978221	-5.831240593
C118	-2.572843777	1.239441699	-5.630169921
C119	-2.780830562	-1.154434646	-5.343991559
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C122	-0.772459704	-0.025690965	-4.605461822
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C124	9.111328701	-6.326176115	-3.795733453
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C138	3.573510395	-0.702900471	-2.234995090
Fe139	3.813469451	-1.978898766	-3.779657341
Fe140	2.260843910	0.567513312	-1.164972956
Fe141	5.055510835	0.458179423	-1.579227544
Fe142	3.692161188	0.538507134	-3.756382143
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Fe144	4.743550177	-2.076620932	-1.406364625
Fe145	2.211049044	-2.382169110	-1.814460684
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H148	-9.726434307	-4.818847408	1.373898796
H149	-8.823538412	-6.150145714	-0.404891502
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H159	-3.799874605	-6.201399606	3.315790907
H160	-4.804798817	-0.124413267	7.212720534
H161	-5.690168093	-2.319271199	5.550676729
H162	-3.519976960	-6.306407400	5.071851496
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H167	-0.725233812	-2.112073331	2.280211167
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H173	-1.745448032	3.188371832	9.544871193
H174	0.905163927	0.289027154	2.973037980
H175	-0.082174710	1.063039530	4.242931953
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H179	-1.074283173	3.569036145	5.807265812
H180	-0.949839041	4.227822395	8.338588748
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H182	0.451242531	2.231093104	7.304017851
H183	-1.278100704	0.069844429	6.422141912
H184	-0.854772610	0.420962590	2.786390927
H185	1.592249402	4.254298615	0.207844510
H186	0.765307031	4.501718840	1.770376769
H187	2.682462052	5.328768488	2.311969922
H188	3.220384747	4.684083066	4.854371526
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H205	-2.275708041	-6.237312974	-8.495568095
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H215	-1.311515947	-5.828932364	-2.435204235
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H220	0.825078306	-5.301545772	-7.583146969
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H266	-6.097226724	-0.957471406	-3.078135335
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H268	-3.398602033	6.975103220	0.275019671
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	H274	-6.921930067	10.360386837	1.237750201
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	H276	-0.487235922	8.021522955	-3.710822391
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	H278	-0.683477568	4.203518868	-4.815629340
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	H281	-0.460557719	9.754443356	0.106540620
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	H288	5.043913598	-5.117761384	-10.403756766
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	H292	4.829577289	8.091126285	-3.607934546
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	H294	6.811562440	8.024887665	-0.535280901
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	H296	5.981008150	6.756370289	-2.327020623
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	H304	4.257362215	-4.521969083	4.480117201
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	H307	4.786363277	-7.320794250	3.314847154
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	H310	-5.189182338	-0.802873837	-6.417696533
	H311	5.938154488	-9.481885803	4.894131098
	H312	4.987795158	-11.789156204	3.122159673
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	H322	6.789524387	-10.535793216	-2.819850617
	H323	4.918816191	2.555319112	-9.528500783
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	H327	3.095327427	-9.199407978	-0.821761352
	H328	3.143750504	-7.050478741	-7.063837334
	H329	2.262385045	-5.556067282	-5.212304099
	H330	6.590572779	-12.438909877	3.485752540
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	H332	8.347527814	-5.800658971	0.809354846
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	H334	8.972624772	-6.857653671	2.793473448
