

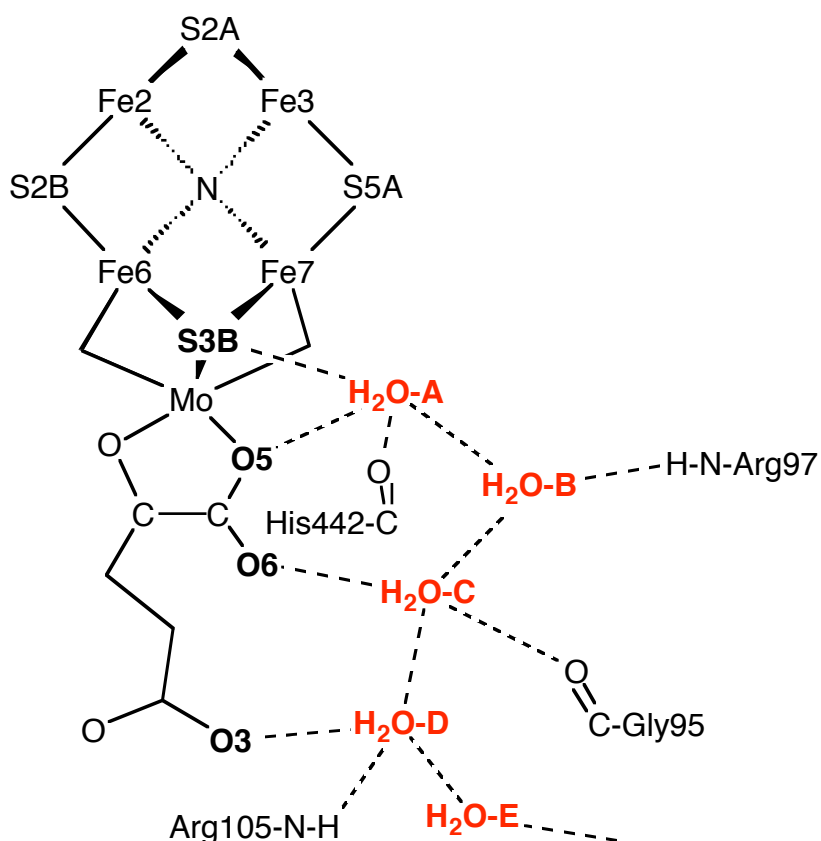
## The chemical mechanism of nitrogenase: calculated details of the intramolecular mechanism for hydrogenation of $\eta^2\text{-N}_2$ on FeMo-co to $\text{NH}_3$ .

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### Electronic Supplementary Information

Details of the penultimate five water molecules in the water chain leading to S3B.



Arranged in order of decreasing diffraction resolution. Distances Å, angles °.

PDB code resolution (Å)	FeMo-co ID	H <sub>2</sub> O-A, distance from S3B	H <sub>2</sub> O-B, distance from previous H <sub>2</sub> O, angle	H <sub>2</sub> O-C, distance from previous H <sub>2</sub> O, angle	H <sub>2</sub> O-D, distance from previous H <sub>2</sub> O, angle	H <sub>2</sub> O-E distance from previous H <sub>2</sub> O, angle
1M1N 1.16Å	CFN6496	HOH679 4.01	HOH15 2.88 94	HOH259 2.84 144	HOH24 2.84 103	HOH50 2.82

1M1N	CFN7496	HOH381 4.04	HOH363 2.85 93	HOH533 2.86 144	HOH86 2.83 104	HOH53 2.80
1M1N	CFN8496	HOH3220 4.01	HOH2552 2.88 94	HOH2796 2.84 144	HOH2561 2.84 103	HOH2587 2.81
1M1N	CFN9496	HOH2920 4.04	HOH2901 2.82 93	HOH3073 2.86 143	HOH2623 2.83 105	HOH2590 2.78
1GQU 1.60Å	CFM503 chain A	HOH10 4.05	HOH12 2.83 95	HOH9 2.86 141	HOH609 2.86 106	HOH7 2.79
1GQU	CFM503 chain C	HOH1396 4.05	HOH1410 2.87 99	HOH1393 2.78 140	HOH1963 2.85 105	HOH1376 2.84
1QH1 1.60Å	CFM503 chain A	HOH13 4.02	HOH12 2.90 93	HOH2 2.85 140	HOH584 2.88 107	HOH3 2.79
1QH1	CFM503 chain C	HOH1335 4.06	HOH1339 2.87 98	HOH1344 2.79 138	HOH1865 2.90 105	HOH1311 2.83
1QH8 1.60	CFM503 chain A	HOH13 3.98	HOH10 2.87 94	HOH7 2.83 140	HOH616 2.88 106	HOH2 2.80
1QH8	CFM503 chain C	HOH1436 4.01	HOH1432 2.82 98	HOH1431 2.92 138	HOH2033 2.86 105	HOH1410 2.80
1H1L 1.90	CFM1480 chain A	HOH310 3.81	HOH68 3.05 92	HOH312 2.75 142	HOH108 2.61 110	HOH294 2.85
1H1L	CFM1480 chain B	HOH282 3.78	HOH70 3.13 96	HOH68 2.72 140	HOH284 2.81 102	HOH264 3.02
2MIN 2.03	CFM496 chain A	HOH47 4.21	HOH32 2.59 101	HOH31 2.70 149	HOH39 2.71 103	HOH64 2.69
2MIN	CFM496 chain C	HOH368 4.23	HOH340 2.67 101	HOH347 3.12 143	HOH373 2.53 98	HOH336 2.62
3MIN	CFM496	HOH47	HOH32	HOH31	HOH39	HOH64

2.03	chain A	4.27	2.63 105	2.69 145	2.68 99	2.60
3MIN	CFM496 chain C	HOH368 4.12	HOH340 2.57 98	HOH347 2.70 146	HOH373 2.54 108	HOH336 2.76
2AFH 2.10	CFN2496	HOH99 4.05	HOH265 2.87 89	HOH309 2.92 146	HOH1456 2.83 107	HOH341 2.70
2AFH	CFN3496	HOH259 3.99	HOH96 2.84 97	HOH1074 2.75 146	HOH314 2.85 102	HOH1491 2.77
1G20 2.20	CFM1496	HOH24 4.16	HOH35 3.06 94	HOH98 2.84 151	HOH144 2.77 100	HOH39 2.82
1G20	CFM3496	HOH1059 3.76	HOH607 3.28	misplaced	HOH778	missing
1M34 2.30	CFM2096	HOH4 4.10	HOH284 2.91 90	HOH330 2.90 153	HOH94 2.95 113	HOH507 2.91
1M34	CFM2296	HOH103 4.23	HOH715 2.99 94	HOH1187 2.99 140	HOH1025 3.01 92	HOH262 2.81
1M34	CFM4096	HOH76 4.30	HOH172 2.95 98	HOH357 2.81 141	HOH54 2.95 106	HOH847 2.90
1M34	CFM4296	HOH53 4.05	HOH374 2.93 87	HOH219 2.96 154	HOH418 3.05 97	HOH517 3.07
2AFK 2.30	CFN496 chain A	HOH67 3.98	HOH497 3.10 95	HOH521 2.70 135	HOH98 3.33 H-bonded (2.93) to O6 of HCA instead of O3	
2AFK	CFN496 chain C	HOH232 4.42	HOH42 2.91 90	HOH562 2.86 138	HOH102 2.86 106	HOH503 2.41

Cartesian coordinates for all intermediate structures and intermediates

Structure/file	Cartesian coordinates Å							
Fig 2 (a)								
<b>1H-a</b> s3b5s3b3tgvd _1a.cmmf	40							
	C1	1.441367897	8.171447479	0.850446657	dmol	1	C	0.000
	H2	2.345407106	7.767365869	0.375081793	dmol	1	H	0.000
	H3	1.479507358	9.273647533	0.826482014	dmol	1	H	0.000
	H4	1.414696105	7.838484307	1.896821206	dmol	1	H	0.000
	S5	-0.093273551	7.588024376	-0.050678863	dmol	1	S	0.000
	C6	0.762296305	-3.455722607	-2.678456171	dmol	1	C	0.000
	H7	1.707927605	-2.930435348	-2.623103862	dmol	1	H	0.000
	N8	-0.190796514	-3.277563154	-1.691711400	dmol	1	N	0.000
	C9	0.286185140	-4.330044309	-3.629313558	dmol	1	C	0.000
	H10	0.717475748	-4.725406849	-4.541032220	dmol	1	H	0.000
	C11	-1.235786322	-4.022037618	-2.017920017	dmol	1	C	0.000
	H12	-2.129862659	-4.105182543	-1.411742797	dmol	1	H	0.000
	N13	-0.994311356	-4.687531245	-3.195218444	dmol	1	N	0.000
	H14	-1.645911166	-5.296662995	-3.675454679	dmol	1	H	0.000
	C15	-0.994638838	-4.621702562	1.619991135	dmol	1	C	0.000
	H16	-1.432292170	-5.601779720	1.330093596	dmol	1	H	0.000
	H17	-1.222147768	-4.483924790	2.703190200	dmol	1	H	0.000
	C18	0.546859746	-4.748048968	1.516376988	dmol	1	C	0.000
	O19	1.127968504	-5.789851198	1.904908438	dmol	1	O	0.000
	O20	1.128481088	-3.692163017	1.019206620	dmol	1	O	0.000
	O21	-1.524279819	-3.578129732	0.846427687	dmol	1	O	0.000
	Fe22	-0.100007843	5.333066772	0.298985890	dmol	1	Fe	0.000
	Fe23	-1.529211270	3.070198019	1.152218039	dmol	1	Fe	0.000
	Fe24	1.176325660	2.987324317	1.297497527	dmol	1	Fe	0.000
	Fe25	-0.063411077	3.031027391	-1.155140184	dmol	1	Fe	0.000
	Fe26	-0.108264629	0.424698733	-1.134485671	dmol	1	Fe	0.000
	Fe27	-1.550254522	0.485252208	1.027948057	dmol	1	Fe	0.000
	Fe28	1.116140044	0.305774862	1.271808073	dmol	1	Fe	0.000
	Mo29	-0.189773299	-2.010504104	0.342586033	dmol	1	Mo	0.000
	S30	-1.919445209	4.387271188	-0.713701525	dmol	1	S	0.000
	S31	-0.207435507	4.522140074	2.413987906	dmol	1	S	0.000
	S32	-0.022349504	1.707334734	-2.970184788	dmol	1	S	0.000
	S33	1.769086333	4.329972502	-0.516703197	dmol	1	S	0.000
	S34	-2.041417666	-0.818050806	-0.682116358	dmol	1	S	0.000
	S35	-3.078529512	1.692656720	2.056454825	dmol	1	S	0.000
	S36	-0.001623923	-1.202276046	2.718054411	dmol	1	S	0.000
	S37	1.747469230	-0.873937684	-0.614004462	dmol	1	S	0.000
	S38	2.582109267	1.620417838	2.373237934	dmol	1	S	0.000
	N39	-0.154536757	1.704715822	0.399187924	dmol	1	N	0.000
	H40	1.080257193	-1.989865450	3.059975243	dmol	1	H	0.000
<b>1H-ab</b> s3b5s3b3thz02 _1_3932.02a.c mmf	40							
	C1	1.401966193	8.122604015	0.963253239	dmol	1	C	0.000
	H2	2.248706035	7.692026288	0.413191631	dmol	1	H	0.000
	H3	1.477954181	9.223586715	0.941181088	dmol	1	H	0.000
	H4	1.455723070	7.783569188	2.007470188	dmol	1	H	0.000
	S5	-0.210884402	7.584323906	0.175171817	dmol	1	S	0.000
	C6	0.803237785	-3.529386346	-2.649976010	dmol	1	C	0.000
	H7	1.771334213	-3.054352815	-2.556535391	dmol	1	H	0.000
	N8	-0.173038753	-3.313150316	-1.691530229	dmol	1	N	0.000
	C9	0.313926148	-4.361770068	-3.630777460	dmol	1	C	0.000
	H10	0.753632459	-4.759877609	-4.537736307	dmol	1	H	0.000
	C11	-1.244937747	-3.997671643	-2.065951851	dmol	1	C	0.000
	H12	-2.168300762	-4.042054517	-1.502707612	dmol	1	H	0.000
	N13	-0.997609337	-4.656910141	-3.245851504	dmol	1	N	0.000
	H14	-1.663113452	-5.218420638	-3.764314358	dmol	1	H	0.000
	C15	-1.002192583	-4.651733692	1.625672051	dmol	1	C	0.000
	H16	-1.485575946	-5.613630934	1.347671392	dmol	1	H	0.000
	H17	-1.199711190	-4.513608109	2.714374007	dmol	1	H	0.000
	C18	0.528520072	-4.832245254	1.481396768	dmol	1	C	0.000
	O19	1.083297401	-5.892455212	1.853023335	dmol	1	O	0.000
	O20	1.136322410	-3.795358255	0.970400333	dmol	1	O	0.000
	O21	-1.509394958	-3.583146754	0.875009054	dmol	1	O	0.000
	Fe22	-0.143198959	5.299901101	0.315697447	dmol	1	Fe	0.000
	Fe23	-1.450574724	2.998671688	1.130299261	dmol	1	Fe	0.000
	Fe24	1.247699118	3.020831525	1.124464221	dmol	1	Fe	0.000
	Fe25	-0.107479695	2.991302326	-1.222231644	dmol	1	Fe	0.000
	Fe26	-0.065174039	0.366855445	-1.167584955	dmol	1	Fe	0.000

	Fe27	-1.459358264	0.377337351	1.176319420	dmol	1	Fe	0.000
	Fe28	1.329916163	0.384555920	1.117601440	dmol	1	Fe	0.000
	Mo29	-0.118361036	-2.075830059	0.340431759	dmol	1	Mo	0.000
	S30	-1.942705724	4.340924286	-0.694050445	dmol	1	S	0.000
	S31	-0.114739544	4.434536733	2.404403166	dmol	1	S	0.000
	S32	-0.071674795	1.636092045	-3.007146625	dmol	1	S	0.000
	S33	1.669151466	4.396276628	-0.697521837	dmol	1	S	0.000
	S34	-1.983214000	-0.862170857	-0.639917639	dmol	1	S	0.000
	S35	-3.025533705	1.674153495	2.060825110	dmol	1	S	0.000
	S36	-0.038132371	-0.818586479	2.556466773	dmol	1	S	0.000
	S37	1.805075298	-0.946431658	-0.686418493	dmol	1	S	0.000
	S38	2.877738262	1.729546856	1.985513786	dmol	1	S	0.000
	N39	-0.079640443	1.682149200	0.351552860	dmol	1	N	0.000
	H40	0.350346156	-1.220453352	3.828862215	dmol	1	H	0.000
<b>1H-b</b> s3b5s3b3tevd_ 1a.cmmf	40							
	C1	1.416863429	8.147306415	0.839003887	dmol	1	C	0.000
	H2	2.285730264	7.766849551	0.284067709	dmol	1	H	0.000
	H3	1.424491091	9.250635729	0.810023214	dmol	1	H	0.000
	H4	1.494538722	7.815564028	1.883369035	dmol	1	H	0.000
	S5	-0.178610579	7.514548329	0.088448433	dmol	1	S	0.000
	C6	0.724602284	-3.479319726	-2.713966175	dmol	1	C	0.000
	H7	1.683386348	-2.976236099	-2.685884442	dmol	1	H	0.000
	N8	-0.195804536	-3.283501907	-1.700081797	dmol	1	N	0.000
	C9	0.202886650	-4.340895306	-3.652427425	dmol	1	C	0.000
	H10	0.599948380	-4.745443414	-4.575416506	dmol	1	H	0.000
	C11	-1.265718249	-4.005696211	-1.996871013	dmol	1	C	0.000
	H12	-2.144555318	-4.072070568	-1.366794202	dmol	1	H	0.000
	N13	-1.072335881	-4.671444832	-3.182626108	dmol	1	N	0.000
	H14	-1.746681383	-5.273866070	-3.639284187	dmol	1	H	0.000
	C15	-0.871996362	-4.643810718	1.620728919	dmol	1	C	0.000
	H16	-1.358957146	-5.610356139	1.370716173	dmol	1	H	0.000
	H17	-1.009130126	-4.495575607	2.716814828	dmol	1	H	0.000
	C18	0.651380637	-4.806910412	1.399286594	dmol	1	C	0.000
	O19	1.229665640	-5.875141165	1.712756279	dmol	1	O	0.000
	O20	1.227569633	-3.751876696	0.892493345	dmol	1	O	0.000
	O21	-1.439015609	-3.587087425	0.890633223	dmol	1	O	0.000
	Fe22	-0.056049224	5.247999327	0.327612192	dmol	1	Fe	0.000
	Fe23	-1.327877825	2.983348966	1.298094013	dmol	1	Fe	0.000
	Fe24	1.317114875	2.977781837	1.194042383	dmol	1	Fe	0.000
	Fe25	-0.083815093	2.890732026	-1.109551761	dmol	1	Fe	0.000
	Fe26	-0.093063187	0.333026971	-1.134347960	dmol	1	Fe	0.000
	Fe27	-1.381078800	0.370366393	1.248878223	dmol	1	Fe	0.000
	Fe28	1.298204313	0.330366728	1.207769165	dmol	1	Fe	0.000
	Mo29	-0.096722757	-2.039205989	0.332432214	dmol	1	Mo	0.000
	S30	-1.851851451	4.222635699	-0.639357309	dmol	1	S	0.000
	S31	0.031894422	4.460774426	2.470210129	dmol	1	S	0.000
	S32	-0.141595282	1.675010747	-2.939219122	dmol	1	S	0.000
	S33	1.696021233	4.250712381	-0.742534203	dmol	1	S	0.000
	S34	-2.004540388	-0.834367528	-0.551559223	dmol	1	S	0.000
	S35	-2.813663952	1.644531656	2.377507323	dmol	1	S	0.000
	S36	0.203838174	-1.207707780	2.711723072	dmol	1	S	0.000
	S37	1.811648170	-0.899112866	-0.663497042	dmol	1	S	0.000
	S38	2.871385692	1.648784234	2.118159309	dmol	1	S	0.000
	N39	-0.034036061	1.675589021	0.437254110	dmol	1	N	0.000
	H40	-1.004070748	-0.606937913	3.061404775	dmol	1	H	0.000
<b>1H-bc</b> s3b2fe6ta9_1_ 3939.97a.cmmf	40							
	C1	1.559009719	8.017849133	0.973269332	dmol	1	C	0.000
	H2	2.380264025	7.579002888	0.389723996	dmol	1	H	0.000
	H3	1.668655493	9.117298339	0.986964295	dmol	1	H	0.000
	H4	1.621276635	7.638297088	2.004028150	dmol	1	H	0.000
	S5	-0.089849024	7.561630299	0.200783159	dmol	1	S	0.000
	C6	0.897912246	-3.613820509	-2.610829196	dmol	1	C	0.000
	H7	1.895643427	-3.211831792	-2.481870177	dmol	1	H	0.000
	N8	-0.086532631	-3.357079033	-1.674293287	dmol	1	N	0.000
	C9	0.381635924	-4.391862844	-3.623429168	dmol	1	C	0.000
	H10	0.814571640	-4.797127976	-4.530274165	dmol	1	H	0.000
	C11	-1.189616095	-3.957525705	-2.090724996	dmol	1	C	0.000
	H12	-2.131558249	-3.940169224	-1.557489435	dmol	1	H	0.000
	N13	-0.957131478	-4.607428765	-3.277827642	dmol	1	N	0.000
	H14	-1.657687877	-5.074798410	-3.841101946	dmol	1	H	0.000
	C15	-0.847128994	-4.587093026	1.727927480	dmol	1	C	0.000
	H16	-1.292830919	-5.586086254	1.533217382	dmol	1	H	0.000
	H17	-1.029821171	-4.360962016	2.805512976	dmol	1	H	0.000
	C18	0.689673752	-4.709949863	1.570489982	dmol	1	C	0.000
	O19	1.294744597	-5.725357518	1.986929527	dmol	1	O	0.000
	O20	1.243007216	-3.674232804	0.997319049	dmol	1	O	0.000
	O21	-1.418079223	-3.607638230	0.899649477	dmol	1	O	0.000

	Fe22	-0.094549511	5.274407726	0.326881570	dmol	1	Fe	0.000
	Fe23	-1.445644815	2.958427842	1.129709020	dmol	1	Fe	0.000
	Fe24	1.275105815	2.974998062	1.161647033	dmol	1	Fe	0.000
	Fe25	-0.074018397	2.997845526	-1.191029928	dmol	1	Fe	0.000
	Fe26	-0.115696715	0.395712009	-1.154953033	dmol	1	Fe	0.000
	Fe27	-1.583031612	0.250350267	1.246801274	dmol	1	Fe	0.000
	Fe28	1.168019284	0.344257785	1.187014265	dmol	1	Fe	0.000
	Mo29	-0.115081203	-2.035979514	0.322666369	dmol	1	Mo	0.000
	S30	-1.937635954	4.331077805	-0.659577141	dmol	1	S	0.000
	S31	-0.096033798	4.393984718	2.409246750	dmol	1	S	0.000
	S32	-0.099101355	1.653593822	-2.996041670	dmol	1	S	0.000
	S33	1.745033776	4.351683996	-0.648248168	dmol	1	S	0.000
	S34	-2.014209885	-0.905626751	-0.659533771	dmol	1	S	0.000
	S35	-3.043465566	1.681786984	2.083202407	dmol	1	S	0.000
	S36	-0.085836301	-1.068372921	2.603952452	dmol	1	S	0.000
	S37	1.767197572	-0.870439440	-0.657853027	dmol	1	S	0.000
	S38	2.739884074	1.596635544	2.164986818	dmol	1	S	0.000
	N39	-0.072641670	1.691417332	0.371205961	dmol	1	N	0.000
	H40	-1.664452756	-0.726874571	2.580348024	dmol	1	H	0.000
<b>1H-c</b>	40							
fe6hs2btb3vd_ 1a.cmmf	C1	1.599205953	8.020739594	1.010438934	dmol	1	C	0.000
	H2	2.449689538	7.593546899	0.464049916	dmol	1	H	0.000
	H3	1.690999848	9.118848854	1.032097529	dmol	1	H	0.000
	H4	1.617933297	7.636645916	2.039202059	dmol	1	H	0.000
	S5	-0.009305054	7.555719181	0.169180289	dmol	1	S	0.000
	C6	0.912882371	-3.717756544	-2.576929362	dmol	1	C	0.000
	H7	1.922807856	-3.369335286	-2.399206446	dmol	1	H	0.000
	N8	-0.102062367	-3.404726978	-1.691225028	dmol	1	N	0.000
	C9	0.411121677	-4.471695402	-3.615380590	dmol	1	C	0.000
	H10	0.867522081	-4.900662934	-4.499672141	dmol	1	H	0.000
	C11	-1.208576301	-3.952966046	-2.162112634	dmol	1	C	0.000
	H12	-2.177852475	-3.891654470	-1.683778100	dmol	1	H	0.000
	N13	-0.951542345	-4.621347080	-3.336947320	dmol	1	N	0.000
	H14	-1.641989404	-5.061970206	-3.934179122	dmol	1	H	0.000
	C15	-0.893460524	-4.564673731	1.734468152	dmol	1	C	0.000
	H16	-1.361697903	-5.549712011	1.532985601	dmol	1	H	0.000
	H17	-1.067339012	-4.338376620	2.811710265	dmol	1	H	0.000
	C18	0.638210949	-4.709905625	1.564107553	dmol	1	C	0.000
	O19	1.229580500	-5.752549245	1.931390719	dmol	1	O	0.000
	O20	1.203744019	-3.661051312	1.034247646	dmol	1	O	0.000
	O21	-1.445803045	-3.567283997	0.913058460	dmol	1	O	0.000
	Fe22	0.014915684	5.283607642	0.371177605	dmol	1	Fe	0.000
	Fe23	-1.375563222	2.966627748	1.177564657	dmol	1	Fe	0.000
	Fe24	1.391668833	2.971981573	1.219838351	dmol	1	Fe	0.000
	Fe25	0.037488332	3.026697185	-1.122419345	dmol	1	Fe	0.000
	Fe26	-0.113876563	0.439787523	-1.112746932	dmol	1	Fe	0.000
	Fe27	-1.597388364	0.161261047	1.329345696	dmol	1	Fe	0.000
	Fe28	1.214900087	0.339463038	1.208880153	dmol	1	Fe	0.000
	Mo29	-0.150106903	-2.005582859	0.392511749	dmol	1	Mo	0.000
	S30	-1.834477487	4.357173118	-0.609163681	dmol	1	S	0.000
	S31	-0.009600406	4.396348398	2.449079058	dmol	1	S	0.000
	S32	-0.057529618	1.713146128	-2.952744731	dmol	1	S	0.000
	S33	1.878277479	4.363479625	-0.575831746	dmol	1	S	0.000
	S34	-1.999450421	-0.827377985	-0.671849746	dmol	1	S	0.000
	S35	-2.992410342	1.729803114	2.090856000	dmol	1	S	0.000
	S36	-0.077737838	-0.983884316	2.574882804	dmol	1	S	0.000
	S37	1.739299100	-0.883518876	-0.666552775	dmol	1	S	0.000
	S38	2.830960083	1.552382623	2.179922508	dmol	1	S	0.000
	N39	0.011267294	1.755131171	0.377483603	dmol	1	N	0.000
H40	-2.594705387	-0.746358953	2.002715232	dmol	1	H	0.000	
<b>1H-cd</b>	40							
fe6hs2btb9_1_ 3943.47a.cmmf	C1	1.612726843	7.961806746	1.078176851	dmol	1	C	0.000
	H2	2.444446958	7.535538668	0.499991549	dmol	1	H	0.000
	H3	1.728436750	9.058893169	1.124317337	dmol	1	H	0.000
	H4	1.652755001	7.552818969	2.097983488	dmol	1	H	0.000
	S5	-0.022720582	7.541843746	0.263842198	dmol	1	S	0.000
	C6	0.939331191	-3.740670835	-2.574238559	dmol	1	C	0.000
	H7	1.954656980	-3.414685895	-2.383649995	dmol	1	H	0.000
	N8	-0.074284577	-3.415690334	-1.692126268	dmol	1	N	0.000
	C9	0.426037792	-4.463234339	-3.629199456	dmol	1	C	0.000
	H10	0.878463625	-4.889637864	-4.516651148	dmol	1	H	0.000
	C11	-1.191662621	-3.923478267	-2.181803258	dmol	1	C	0.000
	H12	-2.163865680	-3.834220415	-1.714355026	dmol	1	H	0.000
	N13	-0.942727573	-4.579868599	-3.364467071	dmol	1	N	0.000
	H14	-1.640758331	-4.985779462	-3.976764742	dmol	1	H	0.000
	C15	-0.894282102	-4.566879380	1.748854299	dmol	1	C	0.000
	H16	-1.368678196	-5.553089854	1.562657320	dmol	1	H	0.000