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	H348	0.458753705	-2.943826571	-7.506522119
	H349	4.272965423	4.166442150	-7.012607305
	H350	7.772979909	0.153555387	3.940337968
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N372	-8.801693594	-4.646593258	1.760926613
N373	-8.161696356	-4.947093561	4.482307925
N374	-5.476425204	-5.793710768	4.486208942
N375	-4.233997908	-3.393573819	3.638497991
N376	-4.905845097	-1.769534659	5.910676601
N377	-3.664836120	-3.113176347	8.140075864
N378	-1.105679325	-4.437767416	7.537769944
N379	0.226417346	-2.527152326	6.144769406
N380	-0.384308182	0.391126858	6.801489330
N381	-0.674099684	0.209201143	9.672479311
N382	5.521485250	-11.531133276	5.142625681
N383	6.397410550	-9.275846363	4.000901877
N384	5.021905657	-3.337854817	2.914976924
N385	4.273913414	-2.011448503	4.698030579
N386	5.403182055	-1.056337140	2.904194671
N387	9.048617045	-6.972128757	3.828687881
N388	-5.869841225	-2.951025211	-2.918221600
N389	-1.945995558	-5.583365063	-3.202480040
N390	-6.084769616	-0.447098480	-2.178700390
N391	-8.346844320	0.662780331	-0.961109012
N392	-7.845977816	0.355254944	1.787156567
N393	-5.694781676	2.093671918	2.270028664
N394	-3.112731746	2.694399544	-1.099961825
N395	-2.406214602	0.695068951	-0.715892096
N396	-6.326069877	4.730411128	2.873817191
N397	-9.757877231	7.736816554	1.592291919
N398	-9.661242635	9.521473015	2.907287516
N399	9.470622651	2.672928562	2.389458599
N400	6.278941578	7.181990929	-0.302755539
N401	4.213004538	8.454145374	-2.885791754
N402	1.556295429	7.844837616	-3.358854873
N403	-3.174931992	6.404471785	-4.457799752
N404	-3.365922545	8.246762390	-5.889633784
N405	-4.454392447	8.242187597	-3.844719210
N406	0.663751371	6.332795689	-1.077039936
N407	0.975954686	8.221144876	0.977144212
N408	-0.367360301	10.606571822	0.658740716
N409	-1.885794888	10.350478966	-3.052326147
N410	-2.747218344	11.618924993	1.708177852
N411	4.096051207	-4.770134132	-10.241167160
N412	2.462346834	-2.573201552	-7.885379004
N413	1.412692909	0.228583276	-7.343623507
N414	3.491204063	2.227834639	-7.372558848
N415	-1.723962375	-2.999470503	-10.085502224
N416	-3.290834354	-1.180256838	-8.509865766
N417	8.149061072	-7.097222846	-5.976388711
N418	4.256571886	-5.715578990	-4.404310366
N419	3.715776072	-6.708799881	-6.295951755
N420	9.244015450	-7.457259521	-3.052367920
N421	0.187919764	2.169026722	0.192074862
N422	2.792518785	-0.513285989	0.516397472
N423	1.025961113	1.592223457	-0.292982061
N424	2.434935092	-0.517520643	1.643265193
O425	-6.579309642	-5.127426983	1.653159263
O426	-7.303513918	-2.833636225	4.504205024
O427	-5.325247792	-5.212033083	6.688610307
O428	-2.466183215	-4.005763972	4.939520516
O429	-3.069339653	-0.528876077	5.419595368
O430	-3.277843738	-1.021534378	8.988804394
O431	-0.544973388	-4.035834269	9.722615367

	O432	2.179496851	-3.747923647	6.061516273
	O433	1.895820714	0.289310734	6.665844704
	O434	0.837097156	1.903267181	9.726040273
	O435	1.536696954	-0.290970046	12.456763213
	O436	7.058404151	-10.337144726	2.055972886
	O437	8.042438795	-7.705921441	5.762194791
	O438	11.568202047	-4.515928725	4.541797306
	O439	-5.631237384	-0.844082578	0.034496669
	O440	-3.709248933	-4.399772946	-4.016280228
	O441	-7.114931153	2.506142662	-0.411918286
	O442	-6.331912675	3.043775433	-3.354057497
	O443	-9.770757807	1.505288326	2.278273431
	O444	-5.637717963	1.491589183	4.473606605
	O445	-4.249753893	5.052892075	3.768715997
	O446	-6.565949021	7.261813238	5.339472915
	O447	10.789296010	-0.067154871	4.155860831
	O448	3.578154199	4.712638643	3.947977348
	O449	3.602216522	8.368673269	-0.691879999
	O450	0.990085233	10.068827497	-3.528969640
	O451	-1.402278745	7.193805510	-1.537051904
	O452	-0.692981040	7.168525238	2.150410462
	O453	2.445161592	5.699908804	1.437559034
	O454	0.855924164	11.607382370	2.317260954
	O455	-2.502996555	13.583678481	0.577492279
	O456	-3.258440359	11.010638992	-1.347588611
	O457	-4.953628392	13.710620450	3.620296552
	O458	-5.503752911	6.843991619	-1.323723848
	O459	1.754975972	-4.576379136	-8.757822230
	O460	-0.275256683	-0.743103802	-8.553715584
	O461	2.121287047	3.603122923	-8.554321047
	O462	5.815405677	4.346491294	-9.137764281
	O463	-5.007321911	-2.635186633	-8.876355508
	O464	-1.485235086	-6.595854457	-6.017387915
	O465	0.446700645	-5.783924934	-6.784598341
	O466	-4.001177637	2.320293228	-8.447846849
	O467	9.938884492	-5.398785979	-3.699809502
	O468	12.673554684	-6.984812657	-2.101289833
	O469	0.300181426	-6.289822590	-1.362282089
	O470	-0.249342570	-7.365085868	0.534526337
	O471	5.160661828	-10.901794049	-3.342030229
	O472	2.899956109	-10.950334789	-3.319629477
	O473	5.076902886	-5.807714042	-1.332706593
	O474	5.030167825	-7.499571971	0.146886301
	O475	2.614103254	-6.122020858	-2.117654182
	O476	8.944207625	-6.556313364	1.033225964
	O477	6.953437691	-4.559866108	0.409396646
	O478	-4.385315932	4.749725561	-2.455116111
	O479	7.740644461	-10.423552733	-2.518393322
	O480	7.511538319	-8.633372984	-0.092183345
	S481	3.610408146	4.957772599	-2.509930338
	S482	1.954720729	1.834999963	-3.146396789
	S483	2.064655559	-3.392489068	-3.750699467
	S484	4.005943002	1.942733141	-0.315517100
	S485	0.514969663	-0.935833807	-1.583062557
	S486	3.989174197	-0.686566062	-5.574204255
	S487	3.380810537	-3.492136329	-0.327688518
	S488	5.616981550	1.635658437	-3.403721312
	S489	5.664400653	-3.074807595	-3.150879540
	S490	6.335270611	-0.910841898	-0.410126151
	end			

Fe6-N-N to Fe6-NH-NH-a

Figure 8, scheme G

reactant **Fe6-N-N** (S=1/2)	bm526hx7hn6n2n147.car_2			
Fe(139) 1.257	C1	-7.736529657	-5.357530967	1.287924563
Fe(140) -1.290	C2	-8.081696689	-6.516056852	0.345073833
Fe(141) 1.973	C3	-8.625326579	-3.464947002	2.578483484
Fe(142) -2.250	C4	-7.988138163	-3.730401790	3.940393160
Fe(143) 2.638	C5	-7.570522466	-5.332511304	5.742366667
Fe(144) -1.640	C6	-6.044454485	-5.446756387	5.682626648
Fe(145) -0.237	C7	-4.063162449	-5.764498047	4.294286300
	C8	-3.516980243	-4.334822411	4.329767962
	C9	-3.911450411	-1.997714912	3.694200158
	C10	-3.918115494	-1.389699254	5.104845734
	C11	-4.952270573	-1.237142312	7.278960474
	C12	-3.876964296	-1.806418311	8.216896463

	C13	-2.872764459	-3.837746638	9.155769846
	C14	-1.397442140	-4.106933968	8.826917204
	C15	0.258828856	-4.719633287	7.107499432
	C16	0.989174280	-3.584332516	6.383984374
	C17	0.670953779	-1.316257601	5.410925155
	C18	0.785691137	-0.101447217	6.345307800
	C19	-0.212550177	-1.099266975	4.160487275
	C20	0.087848248	0.239779546	3.475832509
	C21	-0.084080703	-2.295420879	3.209223605
	C22	-0.387786766	1.610881013	7.658220835
	C23	-0.033523101	1.262676325	9.115033957
	C24	-1.725336075	2.375500492	7.519948432
	C25	-1.806077324	3.538993780	8.513796917
	C26	-1.906460198	2.886062161	6.083912551
	C27	-0.438617231	-0.117634691	11.064269959
	C28	1.025346124	-0.397056886	11.340988422
	C29	5.889131066	-11.622457201	3.704831299
	C30	6.519742048	-10.340945307	3.171010080
	C31	6.811436079	-7.926594019	3.687970781
	C32	8.040113667	-7.542337646	4.531690097
	C33	5.641220737	-6.961763876	3.938985638
	C34	5.983749619	-5.521826086	3.568384702
	C35	4.748582227	-4.626525073	3.535387132
	C36	4.877119114	-2.119648462	3.473725664
	C37	10.282906024	-6.553605398	4.468786855
	C38	10.467336425	-5.052933590	4.466971311
	C39	-5.335701990	-2.672908771	-1.589009254
	C40	-5.701038508	-1.239040985	-1.158539722
	C41	-3.797841753	-2.815961968	-1.521079965
	C42	-3.240784629	-4.250424144	-1.628548950
	C43	-2.970709835	-4.745903301	-3.049797172
	C44	-6.178119255	1.001642818	-2.065695776
	C45	-7.261670205	1.467171166	-1.082609717
	C46	-6.350449786	1.612531918	-3.462024532
	C47	-9.416768782	0.964753988	-0.029896593
	C48	-9.014165129	0.973188562	1.447884153
	C49	-7.308118646	0.429973432	3.120772325
	C50	-6.125745756	1.375644099	3.336920355
	C51	-4.603699423	3.061455381	2.429929859
	C52	-5.039212236	4.367856950	3.132767928
	C53	-4.010900559	3.503043792	1.083025196
	C54	-3.416527050	2.434396792	0.230063573
	C55	-3.037310322	1.136393105	0.460285514
	C56	-2.603817148	1.598909695	-1.677788055
	C57	-6.839342309	6.045714236	3.259154758