	H17	-1.074997081	-4.319887044	2.821424964	dmol	1	H	0.000
	C18	0.636653786	-4.730406257	1.596080332	dmol	1	C	0.000
	O19	1.216995674	-5.763479639	2.004152536	dmol	1	O	0.000
	O20	1.217904997	-3.705427083	1.033509837	dmol	1	O	0.000
	O21	-1.432863652	-3.580912631	0.906775616	dmol	1	O	0.000
	Fe22	-0.104147623	5.263434093	0.375821628	dmol	1	Fe	0.000
	Fe23	-1.395794735	2.921606747	1.124823407	dmol	1	Fe	0.000
	Fe24	1.328033254	2.963565734	1.152866389	dmol	1	Fe	0.000
	Fe25	-0.041134853	2.958773183	-1.175841278	dmol	1	Fe	0.000
	Fe26	-0.060322725	0.352769207	-1.164707784	dmol	1	Fe	0.000
	Fe27	-1.441438682	0.228072443	1.235501485	dmol	1	Fe	0.000
	Fe28	1.268544357	0.314754248	1.170712245	dmol	1	Fe	0.000
	Mo29	-0.103251787	-2.033348420	0.392475868	dmol	1	Mo	0.000
	S30	-1.915854609	4.276377556	-0.646256825	dmol	1	S	0.000
	S31	-0.056279813	4.353572987	2.430635581	dmol	1	S	0.000
	S32	-0.054442497	1.618725746	-3.001709902	dmol	1	S	0.000
	S33	1.727191208	4.384033032	-0.650139342	dmol	1	S	0.000
	S34	-1.956181999	-0.890758471	-0.680957811	dmol	1	S	0.000
	S35	-3.015659951	1.662117100	2.151983268	dmol	1	S	0.000
	S36	-0.037420501	-0.992433654	2.556638841	dmol	1	S	0.000
	S37	1.805080464	-0.930346500	-0.684014587	dmol	1	S	0.000
	S38	2.840011655	1.632254941	2.108416578	dmol	1	S	0.000
	N39	-0.015464611	1.679984907	0.349971666	dmol	1	N	0.000
	H40	-2.673035756	0.053291719	2.249269772	dmol	1	H	0.000
<b>1H-d</b> fe6hs2bta4vd_ 1a.cmmf	40							
	C1	1.546046230	8.008697409	1.003880932	dmol	1	C	0.000
	H2	2.358817397	7.561835865	0.415425346	dmol	1	H	0.000
	H3	1.629287929	9.108584810	0.966798443	dmol	1	H	0.000
	H4	1.647063961	7.676040863	2.046690434	dmol	1	H	0.000
	S5	-0.110363420	7.489160134	0.303962678	dmol	1	S	0.000
	C6	0.947378468	-3.753054926	-2.674543064	dmol	1	C	0.000
	H7	1.951924450	-3.373654727	-2.530840270	dmol	1	H	0.000
	N8	-0.045373662	-3.458811091	-1.759179743	dmol	1	N	0.000
	C9	0.431618881	-4.532179798	-3.687425751	dmol	1	C	0.000
	H10	0.869341622	-4.956770962	-4.583245296	dmol	1	H	0.000
	C11	-1.152186386	-4.042925501	-2.183811515	dmol	1	C	0.000
	H12	-2.101620026	-4.003456026	-1.664664421	dmol	1	H	0.000
	N13	-0.916237130	-4.716582111	-3.359516090	dmol	1	N	0.000
	H14	-1.614862068	-5.180197253	-3.928772573	dmol	1	H	0.000
	C15	-0.922167444	-4.562499426	1.665640551	dmol	1	C	0.000
	H16	-1.404155500	-5.547858372	1.493619219	dmol	1	H	0.000
	H17	-1.112824098	-4.290391871	2.730820029	dmol	1	H	0.000
	C18	0.611144027	-4.746907644	1.540549298	dmol	1	C	0.000
	O19	1.167427711	-5.793118272	1.955510200	dmol	1	O	0.000
	O20	1.214450838	-3.728207900	0.996404143	dmol	1	O	0.000
	O21	-1.435227752	-3.590170952	0.789789908	dmol	1	O	0.000
	Fe22	-0.147024852	5.222667680	0.487147036	dmol	1	Fe	0.000
	Fe23	-1.393832254	2.863763673	1.112758526	dmol	1	Fe	0.000
	Fe24	1.288472928	2.858767579	1.300336705	dmol	1	Fe	0.000
	Fe25	0.038498030	2.987040951	-1.130386491	dmol	1	Fe	0.000
	Fe26	0.025056594	0.368192586	-1.236061209	dmol	1	Fe	0.000
	Fe27	-1.347221616	0.248864925	1.038991599	dmol	1	Fe	0.000
	Fe28	1.306190075	0.197959944	1.176739646	dmol	1	Fe	0.000
	Mo29	-0.095512146	-2.049636785	0.276262809	dmol	1	Mo	0.000
	S30	-1.882970689	4.243187051	-0.638471994	dmol	1	S	0.000
	S31	-0.177175742	4.251924765	2.532077564	dmol	1	S	0.000
	S32	0.154757944	1.757344741	-3.000971151	dmol	1	S	0.000
	S33	1.770752819	4.371342745	-0.406030802	dmol	1	S	0.000
S34	-1.919312778	-0.856751010	-0.855719503	dmol	1	S	0.000	
S35	-3.045024855	1.448040507	2.077905153	dmol	1	S	0.000	
S36	-0.159235129	-1.039257455	2.473546943	dmol	1	S	0.000	
S37	1.854823322	-0.972567809	-0.726487989	dmol	1	S	0.000	
S38	2.803066769	1.509154330	2.233255620	dmol	1	S	0.000	
N39	-0.018136919	1.593894668	0.376187129	dmol	1	N	0.000	
H40	-2.615655530	1.428534665	3.371827953	dmol	1	H	0.000	
Fig 2 (b)								
<b>2H-a</b> s2bhs3bh5te9_ 5a.cmmf	41							
	C1	1.441287229	8.188923932	0.894661725	dmol	1	C	0.000
	H2	2.312053456	7.805705509	0.345171856	dmol	1	H	0.000
	H3	1.483413021	9.290496269	0.910511430	dmol	1	H	0.000
	H4	1.490078581	7.816444489	1.927207514	dmol	1	H	0.000
	S5	-0.146149352	7.654807230	0.062178868	dmol	1	S	0.000
	C6	0.878601076	-3.715965345	-2.643161941	dmol	1	C	0.000
	H7	1.869306066	-3.285055851	-2.564081629	dmol	1	H	0.000
	N8	-0.085679552	-3.421246581	-1.696605658	dmol	1	N	0.000

	C9	0.350814601	-4.559337831	-3.595521493	dmol	1	C	0.000
	H10	0.768062433	-5.010921082	-4.487441672	dmol	1	H	0.000
	C11	-1.189456819	-4.064700275	-2.048077597	dmol	1	C	0.000
	H12	-2.112305193	-4.039496425	-1.482764273	dmol	1	H	0.000
	N13	-0.973472676	-4.779651506	-3.201213746	dmol	1	N	0.000
	H14	-1.672680743	-5.311571978	-3.705397332	dmol	1	H	0.000
	C15	-0.933752555	-4.581548849	1.656461031	dmol	1	C	0.000
	H16	-1.364309247	-5.571083947	1.389162472	dmol	1	H	0.000
	H17	-1.188949084	-4.405530145	2.728321033	dmol	1	H	0.000
	C18	0.610597548	-4.713414716	1.604163672	dmol	1	C	0.000
	O19	1.175350498	-5.736624029	2.063062220	dmol	1	O	0.000
	O20	1.213113237	-3.685023602	1.076028772	dmol	1	O	0.000
	O21	-1.445805341	-3.565021241	0.836143242	dmol	1	O	0.000
	Fe22	0.004376309	5.303064610	0.245076185	dmol	1	Fe	0.000
	Fe23	-1.432810008	3.057586837	0.884186289	dmol	1	Fe	0.000
	Fe24	1.289121507	2.914357247	0.971092563	dmol	1	Fe	0.000
	Fe25	-0.031742411	2.960269111	-1.439288939	dmol	1	Fe	0.000
	Fe26	0.003751536	0.295584876	-1.368425441	dmol	1	Fe	0.000
	Fe27	-1.487109730	0.465962567	0.752490227	dmol	1	Fe	0.000
	Fe28	1.176586035	0.345697675	1.033469038	dmol	1	Fe	0.000
	Mo29	-0.086719943	-2.057794835	0.246775455	dmol	1	Mo	0.000
	S30	-1.849793104	4.364780472	-0.913833332	dmol	1	S	0.000
	S31	-0.078017712	4.315683600	2.307314421	dmol	1	S	0.000
	S32	0.080065865	1.587831870	-3.216170641	dmol	1	S	0.000
	S33	1.849691495	4.254252616	-0.816916162	dmol	1	S	0.000
	S34	-1.941792286	-0.917430894	-0.958530522	dmol	1	S	0.000
	S35	-3.087890017	1.677093004	1.993327061	dmol	1	S	0.000
	S36	-0.024082273	-1.065749577	2.597517524	dmol	1	S	0.000
	S37	1.865894846	-0.967537859	-0.723894978	dmol	1	S	0.000
	S38	2.828149051	1.580784859	1.927833585	dmol	1	S	0.000
	N39	-0.116647504	1.710604590	0.116834976	dmol	1	N	0.000
	H40	1.105040999	-1.698638206	3.049784781	dmol	1	H	0.000
	H41	-2.546190132	1.563413412	3.242549412	dmol	1	H	0.000
<b>2H-ab</b> s2bhs3bh5tc12 9_1a.cmmf	41							
	C1	1.419087685	8.133631525	0.885401665	dmol	1	C	0.000
	H2	2.271496413	7.755122268	0.303796738	dmol	1	H	0.000
	H3	1.456263723	9.235378954	0.903861971	dmol	1	H	0.000
	H4	1.508560277	7.755181038	1.913340448	dmol	1	H	0.000
	S5	-0.198133935	7.603927287	0.110298527	dmol	1	S	0.000
	C6	0.892934846	-3.752771328	-2.635719077	dmol	1	C	0.000
	H7	1.896860391	-3.355767273	-2.546586650	dmol	1	H	0.000
	N8	-0.069432192	-3.425454714	-1.696687447	dmol	1	N	0.000
	C9	0.344923848	-4.574009523	-3.595252678	dmol	1	C	0.000
	H10	0.892934846	-5.033901772	-4.486106202	dmol	1	H	0.000
	C11	-1.191253192	-4.030881502	-2.059407095	dmol	1	C	0.000
	H12	-2.121862406	-3.969914576	-1.509552300	dmol	1	H	0.000
	N13	-0.990003737	-4.749373117	-3.214318959	dmol	1	N	0.000
	H14	-1.702734167	-5.251288249	-3.730538672	dmol	1	H	0.000
	C15	-0.901198001	-4.536043360	1.657870256	dmol	1	C	0.000
	H16	-1.364251712	-5.507585619	1.376706938	dmol	1	H	0.000
	H17	-1.118395759	-4.398970150	2.744842454	dmol	1	H	0.000
	C18	0.635044190	-4.707850974	1.551888530	dmol	1	C	0.000
	O19	1.185325120	-5.755534111	1.970755573	dmol	1	O	0.000
	O20	1.248567630	-3.685949290	1.024293663	dmol	1	O	0.000
	O21	-1.415649297	-3.481596254	0.891034432	dmol	1	O	0.000
	Fe22	-0.040814271	5.252579499	0.261171128	dmol	1	Fe	0.000
	Fe23	-1.372618531	2.936671849	0.895099836	dmol	1	Fe	0.000
	Fe24	1.339075060	2.926050184	0.963248306	dmol	1	Fe	0.000
	Fe25	-0.042717613	2.947440888	-1.408840248	dmol	1	Fe	0.000
	Fe26	0.074296516	0.320503729	-1.314659191	dmol	1	Fe	0.000
	Fe27	-1.366534248	0.394820245	0.912752999	dmol	1	Fe	0.000
	Fe28	1.533922081	0.316249257	0.963293092	dmol	1	Fe	0.000
	Mo29	-0.016341821	-2.017208804	0.221143037	dmol	1	Mo	0.000
	S30	-1.897317294	4.273475510	-0.851629728	dmol	1	S	0.000
	S31	-0.078040408	4.239533319	2.306719115	dmol	1	S	0.000
	S32	0.090755223	1.578092364	-3.174009464	dmol	1	S	0.000
	S33	1.802526071	4.281352850	-0.834676875	dmol	1	S	0.000
	S34	-1.879312733	-0.874172567	-0.872016168	dmol	1	S	0.000
	S35	-3.097162207	1.669068152	1.910889339	dmol	1	S	0.000
	S36	0.015968141	-0.804143090	2.438240530	dmol	1	S	0.000
	S37	1.942013272	-1.026202847	-0.836164501	dmol	1	S	0.000
	S38	3.081505654	1.746195431	1.785199877	dmol	1	S	0.000
	N39	-0.007394918	1.727843653	0.197298937	dmol	1	N	0.000
	H40	0.116648987	-1.851266497	3.346657869	dmol	1	H	0.000
	H41	-2.740298242	1.696767614	3.230359995	dmol	1	H	0.000

<b>2H-b</b> s2bhs3bh5tdd 129_3a.cmmf	41						
	C1	1.556467818	8.097438596	1.022531912	dmol	1	C 0.000
	H2	2.402091251	7.696118736	0.448177897	dmol	1	H 0.000
	H3	1.634095121	9.196902511	1.051891699	dmol	1	H 0.000
	H4	1.617983016	7.709747792	2.048366102	dmol	1	H 0.000
	S5	-0.063527127	7.613895219	0.220796922	dmol	1	S 0.000
	C6	0.856156577	-3.711164942	-2.700919604	dmol	1	C 0.000
	H7	1.863391115	-3.325311685	-2.603718705	dmol	1	H 0.000
	N8	-0.106128254	-3.385700945	-1.761733450	dmol	1	N 0.000
	C9	0.303152305	-4.518640774	-3.669192995	dmol	1	C 0.000
	H10	0.712363683	-4.976717297	-4.561100866	dmol	1	H 0.000
	C11	-1.234543185	-3.974248229	-2.135192243	dmol	1	C 0.000
	H12	-2.164304182	-3.911401387	-1.585037677	dmol	1	H 0.000
	N13	-1.035253566	-4.681993047	-3.295807599	dmol	1	N 0.000
	H14	-1.747189118	-5.191244108	-3.804694568	dmol	1	H 0.000
	C15	-0.948782998	-4.626736237	1.583426212	dmol	1	C 0.000
	H16	-1.455800797	-5.580160874	1.325756781	dmol	1	H 0.000
	H17	-1.143427603	-4.452519318	2.666825342	dmol	1	H 0.000
	C18	0.577287031	-4.849482567	1.450105104	dmol	1	C 0.000
	O19	1.096948850	-5.923443971	1.840760287	dmol	1	O 0.000
	O20	1.215157789	-3.839360370	0.929317963	dmol	1	O 0.000
	O21	-1.438569458	-3.567415957	0.803465241	dmol	1	O 0.000
	Fe22	0.063148555	5.262235560	0.345689107	dmol	1	Fe 0.000
	Fe23	-1.331721846	2.992185374	0.958245675	dmol	1	Fe 0.000
	Fe24	1.396997511	2.863157139	0.997678307	dmol	1	Fe 0.000
	Fe25	0.025835208	2.932915130	-1.381027992	dmol	1	Fe 0.000
	Fe26	0.075341807	0.273133250	-1.330990164	dmol	1	Fe 0.000
	Fe27	-1.318225559	0.408798956	0.888367177	dmol	1	Fe 0.000
	Fe28	1.363963879	0.283485098	1.014717198	dmol	1	Fe 0.000
	Mo29	-0.023135183	-2.122832478	0.197070689	dmol	1	Mo 0.000
	S30	-1.798808968	4.322840791	-0.807487024	dmol	1	S 0.000
	S31	0.034365318	4.235435108	2.383668229	dmol	1	S 0.000
	S32	0.136752030	1.572655348	-3.171135260	dmol	1	S 0.000
	S33	1.894644598	4.238091928	-0.774422115	dmol	1	S 0.000
	S34	-1.890091681	-0.885113564	-0.871020585	dmol	1	S 0.000
	S35	-2.938646686	1.637089192	2.135893532	dmol	1	S 0.000
	S36	0.219513442	-1.162175202	2.583373659	dmol	1	S 0.000
	S37	1.940232189	-1.039330475	-0.778725594	dmol	1	S 0.000
	S38	3.007400765	1.559614956	1.879483870	dmol	1	S 0.000
	N39	-0.008429412	1.681651409	0.170156009	dmol	1	N 0.000
	H40	-0.955290543	-0.516655299	2.907033342	dmol	1	H 0.000
H41	-2.391413217	1.664256633	3.385738183	dmol	1	H 0.000	
<b>2H-bc</b> s2bhs3bh3tffb 129_1_3985.0 0a.cmmf	41						
	C1	1.421130263	8.028063497	0.877104929	dmol	1	C 0.000
	H2	2.211227035	7.608176893	0.240010423	dmol	1	H 0.000
	H3	1.497724561	9.127721682	0.877459379	dmol	1	H 0.000
	H4	1.569835743	7.654866294	1.900659345	dmol	1	H 0.000
	S5	-0.261743942	7.541682473	0.216038890	dmol	1	S 0.000
	C6	0.919260466	-3.784549254	-2.587153922	dmol	1	C 0.000
	H7	1.926761838	-3.418491567	-2.433962126	dmol	1	H 0.000
	N8	-0.087674194	-3.431257329	-1.708051329	dmol	1	N 0.000
	C9	0.405324244	-4.583915423	-3.583162350	dmol	1	C 0.000
	H10	0.852923544	-5.051461130	-4.451590924	dmol	1	H 0.000
	C11	-1.202085921	-4.000281812	-2.139168718	dmol	1	C 0.000
	H12	-2.164850900	-3.913788313	-1.652217316	dmol	1	H 0.000
	N13	-0.954827473	-4.718938534	-3.284261132	dmol	1	N 0.000
	H14	-1.650083410	-5.195551052	-3.846184876	dmol	1	H 0.000
	C15	-0.856975923	-4.575912214	1.692420767	dmol	1	C 0.000
	H16	-1.351322125	-5.549910765	1.488602111	dmol	1	H 0.000
	H17	-1.017609249	-4.363245041	2.776249387	dmol	1	H 0.000
	C18	0.669920403	-4.770846086	1.518657175	dmol	1	C 0.000
	O19	1.225186709	-5.825956399	1.909423524	dmol	1	O 0.000
	O20	1.273475397	-3.754542531	0.966721919	dmol	1	O 0.000
	O21	-1.392717026	-3.556017956	0.890752090	dmol	1	O 0.000
	Fe22	-0.024315559	5.202458544	0.288082383	dmol	1	Fe 0.000
	Fe23	-1.247842525	2.919659354	0.984694332	dmol	1	Fe 0.000
	Fe24	1.384379107	2.914753028	1.025086028	dmol	1	Fe 0.000
	Fe25	0.030407157	2.935923287	-1.400218721	dmol	1	Fe 0.000
	Fe26	0.004514966	0.266071095	-1.290529793	dmol	1	Fe 0.000
	Fe27	-1.229228466	0.268663618	1.066799274	dmol	1	Fe 0.000
	Fe28	1.445694542	0.346297579	0.956013631	dmol	1	Fe 0.000
	Mo29	-0.026121600	-2.066937838	0.263714025	dmol	1	Mo 0.000
	S30	-1.859395101	4.190851767	-0.781105269	dmol	1	S 0.000
	S31	0.023595340	4.209419340	2.394354027	dmol	1	S 0.000
	S32	0.017858634	1.520600996	-3.153490538	dmol	1	S 0.000
	S33	1.869400347	4.249601577	-0.780465498	dmol	1	S 0.000
	S34	-1.922262641	-0.904454011	-0.721206225	dmol	1	S 0.000
S35	-3.017001227	1.571232433	1.787336300	dmol	1	S 0.000	

	S36	0.250078850	-1.025642307	2.500350606	dmol	1	S	0.000
	S37	1.896925888	-1.003679187	-0.836629626	dmol	1	S	0.000
	S38	3.026272623	1.639948534	1.878871457	dmol	1	S	0.000
	N39	0.015634779	1.602334312	0.267750860	dmol	1	N	0.000
	H40	-0.839901829	-0.039161206	2.750990381	dmol	1	H	0.000
	H41	-2.831573326	1.736213790	3.131255117	dmol	1	H	0.000
<b>2H-c</b> s2bhs3bh3tg3 12as_1a.cmmf	41							
	C1	1.573225883	8.046132635	0.828406511	dmol	1	C	0.000
	H2	2.406174580	7.640089684	0.236699463	dmol	1	H	0.000
	H3	1.637166893	9.148301487	0.827515010	dmol	1	H	0.000
	H4	1.668372608	7.685713234	1.862140664	dmol	1	H	0.000
	S5	-0.062430588	7.510088582	0.097041614	dmol	1	S	0.000
	C6	0.832566145	-3.814155625	-2.683069513	dmol	1	C	0.000
	H7	1.847984593	-3.453297504	-2.572505548	dmol	1	H	0.000
	N8	-0.135648114	-3.448055377	-1.767717658	dmol	1	N	0.000
	C9	0.279409395	-4.628220688	-3.646744928	dmol	1	C	0.000
	H10	0.692513605	-5.116993372	-4.521323894	dmol	1	H	0.000
	C11	-1.265863639	-4.019531019	-2.145984418	dmol	1	C	0.000
	H12	-2.206709398	-3.931480101	-1.617168343	dmol	1	H	0.000
	N13	-1.068440664	-4.755396177	-3.291632119	dmol	1	N	0.000
	H14	-1.782774549	-5.253447146	-3.810249486	dmol	1	H	0.000
	C15	-0.867967490	-4.584478335	1.657510051	dmol	1	C	0.000
	H16	-1.405832946	-5.539566877	1.476967328	dmol	1	H	0.000
	H17	-0.967392283	-4.366018215	2.747416711	dmol	1	H	0.000
	C18	0.639270610	-4.833718294	1.406967022	dmol	1	C	0.000
	O19	1.179064094	-5.907359805	1.765445792	dmol	1	O	0.000
	O20	1.250586772	-3.837787487	0.823962928	dmol	1	O	0.000
	O21	-1.403810189	-3.546279178	0.878869092	dmol	1	O	0.000
	Fe22	0.067344335	5.169604422	0.358203157	dmol	1	Fe	0.000
	Fe23	-1.258983303	2.873007605	1.059674465	dmol	1	Fe	0.000
	Fe24	1.377699377	2.844764330	1.121736677	dmol	1	Fe	0.000
	Fe25	0.095080689	2.899171288	-1.306979587	dmol	1	Fe	0.000
	Fe26	0.084493751	0.267611582	-1.239117457	dmol	1	Fe	0.000
	Fe27	-1.174246921	0.255913861	1.386090978	dmol	1	Fe	0.000
	Fe28	1.423312965	0.280195306	1.015794268	dmol	1	Fe	0.000
Mo29	-0.004807912	-2.064758915	0.298489908	dmol	1	Mo	0.000	
S30	-1.776898446	4.204693883	-0.716019039	dmol	1	S	0.000	
S31	0.041428976	4.186320404	2.457131205	dmol	1	S	0.000	
S32	0.108987902	1.526799304	-3.085981917	dmol	1	S	0.000	
S33	1.935776870	4.170789047	-0.656238907	dmol	1	S	0.000	
S34	-1.844010861	-0.826964969	-0.627826139	dmol	1	S	0.000	
S35	-3.157616424	1.484332084	1.674237153	dmol	1	S	0.000	
S36	0.236093584	-1.110317600	2.464163719	dmol	1	S	0.000	
S37	1.935655282	-1.029176373	-0.812111749	dmol	1	S	0.000	
S38	2.958256522	1.549114672	2.025297203	dmol	1	S	0.000	
N39	0.093948197	1.565975660	0.331676045	dmol	1	N	0.000	
H40	-0.896125243	0.983501508	2.696527803	dmol	1	H	0.000	
H41	-3.084854660	1.774882478	3.002705932	dmol	1	H	0.000	
<b>2H-cd</b> s2hfeha9_2a.c mmf	41							
	C1	1.247907479	7.934020038	0.928662258	dmol	1	C	0.000
	H2	2.080026304	7.564384770	0.312459447	dmol	1	H	0.000
	H3	1.258847429	9.038862771	0.934155903	dmol	1	H	0.000
	H4	1.388758026	7.568691573	1.956416552	dmol	1	H	0.000
	S5	-0.382710401	7.318508390	0.240787885	dmol	1	S	0.000
	C6	1.080576366	-3.687413578	-2.652977891	dmol	1	C	0.000
	H7	2.070323821	-3.276797436	-2.494173267	dmol	1	H	0.000
	N8	0.062471017	-3.406986337	-1.762103255	dmol	1	N	0.000
	C9	0.602673142	-4.488221178	-3.665686548	dmol	1	C	0.000
	H10	1.071239911	-4.917369042	-4.542828732	dmol	1	H	0.000
	C11	-1.025158873	-4.012352388	-2.205887720	dmol	1	C	0.000
	H12	-1.989181484	-3.981269417	-1.712966346	dmol	1	H	0.000
	N13	-0.749028523	-4.692830678	-3.368534953	dmol	1	N	0.000
	H14	-1.418102747	-5.205045199	-3.930702331	dmol	1	H	0.000
	C15	-0.785790474	-4.585643542	1.653798042	dmol	1	C	0.000
	H16	-1.283142716	-5.563022832	1.491717676	dmol	1	H	0.000
	H17	-0.937568507	-4.321457587	2.726093403	dmol	1	H	0.000
	C18	0.738454144	-4.780609375	1.474541059	dmol	1	C	0.000
	O19	1.301555996	-5.832807384	1.859950336	dmol	1	O	0.000
	O20	1.337198790	-3.761565778	0.921923833	dmol	1	O	0.000
	O21	-1.325403127	-3.601759378	0.809479071	dmol	1	O	0.000
	Fe22	-0.148896612	5.063338834	0.418395743	dmol	1	Fe	0.000
	Fe23	-1.332686040	2.589341969	1.187304321	dmol	1	Fe	0.000
	Fe24	1.496445858	2.882255383	1.129071024	dmol	1	Fe	0.000
	Fe25	0.148854433	2.940704256	-1.242771780	dmol	1	Fe	0.000
	Fe26	0.100279762	0.340427238	-1.185204450	dmol	1	Fe	0.000
	Fe27	-1.379463030	0.180334429	1.219275696	dmol	1	Fe	0.000
	Fe28	1.436894721	0.277961057	1.127089452	dmol	1	Fe	0.000