	C58	-6.728252098	6.212538311	4.773558440
	C59	-8.320000513	6.102513780	2.813460613
	C60	-8.934334653	7.465940184	2.686847965
	C61	-8.872059666	8.568333768	3.516979719
	C62	-10.163053665	8.993244943	1.767050373
	C63	9.250863037	1.657696144	3.407544706
	C64	10.297184607	0.571833439	3.236769293
	C65	7.865338334	0.995453510	3.209237436
	C66	6.721667485	1.959361255	3.418156006
	C67	6.142226943	2.143599808	4.685746959
	C68	6.209709371	2.711877753	2.345673903
	C69	5.089989279	3.045837804	4.881790818
	C70	5.173374121	3.628467537	2.527972698
	C71	4.609750962	3.789991112	3.796217301
	C72	5.385808824	6.863915523	-1.403603184
	C73	4.325122349	7.960025537	-1.607470315
	C74	4.719911015	5.528322351	-1.077717083
	C75	3.313136854	9.548644658	-3.206824845
	C76	1.838900044	9.170955840	-3.377237909
	C77	0.216862387	7.275999659	-3.338552009
	C78	-0.249714350	6.927545326	-1.901234153
	C79	0.248340008	6.033499250	-4.256712090
	C80	-1.003151060	5.153651543	-4.361273062
	C81	-2.151596501	5.688371043	-5.233452650
	C82	-3.678413560	7.603318288	-4.754351228
	C83	0.270716743	5.959862236	0.285201934
	C84	0.110307745	7.172152040	1.214026817
	C85	1.272797046	4.990029645	0.945797596
	C86	1.183755430	9.237036200	1.969743546
	C87	0.546459361	10.587332000	1.674026663
	C88	-0.849017497	11.880555767	0.147144552
	C89	-2.126150234	12.434643394	0.822206217
	C90	-0.992349649	11.895826079	-1.377332773
	C91	-2.144080721	11.046842553	-1.901833622
	C92	-4.073450764	11.954194049	2.228157735

C93	-3.990944170	13.060814398	3.271643997
C94	-4.733434543	10.689189706	2.842959272
C95	-4.972476763	9.615550291	1.806446619
C96	-6.145354805	9.622244879	1.036590751
C97	-4.012478531	8.625732641	1.541805274
C98	-6.346960030	8.687508523	0.019960524
C99	-4.185399576	7.696506023	0.511153186
C100	-5.353211319	7.744780444	-0.244249483
C101	4.087656132	-3.992202654	-8.988489994
C102	2.662754243	-3.737912617	-8.530118232
C103	1.213551941	-2.199158721	-7.223836877
C104	0.715105595	-0.846637737	-7.746758697
C105	1.130726490	1.576777997	-7.708480066
C106	2.316373567	2.514833800	-7.921423257
C107	4.601851814	3.167366879	-7.435657606
C108	5.112601324	3.392910333	-8.844358207
C109	-2.739364565	-3.496963115	-9.169320266
C110	-3.763557078	-2.401551710	-8.849649318
C111	-2.254063695	-4.163285634	-7.861859632
C112	-1.530924492	-5.491772008	-8.149351083
C113	-0.864888039	-6.016524884	-6.897423164
C114	-4.166673790	-0.084582025	-8.194623061
C115	-3.680661116	1.201510523	-8.832829331
C116	-4.568550431	0.047014487	-6.703712488
C117	-3.344207056	0.071366160	-5.834323783
C118	-2.628739034	1.264621990	-5.634834520
C119	-2.805739280	-1.133904823	-5.355097925
C120	-1.360490486	1.231911956	-5.045534590
C121	-1.539765011	-1.165420319	-4.764057694
C122	-0.800679575	0.015720550	-4.642935039
C123	7.925562595	-6.271061109	-4.814554932
C124	9.110190720	-6.343086721	-3.837164070
C125	6.616064006	-6.580783346	-4.075959609
C126	5.346908465	-6.352511995	-4.831899743
C127	4.953469900	-6.930696526	-6.021578090
C128	3.251019991	-5.805560837	-5.161849187
C129	10.312472328	-7.537300143	-2.108099673
C130	11.671105806	-7.326015417	-2.739342143
C131	0.630353692	-6.901355347	-0.179216779
C132	2.124046354	-6.958299490	0.133903950
C133	3.034266253	-7.084390104	-1.123104091
C134	2.928713602	-8.520004410	-1.705408052
C135	3.965829537	-8.866851603	-2.776979200
C136	3.992473149	-10.359590622	-3.170734638
C137	4.502483987	-6.847879049	-0.728488283
C138	3.584332355	-0.690575566	-2.228495610
Fe139	3.814225626	-1.979617785	-3.599718328
Fe140	2.136667520	0.706333287	-1.580572694
Fe141	5.057199197	0.420859746	-1.584024924
Fe142	3.774613993	0.508842752	-3.765279954
Fe143	3.720276806	2.723072027	-2.380214157
Fe144	4.846378337	-2.073731431	-1.245366539
Fe145	2.201704189	-2.395131284	-1.190575080
H146	-6.289011426	-7.492080653	0.380338348
H147	-6.466179081	-6.505578407	-0.908272076
H148	-9.726653098	-4.836019693	1.364430638
H149	-8.795909913	-6.154989418	-0.412700097
H150	-8.630449501	-7.259734726	0.948586143
H151	-7.986544958	-2.724969447	2.074161096