	Mo29	0.020978908	-2.057722952	0.299252300	dmol	1	Mo	0.000
	S30	-1.838902159	3.986343801	-0.623929413	dmol	1	S	0.000
	S31	-0.072433258	4.088418825	2.449969845	dmol	1	S	0.000
	S32	0.142180093	1.600808092	-3.044842950	dmol	1	S	0.000
	S33	1.813903878	4.436931549	-0.557628593	dmol	1	S	0.000
	S34	-1.809346664	-0.897569477	-0.762832904	dmol	1	S	0.000
	S35	-3.463599155	1.365796505	1.396973743	dmol	1	S	0.000
	S36	0.058323049	-1.053127438	2.471076089	dmol	1	S	0.000
	S37	1.956573498	-0.968121867	-0.727869317	dmol	1	S	0.000
	S38	3.025979807	1.544154411	2.074969646	dmol	1	S	0.000
	N39	0.182375269	1.673898697	0.263638170	dmol	1	N	0.000
	H40	-3.529651816	1.380551203	2.758814854	dmol	1	H	0.000
	H41	-1.151755887	1.315959068	2.375124106	dmol	1	H	0.000
<b>2H-d</b>	41							
nrsvfehbshb9_ 2a.cmmf	C1	1.311857527	8.006659464	1.032666414	dmol	1	C	0.000
	H2	2.117635360	7.632309033	0.387432340	dmol	1	H	0.000
	H3	1.334322063	9.109317049	1.035353391	dmol	1	H	0.000
	H4	1.480140941	7.641052568	2.053970008	dmol	1	H	0.000
	S5	-0.344670707	7.420994589	0.378586198	dmol	1	S	0.000
	C6	1.183014968	-3.778692060	-2.620638060	dmol	1	C	0.000
	H7	2.174529215	-3.426128678	-2.363374130	dmol	1	H	0.000
	N8	0.104222075	-3.464803982	-1.815273472	dmol	1	N	0.000
	C9	0.757379155	-4.527435662	-3.694703946	dmol	1	C	0.000
	H10	1.278573831	-4.958012189	-4.540780941	dmol	1	H	0.000
	C11	-0.966938572	-4.005242678	-2.368621123	dmol	1	C	0.000
	H12	-1.969107263	-3.936791994	-1.964770352	dmol	1	H	0.000
	N13	-0.623518472	-4.671381321	-3.521667881	dmol	1	N	0.000
	H14	-1.266829592	-5.117027563	-4.164888003	dmol	1	H	0.000
	C15	-0.845771752	-4.715718460	1.541348190	dmol	1	C	0.000
	H16	-1.310170538	-5.701513749	1.330610878	dmol	1	H	0.000
	H17	-1.028221441	-4.503374707	2.621219907	dmol	1	H	0.000
	C18	0.685831905	-4.865679623	1.397999931	dmol	1	C	0.000
	O19	1.271563503	-5.908722015	1.770594455	dmol	1	O	0.000
	O20	1.274955257	-3.816630621	0.885778920	dmol	1	O	0.000
	O21	-1.389490351	-3.711316027	0.724407567	dmol	1	O	0.000
	Fe22	-0.202817234	5.144465971	0.332609157	dmol	1	Fe	0.000
	Fe23	-1.260129450	2.778975380	1.421599119	dmol	1	Fe	0.000
	Fe24	1.359057676	2.838919800	1.161490902	dmol	1	Fe	0.000
	Fe25	-0.054475402	2.867254712	-1.173248987	dmol	1	Fe	0.000
	Fe26	0.049982564	0.236676442	-1.201781897	dmol	1	Fe	0.000
	Fe27	-1.407942290	0.228640283	1.055411550	dmol	1	Fe	0.000
	Fe28	1.292474412	0.182879257	1.193135913	dmol	1	Fe	0.000
	Mo29	-0.038004441	-2.134628515	0.270512413	dmol	1	Mo	0.000
	S30	-1.941951164	4.056499672	-0.613799133	dmol	1	S	0.000
	S31	0.037272846	4.338036963	2.414894693	dmol	1	S	0.000
	S32	0.118984736	1.559223618	-2.994679991	dmol	1	S	0.000
	S33	1.680830926	4.315890247	-0.644880448	dmol	1	S	0.000
	S34	-1.859884341	-0.985728326	-0.857348601	dmol	1	S	0.000
	S35	-3.317497516	1.623736115	1.578365116	dmol	1	S	0.000
	S36	-0.148269363	-1.128800446	2.461752633	dmol	1	S	0.000
S37	1.913550638	-1.020482591	-0.667255193	dmol	1	S	0.000	
S38	2.904570417	1.489097036	2.063442979	dmol	1	S	0.000	
N39	-0.030299861	1.547246377	0.427016978	dmol	1	N	0.000	
H40	-1.025293478	2.105488219	2.780294776	dmol	1	H	0.000	
H41	-3.299466784	1.254748410	2.887217726	dmol	1	H	0.000	
<b>2H-de</b>	41							
s2bfe2henextc 94s_2a.cmmf	C1	1.553538967	8.060530579	1.293021977	dmol	1	C	0.000
	H2	2.443910148	7.656887973	0.791500380	dmol	1	H	0.000
	H3	1.580947902	9.162421596	1.243668917	dmol	1	H	0.000
	H4	1.571411958	7.749524296	2.346776725	dmol	1	H	0.000
	S5	-0.004445589	7.453069143	0.446243538	dmol	1	S	0.000
	C6	0.894507601	-3.535914672	-3.032056315	dmol	1	C	0.000
	H7	1.758523478	-2.882715869	-3.069078853	dmol	1	H	0.000
	N8	0.059745347	-3.520610908	-1.930113247	dmol	1	N	0.000
	C9	0.424859219	-4.441712203	-3.957728155	dmol	1	C	0.000
	H10	0.781429624	-4.742725710	-4.935935182	dmol	1	H	0.000
	C11	-0.908484925	-4.391853174	-2.160081276	dmol	1	C	0.000
	H12	-1.706882540	-4.592355234	-1.451739043	dmol	1	H	0.000
	N13	-0.730703424	-4.986117545	-3.387749243	dmol	1	N	0.000
	H14	-1.346248940	-5.670610749	-3.811274045	dmol	1	H	0.000
	C15	-0.812871908	-4.725690509	1.473535638	dmol	1	C	0.000
	H16	-1.264543044	-5.724438220	1.287587021	dmol	1	H	0.000
	H17	-1.010682074	-4.485210594	2.545163788	dmol	1	H	0.000
	C18	0.723182651	-4.868106527	1.342934046	dmol	1	C	0.000
	O19	1.309603983	-5.898984338	1.749720812	dmol	1	O	0.000
	O20	1.304290349	-3.831899012	0.798589064	dmol	1	O	0.000
	O21	-1.356661582	-3.751509719	0.619797198	dmol	1	O	0.000

	Fe22	0.031209014	5.177341263	0.434727854	dmol	1	Fe	0.000
	Fe23	-1.317344703	2.909958199	1.537220123	dmol	1	Fe	0.000
	Fe24	1.407828560	2.773791419	1.210449443	dmol	1	Fe	0.000
	Fe25	-0.052917239	2.932362406	-1.102813129	dmol	1	Fe	0.000
	Fe26	0.068901420	0.300208496	-1.237560103	dmol	1	Fe	0.000
	Fe27	-1.370599932	0.194372315	0.958844072	dmol	1	Fe	0.000
	Fe28	1.286997165	0.132477058	1.119888479	dmol	1	Fe	0.000
	Mo29	-0.007959303	-2.153119902	0.153950316	dmol	1	Mo	0.000
	S30	-1.835958445	4.218213621	-0.443924806	dmol	1	S	0.000
	S31	0.210245194	4.316200169	2.509233685	dmol	1	S	0.000
	S32	0.022017955	1.688359206	-2.980151272	dmol	1	S	0.000
	S33	1.818413701	4.229409330	-0.581835559	dmol	1	S	0.000
	S34	-1.807339852	-0.988899316	-0.972041170	dmol	1	S	0.000
	S35	-3.271323465	1.549586136	1.387001077	dmol	1	S	0.000
	S36	-0.158054962	-1.183928957	2.359195843	dmol	1	S	0.000
	S37	1.929593939	-1.010207936	-0.775918084	dmol	1	S	0.000
	S38	2.897807938	1.351174003	2.092728915	dmol	1	S	0.000
	N39	-0.006677200	1.524109195	0.396897142	dmol	1	N	0.000
	H40	-1.700365215	2.808608802	3.039323163	dmol	1	H	0.000
	H41	-3.408901771	1.198005888	2.692000264	dmol	1	H	0.000
<b>2H-e</b> s2bfe2henextd 9_3a.cmmf	41							
	C1	1.422084191	8.014866980	1.213248800	dmol	1	C	0.000
	H2	2.331940083	7.632637440	0.731445170	dmol	1	H	0.000
	H3	1.457802323	9.116227955	1.227318684	dmol	1	H	0.000
	H4	1.390365870	7.645443911	2.246543301	dmol	1	H	0.000
	S5	-0.106272668	7.476388654	0.281671299	dmol	1	S	0.000
	C6	1.049621899	-3.658139876	-2.838292919	dmol	1	C	0.000
	H7	1.959160660	-3.069419843	-2.814292574	dmol	1	H	0.000
	N8	0.140566980	-3.572081396	-1.799956943	dmol	1	N	0.000
	C9	0.582408032	-4.534058830	-3.792451343	dmol	1	C	0.000
	H10	0.986374934	-4.868920389	-4.740683474	dmol	1	H	0.000
	C11	-0.868784926	-4.373165717	-2.095987521	dmol	1	C	0.000
	H12	-1.726721367	-4.518028412	-1.447362581	dmol	1	H	0.000
	N13	-0.647132075	-4.990662244	-3.305093704	dmol	1	N	0.000
	H14	-1.288322773	-5.616035611	-3.779817394	dmol	1	H	0.000
	C15	-0.825843270	-4.712036933	1.588057705	dmol	1	C	0.000
	H16	-1.271698988	-5.707297162	1.376044377	dmol	1	H	0.000
	H17	-1.058258846	-4.485255402	2.654847285	dmol	1	H	0.000
	C18	0.713236505	-4.858887357	1.508850651	dmol	1	C	0.000
	O19	1.284586422	-5.879988019	1.958731350	dmol	1	O	0.000
	O20	1.315960648	-3.836822002	0.959742688	dmol	1	O	0.000
	O21	-1.341634675	-3.729829958	0.731177125	dmol	1	O	0.000
	Fe22	0.026931224	5.125889987	0.342229178	dmol	1	Fe	0.000
	Fe23	-1.486982428	2.964398051	1.348609988	dmol	1	Fe	0.000
	Fe24	1.405707573	2.816117304	1.087063405	dmol	1	Fe	0.000
	Fe25	-0.019801070	2.836683911	-1.223376667	dmol	1	Fe	0.000
	Fe26	0.113658460	0.200502030	-1.250124684	dmol	1	Fe	0.000
	Fe27	-1.308947188	0.221534008	0.986570319	dmol	1	Fe	0.000
	Fe28	1.362367791	0.169576238	1.072096666	dmol	1	Fe	0.000
	Mo29	0.043000519	-2.168988761	0.240579054	dmol	1	Mo	0.000
	S30	-1.831567961	4.115209966	-0.605774110	dmol	1	S	0.000
	S31	0.122056860	4.166323073	2.445586610	dmol	1	S	0.000
	S32	0.060380505	1.530596109	-3.057965010	dmol	1	S	0.000
	S33	1.818281007	4.207382473	-0.750509371	dmol	1	S	0.000
	S34	-1.782286084	-1.041420000	-0.888895382	dmol	1	S	0.000
	S35	-3.258944722	1.429671516	1.475384037	dmol	1	S	0.000
	S36	-0.063854878	-1.098379581	2.410784149	dmol	1	S	0.000
	S37	1.975661589	-1.090086550	-0.750938563	dmol	1	S	0.000
	S38	2.983229178	1.462317624	1.938292414	dmol	1	S	0.000
	N39	0.061745396	1.476225649	0.296122905	dmol	1	N	0.000
	H40	-2.427659241	3.832882746	2.185946165	dmol	1	H	0.000
	H41	-3.292415492	1.368628417	2.834578916	dmol	1	H	0.000
<b>Fig 3</b>								
<b>3H-c + N<sub>2</sub></b> fe6n2en13hvct a_2a.cmmf	44							
	C1	1.623569261	7.951495890	1.400876280	dmol	1	C	0.000
	H2	2.614398956	7.639682225	1.042074234	dmol	1	H	0.000
	H3	1.630050224	9.038598637	1.578466425	dmol	1	H	0.000
	H4	1.418154915	7.432828779	2.347328178	dmol	1	H	0.000
	S5	0.306991309	7.578236486	0.123692183	dmol	1	S	0.000
	C6	1.312181801	-3.664295685	-2.962536240	dmol	1	C	0.000
	H7	2.308498172	-3.294006463	-2.755691922	dmol	1	H	0.000
	N8	0.279295214	-3.410171307	-2.082854291	dmol	1	N	0.000
	C9	0.841173084	-4.392069110	-4.033048497	dmol	1	C	0.000
	H10	1.322171425	-4.790033715	-4.917842778	dmol	1	H	0.000
	C11	-0.811530229	-3.960859736	-2.588986050	dmol	1	C	0.000

	H12	-1.791221285	-3.917272253	-2.131238607	dmol	1	H	0.000
	N13	-0.522079282	-4.579877642	-3.779927430	dmol	1	N	0.000
	H14	-1.193283697	-5.031712436	-4.389538042	dmol	1	H	0.000
	C15	-0.302727879	-4.971848732	1.141119935	dmol	1	C	0.000
	H16	-0.719959983	-5.945293610	0.814009184	dmol	1	H	0.000
	H17	-0.450037307	-4.912898380	2.244960589	dmol	1	H	0.000
	C18	1.226489072	-4.987050102	0.907715957	dmol	1	C	0.000
	O19	1.888370611	-6.037223380	1.095370022	dmol	1	O	0.000
	O20	1.705051553	-3.834831678	0.532383003	dmol	1	O	0.000
	O21	-0.957271385	-3.913730972	0.487050218	dmol	1	O	0.000
	Fe22	0.303187323	5.239726920	0.206830818	dmol	1	Fe	0.000
	Fe23	-1.384855958	3.092145194	0.768469342	dmol	1	Fe	0.000
	Fe24	1.445927424	2.867409563	1.053824096	dmol	1	Fe	0.000
	Fe25	0.294725725	2.850211674	-1.379697660	dmol	1	Fe	0.000
	Fe26	0.064985130	0.252347104	-1.253870811	dmol	1	Fe	0.000
	Fe27	-1.622813251	-0.465913358	1.034456688	dmol	1	Fe	0.000
	Fe28	1.319259888	0.280307800	1.046267881	dmol	1	Fe	0.000
	Mo29	0.179735926	-2.230445191	0.046950523	dmol	1	Mo	0.000
	S30	-1.463087816	4.380134224	-1.060122943	dmol	1	S	0.000
	S31	0.019803109	4.270752335	2.240745239	dmol	1	S	0.000
	S32	0.172299426	1.484437536	-3.143583408	dmol	1	S	0.000
	S33	2.165829344	4.135449558	-0.715033404	dmol	1	S	0.000
	S34	-1.732353308	-1.201748454	-1.053217497	dmol	1	S	0.000
	S35	-3.013135123	1.398930192	0.846650089	dmol	1	S	0.000
	S36	0.072277496	-1.282971157	2.285791588	dmol	1	S	0.000
	S37	2.008483830	-0.896606083	-0.826008508	dmol	1	S	0.000
	S38	2.833721103	1.495908540	2.161939981	dmol	1	S	0.000
	N39	0.127472405	1.699523130	0.180914306	dmol	1	N	0.000
	N40	-1.939853978	0.602283026	4.068331584	dmol	1	N	0.000
	N41	-2.707654012	-0.154049256	4.338538873	dmol	1	N	0.000
	H42	-3.669600507	1.687333819	2.005417832	dmol	1	H	0.000
	H43	-2.486999306	3.890289974	1.472903597	dmol	1	H	0.000
	H44	-2.715639755	-1.393123910	1.600119444	dmol	1	H	0.000
TS: 3H-c + N <sub>2</sub> → 3HN <sub>2</sub> -a fe6n2en13hvct c_orig.cmmf	44							
	C1	1.476959	6.237320	1.141266	dmol	1	C	0.000
	H2	2.448608	5.932480	0.728317	dmol	1	H	0.000
	H3	1.497330	7.320175	1.343536	dmol	1	H	0.000
	H4	1.314835	5.699249	2.085144	dmol	1	H	0.000
	S5	0.099640	5.883484	-0.076233	dmol	1	S	0.000
	C6	1.071228	-5.363617	-3.126144	dmol	1	C	0.000
	H7	2.074493	-4.999924	-2.941040	dmol	1	H	0.000
	N8	0.051620	-5.075912	-2.239380	dmol	1	N	0.000
	C9	0.582642	-6.122086	-4.167068	dmol	1	C	0.000
	H10	1.050003	-6.548431	-5.046783	dmol	1	H	0.000
	C11	-1.046555	-5.637985	-2.712600	dmol	1	C	0.000
	H12	-2.016693	-5.597641	-2.233704	dmol	1	H	0.000
	N13	-0.778214	-6.293625	-3.891556	dmol	1	N	0.000
	H14	-1.455826	-6.768707	-4.476639	dmol	1	H	0.000
	C15	-0.423294	-6.654938	1.038666	dmol	1	C	0.000
	H16	-0.861420	-7.635651	0.759079	dmol	1	H	0.000
	H17	-0.501526	-6.575700	2.149094	dmol	1	H	0.000
	C18	1.086945	-6.692291	0.715912	dmol	1	C	0.000
	O19	1.767410	-7.725266	0.907425	dmol	1	O	0.000
	O20	1.553619	-5.556641	0.255127	dmol	1	O	0.000
	O21	-1.095444	-5.602905	0.403198	dmol	1	O	0.000
	Fe22	0.093811	3.536407	-0.011276	dmol	1	Fe	0.000
	Fe23	-1.556366	1.396317	0.608047	dmol	1	Fe	0.000
	Fe24	1.319809	1.195053	0.850571	dmol	1	Fe	0.000
	Fe25	0.068878	1.113831	-1.535294	dmol	1	Fe	0.000
	Fe26	-0.044952	-1.433075	-1.406052	dmol	1	Fe	0.000
	Fe27	-1.801727	-2.140594	1.328140	dmol	1	Fe	0.000
	Fe28	1.237473	-1.432098	0.871414	dmol	1	Fe	0.000
	Mo29	0.093704	-3.908768	-0.011261	dmol	1	Mo	0.000
	S30	-1.676910	2.643219	-1.239563	dmol	1	S	0.000
	S31	-0.120895	2.592911	2.043915	dmol	1	S	0.000
	S32	-0.035950	-0.267410	-3.309906	dmol	1	S	0.000
S33	1.939545	2.447845	-0.976166	dmol	1	S	0.000	
S34	-1.868103	-2.798355	-0.846603	dmol	1	S	0.000	
S35	-3.169525	-0.325272	0.766068	dmol	1	S	0.000	
S36	0.125687	-3.037567	2.163376	dmol	1	S	0.000	
S37	1.892456	-2.601608	-1.003220	dmol	1	S	0.000	
S38	2.745880	-0.145508	1.925858	dmol	1	S	0.000	
N39	0.000000	0.000000	0.000000	dmol	1	N	0.000	
N40	-1.810272	-1.090302	3.598267	dmol	1	N	0.000	
N41	-2.543350	-1.936493	3.711777	dmol	1	N	0.000	
H42	-3.749405	0.010254	1.951263	dmol	1	H	0.000	
H43	-2.646469	2.233047	1.290787	dmol	1	H	0.000	
H44	-2.894623	-3.166290	1.590546	dmol	1	H	0.000	

<b>3HN2-a</b> fe6n2en13hvct b_2a.cmmf	44							
	C1	1.627482369	7.977211201	1.304412617	dmol	1	C	0.000
	H2	2.606568716	7.657652087	0.921276080	dmol	1	H	0.000
	H3	1.649103614	9.065468065	1.478486737	dmol	1	H	0.000
	H4	1.441353428	7.465547757	2.258194048	dmol	1	H	0.000
	S5	0.277037058	7.588121030	0.067227600	dmol	1	S	0.000
	C6	1.218345105	-3.654106897	-2.965444281	dmol	1	C	0.000
	H7	2.218598221	-3.277969939	-2.789881081	dmol	1	H	0.000
	N8	0.204237809	-3.390514995	-2.063895649	dmol	1	N	0.000
	C9	0.729665978	-4.407155425	-4.010059716	dmol	1	C	0.000
	H10	1.192317312	-4.814883937	-4.900818363	dmol	1	H	0.000
	C11	-0.890065527	-3.963095654	-2.532653467	dmol	1	C	0.000
	H12	-1.856891560	-3.941199408	-2.045012567	dmol	1	H	0.000
	N13	-0.625131714	-4.602824240	-3.721905042	dmol	1	N	0.000
	H14	-1.303466470	-5.074102181	-4.309372649	dmol	1	H	0.000
	C15	-0.259763096	-4.958303933	1.202458068	dmol	1	C	0.000
	H16	-0.680004023	-5.933767833	0.879453476	dmol	1	H	0.000
	H17	-0.341625736	-4.934040091	2.314646464	dmol	1	H	0.000
	C18	1.250662422	-4.962141556	0.883138753	dmol	1	C	0.000
	O19	1.951247011	-5.982881666	1.060449248	dmol	1	O	0.000
	O20	1.700722121	-3.812827386	0.439797589	dmol	1	O	0.000
	O21	-0.946057492	-3.890822110	0.612511999	dmol	1	O	0.000
	Fe22	0.278293896	5.234405517	0.171300732	dmol	1	Fe	0.000
	Fe23	-1.396191451	3.082084404	0.778955324	dmol	1	Fe	0.000
	Fe24	1.494192295	2.882543396	0.994558546	dmol	1	Fe	0.000
	Fe25	0.238136131	2.820339776	-1.364148362	dmol	1	Fe	0.000
	Fe26	0.054594537	0.278137948	-1.249571008	dmol	1	Fe	0.000
	Fe27	-1.694366886	-0.438359992	1.577495377	dmol	1	Fe	0.000
	Fe28	1.365281964	0.272599139	1.035683763	dmol	1	Fe	0.000
	Mo29	0.231641054	-2.187913543	0.182620520	dmol	1	Mo	0.000
	S30	-1.491465949	4.349306195	-1.058931818	dmol	1	S	0.000
	S31	0.073788424	4.259796096	2.212766328	dmol	1	S	0.000
	S32	0.060389673	1.468979004	-3.146207300	dmol	1	S	0.000
	S33	2.113224602	4.141557070	-0.822139758	dmol	1	S	0.000
	S34	-1.742541670	-1.100066653	-0.624581380	dmol	1	S	0.000
	S35	-3.048050054	1.378105468	0.897347528	dmol	1	S	0.000
	S36	0.291901994	-1.325859355	2.355162381	dmol	1	S	0.000
	S37	2.002581663	-0.878544582	-0.856243924	dmol	1	S	0.000
	S38	2.878195962	1.535415916	2.109478177	dmol	1	S	0.000
	N39	0.148284755	1.697759651	0.164314071	dmol	1	N	0.000
	N40	-1.711891611	0.536397314	3.565996607	dmol	1	N	0.000
	N41	-2.449387502	-0.321517791	3.702082233	dmol	1	N	0.000
	H42	-3.633211852	1.763256114	2.061690404	dmol	1	H	0.000
	H43	-2.471371527	3.895383071	1.517525308	dmol	1	H	0.000
H44	-2.756363994	-1.497167048	1.711836064	dmol	1	H	0.000	
<b>4H-b + N<sub>2</sub></b> fe6n2nhx2b2h 3btfu_2a.cmmf	45							
	C1	1.857496542	7.878243975	1.018609813	dmol	1	C	0.000
	H2	2.778786733	7.518170369	0.539309995	dmol	1	H	0.000
	H3	1.927515898	8.968709372	1.166160553	dmol	1	H	0.000
	H4	1.760354446	7.390226383	1.997685564	dmol	1	H	0.000
	S5	0.367027605	7.516131651	-0.049243702	dmol	1	S	0.000
	C6	0.978418772	-3.632730618	-3.015481563	dmol	1	C	0.000
	H7	1.989311249	-3.271145277	-2.882448416	dmol	1	H	0.000
	N8	0.011865977	-3.342946040	-2.072439182	dmol	1	N	0.000
	C9	0.426981436	-4.389159147	-4.024021285	dmol	1	C	0.000
	H10	0.841807211	-4.815242995	-4.928471985	dmol	1	H	0.000
	C11	-1.117145625	-3.904408764	-2.478402443	dmol	1	C	0.000
	H12	-2.063796076	-3.845169890	-1.957217640	dmol	1	H	0.000
	N13	-0.915494222	-4.558418698	-3.668663055	dmol	1	N	0.000
	H14	-1.625641726	-5.043897427	-4.203126444	dmol	1	H	0.000
	C15	-0.177518666	-4.965186444	1.216105950	dmol	1	C	0.000
	H16	-0.713172272	-5.912833188	1.008804563	dmol	1	H	0.000
	H17	-0.092689313	-4.879716435	2.324067167	dmol	1	H	0.000
	C18	1.268277482	-5.096692987	0.684473594	dmol	1	C	0.000
	O19	1.893234349	-6.177807728	0.801936662	dmol	1	O	0.000
	O20	1.736744135	-4.004541397	0.142344063	dmol	1	O	0.000
	O21	-0.877212449	-3.878418118	0.674414837	dmol	1	O	0.000
	Fe22	0.220767412	5.180447958	0.029630811	dmol	1	Fe	0.000
	Fe23	-1.650170351	3.338325400	0.834646371	dmol	1	Fe	0.000
	Fe24	1.218885215	2.738648008	1.013567904	dmol	1	Fe	0.000
	Fe25	0.107338000	2.811350736	-1.412913891	dmol	1	Fe	0.000
	Fe26	0.099495463	0.191678633	-1.355618967	dmol	1	Fe	0.000
	Fe27	-1.587246300	0.343950838	0.762569688	dmol	1	Fe	0.000
	Fe28	1.294791847	0.122724849	1.061917369	dmol	1	Fe	0.000
	Mo29	0.298535925	-2.276315101	0.004241651	dmol	1	Mo	0.000
	S30	-1.541867249	4.402191541	-1.191674893	dmol	1	S	0.000
S31	-0.056242100	4.271586622	2.154499717	dmol	1	S	0.000	

	S32	0.124773153	1.473106013	-3.214514129	dmol	1	S	0.000
	S33	2.014903664	4.024693453	-0.766447384	dmol	1	S	0.000
	S34	-1.713520787	-1.167737866	-0.864112935	dmol	1	S	0.000
	S35	-3.379780438	1.754748531	0.776897854	dmol	1	S	0.000
	S36	1.082306029	-1.838975921	2.385770885	dmol	1	S	0.000
	S37	2.071283333	-0.879580311	-0.880798576	dmol	1	S	0.000
	S38	2.695880997	1.498487586	2.138743657	dmol	1	S	0.000
	N39	0.013201662	1.382276715	0.175398465	dmol	1	N	0.000
	N40	-1.103347535	0.985979197	3.593181278	dmol	1	N	0.000
	N41	-1.683436415	0.215557043	4.152970351	dmol	1	N	0.000
	H42	-3.726469361	1.770513296	2.090955797	dmol	1	H	0.000
	H43	-0.039320734	-1.567709173	3.105482897	dmol	1	H	0.000
	H44	-2.638427266	4.331220692	1.433939033	dmol	1	H	0.000
	H45	-2.377485649	-0.660335335	1.677270002	dmol	1	H	0.000
TS: 4H-b + N <sub>2</sub> → 4HN <sub>2</sub> -c fe6n2nhx2b2h 3btgu_1_4296. 86a.cmmf	45							
	C1	1.875463008	7.897032010	1.024770776	dmol	1	C	0.000
	H2	2.803046803	7.584514078	0.525412564	dmol	1	H	0.000
	H3	1.904221738	8.987456937	1.184811609	dmol	1	H	0.000
	H4	1.816248251	7.396285498	2.000013204	dmol	1	H	0.000
	S5	0.382399769	7.486850194	-0.020460656	dmol	1	S	0.000
	C6	0.955861137	-3.597895857	-3.004461801	dmol	1	C	0.000
	H7	1.972760199	-3.247576931	-2.882959092	dmol	1	H	0.000
	N8	-0.011784891	-3.266296448	-2.073025640	dmol	1	N	0.000
	C9	0.399554061	-4.383706423	-3.987542403	dmol	1	C	0.000
	H10	0.812138925	-4.846213328	-4.875449389	dmol	1	H	0.000
	C11	-1.142187107	-3.835334137	-2.461350382	dmol	1	C	0.000
	H12	-2.083243603	-3.760709762	-1.932862232	dmol	1	H	0.000
	N13	-0.945203988	-4.529818028	-3.629734002	dmol	1	N	0.000
	H14	-1.655044663	-5.039757750	-4.141258476	dmol	1	H	0.000
	C15	-0.145132451	-4.930685150	1.222272067	dmol	1	C	0.000
	H16	-0.664780826	-5.892120393	1.036503675	dmol	1	H	0.000
	H17	-0.043272591	-4.826302925	2.326920568	dmol	1	H	0.000
	C18	1.296349667	-5.044202828	0.669861301	dmol	1	C	0.000
	O19	1.934527142	-6.120860448	0.773354567	dmol	1	O	0.000
	O20	1.740865780	-3.946272610	0.129105198	dmol	1	O	0.000
	O21	-0.870516076	-3.859019032	0.678001838	dmol	1	O	0.000
	Fe22	0.267480730	5.147255275	0.030652493	dmol	1	Fe	0.000
	Fe23	-1.482829755	3.128339127	0.803266069	dmol	1	Fe	0.000
	Fe24	1.289219892	2.749708743	0.937487035	dmol	1	Fe	0.000
	Fe25	0.073736859	2.785605517	-1.412172515	dmol	1	Fe	0.000
	Fe26	0.033313866	0.210432482	-1.303457611	dmol	1	Fe	0.000
	Fe27	-1.587361335	0.178815192	1.145056415	dmol	1	Fe	0.000
	Fe28	1.211433830	0.161333248	1.041227729	dmol	1	Fe	0.000
	Mo29	0.268128258	-2.226586894	0.023622772	dmol	1	Mo	0.000
	S30	-1.544429079	4.372360898	-1.137234868	dmol	1	S	0.000
	S31	0.043971970	4.254071090	2.143092488	dmol	1	S	0.000
S32	-0.072156910	1.452248282	-3.180021127	dmol	1	S	0.000	
S33	2.006262302	3.983568333	-0.883329758	dmol	1	S	0.000	
S34	-1.760022872	-1.063735272	-0.709155366	dmol	1	S	0.000	
S35	-3.281274747	1.661708172	0.866325645	dmol	1	S	0.000	
S36	1.161420364	-1.765010211	2.366543928	dmol	1	S	0.000	
S37	2.030537360	-0.874213904	-0.874364445	dmol	1	S	0.000	
S38	2.702346456	1.489893415	2.077851441	dmol	1	S	0.000	
N39	-0.006177640	1.482294940	0.202955382	dmol	1	N	0.000	
N40	-1.311133801	1.024725749	3.389070234	dmol	1	N	0.000	
N41	-1.703484659	-0.016277247	3.565801714	dmol	1	N	0.000	
H42	-3.708455480	1.960728001	2.126587610	dmol	1	H	0.000	
H43	0.075750215	-1.556911708	3.162705637	dmol	1	H	0.000	
H44	-2.472495427	4.127886286	1.390396708	dmol	1	H	0.000	
H45	-2.566050681	-0.893606183	1.665169238	dmol	1	H	0.000	
4HN <sub>2</sub> -c fe6n2nhx2b2h 3btgu_2a.cmmf	45							
	C1	1.855238459	7.881949705	0.998961136	dmol	1	C	0.000
	H2	2.768549848	7.517916398	0.508240364	dmol	1	H	0.000
	H3	1.935369456	8.972110148	1.145159242	dmol	1	H	0.000
	H4	1.765123440	7.396553408	1.979272835	dmol	1	H	0.000
	S5	0.347888328	7.512216315	-0.045124865	dmol	1	S	0.000
	C6	0.941236103	-3.593100649	-3.010863062	dmol	1	C	0.000
	H7	1.955603203	-3.234443935	-2.892195742	dmol	1	H	0.000
	N8	-0.019276042	-3.286631453	-2.063443756	dmol	1	N	0.000
	C9	0.382271877	-4.365203958	-4.003470933	dmol	1	C	0.000
	H10	0.790265074	-4.804809764	-4.905516524	dmol	1	H	0.000
	C11	-1.148900749	-3.857953456	-2.451801958	dmol	1	C	0.000
	H12	-2.085962193	-3.804958807	-1.913592012	dmol	1	H	0.000
	N13	-0.957711750	-4.529517270	-3.635565733	dmol	1	N	0.000
	H14	-1.667294138	-5.035346734	-4.152050390	dmol	1	H	0.000
	C15	-0.170604452	-4.965948101	1.224076867	dmol	1	C	0.000
H16	-0.704906851	-5.916151619	1.014584556	dmol	1	H	0.000	

	H17	-0.067136754	-4.894227396	2.331875944	dmol	1	H	0.000
	C18	1.270665339	-5.095290091	0.670745013	dmol	1	C	0.000
	O19	1.895478080	-6.179660047	0.774163774	dmol	1	O	0.000
	O20	1.727849875	-4.002366107	0.129984918	dmol	1	O	0.000
	O21	-0.873171126	-3.865513564	0.704055412	dmol	1	O	0.000
	Fe22	0.198442217	5.176531648	0.061254286	dmol	1	Fe	0.000
	Fe23	-1.563898804	3.203133577	0.839490039	dmol	1	Fe	0.000
	Fe24	1.264934381	2.791062048	0.998566799	dmol	1	Fe	0.000
	Fe25	0.078295113	2.783858272	-1.337676504	dmol	1	Fe	0.000
	Fe26	0.120823929	0.202398152	-1.263663171	dmol	1	Fe	0.000
	Fe27	-1.566252470	0.221516786	1.179387344	dmol	1	Fe	0.000
	Fe28	1.230188507	0.158744752	1.068801813	dmol	1	Fe	0.000
	Mo29	0.293086264	-2.254193236	0.049206218	dmol	1	Mo	0.000
	S30	-1.567248103	4.345381921	-1.139349970	dmol	1	S	0.000
	S31	-0.033130199	4.292320335	2.176272636	dmol	1	S	0.000
	S32	0.073242603	1.465668717	-3.126356706	dmol	1	S	0.000
	S33	1.965347285	4.038469271	-0.814872378	dmol	1	S	0.000
	S34	-1.712579508	-1.037213903	-0.698799627	dmol	1	S	0.000
	S35	-3.295941460	1.671013590	0.878809519	dmol	1	S	0.000
	S36	1.180552671	-1.778595075	2.388677217	dmol	1	S	0.000
	S37	2.091127513	-0.929013392	-0.837215925	dmol	1	S	0.000
	S38	2.715339740	1.528795006	2.083566063	dmol	1	S	0.000
	N39	0.010030909	1.495632750	0.219109112	dmol	1	N	0.000
	N40	-0.941126193	0.973312725	3.110091306	dmol	1	N	0.000
	N41	-1.673474001	0.158935450	3.442092317	dmol	1	N	0.000
	H42	-3.747077223	1.918159731	2.144526082	dmol	1	H	0.000
	H43	0.068219925	-1.618237083	3.159488949	dmol	1	H	0.000
	H44	-2.576270268	4.197506220	1.398022170	dmol	1	H	0.000
	H45	-2.553207856	-0.854811284	1.613077273	dmol	1	H	0.000
<b>4HN<sub>2</sub>-a</b>	45							
<b>fe6n2en13ha3</b>	C1	1.599939949	7.984025124	1.067014805	dmol	1	C	0.000
<b>btgvv_3_4296.</b>	H2	2.577269309	7.658817722	0.685701570	dmol	1	H	0.000
<b>16a.cmmf</b>	H3	1.623695263	9.072090431	1.232941519	dmol	1	H	0.000
	H4	1.412143103	7.478301035	2.023389499	dmol	1	H	0.000
	S5	0.248443789	7.593901068	-0.162172825	dmol	1	S	0.000
	C6	0.879497248	-3.715337602	-3.060917834	dmol	1	C	0.000
	H7	1.898045415	-3.348316824	-3.041129455	dmol	1	H	0.000
	N8	0.011620475	-3.413083589	-2.026725646	dmol	1	N	0.000
	C9	0.233365206	-4.487900556	-3.999878545	dmol	1	C	0.000
	H10	0.559103197	-4.931282293	-4.932299589	dmol	1	H	0.000
	C11	-1.150825136	-3.981920467	-2.314947007	dmol	1	C	0.000
	H12	-2.032998324	-3.935974240	-1.690659125	dmol	1	H	0.000
	N13	-1.066411425	-4.653421005	-3.511053327	dmol	1	N	0.000
	H14	-1.825126298	-5.145008822	-3.967915651	dmol	1	H	0.000
	C15	-0.184213032	-4.997813342	1.271900171	dmol	1	C	0.000
	H16	-0.651469311	-5.958654856	0.974305715	dmol	1	H	0.000
	H17	-0.283829236	-4.925598680	2.378726633	dmol	1	H	0.000
	C18	1.333225203	-5.075620423	0.966559864	dmol	1	C	0.000
	O19	1.972767845	-6.125941080	1.229684780	dmol	1	O	0.000
	O20	1.815394104	-3.983532902	0.452246920	dmol	1	O	0.000
	O21	-0.832570595	-3.920605654	0.642526474	dmol	1	O	0.000
	Fe22	0.172521550	5.253520467	-0.126238472	dmol	1	Fe	0.000
	Fe23	-1.523448844	3.275679570	0.749960831	dmol	1	Fe	0.000
	Fe24	1.379944675	2.851990164	0.911766212	dmol	1	Fe	0.000
	Fe25	0.190853492	2.779943285	-1.442615305	dmol	1	Fe	0.000
	Fe26	0.175070766	0.203278016	-1.303667133	dmol	1	Fe	0.000
	Fe27	-1.511171285	0.176596420	1.185537194	dmol	1	Fe	0.000
	Fe28	1.462279253	0.220615749	0.945276881	dmol	1	Fe	0.000
	Mo29	0.334541531	-2.297831582	0.058421046	dmol	1	Mo	0.000
	S30	-1.545294833	4.326199116	-1.298532786	dmol	1	S	0.000
	S31	-0.038086748	4.395686116	2.035570656	dmol	1	S	0.000
	S32	0.099667403	1.404955552	-3.195789814	dmol	1	S	0.000
	S33	2.023772956	4.100793115	-0.961602252	dmol	1	S	0.000
	S34	-1.641351262	-1.071525584	-0.677087128	dmol	1	S	0.000
	S35	-3.228184134	1.657041235	0.750482079	dmol	1	S	0.000
	S36	0.527409499	-1.443329313	2.451477582	dmol	1	S	0.000
	S37	2.125499262	-1.000034087	-0.919599469	dmol	1	S	0.000
	S38	2.930364888	1.646040491	1.940657619	dmol	1	S	0.000
	N39	0.127595271	1.566213352	0.134822297	dmol	1	N	0.000
	N40	-1.106745471	1.188508850	3.160203188	dmol	1	N	0.000
	N41	-1.890826077	0.407259660	3.427773332	dmol	1	N	0.000
	H42	-3.720739926	1.858343276	2.003930929	dmol	1	H	0.000
	H43	-2.622491489	4.213934245	1.270250575	dmol	1	H	0.000
	H44	-2.486175048	-0.911643252	1.607111732	dmol	1	H	0.000
	H45	1.627919043	-1.989350322	3.074175798	dmol	1	H	0.000

<b>4HN<sub>2</sub>-b</b> fe6n2en13ha3 bthv_2_4287.4 7a.cmmf	45							
	C1	1.622937542	7.973550247	1.055329805	dmol	1	C	0.000
	H2	2.600847633	7.646466812	0.676649504	dmol	1	H	0.000
	H3	1.648903850	9.061711621	1.226062006	dmol	1	H	0.000
	H4	1.429106758	7.463759364	2.007943731	dmol	1	H	0.000
	S5	0.276120130	7.582319386	-0.176769954	dmol	1	S	0.000
	C6	0.905763044	-3.726892428	-3.064147647	dmol	1	C	0.000
	H7	1.922964676	-3.358649839	-3.042151440	dmol	1	H	0.000
	N8	0.033071982	-3.426288033	-2.032529719	dmol	1	N	0.000
	C9	0.261427609	-4.498585951	-4.003786775	dmol	1	C	0.000
	H10	0.590011269	-4.936633549	-4.937483586	dmol	1	H	0.000
	C11	-1.131135992	-3.995618539	-2.324377349	dmol	1	C	0.000
	H12	-2.014040679	-3.950879643	-1.701689987	dmol	1	H	0.000
	N13	-1.040013271	-4.664843108	-3.519454432	dmol	1	N	0.000
	H14	-1.798840750	-5.153675838	-3.978676081	dmol	1	H	0.000
	C15	-0.177607899	-5.040643319	1.262831117	dmol	1	C	0.000
	H16	-0.622773833	-6.021269726	0.993575649	dmol	1	H	0.000
	H17	-0.259975602	-4.948240964	2.368888796	dmol	1	H	0.000
	C18	1.337219481	-5.099274179	0.938085296	dmol	1	C	0.000
	O19	2.004465013	-6.119983569	1.232512851	dmol	1	O	0.000
	O20	1.795016337	-4.022936594	0.369885008	dmol	1	O	0.000
	O21	-0.850114611	-3.982006528	0.622911318	dmol	1	O	0.000
	Fe22	0.186451405	5.235911945	-0.126484857	dmol	1	Fe	0.000
	Fe23	-1.559722140	3.355001169	0.710146253	dmol	1	Fe	0.000
	Fe24	1.414957699	2.867045162	0.907401339	dmol	1	Fe	0.000
	Fe25	0.205108679	2.789795357	-1.452293704	dmol	1	Fe	0.000
	Fe26	0.189244832	0.196095275	-1.302326393	dmol	1	Fe	0.000
	Fe27	-1.371079795	0.077012543	1.348087826	dmol	1	Fe	0.000
	Fe28	1.609289868	0.324975328	0.886431465	dmol	1	Fe	0.000
	Mo29	0.317403153	-2.369750873	-0.005885845	dmol	1	Mo	0.000
	S30	-1.536634484	4.351886640	-1.299154906	dmol	1	S	0.000
	S31	-0.015289013	4.349019421	2.029922904	dmol	1	S	0.000
	S32	0.106335359	1.380632599	-3.193300447	dmol	1	S	0.000
	S33	2.033773749	4.089902888	-0.985177456	dmol	1	S	0.000
	S34	-1.616086892	-1.077719298	-0.663826732	dmol	1	S	0.000
	S35	-3.060665274	1.577508746	0.739232865	dmol	1	S	0.000
	S36	0.685279384	-1.329513848	2.262579725	dmol	1	S	0.000
	S37	2.143721386	-1.027919292	-0.922416137	dmol	1	S	0.000
	S38	3.049250054	1.675108219	1.905211592	dmol	1	S	0.000
	N39	0.190176012	1.469457570	0.192960059	dmol	1	N	0.000
	N40	-1.086339389	1.191980032	3.165989726	dmol	1	N	0.000
	N41	-1.857228230	0.385029449	3.439840190	dmol	1	N	0.000
	H42	-3.658941097	1.806272251	1.940763899	dmol	1	H	0.000
	H43	-2.655766901	4.265337789	1.263866962	dmol	1	H	0.000
	H44	-2.394466372	-0.997918808	1.671948253	dmol	1	H	0.000
H45	0.147873336	-1.366533552	3.512877803	dmol	1	H	0.000	
<b>4HN<sub>2</sub>-c</b> fe6n2en13ha3 bthv_3a.cmmf	45							
	C1	1.653664302	7.998346942	1.057432579	dmol	1	C	0.000
	H2	2.635951569	7.663961199	0.697911297	dmol	1	H	0.000
	H3	1.687247220	9.086436030	1.229857604	dmol	1	H	0.000
	H4	1.435952534	7.492592418	2.006748792	dmol	1	H	0.000
	S5	0.331531039	7.614911988	-0.205745701	dmol	1	S	0.000
	C6	0.938539777	-3.705999687	-3.067888974	dmol	1	C	0.000
	H7	1.954746217	-3.333185146	-3.051062937	dmol	1	H	0.000
	N8	0.077320943	-3.424624060	-2.022328937	dmol	1	N	0.000
	C9	0.288354960	-4.468028436	-4.012041039	dmol	1	C	0.000
	H10	0.607667126	-4.888799739	-4.957721104	dmol	1	H	0.000
	C11	-1.083170866	-3.998146628	-2.305931648	dmol	1	C	0.000
	H12	-1.954394664	-3.969441059	-1.665530569	dmol	1	H	0.000
	N13	-1.006158262	-4.650228894	-3.512833147	dmol	1	N	0.000
	H14	-1.768958169	-5.131375327	-3.974638474	dmol	1	H	0.000
	C15	-0.153537692	-5.027461490	1.267098271	dmol	1	C	0.000
	H16	-0.633006760	-5.983186727	0.965363915	dmol	1	H	0.000
	H17	-0.214764510	-4.986241063	2.378859142	dmol	1	H	0.000
	C18	1.350656909	-5.124124995	0.910852116	dmol	1	C	0.000
	O19	1.993158299	-6.170801070	1.159081183	dmol	1	O	0.000
	O20	1.838956708	-4.048225701	0.356252279	dmol	1	O	0.000
	O21	-0.796655492	-3.927970313	0.680635788	dmol	1	O	0.000
	Fe22	0.177879413	5.268084518	-0.184215582	dmol	1	Fe	0.000
	Fe23	-1.597972185	3.416235903	0.668547033	dmol	1	Fe	0.000
	Fe24	1.375963141	2.811060219	0.886919819	dmol	1	Fe	0.000
	Fe25	0.124382115	2.747081458	-1.433035704	dmol	1	Fe	0.000
	Fe26	0.160887076	0.144654631	-1.251509628	dmol	1	Fe	0.000
	Fe27	-1.464248357	0.136476552	1.392576941	dmol	1	Fe	0.000
	Fe28	1.461372216	0.215629535	0.979729498	dmol	1	Fe	0.000
	Mo29	0.434076904	-2.343186140	0.056903958	dmol	1	Mo	0.000
	S30	-1.548969292	4.392474101	-1.359986750	dmol	1	S	0.000
	S31	-0.049592302	4.382920031	1.972905361	dmol	1	S	0.000

	S32	0.011424183	1.306635606	-3.147127633	dmol	1	S	0.000
	S33	1.990911623	4.035433119	-0.992839267	dmol	1	S	0.000
	S34	-1.603004020	-1.134525770	-0.523860150	dmol	1	S	0.000
	S35	-3.103114244	1.645514664	0.818436292	dmol	1	S	0.000
	S36	0.960813330	-1.665068111	2.424221136	dmol	1	S	0.000
	S37	2.163514113	-0.978032297	-0.930973358	dmol	1	S	0.000
	S38	2.958611419	1.614688188	1.910206865	dmol	1	S	0.000
	N39	0.138035796	1.457313561	0.200521380	dmol	1	N	0.000
	N40	-0.898749402	1.182907070	3.173523221	dmol	1	N	0.000
	N41	-1.713719348	0.456490241	3.532667834	dmol	1	N	0.000
	H42	-3.681976406	1.885895350	2.027538725	dmol	1	H	0.000
	H43	-2.697720022	4.378518642	1.103217328	dmol	1	H	0.000
	H44	-2.495370248	-0.915193236	1.807906193	dmol	1	H	0.000
	H45	-0.286538919	-1.460408166	2.933384507	dmol	1	H	0.000
Fig 4								
TS: 4HN <sub>2</sub> -c → 3HN <sub>2</sub> H-a fe6n2nhx2b2x 3bteua1_1_42 67.26a.cmmf	45							
	C1	1.639030314	7.898592613	0.781517740	dmol	1	C	0.000
	H2	2.492327875	7.597700877	0.158519919	dmol	1	H	0.000
	H3	1.649734262	8.991936861	0.914670583	dmol	1	H	0.000
	H4	1.735107813	7.414567743	1.762694046	dmol	1	H	0.000
	S5	0.035383009	7.411771370	-0.043201922	dmol	1	S	0.000
	C6	1.350276242	-3.895432209	-2.694611197	dmol	1	C	0.000
	H7	2.350894463	-3.556590776	-2.458365943	dmol	1	H	0.000
	N8	0.280569085	-3.500996403	-1.910948782	dmol	1	N	0.000
	C9	0.903590838	-4.706385248	-3.712711069	dmol	1	C	0.000
	H10	1.417355247	-5.216048575	-4.518484193	dmol	1	H	0.000
	C11	-0.807549072	-4.055026051	-2.424324361	dmol	1	C	0.000
	H12	-1.807155523	-3.938389840	-2.026238601	dmol	1	H	0.000
	N13	-0.480070091	-4.804426658	-3.529979468	dmol	1	N	0.000
	H14	-1.134437625	-5.289536687	-4.132379789	dmol	1	H	0.000
	C15	-0.503961692	-4.699126616	1.502810370	dmol	1	C	0.000
	H16	-0.975412688	-5.694127663	1.366825695	dmol	1	H	0.000
	H17	-0.664289576	-4.406011779	2.566532097	dmol	1	H	0.000
	C18	1.025808313	-4.861199373	1.323778586	dmol	1	C	0.000
	O19	1.619284223	-5.876109944	1.757500063	dmol	1	O	0.000
	O20	1.593167954	-3.858247534	0.708887235	dmol	1	O	0.000
	O21	-1.067194572	-3.752820357	0.630369360	dmol	1	O	0.000
	Fe22	0.197039759	5.104281219	0.026563649	dmol	1	Fe	0.000
	Fe23	-1.435995788	3.005644836	0.643411954	dmol	1	Fe	0.000
	Fe24	1.468779549	2.842955556	0.843793822	dmol	1	Fe	0.000
	Fe25	0.297324554	2.823644754	-1.532995582	dmol	1	Fe	0.000
	Fe26	0.189880406	0.235151679	-1.391728797	dmol	1	Fe	0.000
	Fe27	-1.674247331	-0.061465922	1.191224467	dmol	1	Fe	0.000
	Fe28	1.466506418	0.244855360	0.872088247	dmol	1	Fe	0.000
	Mo29	0.241336726	-2.199346697	0.073174406	dmol	1	Mo	0.000
	S30	-1.474406314	4.207752086	-1.255163161	dmol	1	S	0.000
	S31	-0.001848648	4.134297749	2.091646396	dmol	1	S	0.000
	S32	0.225621157	1.480934241	-3.293657981	dmol	1	S	0.000
	S33	2.070322818	4.207329039	-0.921753848	dmol	1	S	0.000
	S34	-1.669790133	-1.041648013	-0.888318628	dmol	1	S	0.000
	S35	-3.192588613	1.520678751	0.498646188	dmol	1	S	0.000
	S36	0.436705465	-1.271556821	2.332411400	dmol	1	S	0.000
	S37	2.097451530	-1.012199706	-0.968720868	dmol	1	S	0.000
	S38	3.003737074	1.577690162	1.835456715	dmol	1	S	0.000
	N39	0.188240697	1.606912719	0.021648705	dmol	1	N	0.000
	N40	-1.347411469	0.712825176	3.079741687	dmol	1	N	0.000
	N41	-2.449049164	0.215214444	3.070813085	dmol	1	N	0.000
	H42	-0.447420040	0.012404643	3.273832920	dmol	1	H	0.000
	H43	-3.710558225	1.781685191	1.730654130	dmol	1	H	0.000
	H44	-2.590559979	-1.223425735	1.391224733	dmol	1	H	0.000
	H45	-2.541529251	3.891291536	1.253145990	dmol	1	H	0.000
3HN <sub>2</sub> H-a fe6n2nhx2b2x 3bteua1_4a.c mmf	45							
	C1	1.753502894	8.026879185	0.789724566	dmol	1	C	0.000
	H2	2.681426906	7.702599073	0.296965563	dmol	1	H	0.000
	H3	1.775319282	9.121740710	0.919893326	dmol	1	H	0.000
	H4	1.696616864	7.549035381	1.777321211	dmol	1	H	0.000
	S5	0.265488582	7.579576569	-0.248697641	dmol	1	S	0.000
	C6	1.311115997	-3.893025759	-2.780692926	dmol	1	C	0.000
	H7	2.308880612	-3.519765041	-2.585207448	dmol	1	H	0.000
	N8	0.263468625	-3.551728818	-1.946413551	dmol	1	N	0.000
	C9	0.852760678	-4.708821235	-3.790901494	dmol	1	C	0.000
	H10	1.346867896	-5.186809299	-4.628028973	dmol	1	H	0.000
	C11	-0.820643491	-4.141378211	-2.419144876	dmol	1	C	0.000
	H12	-1.803803453	-4.076565227	-1.970529259	dmol	1	H	0.000
	N13	-0.516276046	-4.863798782	-3.549082106	dmol	1	N	0.000

	H14	-1.175977503	-5.371880964	-4.126497929	dmol	1	H	0.000
	C15	-0.379416361	-4.856274872	1.442785260	dmol	1	C	0.000
	H16	-0.828658838	-5.853518304	1.257701909	dmol	1	H	0.000
	H17	-0.492277080	-4.651738739	2.532839756	dmol	1	H	0.000
	C18	1.140504791	-4.952064786	1.178410032	dmol	1	C	0.000
	O19	1.792779933	-5.969482212	1.500881171	dmol	1	O	0.000
	O20	1.646870469	-3.881007178	0.614434123	dmol	1	O	0.000
	O21	-1.008767265	-3.867937269	0.671179912	dmol	1	O	0.000
	Fe22	0.266733977	5.240047155	-0.152057695	dmol	1	Fe	0.000
	Fe23	-1.343275454	3.112722585	0.574196257	dmol	1	Fe	0.000
	Fe24	1.377162345	2.897992684	0.870371505	dmol	1	Fe	0.000
	Fe25	0.257775892	2.803215623	-1.516509214	dmol	1	Fe	0.000
	Fe26	0.112207895	0.190617918	-1.361570339	dmol	1	Fe	0.000
	Fe27	-1.667825201	-0.284744576	1.363090400	dmol	1	Fe	0.000
	Fe28	1.413739595	0.283757249	1.025712906	dmol	1	Fe	0.000
	Mo29	0.231614227	-2.230848484	0.180260691	dmol	1	Mo	0.000
	S30	-1.441259072	4.360042875	-1.348221453	dmol	1	S	0.000
	S31	-0.000127058	4.361094567	1.981904228	dmol	1	S	0.000
	S32	0.160440213	1.382726096	-3.260785624	dmol	1	S	0.000
	S33	2.115230019	4.138476864	-0.971875145	dmol	1	S	0.000
	S34	-1.693747473	-1.151158842	-0.777829124	dmol	1	S	0.000
	S35	-3.036459647	1.450356283	0.487031892	dmol	1	S	0.000
	S36	0.246305517	-1.279808315	2.319512508	dmol	1	S	0.000
	S37	2.069188670	-0.989498222	-0.852554185	dmol	1	S	0.000
	S38	2.836757557	1.662237805	2.064164745	dmol	1	S	0.000
	N39	0.177251875	1.613147329	0.042931840	dmol	1	N	0.000
	N40	-1.668967980	0.804269004	3.125594442	dmol	1	N	0.000
	N41	-2.548303450	-0.083810973	3.247574561	dmol	1	N	0.000
	H42	-0.819189476	0.710288483	3.738063431	dmol	1	H	0.000
	H43	-3.705185160	1.784642058	1.620739948	dmol	1	H	0.000
	H44	-2.681740395	-1.376240358	1.491590300	dmol	1	H	0.000
	H45	-2.468111165	3.966440972	1.171722495	dmol	1	H	0.000
<b>3HN<sub>2</sub>H-b</b> fe6n2hihx2b2 htetau_4a.cm mf	45							
	C1	1.718620343	7.940309188	0.788307518	dmol	1	C	0.000
	H2	2.645753154	7.543320201	0.352603885	dmol	1	H	0.000
	H3	1.766909446	9.041518998	0.798291755	dmol	1	H	0.000
	H4	1.633471420	7.576599915	1.821003222	dmol	1	H	0.000
	S5	0.232900453	7.413419522	-0.221247447	dmol	1	S	0.000
	C6	1.270986424	-3.820938589	-2.843559097	dmol	1	C	0.000
	H7	2.250822913	-3.376675337	-2.714888784	dmol	1	H	0.000
	N8	0.271937412	-3.579676447	-1.919705509	dmol	1	N	0.000
	C9	0.792896810	-4.640358920	-3.842375393	dmol	1	C	0.000
	H10	1.249149903	-5.055803672	-4.733220063	dmol	1	H	0.000
	C11	-0.802862334	-4.229463344	-2.329290413	dmol	1	C	0.000
	H12	-1.750842799	-4.242000990	-1.805546869	dmol	1	H	0.000
	N13	-0.539359880	-4.898134480	-3.502316401	dmol	1	N	0.000
	H14	-1.204625922	-5.436652064	-4.045026420	dmol	1	H	0.000
	C15	-0.352183481	-4.925550380	1.411474759	dmol	1	C	0.000
	H16	-0.766286453	-5.917631185	1.133933502	dmol	1	H	0.000
	H17	-0.482716295	-4.827065381	2.515048789	dmol	1	H	0.000
	C18	1.170628554	-4.961799092	1.163735207	dmol	1	C	0.000
	O19	1.852352437	-5.976243954	1.426280885	dmol	1	O	0.000
	O20	1.653594297	-3.840709840	0.679980534	dmol	1	O	0.000
	O21	-1.002345997	-3.892055803	0.722642850	dmol	1	O	0.000
	Fe22	0.267298098	5.096725478	-0.043103783	dmol	1	Fe	0.000
	Fe23	-1.444765333	2.862998321	0.932980169	dmol	1	Fe	0.000
	Fe24	1.443743884	2.820758645	1.040204274	dmol	1	Fe	0.000
	Fe25	0.207724121	2.715897613	-1.480449315	dmol	1	Fe	0.000
	Fe26	0.191969030	0.142564806	-1.254159822	dmol	1	Fe	0.000
	Fe27	-1.650016982	-0.079063538	1.212073944	dmol	1	Fe	0.000
	Fe28	1.410840882	0.218423361	1.019083991	dmol	1	Fe	0.000
	Mo29	0.232565370	-2.231910995	0.245329636	dmol	1	Mo	0.000
	S30	-1.522748313	4.149352360	-1.054106724	dmol	1	S	0.000
	S31	0.031801595	4.257900859	2.121837394	dmol	1	S	0.000
S32	0.229025048	1.280084771	-3.193218300	dmol	1	S	0.000	
S33	2.095984654	4.015182269	-0.893763470	dmol	1	S	0.000	
S34	-1.662719723	-1.196624078	-0.792199227	dmol	1	S	0.000	
S35	-3.212154633	1.432355111	0.225501950	dmol	1	S	0.000	
S36	0.113119401	-1.206706064	2.350913474	dmol	1	S	0.000	
S37	2.098957977	-1.060129336	-0.776528869	dmol	1	S	0.000	
S38	2.883678314	1.505117832	2.124977469	dmol	1	S	0.000	
N39	0.186974067	1.531181884	0.139265708	dmol	1	N	0.000	
N40	-1.443303079	1.456123609	2.551029067	dmol	1	N	0.000	
N41	-2.346017617	0.709817687	3.026770759	dmol	1	N	0.000	
H42	-0.541127654	1.520898151	3.072446464	dmol	1	H	0.000	
H43	-3.954583635	1.585384635	1.353756161	dmol	1	H	0.000	
H44	-2.647122715	-1.109707260	1.666272393	dmol	1	H	0.000	
H45	-2.577923163	3.688965533	1.549050147	dmol	1	H	0.000	