H152	-8.749474110	-5.632178583	3.967865963
H153	-9.609301322	-3.004693101	2.741761524
H154	-7.987421326	-6.296851937	6.060700144
H155	-6.100529909	-5.872910786	3.665103491
H156	-7.798186071	-4.590437523	6.518604744
H157	-2.909601987	-1.829250596	3.278963981
H158	-5.074034046	-3.709097572	3.136457047
H159	-3.829384519	-6.224977263	3.324930703
H160	-4.803638673	-0.149681053	7.247663523
H161	-5.699890176	-2.326683300	5.569792667
H162	-3.552715828	-6.331924199	5.081366117
H163	-4.636418600	-1.464401994	3.063514933
H164	-4.263992837	-3.712835466	7.533595109
H165	-5.940096264	-1.445824860	7.713197238
H166	-0.457775149	-3.217526142	3.674632964
H167	-0.669286779	-2.124312329	2.291311151
H168	0.959398501	-2.457692564	2.906155055
H169	-1.253758640	-1.053704654	4.509617578
H170	-3.344252488	-4.809340905	9.365357692
H171	-1.914714352	2.069044867	5.350107902
H172	-1.470785266	-0.246744375	9.202299638

	H173	-1.768185521	3.201607726	9.559367175
	H174	1.110746552	0.283511667	3.081927890
	H175	-0.056132034	1.087793895	4.161151349
	H176	9.311608856	2.011668002	4.454635220
	H177	-2.860556635	3.423687897	5.986675314
	H178	-2.749585809	4.084740758	8.366876252
	H179	-1.094775698	3.584116581	5.820118669
	H180	-0.975798302	4.245476182	8.354872499
	H181	-2.543248882	1.667106001	7.746211500
	H182	0.433696460	2.263762200	7.326708104
	H183	-1.275285295	0.080150121	6.437976513
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Fe(143)	2.668	C5	-7.502409756	-5.303465811	5.736347225
Fe(144)	-1.860	C6	-5.977203747	-5.423836124	5.668583404
Fe(145)	-0.418	C7	-4.004646804	-5.728710984	4.268955515
		C8	-3.479991546	-4.290847449	4.302065466
		C9	-3.899757709	-1.965014472	3.630383954
		C10	-3.912145439	-1.340223028	5.034415066
		C11	-4.935526933	-1.180333303	7.212888407
		C12	-3.865944088	-1.734464251	8.165626874
		C13	-2.862700825	-3.751137979	9.138442429
		C14	-1.393454159	-4.058619166	8.815060272
		C15	0.246748842	-4.776472508	7.122575097
		C16	0.987017071	-3.637754109	6.410262000
		C17	0.657583089	-1.388327415	5.389269127
		C18	0.780475987	-0.179613650	6.332281177
		C19	-0.244277785	-1.172126807	4.154351494
		C20	-0.021328335	0.190381438	3.482295677
		C21	-0.088179129	-2.342318822	3.173719802
		C22	-0.364751636	1.564285135	7.624960537
		C23	-0.001467762	1.235544749	9.083438776
		C24	-1.695073548	2.343271266	7.489828202
		C25	-1.763437572	3.508985474	8.482345521
		C26	-1.874485826	2.856123806	6.054200185
		C27	-0.408489240	-0.095993477	11.063539355
		C28	1.055486297	-0.366970880	11.347867772
		C29	5.886465780	-11.602313439	3.731643448
		C30	6.509548836	-10.323897171	3.183705997
		C31	6.793595324	-7.903940313	3.686070544
		C32	8.017265657	-7.513128139	4.534299118
		C33	5.618299678	-6.944096486	3.930209817
		C34	5.959080318	-5.503790426	3.560739187
		C35	4.721547256	-4.612584949	3.512256883
		C36	4.897760444	-2.106888429	3.493335055
		C37	10.271771857	-6.552765515	4.479714406
		C38	10.483477767	-5.055947506	4.466485870
		C39	-5.323660085	-2.671589851	-1.570075403
		C40	-5.688532004	-1.238016651	-1.137791159
		C41	-3.787847348	-2.819775836	-1.508295838
		C42	-3.241001490	-4.257144360	-1.624246915
		C43	-2.975923500	-4.745838273	-3.048757069
		C44	-6.182530595	0.999781962	-2.042091874
		C45	-7.270377120	1.456650123	-1.059765526
		C46	-6.356570467	1.610518379	-3.438066067
		C47	-9.424123271	0.939162381	-0.011138524
		C48	-9.025343508	0.956170100	1.467695540
		C49	-7.319387567	0.440093513	3.148262285
		C50	-6.149129575	1.402089639	3.361074484
		C51	-4.601883137	3.052674742	2.435799763
		C52	-5.044502964	4.358699035	3.134657115
		C53	-4.013240102	3.492413910	1.086334528
		C54	-3.409381329	2.426647488	0.234898032
		C55	-3.016648027	1.132543730	0.464964541
		C56	-2.589277045	1.596344833	-1.672482833
		C57	-6.844051909	6.036555584	3.242990785
		C58	-6.748696852	6.195396977	4.759479922
		C59	-8.320303574	6.093626165	2.783238699
		C60	-8.941512512	7.455046668	2.665734136
		C61	-8.872452504	8.558213343	3.494319618
		C62	-10.191797446	8.975232245	1.763560395