<b>4HN<sub>2</sub>H-a</b> fe626n2h262b 3btjvab_2a.cm mf	46							
	C1	1.452477197	8.191579382	0.517843335	dmol	1	C	0.000
	H2	2.429911083	7.939136346	0.084128044	dmol	1	H	0.000
	H3	1.315079891	9.284935081	0.482619802	dmol	1	H	0.000
	H4	1.434467284	7.867668105	1.567251004	dmol	1	H	0.000
	S5	0.067071117	7.379077105	-0.443567859	dmol	1	S	0.000
	C6	1.496185453	-3.828347883	-2.876662935	dmol	1	C	0.000
	H7	2.459232965	-3.350180036	-2.751922243	dmol	1	H	0.000
	N8	0.479575479	-3.595687917	-1.963756826	dmol	1	N	0.000
	C9	1.054120449	-4.685592843	-3.858507422	dmol	1	C	0.000
	H10	1.544189205	-5.123525632	-4.719518738	dmol	1	H	0.000
	C11	-0.577442448	-4.287113535	-2.376881813	dmol	1	C	0.000
	H12	-1.532028213	-4.309839005	-1.869099588	dmol	1	H	0.000
	N13	-0.273861270	-4.972748739	-3.530821453	dmol	1	N	0.000
	H14	-0.907566415	-5.571647222	-4.045086959	dmol	1	H	0.000
	C15	-0.180123416	-5.076714927	1.394431947	dmol	1	C	0.000
	H16	-0.538048170	-6.098248683	1.150864423	dmol	1	H	0.000
	H17	-0.482167657	-4.877991991	2.449045243	dmol	1	H	0.000
	C18	1.368364772	-5.086385497	1.384402297	dmol	1	C	0.000
	O19	1.990184586	-6.071757827	1.861717105	dmol	1	O	0.000
	O20	1.886030883	-4.010526808	0.878780640	dmol	1	O	0.000
	O21	-0.739665133	-4.118607674	0.530193228	dmol	1	O	0.000
	Fe22	0.331693179	5.174689767	-0.043799186	dmol	1	Fe	0.000
	Fe23	-1.523782148	2.854808111	0.774105649	dmol	1	Fe	0.000
	Fe24	1.402380497	2.786926754	0.910969631	dmol	1	Fe	0.000
	Fe25	0.191814194	2.744293050	-1.461923526	dmol	1	Fe	0.000
	Fe26	0.133239297	0.130273834	-1.341010115	dmol	1	Fe	0.000
	Fe27	-1.971837841	0.120071522	1.179908248	dmol	1	Fe	0.000
	Fe28	1.393339800	0.212573451	0.937458078	dmol	1	Fe	0.000
	Mo29	0.425383150	-2.455114126	0.043637988	dmol	1	Mo	0.000
	S30	-1.464841942	4.285432425	-1.005347629	dmol	1	S	0.000
	S31	0.075540674	4.286107776	1.985494307	dmol	1	S	0.000
	S32	0.061502453	1.395532238	-3.223633138	dmol	1	S	0.000
	S33	2.047076567	4.072505757	-0.944605181	dmol	1	S	0.000
	S34	-1.631994121	-1.286614095	-0.707583008	dmol	1	S	0.000
	S35	-0.332755157	1.543224492	-0.039680092	dmol	1	S	0.000
	S36	-0.173862525	-1.217173557	2.078147139	dmol	1	S	0.000
	S37	2.146666566	-1.050165013	-0.875924424	dmol	1	S	0.000
	S38	2.806826747	1.516125603	2.099573100	dmol	1	S	0.000
	N39	0.126358153	1.519296403	0.07666240	dmol	1	N	0.000
	N40	-1.726725840	1.681584901	2.453702994	dmol	1	N	0.000
	N41	-2.645839450	0.892031591	2.882975450	dmol	1	N	0.000
	H42	-0.921700410	1.826715713	3.098007035	dmol	1	H	0.000
	H43	0.293388323	-1.361422099	3.368797090	dmol	1	H	0.000
	H44	-2.586206149	3.784547009	1.376604449	dmol	1	H	0.000
	H45	-4.208183728	1.868877813	0.950229935	dmol	1	H	0.000
H46	-2.993467542	-0.922609124	1.561777228	dmol	1	H	0.000	
<b>TS: 4HN<sub>2</sub>H-a</b> <b>→ 4HN<sub>2</sub>H-b</b> fe626n2h262b 3btmab_1_431 2.23a.cmmf	46							
	C1	1.481315110	8.198108631	0.483021340	dmol	1	C	0.000
	H2	2.450624227	7.942542205	0.033058324	dmol	1	H	0.000
	H3	1.342384928	9.290824946	0.440359276	dmol	1	H	0.000
	H4	1.485144490	7.884319685	1.535945608	dmol	1	H	0.000
	S5	0.076451886	7.382621708	-0.448902559	dmol	1	S	0.000
	C6	1.444759532	-3.881697664	-2.876948575	dmol	1	C	0.000
	H7	2.421193781	-3.431096265	-2.754627742	dmol	1	H	0.000
	N8	0.427345409	-3.615644729	-1.967228826	dmol	1	N	0.000
	C9	0.988411493	-4.750431306	-3.841731669	dmol	1	C	0.000
	H10	1.466272711	-5.191066892	-4.707875064	dmol	1	H	0.000
	C11	-0.640577691	-4.307916110	-2.369506135	dmol	1	C	0.000
	H12	-1.592063266	-4.319576611	-1.856380436	dmol	1	H	0.000
	N13	-0.337450735	-5.026263420	-3.504260096	dmol	1	N	0.000
	H14	-0.992034390	-5.587018508	-4.033613281	dmol	1	H	0.000
	C15	-0.240034651	-5.001233691	1.423987762	dmol	1	C	0.000
	H16	-0.619314414	-6.018895614	1.200516669	dmol	1	H	0.000
	H17	-0.517226363	-4.775069908	2.477021005	dmol	1	H	0.000
	C18	1.310376065	-5.025579616	1.365327963	dmol	1	C	0.000
	O19	1.932200507	-6.002991102	1.859392162	dmol	1	O	0.000
	O20	1.820361555	-3.982079497	0.797052538	dmol	1	O	0.000
	O21	-0.822860882	-4.049445604	0.562203701	dmol	1	O	0.000
	Fe22	0.344808534	5.180710341	-0.062973785	dmol	1	Fe	0.000
	Fe23	-1.488942524	2.848562976	0.788554265	dmol	1	Fe	0.000
	Fe24	1.411797658	2.807879015	0.861472787	dmol	1	Fe	0.000
	Fe25	0.184232150	2.720770846	-1.487182776	dmol	1	Fe	0.000
	Fe26	0.111233097	0.118880257	-1.338127326	dmol	1	Fe	0.000
	Fe27	-1.771991931	0.105467406	1.114567034	dmol	1	Fe	0.000
	Fe28	1.402312237	0.241648397	0.958316339	dmol	1	Fe	0.000
	Mo29	0.327777261	-2.459830430	-0.063044837	dmol	1	Mo	0.000

	S30	-1.464275338	4.276756602	-1.001428661	dmol	1	S	0.000
	S31	0.107113181	4.300107185	1.959970607	dmol	1	S	0.000
	S32	0.068913592	1.354812334	-3.234918086	dmol	1	S	0.000
	S33	2.036621757	4.076132978	-0.993085847	dmol	1	S	0.000
	S34	-1.656670701	-1.279929916	-0.759121103	dmol	1	S	0.000
	S35	-3.291493929	1.516130690	0.028790508	dmol	1	S	0.000
	S36	0.219744101	-1.243713453	2.323972456	dmol	1	S	0.000
	S37	2.115479397	-1.043866364	-0.844412547	dmol	1	S	0.000
	S38	2.862207755	1.583886881	2.018403463	dmol	1	S	0.000
	N39	0.114967721	1.498873215	0.075791486	dmol	1	N	0.000
	N40	-1.561831492	1.619728100	2.447787887	dmol	1	N	0.000
	N41	-2.432367801	0.770100792	2.873894457	dmol	1	N	0.000
	H42	-0.708151554	1.712452655	3.034687727	dmol	1	H	0.000
	H43	-0.406119117	-0.977873920	3.494196915	dmol	1	H	0.000
	H44	-2.550247131	3.760399409	1.415371648	dmol	1	H	0.000
	H45	-4.118604810	1.767317540	1.080074111	dmol	1	H	0.000
	H46	-2.741791415	-0.987814176	1.491631315	dmol	1	H	0.000
<b>4HN<sub>2</sub>H-b</b> fe626n2h262b 3btkvab_4a.c mmf	46							
	C1	1.594320890	8.152990950	0.408061264	dmol	1	C	0.000
	H2	2.563071238	7.862941064	-0.021876070	dmol	1	H	0.000
	H3	1.487802843	9.248672526	0.347319361	dmol	1	H	0.000
	H4	1.570617368	7.854600992	1.464721315	dmol	1	H	0.000
	S5	0.181684756	7.355017635	-0.526386185	dmol	1	S	0.000
	C6	1.372283720	-3.767341081	-2.791352948	dmol	1	C	0.000
	H7	2.331290033	-3.277650792	-2.679804166	dmol	1	H	0.000
	N8	0.363712221	-3.547126969	-1.867969563	dmol	1	N	0.000
	C9	0.930404126	-4.635954251	-3.762588232	dmol	1	C	0.000
	H10	1.409122207	-5.054725631	-4.639445078	dmol	1	H	0.000
	C11	-0.682453250	-4.265058525	-2.254861365	dmol	1	C	0.000
	H12	-1.622808771	-4.314283531	-1.721896701	dmol	1	H	0.000
	N13	-0.384791846	-4.951624108	-3.408611153	dmol	1	N	0.000
	H14	-1.021638337	-5.545313241	-3.925370664	dmol	1	H	0.000
	C15	-0.190299571	-5.009741192	1.447236584	dmol	1	C	0.000
	H16	-0.573577977	-6.009491966	1.154771650	dmol	1	H	0.000
	H17	-0.400235682	-4.893067685	2.533528422	dmol	1	H	0.000
	C18	1.350840831	-5.026264350	1.295245214	dmol	1	C	0.000
	O19	2.003428201	-6.037538189	1.656165087	dmol	1	O	0.000
	O20	1.841384167	-3.934873887	0.790094003	dmol	1	O	0.000
	O21	-0.818469033	-3.990963454	0.707701877	dmol	1	O	0.000
	Fe22	0.365714832	5.161157987	-0.053823578	dmol	1	Fe	0.000
	Fe23	-1.544317952	2.906960006	0.816454126	dmol	1	Fe	0.000
	Fe24	1.354713530	2.745998343	0.891663779	dmol	1	Fe	0.000
	Fe25	0.127609651	2.694636235	-1.449944177	dmol	1	Fe	0.000
	Fe26	0.145616835	0.100756711	-1.322854102	dmol	1	Fe	0.000
	Fe27	-1.842848708	0.201959908	0.916202920	dmol	1	Fe	0.000
	Fe28	1.303322639	0.152869975	1.011071016	dmol	1	Fe	0.000
	Mo29	0.346814618	-2.358170172	0.146526929	dmol	1	Mo	0.000
	S30	-1.473834845	4.312853191	-0.986738896	dmol	1	S	0.000
	S31	0.106152789	4.293671445	1.981331479	dmol	1	S	0.000
	S32	0.071052957	1.331021887	-3.212544726	dmol	1	S	0.000
	S33	2.020722024	3.990419076	-0.961426669	dmol	1	S	0.000
	S34	-1.645949427	-1.276862143	-0.790298931	dmol	1	S	0.000
	S35	-3.362111396	1.659303350	-0.010372253	dmol	1	S	0.000
S36	0.614289096	-1.559082901	2.563290076	dmol	1	S	0.000	
S37	2.124081925	-1.034467181	-0.802337701	dmol	1	S	0.000	
S38	2.782334504	1.508994274	2.045479306	dmol	1	S	0.000	
N39	0.025091883	1.458173549	0.098996016	dmol	1	N	0.000	
N40	-1.581350625	1.579146395	2.420651697	dmol	1	N	0.000	
N41	-2.365587333	0.605474887	2.758876986	dmol	1	N	0.000	
H42	-0.693278321	1.623534184	2.963066726	dmol	1	H	0.000	
H43	-0.585040573	-1.083039554	3.009230530	dmol	1	H	0.000	
H44	-2.573606117	3.836144941	1.465368050	dmol	1	H	0.000	
H45	-4.166872665	1.802878541	1.076935302	dmol	1	H	0.000	
H46	-2.858407456	-0.867537248	1.220513441	dmol	1	H	0.000	
<b>TS: 4HN<sub>2</sub>H-b</b> → 3HN <sub>2</sub> H <sub>2</sub> -a fe626n2h2h6h 2b3btkfv_orig a.cmmf	45							
	C1	1.426575	6.867172	0.542404	dmol	1	C	0.000
	H2	2.377533	6.625610	0.048569	dmol	1	H	0.000
	H3	1.284744	7.960266	0.530273	dmol	1	H	0.000
	H4	1.471497	6.525635	1.585144	dmol	1	H	0.000
	S5	-0.009293	6.071106	-0.360718	dmol	1	S	0.000
	C6	1.369659	-5.204666	-3.032150	dmol	1	C	0.000
	H7	2.346054	-4.747467	-2.934372	dmol	1	H	0.000
	N8	0.389206	-4.977798	-2.081390	dmol	1	N	0.000
	C9	0.882431	-6.038452	-4.014084	dmol	1	C	0.000
	H10	1.325378	-6.450700	-4.913300	dmol	1	H	0.000
	C11	-0.684998	-5.652756	-2.463806	dmol	1	C	0.000
H12	-1.615479	-5.687912	-1.912308	dmol	1	H	0.000	

	N13	-0.434738	-6.321442	-3.638260	dmol	1	N	0.000
	H14	-1.106781	-6.868942	-4.163391	dmol	1	H	0.000
	C15	-0.210037	-6.360519	1.279419	dmol	1	C	0.000
	H16	-0.576645	-7.379013	1.035004	dmol	1	H	0.000
	H17	-0.432755	-6.183868	2.356140	dmol	1	H	0.000
	C18	1.333511	-6.365219	1.150070	dmol	1	C	0.000
	O19	2.000961	-7.353317	1.539719	dmol	1	O	0.000
	O20	1.818130	-5.273071	0.629135	dmol	1	O	0.000
	O21	-0.838989	-5.391525	0.476944	dmol	1	O	0.000
	Fe22	0.210739	3.853943	-0.115295	dmol	1	Fe	0.000
	Fe23	-1.624817	1.543167	0.970505	dmol	1	Fe	0.000
	Fe24	1.235580	1.350204	0.802155	dmol	1	Fe	0.000
	Fe25	0.042313	1.297195	-1.550766	dmol	1	Fe	0.000
	Fe26	0.130951	-1.283752	-1.487473	dmol	1	Fe	0.000
	Fe27	-1.716600	-1.083771	0.780731	dmol	1	Fe	0.000
	Fe28	1.372711	-1.236328	0.844864	dmol	1	Fe	0.000
	Mo29	0.331741	-3.725357	-0.022659	dmol	1	Mo	0.000
	S30	-1.578171	2.867142	-1.030060	dmol	1	S	0.000
	S31	-0.014557	2.932449	1.908051	dmol	1	S	0.000
	S32	-0.016220	-0.032562	-3.343964	dmol	1	S	0.000
	S33	1.852127	2.691544	-0.994812	dmol	1	S	0.000
	S34	-1.639465	-2.623245	-0.954773	dmol	1	S	0.000
	S35	-3.412445	0.307373	0.131622	dmol	1	S	0.000
	S36	0.354523	-2.815338	2.315109	dmol	1	S	0.000
	S37	2.119293	-2.400284	-0.997375	dmol	1	S	0.000
	S38	2.773071	0.162277	1.888046	dmol	1	S	0.000
	N39	0.000000	0.000000	0.000000	dmol	1	N	0.000
	N40	-1.400345	0.142334	2.433975	dmol	1	N	0.000
	N41	-2.056442	-0.946960	2.773804	dmol	1	N	0.000
	H42	-0.417603	0.153564	2.783554	dmol	1	H	0.000
	H43	-0.832703	-2.097717	2.690659	dmol	1	H	0.000
	H44	-2.667969	2.350403	1.723328	dmol	1	H	0.000
	H45	-4.133575	0.196259	1.281387	dmol	1	H	0.000
	H46	-2.780167	-2.109985	1.094345	dmol	1	H	0.000
<b>3HN<sub>2</sub>H<sub>2</sub>-a</b> fe626n2h2h6h 2b3btkfv_4a.c mmf	46							
	C1	1.482625197	8.207395271	0.640294296	dmol	1	C	0.000
	H2	2.440049149	7.960268347	0.161570713	dmol	1	H	0.000
	H3	1.355959088	9.302476086	0.642827854	dmol	1	H	0.000
	H4	1.501123092	7.848315469	1.677693896	dmol	1	H	0.000
	S5	0.053097392	7.438961964	-0.295822245	dmol	1	S	0.000
	C6	1.419623769	-3.860996263	-3.056658503	dmol	1	C	0.000
	H7	2.385509553	-3.375018962	-2.992891670	dmol	1	H	0.000
	N8	0.476988195	-3.675702216	-2.061505766	dmol	1	N	0.000
	C9	0.912393672	-4.693753480	-4.029288809	dmol	1	C	0.000
	H10	1.326718702	-5.082260607	-4.951920148	dmol	1	H	0.000
	C11	-0.594547874	-4.373556811	-2.405140647	dmol	1	C	0.000
	H12	-1.494410041	-4.441557280	-1.806142174	dmol	1	H	0.000
	N13	-0.379037095	-5.018060134	-3.600284665	dmol	1	N	0.000
	H14	-1.060354358	-5.571604189	-4.106139524	dmol	1	H	0.000
	C15	-0.145554151	-5.013147293	1.341666710	dmol	1	C	0.000
	H16	-0.507623963	-6.037861920	1.114047764	dmol	1	H	0.000
	H17	-0.386140539	-4.821877909	2.413679191	dmol	1	H	0.000
	C18	1.398530118	-5.017118601	1.240801384	dmol	1	C	0.000
	O19	2.065609257	-6.000036732	1.642929535	dmol	1	O	0.000
	O20	1.888505311	-3.922169746	0.726841238	dmol	1	O	0.000
	O21	-0.752767836	-4.060645834	0.510057292	dmol	1	O	0.000
	Fe22	0.276257973	5.219946880	-0.054458520	dmol	1	Fe	0.000
	Fe23	-1.541532036	2.899942055	1.093415038	dmol	1	Fe	0.000
	Fe24	1.355609080	2.739737037	0.855337680	dmol	1	Fe	0.000
	Fe25	0.086538129	2.657351677	-1.457794475	dmol	1	Fe	0.000
	Fe26	0.205942705	0.092486746	-1.415440184	dmol	1	Fe	0.000
	Fe27	-1.570992788	0.141827333	1.121829335	dmol	1	Fe	0.000
	Fe28	1.486049887	0.158604820	0.871216283	dmol	1	Fe	0.000
	Mo29	0.443399983	-2.385105898	0.013500566	dmol	1	Mo	0.000
	S30	-1.541042258	4.223743204	-0.898534793	dmol	1	S	0.000
	S31	0.096494173	4.305971324	1.978712406	dmol	1	S	0.000
	S32	0.020164873	1.344685479	-3.264091685	dmol	1	S	0.000
S33	1.892664798	4.072926934	-0.990249837	dmol	1	S	0.000	
S34	-1.556400320	-1.272240697	-0.812217111	dmol	1	S	0.000	
S35	-3.287362801	1.569600696	0.241699982	dmol	1	S	0.000	
S36	0.169790999	-1.268055927	2.140787926	dmol	1	S	0.000	
S37	2.201037926	-1.033364268	-0.990692146	dmol	1	S	0.000	
S38	2.884502738	1.544217783	1.956675139	dmol	1	S	0.000	
N39	0.113710958	1.377481541	0.092786959	dmol	1	N	0.000	
N40	-1.357148292	1.552554772	2.536802879	dmol	1	N	0.000	
N41	-2.315182591	0.666362748	2.951970991	dmol	1	N	0.000	
H42	-0.438250065	1.431280915	2.989104280	dmol	1	H	0.000	
H43	-1.850902604	0.000065353	3.594069194	dmol	1	H	0.000	

	H44	-2.608381443	3.685740351	1.839106623	dmol	1	H	0.000
	H45	-4.021119638	1.466383554	1.381079994	dmol	1	H	0.000
	H46	-2.530146023	-0.984193571	1.418767748	dmol	1	H	0.000
<b>Fig 5</b>								
<b>4HN<sub>2</sub>-c</b> fe6n2enhx3b2 bfe2h3v_7a.c mmf	45							
	C1	1.901907098	7.913521600	1.037688295	dmol	1	C	0.000
	H2	2.809574244	7.522069226	0.559514746	dmol	1	H	0.000
	H3	2.015391349	8.998513985	1.197080179	dmol	1	H	0.000
	H4	1.778320977	7.419779084	2.010171541	dmol	1	H	0.000
	S5	0.407022988	7.601671354	-0.044435093	dmol	1	S	0.000
	C6	0.947669066	-3.598975977	-3.037360464	dmol	1	C	0.000
	H7	1.966833517	-3.249481266	-2.934507354	dmol	1	H	0.000
	N8	0.002147411	-3.290946539	-2.075269278	dmol	1	N	0.000
	C9	0.369516401	-4.361333982	-4.026718961	dmol	1	C	0.000
	H10	0.761416283	-4.798092649	-4.937068208	dmol	1	H	0.000
	C11	-1.136829887	-3.851846492	-2.452157746	dmol	1	C	0.000
	H12	-2.064671054	-3.792305432	-1.899094141	dmol	1	H	0.000
	N13	-0.966097266	-4.518286200	-3.641036822	dmol	1	N	0.000
	H14	-1.688086963	-5.013844444	-4.149809100	dmol	1	H	0.000
	C15	-0.137378571	-4.996956256	1.196685958	dmol	1	C	0.000
	H16	-0.650410478	-5.957526179	0.990104023	dmol	1	H	0.000
	H17	-0.077794389	-4.890590948	2.303091182	dmol	1	H	0.000
	C18	1.322403367	-5.096180200	0.691307548	dmol	1	C	0.000
	O19	1.957875920	-6.174108469	0.801386078	dmol	1	O	0.000
	O20	1.774661563	-3.987274057	0.184481573	dmol	1	O	0.000
	O21	-0.845749449	-3.918357252	0.634841927	dmol	1	O	0.000
	Fe22	0.181240460	5.266247235	-0.052051461	dmol	1	Fe	0.000
	Fe23	-1.421126089	3.175171395	0.829213885	dmol	1	Fe	0.000
	Fe24	1.282013961	2.788328149	1.007351742	dmol	1	Fe	0.000
	Fe25	0.142735615	2.822101365	-1.390921072	dmol	1	Fe	0.000
	Fe26	0.012770749	0.234661061	-1.237790635	dmol	1	Fe	0.000
	Fe27	-1.658100110	0.063592953	1.274939208	dmol	1	Fe	0.000
	Fe28	1.255158076	0.180877143	1.046406550	dmol	1	Fe	0.000
	Mo29	0.279016301	-2.275045834	0.039842540	dmol	1	Mo	0.000
	S30	-1.557830374	4.392034218	-1.178331362	dmol	1	S	0.000
	S31	-0.016125878	4.363228402	2.139445949	dmol	1	S	0.000
	S32	0.004350565	1.439555222	-3.134346246	dmol	1	S	0.000
	S33	2.006133317	4.028427249	-0.877231309	dmol	1	S	0.000
	S34	-1.768500906	-1.094693757	-0.644404647	dmol	1	S	0.000
	S35	-3.270256346	1.674306060	0.940222093	dmol	1	S	0.000
	S36	1.078427312	-1.810335710	2.411266652	dmol	1	S	0.000
	S37	2.002261462	-0.893073903	-0.907169550	dmol	1	S	0.000
	S38	2.726222274	1.545516510	2.111311723	dmol	1	S	0.000
	N39	-0.031726217	1.590809690	0.231582835	dmol	1	N	0.000
	N40	-1.073498657	0.923507387	3.132939022	dmol	1	N	0.000
N41	-1.747067944	0.042511873	3.442002238	dmol	1	N	0.000	
H42	-3.686786101	1.973802730	2.205439762	dmol	1	H	0.000	
H43	-0.010956286	-1.533655483	3.172369147	dmol	1	H	0.000	
H44	-2.468500125	4.122640455	1.417430627	dmol	1	H	0.000	
H45	-2.707576712	-0.979963318	1.611586429	dmol	1	H	0.000	
<b>TS: 4HN<sub>2</sub>-c</b> → <b>3HN<sub>2</sub>H-c</b> fe6n2hx2h2b3 btevj_1_4272. 25a.cmmf	45							
	C1	1.934688745	7.895476019	1.135496111	dmol	1	C	0.000
	H2	2.858915586	7.555000631	0.648852914	dmol	1	H	0.000
	H3	2.013556700	8.974628493	1.345637899	dmol	1	H	0.000
	H4	1.816848512	7.354582695	2.083178574	dmol	1	H	0.000
	S5	0.458182593	7.595449403	0.028579418	dmol	1	S	0.000
	C6	1.025839688	-3.593084467	-3.133877255	dmol	1	C	0.000
	H7	2.045408279	-3.249659123	-3.014970912	dmol	1	H	0.000
	N8	0.075692505	-3.302971173	-2.172310578	dmol	1	N	0.000
	C9	0.454621701	-4.337653900	-4.141613545	dmol	1	C	0.000
	H10	0.852402192	-4.761658746	-5.055392460	dmol	1	H	0.000
	C11	-1.061574851	-3.853035921	-2.568388111	dmol	1	C	0.000
	H12	-1.991918159	-3.812345980	-2.016691248	dmol	1	H	0.000
	N13	-0.884180612	-4.498526838	-3.768683726	dmol	1	N	0.000
	H14	-1.605169833	-4.976804770	-4.295956148	dmol	1	H	0.000
	C15	-0.129788719	-5.012824890	1.080089866	dmol	1	C	0.000
	H16	-0.594246672	-6.001247217	0.888652391	dmol	1	H	0.000
	H17	-0.109531126	-4.866463203	2.185012751	dmol	1	H	0.000
	C18	1.348333416	-5.059450727	0.624922320	dmol	1	C	0.000
	O19	2.019336880	-6.115691422	0.710654227	dmol	1	O	0.000
	O20	1.786613109	-3.913248760	0.182611320	dmol	1	O	0.000
	O21	-0.854710529	-3.981121158	0.458199296	dmol	1	O	0.000
	Fe22	0.243883075	5.268521054	-0.009272157	dmol	1	Fe	0.000
	Fe23	-1.334721917	3.111361649	0.836359185	dmol	1	Fe	0.000
	Fe24	1.378412811	2.792656380	0.998513041	dmol	1	Fe	0.000

	Fe25	0.224711651	2.863430432	-1.401922528	dmol	1	Fe	0.000
	Fe26	0.005756456	0.267245694	-1.247145627	dmol	1	Fe	0.000
	Fe27	-1.662784830	-0.182968981	1.561051912	dmol	1	Fe	0.000
	Fe28	1.267151537	0.197385341	1.065564407	dmol	1	Fe	0.000
	Mo29	0.262359315	-2.271418428	-0.000691851	dmol	1	Mo	0.000
	S30	-1.494143468	4.409454721	-1.141231574	dmol	1	S	0.000
	S31	0.046813761	4.322958794	2.154575256	dmol	1	S	0.000
	S32	0.010966419	1.479253884	-3.142717707	dmol	1	S	0.000
	S33	2.089495129	4.074273984	-0.858647224	dmol	1	S	0.000
	S34	-1.774909151	-1.060893726	-0.590522987	dmol	1	S	0.000
	S35	-3.153907481	1.524908822	0.936940520	dmol	1	S	0.000
	S36	0.462164458	-1.587827295	2.306949067	dmol	1	S	0.000
	S37	1.986675864	-0.849299664	-0.915597395	dmol	1	S	0.000
	S38	2.792323344	1.489134191	2.102737463	dmol	1	S	0.000
	N39	0.064299751	1.648182922	0.202902459	dmol	1	N	0.000
	N40	-1.370571044	0.886086493	3.238165207	dmol	1	N	0.000
	N41	-1.756120459	-0.222973571	-3.651886783	dmol	1	N	0.000
	H42	-3.611833190	1.930549378	2.150862641	dmol	1	H	0.000
	H43	-0.946567846	-0.928636272	3.706469454	dmol	1	H	0.000
	H44	-2.432079637	4.006501035	1.427309954	dmol	1	H	0.000
	H45	-2.756693952	-1.207235499	1.763458434	dmol	1	H	0.000
<b>3HN<sub>2</sub>H-c</b> fe6n2hx2h2b3 btcvg_5a.cmm f	45							
	C1	1.925586183	7.904566040	1.040063692	dmol	1	C	0.000
	H2	2.838253255	7.522991614	0.562202447	dmol	1	H	0.000
	H3	2.035674098	8.987654237	1.214985073	dmol	1	H	0.000
	H4	1.797709367	7.397937222	2.005709082	dmol	1	H	0.000
	S5	0.434922542	7.609608900	-0.050952266	dmol	1	S	0.000
	C6	0.989551964	-3.568269825	-3.121385393	dmol	1	C	0.000
	H7	1.997457545	-3.183934186	-3.023984816	dmol	1	H	0.000
	N8	0.048716771	-3.306231685	-2.144149061	dmol	1	N	0.000
	C9	0.426102283	-4.332107890	-4.119590747	dmol	1	C	0.000
	H10	0.821285590	-4.744024599	-5.040308306	dmol	1	H	0.000
	C11	-1.075552586	-3.888953346	-2.521209970	dmol	1	C	0.000
	H12	-2.001058313	-3.872058620	-1.958760244	dmol	1	H	0.000
	N13	-0.900889944	-4.533034733	-3.724974053	dmol	1	N	0.000
	H14	-1.615388411	-5.026957429	-4.247043450	dmol	1	H	0.000
	C15	-0.163355847	-4.942396611	1.101631296	dmol	1	C	0.000
	H16	-0.625040469	-5.900687307	0.784147884	dmol	1	H	0.000
	H17	-0.155427883	-4.950192418	2.217512018	dmol	1	H	0.000
	C18	1.317899449	-4.958898964	0.661685454	dmol	1	C	0.000
	O19	2.009166116	-5.997912609	0.751774824	dmol	1	O	0.000
	O20	1.750054665	-3.803127453	0.219539229	dmol	1	O	0.000
	O21	-0.882638164	-3.846119536	0.603508098	dmol	1	O	0.000
	Fe22	0.226552672	5.272912127	-0.101819297	dmol	1	Fe	0.000
	Fe23	-1.265516380	3.076443091	0.827322656	dmol	1	Fe	0.000
	Fe24	1.458774227	2.896883809	0.887756185	dmol	1	Fe	0.000
	Fe25	0.274168685	2.859172367	-1.508959505	dmol	1	Fe	0.000
	Fe26	0.131795012	0.272290613	-1.271221298	dmol	1	Fe	0.000
	Fe27	-1.555819906	-0.347640225	1.642297311	dmol	1	Fe	0.000
	Fe28	1.474045855	0.320252711	0.984071710	dmol	1	Fe	0.000
	Mo29	0.289702405	-2.153377401	0.138725089	dmol	1	Mo	0.000
	S30	-1.503178249	4.333737393	-1.188112757	dmol	1	S	0.000
	S31	0.091256465	4.352009290	2.086708974	dmol	1	S	0.000
	S32	0.042807253	1.407528640	-3.196136189	dmol	1	S	0.000
	S33	2.102507155	4.150321038	-1.006177862	dmol	1	S	0.000
	S34	-1.672381262	-0.966887416	-0.581269863	dmol	1	S	0.000
	S35	-3.014936617	1.419034963	1.021377346	dmol	1	S	0.000
	S36	0.460041205	-1.354521868	2.324655200	dmol	1	S	0.000
	S37	2.066037394	-0.870558066	-0.914004919	dmol	1	S	0.000
	S38	2.977019676	1.665835502	1.970545012	dmol	1	S	0.000
	N39	0.207778715	1.687246435	0.124775158	dmol	1	N	0.000
	N40	-1.341720061	0.612502435	3.448368172	dmol	1	N	0.000
	N41	-2.208091326	-0.290750504	3.613231620	dmol	1	N	0.000
	H42	-3.442358845	1.785531758	2.256989119	dmol	1	H	0.000
	H43	-1.840684441	-1.146787685	4.104328350	dmol	1	H	0.000
	H44	-2.407445040	3.935995159	1.393353151	dmol	1	H	0.000
	H45	-2.523382805	-1.485024969	1.732795848	dmol	1	H	0.000
<b>4HN<sub>2</sub>H-c</b> fe6n2hhx2b2h 3bptbu_2a.cm mf	46							
	C1	1.653831393	8.108511215	0.898724434	dmol	1	C	0.000
	H2	2.623657563	7.826617703	0.464606646	dmol	1	H	0.000
	H3	1.608768284	9.205565219	0.995335102	dmol	1	H	0.000
	H4	1.568679446	7.657149235	1.896258660	dmol	1	H	0.000
	S5	0.246143570	7.531372132	-0.193725922	dmol	1	S	0.000
	C6	1.421174323	-3.750272447	-2.834590421	dmol	1	C	0.000
	H7	2.424051468	-3.414815954	-2.602766302	dmol	1	H	0.000
	N8	0.353671955	-3.375012782	-2.036321955	dmol	1	N	0.000
	C9	0.976348843	-4.548513995	-3.864585357	dmol	1	C	0.000

	H10	1.487504783	-5.040075125	-4.683910138	dmol	1	H	0.000
	C11	-0.731178867	-3.926897621	-2.558616009	dmol	1	C	0.000
	H12	-1.731669303	-3.818936232	-2.161409165	dmol	1	H	0.000
	N13	-0.405390617	-4.656896957	-3.678054468	dmol	1	N	0.000
	H14	-1.055564589	-5.158670460	-4.271320626	dmol	1	H	0.000
	C15	-0.382072585	-4.811672049	1.304883864	dmol	1	C	0.000
	H16	-0.859947627	-5.785522268	1.074063157	dmol	1	H	0.000
	H17	-0.544112540	-4.613438457	2.389838493	dmol	1	H	0.000
	C18	1.149127953	-4.948010029	1.117447789	dmol	1	C	0.000
	O19	1.741147578	-6.011117072	1.429126181	dmol	1	O	0.000
	O20	1.709451957	-3.869065179	0.646914939	dmol	1	O	0.000
	O21	-0.946269684	-3.783758567	0.534208127	dmol	1	O	0.000
	Fe22	0.395890718	5.291061708	0.063195160	dmol	1	Fe	0.000
	Fe23	-1.345338942	2.964617907	0.697619310	dmol	1	Fe	0.000
	Fe24	1.441627042	2.875152259	0.961152427	dmol	1	Fe	0.000
	Fe25	0.240017847	2.835155392	-1.533741869	dmol	1	Fe	0.000
	Fe26	0.214160160	0.265678357	-1.322510482	dmol	1	Fe	0.000
	Fe27	-2.137278649	-0.048115687	0.924609675	dmol	1	Fe	0.000
	Fe28	1.397213322	0.252287126	0.961364611	dmol	1	Fe	0.000
	Mo29	0.313891368	-2.185930761	0.074186559	dmol	1	Mo	0.000
	S30	-1.370025687	4.443135494	-1.013733289	dmol	1	S	0.000
	S31	0.044853250	4.317972372	2.050910183	dmol	1	S	0.000
	S32	0.175260184	1.452677409	-3.259094874	dmol	1	S	0.000
	S33	2.067705548	4.212257549	-0.908156131	dmol	1	S	0.000
	S34	-1.625613899	-1.092539927	-0.946504174	dmol	1	S	0.000
	S35	-3.349636015	1.747118106	0.200188985	dmol	1	S	0.000
	S36	0.483673232	-1.379207959	2.484863199	dmol	1	S	0.000
	S37	2.146833310	-0.948282011	-0.867887238	dmol	1	S	0.000
	S38	2.951834456	1.571792054	1.935786994	dmol	1	S	0.000
	N39	0.217151133	1.634987220	0.051835605	dmol	1	N	0.000
	N40	-1.549105208	0.713059139	2.471474869	dmol	1	N	0.000
	N41	-2.654318927	0.231074429	2.936472183	dmol	1	N	0.000
	H42	-3.216095185	-1.093033725	1.000309753	dmol	1	H	0.000
	H43	-2.445075555	-0.596105709	3.542987647	dmol	1	H	0.000
	H44	-3.914271891	2.000857537	1.413005254	dmol	1	H	0.000
	H45	-2.388005788	3.830774066	1.412005716	dmol	1	H	0.000
	H46	1.597301073	-2.112982658	2.803552898	dmol	1	H	0.000
<b>TS: 4HN<sub>2</sub>H-c</b> <b>→ 4HN<sub>2</sub>H-d</b> fe6n2hxx2b2h 3bptcu_3_430 1.70a.cmmf	46							
	C1	1.623904856	8.109928918	0.845214412	dmol	1	C	0.000
	H2	2.591988741	7.822085303	0.413499877	dmol	1	H	0.000
	H3	1.579051368	9.207246920	0.938255303	dmol	1	H	0.000
	H4	1.533161013	7.659861152	1.841581669	dmol	1	H	0.000
	S5	0.209621819	7.522277657	-0.237879160	dmol	1	S	0.000
	C6	1.400006364	-3.776890246	-2.910328485	dmol	1	C	0.000
	H7	2.401287153	-3.436898991	-2.678282056	dmol	1	H	0.000
	N8	0.344819018	-3.404234368	-2.098415676	dmol	1	N	0.000
	C9	0.933252465	-4.567186236	-3.934057018	dmol	1	C	0.000
	H10	1.435816253	-5.056266607	-4.758340551	dmol	1	H	0.000
	C11	-0.756710961	-3.950218103	-2.597685654	dmol	1	C	0.000
	H12	-1.745307678	-3.838368636	-2.171661568	dmol	1	H	0.000
	N13	-0.446406653	-4.672899239	-3.725950241	dmol	1	N	0.000
	H14	-1.110205448	-5.162449084	-4.312537729	dmol	1	H	0.000
	C15	-0.392430173	-4.864397753	1.251899671	dmol	1	C	0.000
	H16	-0.880531451	-5.845708360	1.069665857	dmol	1	H	0.000
	H17	-0.558635230	-4.638536647	2.334978248	dmol	1	H	0.000
	C18	1.137516371	-5.039768917	1.077615920	dmol	1	C	0.000
	O19	1.705748460	-6.095804893	1.451086733	dmol	1	O	0.000
	O20	1.724691546	-4.005596774	0.542778047	dmol	1	O	0.000
	O21	-0.928935082	-3.864831468	0.429903992	dmol	1	O	0.000
	Fe22	0.393068611	5.302826155	-0.046960593	dmol	1	Fe	0.000
Fe23	-1.296458786	2.923893425	0.852776564	dmol	1	Fe	0.000	
Fe24	1.383963590	2.911953554	0.848962369	dmol	1	Fe	0.000	
Fe25	0.248273105	2.835625118	-1.505289292	dmol	1	Fe	0.000	
Fe26	0.197025881	0.216221875	-1.407705882	dmol	1	Fe	0.000	
Fe27	-1.763541750	-0.005710384	1.221573122	dmol	1	Fe	0.000	
Fe28	1.583530912	0.316895926	0.831592521	dmol	1	Fe	0.000	
Mo29	0.410669101	-2.306393121	-0.114609427	dmol	1	Mo	0.000	
S30	-1.428658646	4.370958487	-0.967371117	dmol	1	S	0.000	
S31	0.099726609	4.409328540	1.987922153	dmol	1	S	0.000	
S32	0.198367925	1.492577330	-3.287947839	dmol	1	S	0.000	
S33	2.083137975	4.234403274	-0.949543994	dmol	1	S	0.000	
S34	-1.598771768	-1.105835471	-0.852058767	dmol	1	S	0.000	
S35	-3.192973961	1.590928758	0.351834672	dmol	1	S	0.000	
S36	0.215140235	-1.153005155	2.037743931	dmol	1	S	0.000	
S37	2.214539704	-0.968365527	-1.009299786	dmol	1	S	0.000	
S38	3.042300806	1.730276633	1.759360657	dmol	1	S	0.000	
N39	0.178969681	1.603543222	0.063412621	dmol	1	N	0.000	
N40	-1.432490744	1.059245074	2.902067708	dmol	1	N	0.000	

	N41	-2.446942265	0.305440640	3.086459107	dmol	1	N	0.000
	H42	-2.704831279	-1.192769588	1.361155995	dmol	1	H	0.000
	H43	-2.261303318	-0.527978551	3.696751158	dmol	1	H	0.000
	H44	-3.797465512	1.815286247	1.547007830	dmol	1	H	0.000
	H45	-2.379497001	3.762766711	1.535891604	dmol	1	H	0.000
	H46	0.252518138	-1.723456797	3.284933093	dmol	1	H	0.000
<b>4HN<sub>2</sub>H-d</b> fe6n2hxx2b2h 3bto2u_2a.cm mf	46							
	C1	1.619925713	8.139541758	0.963352702	dmol	1	C	0.000
	H2	2.579618285	7.848791104	0.512686826	dmol	1	H	0.000
	H3	1.569598404	9.239891366	1.011869901	dmol	1	H	0.000
	H4	1.570594604	7.733823125	1.983981275	dmol	1	H	0.000
	S5	0.189961607	7.517688443	-0.076334020	dmol	1	S	0.000
	C6	1.434242697	-3.761787428	-2.835749031	dmol	1	C	0.000
	H7	2.433673878	-3.417241707	-2.603524795	dmol	1	H	0.000
	N8	0.370075095	-3.410742503	-2.023129542	dmol	1	N	0.000
	C9	0.987332374	-4.547090908	-3.873242149	dmol	1	C	0.000
	H10	1.497288000	-5.015607157	-4.706030362	dmol	1	H	0.000
	C11	-0.714273544	-3.968940820	-2.539339977	dmol	1	C	0.000
	H12	-1.711614365	-3.874887291	-2.130587739	dmol	1	H	0.000
	N13	-0.390605981	-4.678800029	-3.672361388	dmol	1	N	0.000
	H14	-1.044101499	-5.161048888	-4.277506960	dmol	1	H	0.000
	C15	-0.215740450	-4.876788371	1.311762063	dmol	1	C	0.000
	H16	-0.694767480	-5.843638711	1.048375107	dmol	1	H	0.000
	H17	-0.334673485	-4.745394749	2.412555301	dmol	1	H	0.000
	C18	1.307042915	-5.001824369	1.048495934	dmol	1	C	0.000
	O19	1.913332891	-6.064656605	1.330534996	dmol	1	O	0.000
	O20	1.840174800	-3.929118538	0.537098799	dmol	1	O	0.000
	O21	-0.814327454	-3.813182589	0.616317465	dmol	1	O	0.000
	Fe22	0.433911070	5.272574423	0.074548434	dmol	1	Fe	0.000
	Fe23	-1.236355320	2.932246368	0.692956959	dmol	1	Fe	0.000
	Fe24	1.501608853	2.875832109	0.923012034	dmol	1	Fe	0.000
	Fe25	0.245323847	2.795970843	-1.524709428	dmol	1	Fe	0.000
	Fe26	0.180633307	0.211519215	-1.302885204	dmol	1	Fe	0.000
	Fe27	-2.222745830	-0.138084967	0.978837235	dmol	1	Fe	0.000
	Fe28	1.574548055	0.270363527	0.876258596	dmol	1	Fe	0.000
	Mo29	0.424770222	-2.242812973	0.054333691	dmol	1	Mo	0.000
	S30	-1.337120476	4.410594146	-0.983941505	dmol	1	S	0.000
	S31	0.121229950	4.274137951	2.059910676	dmol	1	S	0.000
	S32	0.060577790	1.416637689	-3.237064644	dmol	1	S	0.000
	S33	2.069357284	4.203179769	-0.988548382	dmol	1	S	0.000
	S34	-1.608997554	-1.196604711	-0.855216615	dmol	1	S	0.000
S35	-3.215141970	1.738391172	0.172097134	dmol	1	S	0.000	
S36	0.980755296	-1.497289505	2.400116835	dmol	1	S	0.000	
S37	2.172743031	-0.945071732	-1.007751995	dmol	1	S	0.000	
S38	3.068660543	1.639381525	1.879443128	dmol	1	S	0.000	
N39	0.286670678	1.617669585	0.046569625	dmol	1	N	0.000	
N40	-1.566195236	0.403310556	2.577674340	dmol	1	N	0.000	
N41	-2.777580033	0.193283948	2.998216056	dmol	1	N	0.000	
H42	-3.463362304	-1.021626192	0.903290635	dmol	1	H	0.000	
H43	-2.804651808	-0.659490331	3.603519609	dmol	1	H	0.000	
H44	-3.939222007	2.070319499	1.278666831	dmol	1	H	0.000	
H45	-2.281576726	3.751718072	1.451617019	dmol	1	H	0.000	
H46	-0.060597350	-0.745134922	2.889825437	dmol	1	H	0.000	
<b>TS: 4HN<sub>2</sub>H-d</b> → 3HN <sub>2</sub> H <sub>2</sub> -a fe6n2hxx2b2h 3btuv_origa.c mmf	45							
	C1	1.298264	6.476746	0.948166	dmol	1	C	0.000
	H2	2.278305	6.195511	0.542023	dmol	1	H	0.000
	H3	1.247269	7.572037	1.057709	dmol	1	H	0.000
	H4	1.174011	6.008652	1.932053	dmol	1	H	0.000
	S5	-0.074371	5.897415	-0.189163	dmol	1	S	0.000
	C6	1.305389	-5.365219	-2.865494	dmol	1	C	0.000
	H7	2.292526	-5.024521	-2.579605	dmol	1	H	0.000
	N8	0.198730	-4.982712	-2.129532	dmol	1	N	0.000
	C9	0.914307	-6.170349	-3.910446	dmol	1	C	0.000
	H10	1.467163	-6.673828	-4.694200	dmol	1	H	0.000
	C11	-0.859848	-5.536804	-2.700180	dmol	1	C	0.000
	H12	-1.878677	-5.425018	-2.352386	dmol	1	H	0.000
	N13	-0.476746	-6.274658	-3.795959	dmol	1	N	0.000
	H14	-1.096771	-6.777786	-4.419342	dmol	1	H	0.000
	C15	-0.746918	-6.382385	1.176208	dmol	1	C	0.000
	H16	-1.244751	-7.344131	0.937561	dmol	1	H	0.000
	H17	-0.959442	-6.162415	2.247559	dmol	1	H	0.000
	C18	0.783234	-6.574524	1.068054	dmol	1	C	0.000
	O19	1.320175	-7.638657	1.461166	dmol	1	O	0.000
	O20	1.403793	-5.547287	0.557587	dmol	1	O	0.000
	O21	-1.235900	-5.353256	0.359955	dmol	1	O	0.000
	Fe22	0.078064	3.670425	-0.055710	dmol	1	Fe	0.000
	Fe23	-1.620422	1.317612	0.560532	dmol	1	Fe	0.000

	Fe24	1.162170	1.236542	0.961456	dmol	1	Fe	0.000
	Fe25	0.003189	1.251129	-1.567093	dmol	1	Fe	0.000
	Fe26	-0.028061	-1.339386	-1.394608	dmol	1	Fe	0.000
	Fe27	-2.428986	-1.759796	0.836105	dmol	1	Fe	0.000
	Fe28	1.242889	-1.382400	0.961868	dmol	1	Fe	0.000
	Mo29	0.113571	-3.804000	-0.044968	dmol	1	Mo	0.000
	S30	-1.679626	2.803970	-1.146652	dmol	1	S	0.000
	S31	-0.313812	2.724686	1.927917	dmol	1	S	0.000
	S32	0.005890	-0.125198	-3.314636	dmol	1	S	0.000
	S33	1.867600	2.624466	-0.823273	dmol	1	S	0.000
	S34	-1.850418	-2.724716	-1.077271	dmol	1	S	0.000
	S35	-3.549988	0.030930	0.091690	dmol	1	S	0.000
	S36	0.351547	-3.092957	2.316452	dmol	1	S	0.000
	S37	1.964400	-2.529968	-0.953690	dmol	1	S	0.000
	S38	2.614868	0.008209	2.095963	dmol	1	S	0.000
	N39	0.000000	0.000000	0.000000	dmol	1	N	0.000
	N40	-1.785034	-1.102875	2.494202	dmol	1	N	0.000
	N41	-2.994400	-1.495895	2.806473	dmol	1	N	0.000
	H42	-3.482742	-2.843094	0.852966	dmol	1	H	0.000
	H43	-2.987961	-2.381195	3.360733	dmol	1	H	0.000
	H44	-4.206985	0.348694	1.242920	dmol	1	H	0.000
	H45	-2.706360	2.161224	1.227982	dmol	1	H	0.000
	H46	-0.672180	-2.080154	2.715210	dmol	1	H	0.000
<b>3HN<sub>2</sub>H<sub>2</sub>-a</b> fe6n2hxx2b2h 3btuu_7a.cmm f	46							
	C1	1.639305047	8.085925847	1.043785502	dmol	1	C	0.000
	H2	2.586796469	7.753286256	0.598959538	dmol	1	H	0.000
	H3	1.592126998	9.186560039	1.011878099	dmol	1	H	0.000
	H4	1.603994913	7.758790519	2.091559992	dmol	1	H	0.000
	S5	0.180976079	7.392906898	0.093546999	dmol	1	S	0.000
	C6	1.626095651	-3.867192648	-2.950981085	dmol	1	C	0.000
	H7	2.613923850	-3.503963069	-2.695710583	dmol	1	H	0.000
	N8	0.544469173	-3.561900547	-2.146315929	dmol	1	N	0.000
	C9	1.210810743	-4.635864929	-4.015359644	dmol	1	C	0.000
	H10	1.739053839	-5.078246958	-4.851121707	dmol	1	H	0.000
	C11	-0.520586643	-4.126619556	-2.691158355	dmol	1	C	0.000
	H12	-1.522292755	-4.073968568	-2.284041650	dmol	1	H	0.000
	N13	-0.167740028	-4.797575519	-3.837907916	dmol	1	N	0.000
	H14	-0.804426867	-5.271231448	-4.467691239	dmol	1	H	0.000
	C15	-0.306572997	-4.998221707	1.196382161	dmol	1	C	0.000
	H16	-0.701725835	-6.012748730	0.982309251	dmol	1	H	0.000
	H17	-0.555397846	-4.774171995	2.261690717	dmol	1	H	0.000
	C18	1.237017565	-5.053439528	1.121756095	dmol	1	C	0.000
	O19	1.869515116	-6.061431125	1.515562369	dmol	1	O	0.000
	O20	1.772888826	-3.963564885	0.634447610	dmol	1	O	0.000
	O21	-0.863568868	-4.047535314	0.330790801	dmol	1	O	0.000
	Fe22	0.442940570	5.171176554	0.219852176	dmol	1	Fe	0.000
	Fe23	-1.512027225	2.800892065	0.970612401	dmol	1	Fe	0.000
	Fe24	1.344565689	2.668326544	1.071956835	dmol	1	Fe	0.000
	Fe25	0.247252151	2.752275866	-1.300396798	dmol	1	Fe	0.000
	Fe26	0.217566912	0.144812037	-1.396642321	dmol	1	Fe	0.000
	Fe27	-1.762413028	0.050680355	0.981425920	dmol	1	Fe	0.000
	Fe28	1.381998135	0.045863281	1.074452666	dmol	1	Fe	0.000
	Mo29	0.373124008	-2.367044979	-0.028833151	dmol	1	Mo	0.000
	S30	-1.370907955	4.352566426	-0.827354315	dmol	1	S	0.000
	S31	0.025565828	4.196287610	2.171358188	dmol	1	S	0.000
	S32	0.254227117	1.527893482	-3.175042816	dmol	1	S	0.000
	S33	2.126102162	4.046411302	-0.645846854	dmol	1	S	0.000
	S34	-1.575481626	-1.243725376	-0.986919168	dmol	1	S	0.000
	S35	-3.255562907	1.584553022	-0.060300951	dmol	1	S	0.000
S36	-0.111375100	-1.372043251	2.117650672	dmol	1	S	0.000	
S37	2.216378352	-1.002400041	-0.844839218	dmol	1	S	0.000	
S38	2.713224731	1.387754223	2.293998265	dmol	1	S	0.000	
N39	0.143516717	1.424184049	0.143846266	dmol	1	N	0.000	
N40	-1.564331470	1.443407939	2.400791807	dmol	1	N	0.000	
N41	-2.620970555	0.639739814	2.737951291	dmol	1	N	0.000	
H42	-2.763741728	-1.058561565	1.206595410	dmol	1	H	0.000	
H43	-2.262345475	-0.055237920	3.417530899	dmol	1	H	0.000	
H44	-4.117921035	1.631002564	0.988595034	dmol	1	H	0.000	
H45	-2.638978462	3.621121621	1.587895414	dmol	1	H	0.000	
H46	-0.705068071	1.260271344	2.939281320	dmol	1	H	0.000	
Fig 6								
<b>3HN<sub>2</sub>H<sub>2</sub>-a</b>	46							
	C1	1.488702723	8.216159705	0.623565643	dmol	1	C	0.000
	H2	2.469930288	7.980472901	0.188908913	dmol	1	H	0.000