		C63	9.243729074	1.639162254	3.427534809
		C64	10.279721430	0.542677722	3.258186968
		C65	7.852283981	0.987264145	3.239066374
		C66	6.713642366	1.958244031	3.448475680
		C67	6.139640320	2.151392134	4.717535612
		C68	6.197782973	2.705410032	2.373756889
		C69	5.088241094	3.055072357	4.912057846
		C70	5.162622802	3.623235893	2.554658606
		C71	4.602333670	3.791358052	3.823658510
		C72	5.377482837	6.870909145	-1.392424910
		C73	4.319661556	7.967393168	-1.601376011
		C74	4.712051343	5.530517734	-1.083132652
		C75	3.309542051	9.549475277	-3.205929670
		C76	1.835346453	9.171673802	-3.370994466
		C77	0.214737826	7.277644376	-3.331426472
		C78	-0.248466552	6.932622452	-1.892351248
		C79	0.244066899	6.033042901	-4.247359918
		C80	-1.008243452	5.153782926	-4.349653221

	C81	-2.154596408	5.685118371	-5.226759044
	C82	-3.678407813	7.603829624	-4.747110052
	C83	0.272847372	5.974382642	0.297614192
	C84	0.118801596	7.192205535	1.221168769
	C85	1.268500772	5.001846178	0.963194494
	C86	1.193746552	9.259873767	1.965935953
	C87	0.550824253	10.605062827	1.661983709
	C88	-0.856249804	11.880622838	0.134207384
	C89	-2.131864416	12.433423673	0.813951196
	C90	-1.010242182	11.890358756	-1.389175302
	C91	-2.155804872	11.025172741	-1.899335514
	C92	-4.075231213	11.950812667	2.225526553
	C93	-3.991261749	13.053294641	3.273168501
	C94	-4.733281601	10.683934357	2.839020175
	C95	-4.972633963	9.610531498	1.802238139
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	C97	-4.008379940	8.626866842	1.529666447
	C98	-6.354748991	8.674364954	0.025476344
	C99	-4.182884345	7.697442109	0.499508287
	C100	-5.356731516	7.738233054	-0.247001309
	C101	4.088168463	-3.982041006	-8.998045676
	C102	2.663038861	-3.730275500	-8.538652584
	C103	1.215440354	-2.193487645	-7.226884510
	C104	0.718972720	-0.839497198	-7.747607372
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	C108	5.158337546	3.383408703	-8.811483281
	C109	-2.756032060	-3.492103214	-9.151730260
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	C116	-4.579860469	0.047102566	-6.670613177
	C117	-3.347582277	0.068440733	-5.812127982
	C118	-2.626642173	1.259810788	-5.619879101
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	C121	-1.519571561	-1.176855891	-4.792039050
	C122	-0.775573379	0.001984435	-4.678949354
	C123	7.915813618	-6.244287900	-4.784407407
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	Fe140	2.173620458	0.704806220	-1.565097140
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	Fe143	3.764682668	2.714488338	-2.388838640
	Fe144	4.836563846	-2.090761951	-1.284154651
	Fe145	2.313990946	-2.419951036	-1.383991924
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	H150	-8.672569226	-7.240581466	0.946217090
	H151	-7.905618635	-2.727265426	2.056041362
	H152	-8.679099064	-5.613247203	3.961327038
	H153	-9.533685369	-2.954050708	2.728178322
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	H159	-3.769342759	-6.189038884	3.299949854
	H160	-4.788131128	-0.093364780	7.166430829

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	H162	-3.484517730	-6.287245132	5.055842748
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	H165	-5.924822590	-1.383842584	7.646430251
	H166	-0.432408278	-3.284595956	3.621879326
	H167	-0.682290256	-2.167627035	2.262724854
	H168	0.957373109	-2.462164421	2.854107587
	H169	-1.276095133	-1.177471104	4.529132801
	H170	-3.354615006	-4.703712622	9.385657503
	H171	-1.879393234	2.040956692	5.318672105
	H172	-1.447432737	-0.260357987	9.205634232
	H173	-1.726238148	3.173880626	9.528689304
	H174	0.828113902	0.168173438	2.792173750
	H175	0.139535059	0.998108750	4.210298358
	H176	9.312541894	1.998185224	4.472196859
	H177	-2.829245120	3.392889356	5.957432731
	H178	-2.702813815	4.062233860	8.336382477
	H179	-1.063192248	3.556306866	5.794518543
	H180	-0.928035453	4.208641600	8.320384995
	H181	-2.518545618	1.642409233	7.718546679
	H182	0.461280075	2.203866378	7.278388816
	H183	-1.276246338	0.050794716	6.401499019
	H184	-0.917426790	0.464515871	2.903471307