fe626n2h26x2 x2btgas_2a.cm mf	H3	1.350844068	9.309935264	0.623144663	dmol	1	H	0.000	
	H4	1.462938312	7.854681291	1.659839414	dmol	1	H	0.000	
	S5	0.109255859	7.435154531	-0.376128633	dmol	1	S	0.000	
	C6	1.469417008	-3.841823901	-3.031455291	dmol	1	C	0.000	
	H7	2.433930135	-3.356963098	-2.943624106	dmol	1	H	0.000	
	N8	0.497589548	-3.645634010	-2.066561696	dmol	1	N	0.000	
	C9	0.989679912	-4.682374364	-4.011435529	dmol	1	C	0.000	
	H10	1.431568547	-5.083056752	-4.916059452	dmol	1	H	0.000	
	C11	-0.564826273	-4.342906243	-2.437319453	dmol	1	C	0.000	
	H12	-1.483832952	-4.403027625	-1.867736572	dmol	1	H	0.000	
	N13	-0.315384832	-4.998498690	-3.619689732	dmol	1	N	0.000	
	H14	-0.978769354	-5.563214040	-4.136920897	dmol	1	H	0.000	
	C15	-0.156787013	-5.030996917	1.319363273	dmol	1	C	0.000	
	H16	-0.494362367	-6.057855474	1.064285234	dmol	1	H	0.000	
	H17	-0.426979044	-4.864310785	2.388611817	dmol	1	H	0.000	
	C18	1.389265615	-5.006314501	1.256928674	dmol	1	C	0.000	
	O19	2.063604878	-5.975624115	1.679380466	dmol	1	O	0.000	
	O20	1.871961534	-3.904436786	0.750566864	dmol	1	O	0.000	
	O21	-0.762453715	-4.075365317	0.490249145	dmol	1	O	0.000	
	Fe22	0.305180844	5.216779150	-0.089252363	dmol	1	Fe	0.000	
	Fe23	-1.497339925	2.846003969	1.044092893	dmol	1	Fe	0.000	
	Fe24	1.344223007	2.748506997	0.879458381	dmol	1	Fe	0.000	
	Fe25	0.129903186	2.653819634	-1.468714435	dmol	1	Fe	0.000	
	Fe26	0.166005696	0.094502785	-1.378164757	dmol	1	Fe	0.000	
	Fe27	-1.646226069	0.082380713	1.150502085	dmol	1	Fe	0.000	
	Fe28	1.434735134	0.164694533	0.918221409	dmol	1	Fe	0.000	
	Mo29	0.417469253	-2.379186489	0.034854038	dmol	1	Mo	0.000	
	S30	-1.497559938	4.210673911	-0.946875384	dmol	1	S	0.000	
	S31	0.059164004	4.323421188	1.951072639	dmol	1	S	0.000	
	S32	0.024076543	1.316514045	-3.250294017	dmol	1	S	0.000	
	S33	1.940909774	4.049918364	-0.969852931	dmol	1	S	0.000	
	S34	-1.596192536	-1.287211281	-0.793531953	dmol	1	S	0.000	
	S35	-3.291198033	1.559295209	0.221909886	dmol	1	S	0.000	
	S36	0.106578212	-1.282618838	2.162309179	dmol	1	S	0.000	
	S37	2.173008841	-1.010875641	-0.939449795	dmol	1	S	0.000	
	S38	2.822587990	1.538284923	2.032587265	dmol	1	S	0.000	
	N39	0.096381094	1.419451469	0.105072372	dmol	1	N	0.000	
	N40	-1.371478005	1.515627490	2.517332229	dmol	1	N	0.000	
	N41	-2.366287766	0.690905790	2.968256492	dmol	1	N	0.000	
	H42	-0.456740273	1.362309111	2.967724582	dmol	1	H	0.000	
	H43	-1.924883215	0.024933201	3.628530018	dmol	1	H	0.000	
	H44	-2.570418671	3.642137434	1.770585028	dmol	1	H	0.000	
	H45	-4.043023358	1.570541346	1.356006878	dmol	1	H	0.000	
	H46	-2.604168743	-1.034810086	1.489707519	dmol	1	H	0.000	
	TS: 3HN <sub>2</sub> H <sub>2</sub> - a → 2HN <sub>2</sub> H <sub>3</sub> - b fe626n2h26x2 x2btg9_1_434 5.66a.cmmf	46							
		C1	1.459522098	8.224948427	0.625412525	dmol	1	C	0.000
H2		2.420343712	7.981107513	0.152264569	dmol	1	H	0.000	
H3		1.324665548	9.319134115	0.619931621	dmol	1	H	0.000	
H4		1.477620805	7.873669243	1.665894033	dmol	1	H	0.000	
S5		0.044569395	7.439573342	-0.317842518	dmol	1	S	0.000	
C6		1.483333443	-3.898601040	-2.992900967	dmol	1	C	0.000	
H7		2.463412735	-3.452199784	-2.878572142	dmol	1	H	0.000	
N8		0.491429446	-3.656925417	-2.059623363	dmol	1	N	0.000	
C9		1.000726479	-4.728864635	-3.980174731	dmol	1	C	0.000	
H10		1.451802924	-5.150417054	-4.870542701	dmol	1	H	0.000	
C11		-0.584668823	-4.319079090	-2.454247805	dmol	1	C	0.000	
H12		-1.521601310	-4.341264305	-1.912363063	dmol	1	H	0.000	
N13		-0.325996933	-4.993429130	-3.623943442	dmol	1	N	0.000	
H14		-0.997814976	-5.530018101	-4.159985628	dmol	1	H	0.000	
C15		-0.172351588	-5.000831310	1.328455354	dmol	1	C	0.000	
H16		-0.525328354	-6.029308970	1.103633094	dmol	1	H	0.000	
H17		-0.417541199	-4.806863515	2.399562191	dmol	1	H	0.000	
C18		1.373000603	-4.995342720	1.235817013	dmol	1	C	0.000	
O19		2.044648118	-5.971687067	1.647235050	dmol	1	O	0.000	
O20		1.858758988	-3.900213630	0.718471058	dmol	1	O	0.000	
O21		-0.781979417	-4.056851355	0.489008022	dmol	1	O	0.000	
Fe22		0.286553903	5.227405285	-0.056363693	dmol	1	Fe	0.000	
Fe23		-1.469457511	2.835922404	0.932870695	dmol	1	Fe	0.000	
Fe24		1.350552077	2.764473522	0.894960373	dmol	1	Fe	0.000	
Fe25		0.147184278	2.682892062	-1.481294222	dmol	1	Fe	0.000	
Fe26		0.193643728	0.122095467	-1.418226223	dmol	1	Fe	0.000	
Fe27		-1.650990331	0.056629244	1.091707206	dmol	1	Fe	0.000	
Fe28		1.438816574	0.164494531	0.903504886	dmol	1	Fe	0.000	
Mo29		0.405337656	-2.367955284	0.009293103	dmol	1	Mo	0.000	
S30		-1.486486884	4.236891331	-0.985690677	dmol	1	S	0.000	
S31		0.043742691	4.316708821	1.970352195	dmol	1	S	0.000	
S32		0.082040694	1.363823326	-3.281015904	dmol	1	S	0.000	
S33	1.950516302	4.087117449	-0.939226935	dmol	1	S	0.000		

	S34	-1.592395104	-1.257874112	-0.858642861	dmol	1	S	0.000
	S35	-3.384030489	1.608940781	0.396271373	dmol	1	S	0.000
	S36	0.090800415	-1.280726495	2.139599029	dmol	1	S	0.000
	S37	2.176860711	-1.014513095	-0.954764871	dmol	1	S	0.000
	S38	2.809061136	1.522845537	2.052845784	dmol	1	S	0.000
	N39	0.124062572	1.445973361	0.057655350	dmol	1	N	0.000
	N40	-1.352046500	1.499813437	2.425884361	dmol	1	N	0.000
	N41	-2.448709501	0.750067319	2.789895920	dmol	1	N	0.000
	H42	-0.523157213	1.319020623	3.001022751	dmol	1	H	0.000
	H43	-2.291354671	0.103113173	3.575241503	dmol	1	H	0.000
	H44	-2.516468954	3.736301300	1.561983745	dmol	1	H	0.000
	H45	-3.382737800	1.180191192	2.053912778	dmol	1	H	0.000
	H46	-2.567889213	-1.110186695	1.382735778	dmol	1	H	0.000
<b>2HN<sub>2</sub>H<sub>3</sub>-b</b> fe626n2h26x2 x2btf9_3a.cm mf	46							
	C1	1.489223907	8.216617033	0.602623134	dmol	1	C	0.000
	H2	2.463936458	7.971732115	0.156739512	dmol	1	H	0.000
	H3	1.361306717	9.311917420	0.601467752	dmol	1	H	0.000
	H4	1.478010786	7.862274284	1.642452774	dmol	1	H	0.000
	S5	0.084374393	7.446467020	-0.370075062	dmol	1	S	0.000
	C6	1.460901320	-3.829565333	-3.029180582	dmol	1	C	0.000
	H7	2.423632393	-3.341544470	-2.941077508	dmol	1	H	0.000
	N8	0.486933284	-3.631036235	-2.067046916	dmol	1	N	0.000
	C9	0.986228253	-4.677231501	-4.005385170	dmol	1	C	0.000
	H10	1.430814673	-5.078812825	-4.908317154	dmol	1	H	0.000
	C11	-0.571420803	-4.335828633	-2.434787519	dmol	1	C	0.000
	H12	-1.490825828	-4.398976699	-1.866086718	dmol	1	H	0.000
	N13	-0.317458761	-4.997774020	-3.613066496	dmol	1	N	0.000
	H14	-0.978755470	-5.563611297	-4.131702966	dmol	1	H	0.000
	C15	-0.173074083	-4.998058754	1.305612827	dmol	1	C	0.000
	H16	-0.510489566	-6.024021296	1.042574377	dmol	1	H	0.000
	H17	-0.436455970	-4.844342989	2.378823965	dmol	1	H	0.000
	C18	1.372787846	-4.973405669	1.233708154	dmol	1	C	0.000
	O19	2.050468217	-5.940795074	1.655498982	dmol	1	O	0.000
	O20	1.853029576	-3.874067032	0.720509997	dmol	1	O	0.000
	O21	-0.782264946	-4.032505086	0.491976910	dmol	1	O	0.000
	Fe22	0.309941034	5.223370722	-0.022626711	dmol	1	Fe	0.000
	Fe23	-1.495743670	2.695831191	0.817361669	dmol	1	Fe	0.000
	Fe24	1.447135216	2.834988652	0.874164455	dmol	1	Fe	0.000
	Fe25	0.284996342	2.736156343	-1.500161313	dmol	1	Fe	0.000
	Fe26	0.165484414	0.165727242	-1.390305996	dmol	1	Fe	0.000
	Fe27	-1.909880435	-0.100099489	1.132355983	dmol	1	Fe	0.000
	Fe28	1.466818139	0.208615223	0.910678814	dmol	1	Fe	0.000
	Mo29	0.401285333	-2.336375860	0.034180153	dmol	1	Mo	0.000
	S30	-1.413831784	4.215575092	-1.010296036	dmol	1	S	0.000
	S31	0.016120493	4.251986950	1.981583502	dmol	1	S	0.000
	S32	0.142429716	1.404421086	-3.272140829	dmol	1	S	0.000
	S33	2.030061268	4.188858176	-0.955858963	dmol	1	S	0.000
	S34	-1.611400692	-1.265692504	-0.842466976	dmol	1	S	0.000
	S35	-3.316821735	1.466373718	0.148889834	dmol	1	S	0.000
	S36	0.089628456	-1.253494473	2.152869001	dmol	1	S	0.000
	S37	2.152497575	-0.991421572	-0.956880320	dmol	1	S	0.000
	S38	2.885921866	1.550011970	2.019693156	dmol	1	S	0.000
	N39	0.237647919	1.559523988	0.010231200	dmol	1	N	0.000
	N40	-1.412672731	1.400110473	2.299778528	dmol	1	N	0.000
	N41	-2.541096208	0.729095033	2.835449618	dmol	1	N	0.000
	H42	-0.582193843	1.253133129	2.884772403	dmol	1	H	0.000
	H43	-2.408385040	0.251527508	3.733565036	dmol	1	H	0.000
	H44	-2.550071726	3.623686852	1.424025300	dmol	1	H	0.000
	H45	-3.405714572	1.259116380	2.654476269	dmol	1	H	0.000
	H46	-2.663057732	-1.338456791	1.571400198	dmol	1	H	0.000
<b>TS: 2HN<sub>2</sub>H<sub>3</sub>-b</b> → <b>1HN<sub>2</sub>H<sub>4</sub>-a</b> fe626n2h36x2 xtvk_origa.cm mf	46							
	C1	1.332397	6.553680	0.601334	dmol	1	C	0.000
	H2	2.293000	6.285217	0.139160	dmol	1	H	0.000
	H3	1.231049	7.651611	0.603729	dmol	1	H	0.000
	H4	1.330414	6.196503	1.640228	dmol	1	H	0.000
	S5	-0.106506	5.818893	-0.352097	dmol	1	S	0.000
	C6	1.151627	-5.451233	-3.111633	dmol	1	C	0.000
	H7	2.118851	-4.970718	-3.029404	dmol	1	H	0.000
	N8	0.188248	-5.253128	-2.139832	dmol	1	N	0.000
	C9	0.662964	-6.289108	-4.090271	dmol	1	C	0.000
	H10	1.095154	-6.687088	-5.000809	dmol	1	H	0.000
	C11	-0.877914	-5.948196	-2.502747	dmol	1	C	0.000
	H12	-1.792770	-6.007400	-1.926010	dmol	1	H	0.000
	N13	-0.639481	-6.603683	-3.687988	dmol	1	N	0.000
	H14	-1.310135	-7.162292	-4.202972	dmol	1	H	0.000
	C15	-0.477051	-6.636154	1.219223	dmol	1	C	0.000
	H16	-0.824448	-7.656021	0.949661	dmol	1	H	0.000

	H17	-0.739349	-6.484146	2.292572	dmol	1	H	0.000
	C18	1.068008	-6.623306	1.147003	dmol	1	C	0.000
	O19	1.735443	-7.600937	1.562332	dmol	1	O	0.000
	O20	1.556183	-5.523438	0.641724	dmol	1	O	0.000
	O21	-1.081345	-5.663910	0.408569	dmol	1	O	0.000
	Fe22	0.111191	3.591995	-0.041855	dmol	1	Fe	0.000
	Fe23	-1.637650	0.935562	0.638306	dmol	1	Fe	0.000
	Fe24	1.284561	1.190887	0.822510	dmol	1	Fe	0.000
	Fe25	0.122620	1.114578	-1.550247	dmol	1	Fe	0.000
	Fe26	-0.125641	-1.448441	-1.411270	dmol	1	Fe	0.000
	Fe27	-2.239700	-1.840927	1.100555	dmol	1	Fe	0.000
	Fe28	1.172043	-1.439865	0.905045	dmol	1	Fe	0.000
	Mo29	0.095932	-3.960342	-0.012619	dmol	1	Mo	0.000
	S30	-1.616882	2.563232	-1.045364	dmol	1	S	0.000
	S31	-0.116714	2.618408	1.924545	dmol	1	S	0.000
	S32	-0.068771	-0.227020	-3.310715	dmol	1	S	0.000
	S33	1.840759	2.574844	-0.989258	dmol	1	S	0.000
	S34	-1.889206	-2.895233	-0.945587	dmol	1	S	0.000
	S35	-3.552887	-0.117462	0.142136	dmol	1	S	0.000
	S36	-0.219437	-2.919785	2.106918	dmol	1	S	0.000
	S37	1.858704	-2.601181	-0.978134	dmol	1	S	0.000
	S38	2.658707	-0.144119	1.988403	dmol	1	S	0.000
	N39	0.000000	0.000000	0.000000	dmol	1	N	0.000
	N40	-1.663406	-0.159912	2.400085	dmol	1	N	0.000
	N41	-2.780823	-0.971786	2.810303	dmol	1	N	0.000
	H42	-0.835052	-0.339066	2.973938	dmol	1	H	0.000
	H43	-2.653473	-1.362625	3.743011	dmol	1	H	0.000
	H44	-2.111649	1.241776	2.099503	dmol	1	H	0.000
	H45	-3.644897	-0.425552	2.699631	dmol	1	H	0.000
	H46	-3.096695	-3.069229	1.440521	dmol	1	H	0.000
<b>1HN<sub>2</sub>H<sub>4</sub>-a</b>	46							
fe626n2h36x2	C1	1.535254386	8.195982812	0.574863846	dmol	1	C	0.000
xtvk_4a.cmmf	H2	2.497591080	7.898193653	0.135930392	dmol	1	H	0.000
	H3	1.471294975	9.296885614	0.587404831	dmol	1	H	0.000
	H4	1.492321196	7.826130367	1.608248562	dmol	1	H	0.000
	S5	0.107423511	7.507825022	-0.430061411	dmol	1	S	0.000
	C6	1.359873078	-3.756303966	-3.051933523	dmol	1	C	0.000
	H7	2.308221159	-3.238961978	-2.967577076	dmol	1	H	0.000
	N8	0.394304427	-3.613055372	-2.072863204	dmol	1	N	0.000
	C9	0.897335686	-4.592185074	-4.045549365	dmol	1	C	0.000
	H10	1.336239049	-4.951920059	-4.969194349	dmol	1	H	0.000
	C11	-0.645750805	-4.339242121	-2.445062205	dmol	1	C	0.000
	H12	-1.558193240	-4.435359406	-1.868865815	dmol	1	H	0.000
	N13	-0.389743174	-4.964856143	-3.643098964	dmol	1	N	0.000
	H14	-1.045526432	-5.528296080	-4.171789219	dmol	1	H	0.000
	C15	-0.286967938	-4.968514200	1.248988001	dmol	1	C	0.000
	H16	-0.602760410	-5.989896810	0.944015906	dmol	1	H	0.000
	H17	-0.531378044	-4.873167254	2.333639906	dmol	1	H	0.000
	C18	1.256746899	-4.899493789	1.148188032	dmol	1	C	0.000
	O19	1.966403144	-5.862008269	1.527268359	dmol	1	O	0.000
	O20	1.699592996	-3.772694959	0.663784680	dmol	1	O	0.000
	O21	-0.944718516	-3.986233499	0.489450166	dmol	1	O	0.000
	Fe22	0.318390844	5.279474259	-0.103205778	dmol	1	Fe	0.000
	Fe23	-1.299943524	2.708786650	0.703488591	dmol	1	Fe	0.000
	Fe24	1.479126657	2.885024707	0.864257413	dmol	1	Fe	0.000
	Fe25	0.427094557	2.757332747	-1.560731088	dmol	1	Fe	0.000
	Fe26	0.129719350	0.206483024	-1.406825544	dmol	1	Fe	0.000
	Fe27	-1.846183006	-0.382653231	0.951860620	dmol	1	Fe	0.000
	Fe28	1.311424306	0.260954757	0.959885453	dmol	1	Fe	0.000
	Mo29	0.177649952	-2.252363939	0.069340538	dmol	1	Mo	0.000
	S30	-1.342428945	4.179031503	-1.128449302	dmol	1	S	0.000
	S31	0.044236197	4.361694859	1.915164546	dmol	1	S	0.000
	S32	0.313544871	1.384161894	-3.308870251	dmol	1	S	0.000
	S33	2.106258264	4.234350401	-0.930327420	dmol	1	S	0.000
	S34	-1.669645067	-1.265539061	-1.103674562	dmol	1	S	0.000
	S35	-3.134427661	1.434534424	0.098478459	dmol	1	S	0.000
	S36	-0.074559046	-1.242208470	2.173991862	dmol	1	S	0.000
	S37	2.037993182	-0.986425099	-0.841952794	dmol	1	S	0.000
	S38	2.762169395	1.531011836	2.125610401	dmol	1	S	0.000
	N39	0.188917545	1.651682798	0.037080248	dmol	1	N	0.000
	N40	-1.397019057	1.816727782	2.662389456	dmol	1	N	0.000
	N41	-2.305925488	0.672051130	2.677815052	dmol	1	N	0.000
	H42	-0.449994215	1.468140613	2.858974239	dmol	1	H	0.000
	H43	-2.333875983	0.202140538	3.591841704	dmol	1	H	0.000
	H44	-1.638921327	2.512580643	3.377910337	dmol	1	H	0.000
	H45	-3.218987123	1.036321149	2.344866850	dmol	1	H	0.000
	H46	-2.902177871	-1.406124403	1.375293419	dmol	1	H	0.000

<b>TS: 3HN<sub>2</sub>H<sub>2</sub>-a</b> <b>→ 2HN<sub>2</sub>H<sub>3</sub>-a</b> fe6n2h2n2x2b 6htun_1_4335. 62a.cmmf	46						
	C1	1.514448761	8.225688466	0.699325283	dmol	1	C 0.000
	H2	2.463845995	7.974100332	0.209378796	dmol	1	H 0.000
	H3	1.385372303	9.319446423	0.694503216	dmol	1	H 0.000
	H4	1.548105830	7.877119782	1.739016776	dmol	1	H 0.000
	S5	0.066867283	7.440537634	-0.199395776	dmol	1	S 0.000
	C6	1.483887742	-3.852045193	-3.031551872	dmol	1	C 0.000
	H7	2.467068378	-3.413508573	-2.911884542	dmol	1	H 0.000
	N8	0.492930965	-3.611852154	-2.096913677	dmol	1	N 0.000
	C9	0.996588792	-4.671098483	-4.026425815	dmol	1	C 0.000
	H10	1.444862497	-5.089097566	-4.920160287	dmol	1	H 0.000
	C11	-0.586395412	-4.264867058	-2.496661951	dmol	1	C 0.000
	H12	-1.522757411	-4.287590177	-1.953347945	dmol	1	H 0.000
	N13	-0.332169965	-4.930337432	-3.672552388	dmol	1	N 0.000
	H14	-1.006811250	-5.458408490	-4.213587447	dmol	1	H 0.000
	C15	-0.182231788	-4.984709129	1.274411877	dmol	1	C 0.000
	H16	-0.534423257	-6.012639818	1.0426758671	dmol	1	H 0.000
	H17	-0.422043605	-4.801963090	2.349491379	dmol	1	H 0.000
	C18	1.361953762	-4.976771805	1.176166458	dmol	1	C 0.000
	O19	2.037531813	-5.957733684	1.568268052	dmol	1	O 0.000
	O20	1.851136714	-3.872190000	0.675305271	dmol	1	O 0.000
	O21	-0.798778661	-4.036710044	0.446967162	dmol	1	O 0.000
	Fe22	0.400021962	5.228600894	0.011479305	dmol	1	Fe 0.000
	Fe23	-1.358835487	2.739812674	0.851995086	dmol	1	Fe 0.000
	Fe24	1.393726642	2.800938733	0.932960457	dmol	1	Fe 0.000
	Fe25	0.239145225	2.766580503	-1.441940183	dmol	1	Fe 0.000
	Fe26	0.127093130	0.141958037	-1.375505204	dmol	1	Fe 0.000
	Fe27	-1.734769629	0.001001731	1.122020455	dmol	1	Fe 0.000
	Fe28	1.411410192	0.167032641	0.959410531	dmol	1	Fe 0.000
	Mo29	0.399272538	-2.335417074	0.007272488	dmol	1	Mo 0.000
	S30	-1.440449333	4.297661506	-0.886156709	dmol	1	S 0.000
	S31	0.040670404	4.308566768	2.023783088	dmol	1	S 0.000
	S32	0.109210589	1.443055887	-3.233107135	dmol	1	S 0.000
	S33	2.085327726	4.116004248	-0.886404310	dmol	1	S 0.000
	S34	-1.638749132	-1.255361440	-0.841263592	dmol	1	S 0.000
	S35	-3.283262612	1.593514901	0.107403748	dmol	1	S 0.000
	S36	0.037182832	-1.284882127	2.161708911	dmol	1	S 0.000
	S37	2.156876226	-0.956703743	-0.951111917	dmol	1	S 0.000
	S38	2.839882041	1.531340907	2.060663834	dmol	1	S 0.000
	N39	0.148297689	1.543319174	0.095133951	dmol	1	N 0.000
	N40	-1.510156510	1.421957815	2.521019525	dmol	1	N 0.000
	N41	-2.545819231	0.558900714	2.864288404	dmol	1	N 0.000
	H42	-0.681214235	1.416265861	3.128592578	dmol	1	H 0.000
	H43	-2.130781165	-0.096778653	3.549927715	dmol	1	H 0.000
	H44	-2.063842137	2.719114610	2.271876413	dmol	1	H 0.000
	H45	-4.045019594	1.659937092	1.234313203	dmol	1	H 0.000
H46	-2.684207618	-1.141791598	1.358528118	dmol	1	H 0.000	
<b>2HN<sub>2</sub>H<sub>3</sub>-a</b> fe6n2h2n2x2b 6htum_6a.cm mf	46						
	C1	1.501962445	8.213690352	0.679417107	dmol	1	C 0.000
	H2	2.447757944	7.937034308	0.194337568	dmol	1	H 0.000
	H3	1.399842332	9.311492730	0.674522909	dmol	1	H 0.000
	H4	1.523816154	7.864287820	1.720349385	dmol	1	H 0.000
	S5	0.045256752	7.457600189	-0.223549390	dmol	1	S 0.000
	C6	1.456097910	-3.811104459	-3.020268383	dmol	1	C 0.000
	H7	2.420726063	-3.331402230	-2.905184639	dmol	1	H 0.000
	N8	0.467029661	-3.627390443	-2.072247767	dmol	1	N 0.000
	C9	0.993359428	-4.634202555	-4.024716358	dmol	1	C 0.000
	H10	1.446068577	-5.014951118	-4.932944934	dmol	1	H 0.000
	C11	-0.586518292	-4.318405122	-2.472083849	dmol	1	C 0.000
	H12	-1.517994650	-4.383009807	-1.923028472	dmol	1	H 0.000
	N13	-0.317951822	-4.957956138	-3.659720907	dmol	1	N 0.000
	H14	-0.978576570	-5.497367223	-4.207223389	dmol	1	H 0.000
	C15	-0.236604452	-4.949043813	1.257521003	dmol	1	C 0.000
	H16	-0.552012312	-5.977930017	0.979962712	dmol	1	H 0.000
	H17	-0.473955447	-4.829318575	2.341322041	dmol	1	H 0.000
	C18	1.305449499	-4.882726552	1.146013475	dmol	1	C 0.000
	O19	2.021689108	-5.841730417	1.518864179	dmol	1	O 0.000
	O20	1.748407760	-3.755553602	0.656550669	dmol	1	O 0.000
O21	-0.897174204	-3.984944056	0.479358607	dmol	1	O 0.000	
Fe22	0.334028546	5.220361560	-0.110590000	dmol	1	Fe 0.000	
Fe23	-1.305514360	2.609144611	0.784965664	dmol	1	Fe 0.000	
Fe24	1.493893018	2.839604924	0.981681407	dmol	1	Fe 0.000	
Fe25	0.266824284	2.812742676	-1.498069149	dmol	1	Fe 0.000	
Fe26	0.185384647	0.214814790	-1.364147797	dmol	1	Fe 0.000	
Fe27	-1.765645489	-0.326654246	0.952660785	dmol	1	Fe 0.000	
Fe28	1.298847756	0.211130687	0.999252079	dmol	1	Fe 0.000	
Mo29	0.236234422	-2.243896480	0.049525434	dmol	1	Mo 0.000	
S30	-1.475759770	4.206028916	-1.021132924	dmol	1	S 0.000	