	H185	1.561101351	4.236646493	0.228655102
	H186	0.733492751	4.507430762	1.786980139
	H187	2.666558887	5.313045516	2.319196989
	H188	3.217217054	4.678781572	4.855461806
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	H191	6.510512299	1.578649611	5.572308882
	H192	-0.771170625	-2.638856574	6.344790442
	H193	0.231661262	-5.637685459	6.439052459
	H194	0.835663768	-5.056713503	8.005112804
	H195	-1.848560609	-4.508250865	6.832790798
	H196	-2.849577185	-3.126010073	10.039375379
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	H198	1.683855535	-1.591921924	5.062639143
	H199	-0.751754752	0.709084533	11.733617375
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	H201	1.651468145	-0.728257035	10.477886153
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	H203	-1.749835429	-5.982549847	-4.125553733
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	H205	-2.270733769	-6.237649566	-8.482617310
	H206	-0.801567062	-5.343425290	-8.952110000
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	H208	-3.090991687	1.046560673	-9.727011484
	H209	-3.344959060	-4.237600428	-9.708045690
	H210	-3.343108463	-2.191802481	-2.298785192
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	H212	-2.273656333	-1.027684420	-8.425372420
	H213	-5.120092067	-0.322715414	-8.715210573
	H214	-1.034163264	-2.406936097	-9.570571353
	H215	-1.317232513	-5.845965176	-2.424186134
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	H218	-6.737076782	-3.456591338	-2.856274125
	H219	-3.465005790	-2.415857855	-0.537092312
	H220	0.829854346	-5.290825491	-7.584383546
	H221	-2.313347646	-4.335448903	-1.039479925
	H222	-3.830297516	2.609660152	3.081242035
	H223	-3.065309306	0.520786359	1.356254550
	H224	-8.133248876	0.779074518	3.803793622
	H225	-7.262045333	-0.072136579	1.075780395
	H226	-6.928899541	4.082769163	2.370528143
	H227	-8.331179459	8.747203500	4.413922397
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	H232	-3.246562961	4.253494581	1.302911938
	H233	-4.802927023	3.992337358	0.502471260
	H234	-9.835874532	10.452604186	3.255770146
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	H237	-7.011179437	-0.550755692	3.513848919
	H238	-9.864429929	1.924741129	-0.218077459
	H239	-2.259435496	1.493060715	-2.703870555
	H240	-10.211497188	0.186817660	-0.148730788

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	H244	-0.713052195	5.487830385	0.269314188
	H245	1.732548381	8.069911713	0.303577037
	H246	-3.434947356	3.551930008	-1.608497230
	H247	-5.109868073	4.160761718	-2.784943112
	H248	-6.705878158	3.397591432	-4.168901096
	H249	-4.796881636	5.412743211	-1.850904529
	H250	-5.529436686	1.254427739	-4.074138422
	H251	-7.310622039	1.280587674	-3.877076800
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	H254	-0.907850720	10.187083437	-3.325508918
	H255	-2.584434456	9.640688067	-3.300472659
	H256	-3.694637782	9.198549832	-6.039741663
	H257	-2.649381327	4.849855905	-5.745438711
	H258	-7.283596254	8.678231841	-0.550880858
	H259	-3.095934768	8.563104649	2.127878072
	H260	-4.690696978	7.775879864	-2.960599187
	H261	1.067516327	5.389970817	-3.896800817
	H262	2.343586420	7.203942784	-3.227858333
	H263	-1.391906486	4.893908433	-3.350663003
	H264	-8.368337631	-0.212225758	-1.485673477
	H265	3.644855059	10.014433402	-4.142665428
	H266	-6.096953690	-0.953692704	-3.068924829
	H267	0.531991209	6.372197965	-5.255845302
	H268	-3.392362639	6.983410178	0.264870208
	H269	3.341520011	10.315707544	-2.417880737
	H270	-2.953388336	7.764824972	-6.672652142
	H271	-5.109981241	8.945522398	-4.166876785
	H272	-5.172093438	-3.520338366	-3.441003319
	H273	-5.755193093	-3.330611322	-0.793720817
	H274	-6.929913173	10.349027370	1.244120471
	H275	-5.253736625	1.390836047	-1.603378174
	H276	-0.485382702	8.032812368	-3.701129263
	H277	-1.742168942	6.343099222	-6.001901119
	H278	-0.676224091	4.209961717	-4.803765541
	H279	-3.600249656	5.875773912	-3.675264055
	H280	0.802399986	8.918248648	2.935854101
	H281	-0.465682053	9.762226949	0.099855600
	H282	-0.088165750	12.627380717	0.387679607
	H283	2.271609390	9.439075742	2.075538448
	H284	-2.443762202	10.654201505	1.735981425
	H285	4.605560586	-3.024180127	-9.153971164
	H286	4.591161753	-4.483251936	-8.144082037
	H287	7.882640206	-5.190455558	-5.098624584
	H288	5.045311712	-5.095727642	-10.410866992
	H289	3.509296548	-5.581796909	-10.117482731
	H290	5.501365289	4.781190453	-0.948564062
	H291	5.723855113	7.427799613	0.538850514
	H292	4.821633261	8.091126978	-3.593633604
	H293	4.125061204	5.612702255	-0.157923406
	H294	6.810857541	8.051944848	-0.512777619
	H295	5.400401313	2.849006942	-6.771451570
	H296	5.979094644	6.766543937	-2.308776580
	H297	5.310291743	-7.013432231	4.986644429
	H298	7.057270390	-7.886891631	2.620648120
	H299	3.644164803	1.398523599	-6.788625518
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product **Fe6-NH-NH-a** (S=1/2) Fe(139) 2.461 Fe(140) -1.040 Fe(141) 1.764 Fe(142) -2.305 Fe(143) 2.402 Fe(144) -2.171 Fe(145) -0.246	bm526n2nto6nhnha147ta.car_5 C1 -7.720508147 -5.349580030 1.283776640 C2 -8.064739808 -6.509010019 0.340976115 C3 -8.617737589 -3.461151739 2.576094190 C4 -7.986555031 -3.729263148 3.940446197 C5 -7.572345691 -5.334918996 5.739455727 C6 -6.045776840 -5.448642064 5.683220244 C7 -4.062225459 -5.760825909 4.295762420 C8 -3.519132116 -4.329732372 4.330877604 C9 -3.918529422 -1.993344568 3.698106593 C10 -3.927633799 -1.385956285 5.108732143 C11 -4.957817594 -1.240505116 7.284971142 C12 -3.878085202 -1.807408108 8.219272975 C13 -2.867953442 -3.837533405 9.154077539 C14 -1.391871947 -4.100942930 8.823305343 C15 0.264189267 -4.706657763 7.101061555 C16 0.989926333 -3.573809022 6.369524412 C17 0.653165868 -1.308176969 5.382962003 C18 0.778626071 -0.100955328 6.327329848 C19 -0.250243788 -1.084620826 4.154501854 C20 0.021499162 0.279631281 3.510428407 C21 -0.112445610 -2.265286638 3.185004163 C22 -0.386530518 1.611334129 7.648928091 C23 -0.028638240 1.258755022 9.103373695 C24 -1.724275640 2.377565977 7.517159603 C25 -1.802832582 3.538206685 8.514632413 C26 -1.911728783 2.892618961 6.083569102 C27 -0.430472909 -0.130648378 11.046906086 C28 1.034325723 -0.403799646 11.324616876 C29 5.878889587 -11.623684319 3.693440642 C30 6.518810584 -10.345441515 3.164107263 C31 6.819531494 -7.933926448 3.686933625 C32 8.047378776 -7.546609206 4.530851294 C33 5.647787698 -6.971307095 3.937825349 C34 5.988731458 -5.531269635 3.566021211 C35 4.751656642 -4.639288962 3.527967559 C36 4.882709144 -2.134281513 3.507190270 C37 10.286983407 -6.548942047 4.466426293 C38 10.467471395 -5.047664217 4.462579916 C39 -5.320432397 -2.666375633 -1.585838181 C40 -5.691469802 -1.234195441 -1.155174530 C41 -3.783831294 -2.810117511 -1.519131563 C42 -3.233949149 -4.247283308 -1.628641520 C43 -2.967689963 -4.748182351 -3.048457094 C44 -6.174135213 1.003749545 -2.064902726 C45 -7.260066732 1.466832089 -1.083249000 C46 -6.349244150 1.611699897 -3.462120831 C47 -9.414907424 0.961186395 -0.032598678 C48 -9.016029974 0.967761433 1.446074393 C49 -7.316409155 0.421519495 3.123840869 C50 -6.134564158 1.367045425 3.342195957 C51 -4.601129415 3.036380550 2.422564879 C52 -5.029617602 4.353533363 3.114303692 C53 -4.006223593 3.452756337 1.068739850 C54 -3.381656587 2.382700395 0.233215551 C55 -2.882738351 1.128781847 0.487043539 C56 -2.515504128 1.568905596 -1.660632518 C57 -6.827871680 6.038207089 3.247753125 C58 -6.713199723 6.204670027 4.761678001 C59 -8.309547018 6.097494670 2.806391580 C60 -8.924440979 7.461276160 2.683328965 C61 -8.864105240 8.562090205 3.515850902 C62 -10.157077171 8.987975621 1.767433075 C63 9.248778574 1.659280473 3.408735630 C64 10.295916603 0.574045721 3.237740771 C65 7.864153137 0.992963621 3.210863698 C66 6.716095750 1.953012904 3.416106585 C67 6.135508542 2.138652249 4.683269893 C68 6.204674012 2.704855620 2.342075314

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	H152	-8.744517295	-5.632814685	3.959789198
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	H240	-10.209643174	0.216759479	-0.172187907
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