	S31	-0.012352927	4.331587414	1.908493741	dmol	1	S	0.000
	S32	0.232271110	1.425783607	-3.252802013	dmol	1	S	0.000
	S33	2.149641260	4.141481799	-0.882308136	dmol	1	S	0.000
	S34	-1.589615254	-1.246512637	-1.142165494	dmol	1	S	0.000
	S35	-3.205830812	1.382883432	0.050768360	dmol	1	S	0.000
	S36	-0.068683610	-1.257138393	2.183451418	dmol	1	S	0.000
	S37	2.099959344	-0.954525552	-0.823377239	dmol	1	S	0.000
	S38	2.758103714	1.451824922	2.196222040	dmol	1	S	0.000
	N39	0.170323774	1.593414711	0.105640206	dmol	1	N	0.000
	N40	-1.513235093	1.799483058	2.682062479	dmol	1	N	0.000
	N41	-2.363200635	0.577846691	2.687020675	dmol	1	N	0.000
	H42	-0.551129748	1.600311144	2.990469831	dmol	1	H	0.000
	H43	-2.001629513	0.010889255	3.468015487	dmol	1	H	0.000
	H44	-1.892973510	2.505507095	3.327111928	dmol	1	H	0.000
	H45	-3.849029864	1.447065722	1.248552975	dmol	1	H	0.000
	H46	-2.847587174	-1.340248976	1.271446675	dmol	1	H	0.000
TS: 2HN <sub>2</sub> H <sub>3</sub> - a → 1HN <sub>2</sub> H <sub>4</sub> -a fe6n2h3266xs btuk_orig.cm mf	46							
	C1	1.289856	6.654724	0.483200	dmol	1	C	0.000
	H2	2.228058	6.392532	-0.025146	dmol	1	H	0.000
	H3	1.171555	7.751297	0.475677	dmol	1	H	0.000
	H4	1.346710	6.313507	1.525681	dmol	1	H	0.000
	S5	-0.182434	5.874969	-0.376450	dmol	1	S	0.000
	C6	1.257507	-5.449478	-3.111313	dmol	1	C	0.000
	H7	2.234177	-4.990692	-3.013779	dmol	1	H	0.000
	N8	0.279800	-5.225174	-2.159744	dmol	1	N	0.000
	C9	0.767487	-6.278992	-4.097488	dmol	1	C	0.000
	H10	1.205154	-6.689575	-5.000092	dmol	1	H	0.000
	C11	-0.793259	-5.896408	-2.540512	dmol	1	C	0.000
	H12	-1.723785	-5.924042	-1.987442	dmol	1	H	0.000
	N13	-0.549408	-6.562027	-3.718704	dmol	1	N	0.000
	H14	-1.226654	-7.098679	-4.248093	dmol	1	H	0.000
	C15	-0.348114	-6.528809	1.218307	dmol	1	C	0.000
	H16	-0.679688	-7.562439	0.980972	dmol	1	H	0.000
	H17	-0.552887	-6.373810	2.304565	dmol	1	H	0.000
	C18	1.190125	-6.477112	1.061768	dmol	1	C	0.000
	O19	1.909302	-7.434067	1.435104	dmol	1	O	0.000
	O20	1.627533	-5.364395	0.536331	dmol	1	O	0.000
	O21	-1.021103	-5.583084	0.429733	dmol	1	O	0.000
	Fe22	0.148895	3.638855	-0.183746	dmol	1	Fe	0.000
	Fe23	-1.468262	1.041214	0.693054	dmol	1	Fe	0.000
	Fe24	1.339005	1.268509	0.794891	dmol	1	Fe	0.000
	Fe25	0.017761	1.209274	-1.628906	dmol	1	Fe	0.000
	Fe26	-0.041595	-1.401840	-1.461853	dmol	1	Fe	0.000
	Fe27	-1.876511	-1.967102	0.893967	dmol	1	Fe	0.000
	Fe28	1.188828	-1.372040	0.844360	dmol	1	Fe	0.000
	Mo29	0.098907	-3.851196	-0.042084	dmol	1	Mo	0.000
	S30	-1.694229	2.636627	-1.040726	dmol	1	S	0.000
	S31	-0.088882	2.743546	1.846481	dmol	1	S	0.000
	S32	-0.070633	-0.193771	-3.358063	dmol	1	S	0.000
	S33	1.899155	2.577225	-1.088821	dmol	1	S	0.000
	S34	-1.796295	-2.888367	-1.164276	dmol	1	S	0.000
	S35	-3.391495	-0.150375	0.171783	dmol	1	S	0.000
S36	-0.120407	-2.853607	2.099976	dmol	1	S	0.000	
S37	1.920502	-2.555862	-1.006241	dmol	1	S	0.000	
S38	2.695511	-0.086609	1.936737	dmol	1	S	0.000	
N39	0.000000	0.000000	0.000000	dmol	1	N	0.000	
N40	-1.605026	0.210388	2.650100	dmol	1	N	0.000	
N41	-2.464981	-0.970169	2.579071	dmol	1	N	0.000	
H42	-0.648727	-0.041412	2.933456	dmol	1	H	0.000	
H43	-2.423096	-1.494202	3.467331	dmol	1	H	0.000	
H44	-1.968750	0.907898	3.312836	dmol	1	H	0.000	
H45	-3.432678	-0.548782	1.681702	dmol	1	H	0.000	
H46	-2.930817	-2.993576	1.283829	dmol	1	H	0.000	
1HN <sub>2</sub> H <sub>4</sub> -a fe6n2h3266xs btuk_3a.cmmf	46							
	C1	1.439314263	8.201005505	0.451183070	dmol	1	C	0.000
	H2	2.377394988	7.898421959	-0.035674181	dmol	1	H	0.000
	H3	1.353413048	9.300292789	0.422406818	dmol	1	H	0.000
	H4	1.470002074	7.877125866	1.500939452	dmol	1	H	0.000
	S5	-0.041445626	7.451873202	-0.419094081	dmol	1	S	0.000
	C6	1.389829182	-3.720467762	-3.055959364	dmol	1	C	0.000
	H7	2.328954930	-3.185104411	-2.984153864	dmol	1	H	0.000
	N8	0.423590346	-3.564835225	-2.080434631	dmol	1	N	0.000
	C9	0.939523360	-4.594850218	-4.021222213	dmol	1	C	0.000
	H10	1.383569120	-4.976032428	-4.933083813	dmol	1	H	0.000
	C11	-0.605199210	-4.320611489	-2.425544913	dmol	1	C	0.000
	H12	-1.508505523	-4.420222697	-1.835796643	dmol	1	H	0.000
N13	-0.340271816	-4.976384502	-3.603966919	dmol	1	N	0.000	

H14	-0.984748397	-5.574621140	-4.107175174	dmol	1	H	0.000
C15	-0.258753811	-4.916316361	1.246896513	dmol	1	C	0.000
H16	-0.589158665	-5.947268924	0.993397714	dmol	1	H	0.000
H17	-0.483408509	-4.770705143	2.331098511	dmol	1	H	0.000
C18	1.283236131	-4.872168494	1.117539524	dmol	1	C	0.000
O19	1.990192365	-5.833901077	1.502462071	dmol	1	O	0.000
O20	1.737597472	-3.763591535	0.600352392	dmol	1	O	0.000
O21	-0.912294451	-3.960945334	0.454253557	dmol	1	O	0.000
Fe22	0.240767995	5.222860182	-0.115072774	dmol	1	Fe	0.000
Fe23	-1.345142725	2.633209622	0.683574343	dmol	1	Fe	0.000
Fe24	1.414677288	2.911180086	0.968008012	dmol	1	Fe	0.000
Fe25	0.269553824	2.851947572	-1.547108660	dmol	1	Fe	0.000
Fe26	0.207294692	0.241838979	-1.324515586	dmol	1	Fe	0.000
Fe27	-1.844218704	-0.391577381	0.956885902	dmol	1	Fe	0.000
Fe28	1.313607387	0.234592185	0.973941902	dmol	1	Fe	0.000
Mo29	0.233320176	-2.230544497	0.014480749	dmol	1	Mo	0.000
S30	-1.549854746	4.202444921	-1.062907343	dmol	1	S	0.000
S31	-0.128915808	4.364881138	1.913847567	dmol	1	S	0.000
S32	0.346458876	1.465999589	-3.285370249	dmol	1	S	0.000
S33	2.099755259	4.219303194	-0.875260183	dmol	1	S	0.000
S34	-1.616342717	-1.209622406	-1.140878898	dmol	1	S	0.000
S35	-3.184274587	1.425509157	0.182109403	dmol	1	S	0.000
S36	-0.052303722	-1.280799656	2.158931600	dmol	1	S	0.000
S37	2.114802253	-0.950835924	-0.849709988	dmol	1	S	0.000
S38	2.669039743	1.548735835	2.231084840	dmol	1	S	0.000
N39	0.171996715	1.623061574	0.067044120	dmol	1	N	0.000
N40	-1.329879470	1.735806958	2.655298742	dmol	1	N	0.000
N41	-2.245196109	0.596674494	2.721440780	dmol	1	N	0.000
H42	-0.377555146	1.364866869	2.785265333	dmol	1	H	0.000
H43	-2.175057445	0.090484384	3.614937649	dmol	1	H	0.000
H44	-1.505422126	2.429301441	3.391961664	dmol	1	H	0.000
H45	-3.184171169	0.969988752	2.513397871	dmol	1	H	0.000
H46	-2.935771016	-1.399999650	1.320189879	dmol	1	H	0.000

Fig 7

<b>1HN<sub>2</sub>H<sub>4</sub>-a</b>	46							
fe26n2h46htee	C1	1.231190128	8.290025011	0.649002537	dmol	1	C	0.000
qs_3a.cmmf	H2	2.188391990	8.068491508	0.156761419	dmol	1	H	0.000
	H3	1.085864268	9.383275980	0.673725690	dmol	1	H	0.000
	H4	1.272020811	7.914757812	1.680680753	dmol	1	H	0.000
	S5	-0.191713024	7.501433291	-0.284308088	dmol	1	S	0.000
	C6	1.385471231	-3.561199858	-3.204321933	dmol	1	C	0.000
	H7	2.290905286	-2.969084904	-3.141791241	dmol	1	H	0.000
	N8	0.443541901	-3.507462740	-2.194281180	dmol	1	N	0.000
	C9	0.960810335	-4.422163700	-4.193210438	dmol	1	C	0.000
	H10	1.399063331	-4.737456382	-5.133094472	dmol	1	H	0.000
	C11	-0.546622387	-4.311127096	-2.542883275	dmol	1	C	0.000
	H12	-1.423875097	-4.490685929	-1.932394500	dmol	1	H	0.000
	N13	-0.279077874	-4.901047252	-3.756314764	dmol	1	N	0.000
	H14	-0.898734237	-5.519013254	-4.267328230	dmol	1	H	0.000
	C15	-0.146622682	-5.018219804	1.074808282	dmol	1	C	0.000
	H16	-0.457031906	-6.032360877	0.745378683	dmol	1	H	0.000
	H17	-0.364309875	-4.958795722	2.166745196	dmol	1	H	0.000
	C18	1.391441108	-4.924282762	0.936421505	dmol	1	C	0.000
	O19	2.123759737	-5.892254826	1.252598823	dmol	1	O	0.000
	O20	1.807452023	-3.770806787	0.493410727	dmol	1	O	0.000
	O21	-0.836527318	-4.022800509	0.364294991	dmol	1	O	0.000
	Fe22	0.142030654	5.290023065	0.064245945	dmol	1	Fe	0.000
	Fe23	-1.348222169	2.633532074	0.853793625	dmol	1	Fe	0.000
	Fe24	1.407330544	2.918265534	0.955008483	dmol	1	Fe	0.000
	Fe25	0.333543588	2.821323239	-1.461010124	dmol	1	Fe	0.000
	Fe26	0.094564569	0.263212843	-1.374156624	dmol	1	Fe	0.000
	Fe27	-1.796708914	-0.481620784	1.015184166	dmol	1	Fe	0.000
	Fe28	1.324465454	0.270713935	0.966239079	dmol	1	Fe	0.000
	Mo29	0.245451253	-2.251157724	-0.001672885	dmol	1	Mo	0.000
	S30	-1.487590146	4.144003307	-0.953292085	dmol	1	S	0.000
	S31	-0.068243463	4.312984035	2.072194782	dmol	1	S	0.000
	S32	0.219283516	1.499997559	-3.245915133	dmol	1	S	0.000
	S33	1.966634098	4.341231807	-0.810535429	dmol	1	S	0.000
	S34	-1.662316250	-1.260454847	-1.078106507	dmol	1	S	0.000
	S35	-3.162536636	1.330231651	0.280044658	dmol	1	S	0.000
	S36	0.030055610	-1.339659702	2.153261894	dmol	1	S	0.000
	S37	2.048456920	-0.895839568	-0.892153306	dmol	1	S	0.000
	S38	2.730813058	1.552369465	2.172957626	dmol	1	S	0.000
	N39	0.149214772	1.663108705	0.108133399	dmol	1	N	0.000
	N40	-1.329145710	1.655519574	2.769843459	dmol	1	N	0.000
	N41	-2.214165210	0.493254063	2.791206161	dmol	1	N	0.000

	H42	-0.370508971	1.306723762	2.910102044	dmol	1	H	0.000
	H43	-2.162203352	-0.019067853	3.680254251	dmol	1	H	0.000
	H44	-1.540600869	2.323294268	3.521741462	dmol	1	H	0.000
	H45	-3.157203047	0.839410596	2.534492324	dmol	1	H	0.000
	H46	-2.827796963	-1.530620206	1.424148027	dmol	1	H	0.000
<b>TS:</b> <b>1HN<sub>2</sub>H<sub>4</sub>-a →</b> <b>1H(NH<sub>2</sub>)<sub>2</sub></b> fe26n2h46hted qs_1_4367.43 a.cmmf	46							
	C1	1.245212189	8.321281693	0.745983994	dmol	1	C	0.000
	H2	2.231914671	8.119732842	0.306412931	dmol	1	H	0.000
	H3	1.087623966	9.411344354	0.793213219	dmol	1	H	0.000
	H4	1.222347139	7.910434610	1.763926962	dmol	1	H	0.000
	S5	-0.113491530	7.552694721	-0.289801792	dmol	1	S	0.000
	C6	1.482989707	-3.625345498	-3.170623035	dmol	1	C	0.000
	H7	2.418662500	-3.089135651	-3.067051612	dmol	1	H	0.000
	N8	0.501149812	-3.512056385	-2.205046358	dmol	1	N	0.000
	C9	1.055958029	-4.466610826	-4.175654762	dmol	1	C	0.000
	H10	1.517431724	-4.812345296	-5.093324950	dmol	1	H	0.000
	C11	-0.514891861	-4.262208954	-2.595298329	dmol	1	C	0.000
	H12	-1.430037651	-4.391128878	-2.030540394	dmol	1	H	0.000
	N13	-0.227541931	-4.872119974	-3.793585148	dmol	1	N	0.000
	H14	-0.857234716	-5.458725274	-4.328432426	dmol	1	H	0.000
	C15	-0.111878089	-4.994002164	1.088681831	dmol	1	C	0.000
	H16	-0.411297339	-6.021087424	0.791690230	dmol	1	H	0.000
	H17	-0.342728833	-4.897171569	2.175035584	dmol	1	H	0.000
	C18	1.426961066	-4.888955912	0.962279778	dmol	1	C	0.000
	O19	2.166539613	-5.841762957	1.304009756	dmol	1	O	0.000
	O20	1.836072273	-3.740177967	0.498718851	dmol	1	O	0.000
	O21	-0.799376632	-4.026508125	0.337325396	dmol	1	O	0.000
	Fe22	0.260178342	5.344718784	-0.012267990	dmol	1	Fe	0.000
	Fe23	-1.372915946	2.633612419	0.922611304	dmol	1	Fe	0.000
	Fe24	1.469501435	2.929492525	0.894910280	dmol	1	Fe	0.000
	Fe25	0.273503957	2.826787654	-1.450994328	dmol	1	Fe	0.000
	Fe26	0.091877110	0.271600414	-1.340294656	dmol	1	Fe	0.000
	Fe27	-1.865064175	-0.563765280	0.987718819	dmol	1	Fe	0.000
	Fe28	1.308783988	0.302351319	1.003577563	dmol	1	Fe	0.000
	Mo29	0.263637146	-2.246684016	-0.015474288	dmol	1	Mo	0.000
	S30	-1.472212856	4.234112370	-0.884676425	dmol	1	S	0.000
	S31	0.124449038	4.419404965	1.999314655	dmol	1	S	0.000
	S32	0.146657893	1.483190424	-3.222170373	dmol	1	S	0.000
	S33	1.999125162	4.306211862	-0.928035185	dmol	1	S	0.000
	S34	-1.622169987	-1.265101712	-1.143486634	dmol	1	S	0.000
	S35	-3.105510113	1.355838852	0.255884914	dmol	1	S	0.000
	S36	-0.006590231	-1.354389222	2.132961328	dmol	1	S	0.000
	S37	2.062015368	-0.849663192	-0.857342355	dmol	1	S	0.000
	S38	2.790786360	1.575429395	2.119009367	dmol	1	S	0.000
	N39	0.142018345	1.685840094	0.151499662	dmol	1	N	0.000
	N40	-1.419886611	1.935270066	2.695641413	dmol	1	N	0.000
	N41	-2.465306570	0.042487762	2.702123031	dmol	1	N	0.000
	H42	-0.536436883	1.668933755	3.154170456	dmol	1	H	0.000
	H43	-2.099435216	-0.287920699	3.597109169	dmol	1	H	0.000
	H44	-2.015127635	2.398566342	3.389221352	dmol	1	H	0.000
	H45	-3.417974235	0.408705135	2.780873464	dmol	1	H	0.000
H46	-2.918287295	-1.671175381	1.050195957	dmol	1	H	0.000	
<b>1H(NH<sub>2</sub>)<sub>2</sub></b> fe26n2h46hted qs_2a.cmmf	46							
	C1	1.272377758	8.357411450	0.709442379	dmol	1	C	0.000
	H2	2.264913751	8.163576630	0.281335649	dmol	1	H	0.000
	H3	1.109891866	9.447193519	0.754712304	dmol	1	H	0.000
	H4	1.235082579	7.943454966	1.725290400	dmol	1	H	0.000
	S5	-0.060620925	7.568271520	-0.343885923	dmol	1	S	0.000
	C6	1.467873130	-3.571414648	-3.203838155	dmol	1	C	0.000
	H7	2.379903711	-2.993749316	-3.112760033	dmol	1	H	0.000
	N8	0.499653264	-3.506475849	-2.220435164	dmol	1	N	0.000
	C9	1.061830544	-4.426189998	-4.206431882	dmol	1	C	0.000
	H10	1.522572066	-4.747352468	-5.133532566	dmol	1	H	0.000
	C11	-0.488491084	-4.299708020	-2.597322338	dmol	1	C	0.000
	H12	-1.384556329	-4.476630082	-2.013771432	dmol	1	H	0.000
	N13	-0.195194723	-4.889764195	-3.805064214	dmol	1	N	0.000
	H14	-0.802739881	-5.507781767	-4.330283698	dmol	1	H	0.000
	C15	-0.128880547	-5.019711424	1.056039757	dmol	1	C	0.000
	H16	-0.425812323	-6.041609361	0.739141196	dmol	1	H	0.000
	H17	-0.362244158	-4.941845851	2.141633786	dmol	1	H	0.000
	C18	1.407290435	-4.907658132	0.933304550	dmol	1	C	0.000
	O19	2.151463394	-5.860223419	1.259051563	dmol	1	O	0.000
	O20	1.813443239	-3.747243914	0.490551729	dmol	1	O	0.000
	O21	-0.814278255	-4.033752458	0.321853536	dmol	1	O	0.000
	Fe22	0.364883409	5.359146750	-0.118710954	dmol	1	Fe	0.000
	Fe23	-1.321327904	2.633035381	0.961585534	dmol	1	Fe	0.000
Fe24	1.560213698	2.938771165	0.846164614	dmol	1	Fe	0.000	

	Fe25	0.249761826	2.831240365	-1.446522835	dmol	1	Fe	0.000
	Fe26	0.090987144	0.284227848	-1.303629357	dmol	1	Fe	0.000
	Fe27	-1.970182351	-0.631470432	1.118647851	dmol	1	Fe	0.000
	Fe28	1.273938882	0.312692604	1.070309556	dmol	1	Fe	0.000
	Mo29	0.252480532	-2.243749583	0.018981435	dmol	1	Mo	0.000
	S30	-1.436260231	4.245481557	-0.833612809	dmol	1	S	0.000
	S31	0.338597194	4.529148769	1.916052895	dmol	1	S	0.000
	S32	0.102195260	1.460835512	-3.199143305	dmol	1	S	0.000
	S33	2.052480532	4.250882198	-1.057669916	dmol	1	S	0.000
	S34	-1.624188212	-1.244831258	-1.096578117	dmol	1	S	0.000
	S35	-3.094169672	1.336415588	0.396512376	dmol	1	S	0.000
	S36	-0.022637481	-1.372583143	2.171509653	dmol	1	S	0.000
	S37	2.052480532	-0.842323596	-0.788715237	dmol	1	S	0.000
	S38	2.811471047	1.580952549	2.118922774	dmol	1	S	0.000
	N39	0.180784558	1.725739401	0.162090831	dmol	1	N	0.000
	N40	-1.361119771	2.186676462	2.799198327	dmol	1	N	0.000
	N41	-2.849215568	-0.564301279	2.811256172	dmol	1	N	0.000
	H42	-0.536806615	2.337343700	3.382002680	dmol	1	H	0.000
	H43	-2.192634935	-0.504727717	3.595787920	dmol	1	H	0.000
	H44	-2.201167891	2.442140291	3.323357684	dmol	1	H	0.000
	H45	-3.428010683	0.278571965	2.845588536	dmol	1	H	0.000
	H46	-2.812684940	-1.838112282	0.861582249	dmol	1	H	0.000
TS: 1H(NH <sub>2</sub> ) <sub>2</sub> → NH <sub>2</sub> fe2nh26nh26h tfqb9_1_4372. 22a.cmmf	46							
	C1	1.340471323	8.295521420	0.775305029	dmol	1	C	0.000
	H2	2.304560276	8.086534207	0.292428818	dmol	1	H	0.000
	H3	1.192359591	9.386497122	0.826117965	dmol	1	H	0.000
	H4	1.360060223	7.887306915	1.794187907	dmol	1	H	0.000
	S5	-0.068344604	7.539160355	-0.201637700	dmol	1	S	0.000
	C6	1.428609575	-3.607791832	-3.250705570	dmol	1	C	0.000
	H7	2.373617069	-3.083786490	-3.171812141	dmol	1	H	0.000
	N8	0.477929877	-3.492836971	-2.253755966	dmol	1	N	0.000
	C9	0.961591455	-4.433258051	-4.251255249	dmol	1	C	0.000
	H10	1.391588363	-4.773951042	-5.186148734	dmol	1	H	0.000
	C11	-0.556703911	-4.228560013	-2.621366914	dmol	1	C	0.000
	H12	-1.457522910	-4.353510223	-2.032777711	dmol	1	H	0.000
	N13	-0.313380217	-4.829109841	-3.834983263	dmol	1	N	0.000
	H14	-0.965043229	-5.404044668	-4.356437010	dmol	1	H	0.000
	C15	-0.066863328	-4.982360309	1.048938585	dmol	1	C	0.000
	H16	-0.383730006	-5.997034677	0.731467704	dmol	1	H	0.000
	H17	-0.268464923	-4.908579475	2.141155928	dmol	1	H	0.000
	C18	1.466335528	-4.880672151	0.882096234	dmol	1	C	0.000
	O19	2.212638342	-5.842765017	1.174350905	dmol	1	O	0.000
	O20	1.865189413	-3.717060766	0.441193996	dmol	1	O	0.000
	O21	-0.769580376	-3.990086852	0.341179056	dmol	1	O	0.000
	Fe22	0.294413599	5.331817713	-0.006105012	dmol	1	Fe	0.000
	Fe23	-1.322898083	2.573936181	0.952401391	dmol	1	Fe	0.000
	Fe24	1.523810102	2.917521135	0.876577371	dmol	1	Fe	0.000
	Fe25	0.263479640	2.854075983	-1.447163085	dmol	1	Fe	0.000
	Fe26	0.090802092	0.280539993	-1.361642776	dmol	1	Fe	0.000
	Fe27	-1.884988689	-0.491216122	1.106421791	dmol	1	Fe	0.000
	Fe28	1.336551458	0.307627485	0.983961236	dmol	1	Fe	0.000
	Mo29	0.287800976	-2.213524410	0.002693273	dmol	1	Mo	0.000
	S30	-1.476493015	4.225247543	-0.813017848	dmol	1	S	0.000
	S31	0.230128625	4.429849174	1.985306084	dmol	1	S	0.000
	S32	0.156768735	1.527541447	-3.229287777	dmol	1	S	0.000
	S33	2.015030975	4.296293595	-0.946433493	dmol	1	S	0.000
	S34	-1.647551413	-1.255447440	-1.040917516	dmol	1	S	0.000
	S35	-3.125562927	1.334570500	0.431862906	dmol	1	S	0.000
	S36	0.054869143	-1.308994000	2.156880108	dmol	1	S	0.000
	S37	2.063735832	-0.833552670	-0.902896155	dmol	1	S	0.000
	S38	2.857058785	1.562758441	2.061572916	dmol	1	S	0.000
	N39	0.182933680	1.703484601	0.126483140	dmol	1	N	0.000
	N40	-1.309791173	2.008068585	2.759154840	dmol	1	N	0.000
	N41	-2.973611633	-0.681189291	2.860414767	dmol	1	N	0.000
	H42	-0.465922534	2.249267089	3.285194360	dmol	1	H	0.000
	H43	-2.172114068	-0.477877665	3.470298857	dmol	1	H	0.000
	H44	-2.137376280	2.290480479	3.294826742	dmol	1	H	0.000
	H45	-3.459113724	0.217943644	2.745117127	dmol	1	H	0.000
	H46	-2.907277997	-1.518833270	1.360754884	dmol	1	H	0.000
NH <sub>2</sub> fe2nh26nh26h tfqa9_3a.cmm	46							
	C1	1.379637249	8.338798034	0.740028783	dmol	1	C	0.000
	H2	2.349193464	8.137999042	0.265423482	dmol	1	H	0.000
	H3	1.229265173	9.428748252	0.806874903	dmol	1	H	0.000
	H4	1.388019988	7.915876192	1.752320894	dmol	1	H	0.000
	S5	-0.014364841	7.579175401	-0.253538086	dmol	1	S	0.000
	C6	1.376373500	-3.558119030	-3.228156809	dmol	1	C	0.000
	H7	2.310294568	-3.012538847	-3.162036482	dmol	1	H	0.000

f	N8	0.433016848	-3.461638986	-2.220252127	dmol	1	N	0.000	
	C9	0.919202724	-4.396702790	-4.221634429	dmol	1	C	0.000	
	H10	1.346699030	-4.728133055	-5.161472568	dmol	1	H	0.000	
	C11	-0.585156490	-4.224015514	-2.575549936	dmol	1	C	0.000	
	H12	-1.474050526	-4.376575125	-1.974683902	dmol	1	H	0.000	
	N13	-0.341042949	-4.822978321	-3.792457682	dmol	1	N	0.000	
	H14	-0.979898604	-5.414403828	-4.311649432	dmol	1	H	0.000	
	C15	-0.104536491	-4.946124006	1.079379640	dmol	1	C	0.000	
	H16	-1.835602643	-5.925391952	0.669313511	dmol	1	H	0.000	
	H17	-0.289586270	-4.997150881	2.176937543	dmol	1	H	0.000	
	C18	1.427081008	-4.857552378	0.898860450	dmol	1	C	0.000	
	O19	2.166326750	-5.836870632	1.147628507	dmol	1	O	0.000	
	O20	1.835600240	-3.682857306	0.490195001	dmol	1	O	0.000	
	O21	-0.803104282	-3.876480883	0.496584329	dmol	1	O	0.000	
	Fe22	0.374892355	5.375328333	-0.026392276	dmol	1	Fe	0.000	
	Fe23	-1.234226580	2.750694573	0.881864856	dmol	1	Fe	0.000	
	Fe24	1.625475235	2.933720467	0.803503729	dmol	1	Fe	0.000	
	Fe25	0.175577123	2.872846892	-1.483235148	dmol	1	Fe	0.000	
	Fe26	0.118850294	0.312679492	-1.415359109	dmol	1	Fe	0.000	
	Fe27	-1.189255152	0.267479677	1.133240894	dmol	1	Fe	0.000	
	Fe28	1.501792596	0.303019559	0.917569704	dmol	1	Fe	0.000	
	Mo29	0.325463784	-2.108146920	0.106246059	dmol	1	Mo	0.000	
	S30	-1.465237985	4.356548053	-0.798883082	dmol	1	S	0.000	
	S31	0.271779579	4.374365738	1.968941651	dmol	1	S	0.000	
	S32	0.009597001	1.534268808	-3.281270692	dmol	1	S	0.000	
	S33	2.013777876	4.276836359	-1.058912753	dmol	1	S	0.000	
	S34	-1.625598303	-1.069633943	-0.767643114	dmol	1	S	0.000	
	S35	-3.085984556	1.536538553	0.421411788	dmol	1	S	0.000	
	S36	0.268308030	-1.143668937	2.266301799	dmol	1	S	0.000	
	S37	2.070365706	-0.814310041	-0.999496758	dmol	1	S	0.000	
	S38	3.019612358	1.587720493	1.942671934	dmol	1	S	0.000	
	N39	0.209501924	1.722681428	0.092023189	dmol	1	N	0.000	
	N40	-1.291996379	1.680166570	2.547994481	dmol	1	N	0.000	
	N41	-3.359938899	-1.029032081	2.946111196	dmol	1	N	0.000	
	H42	-0.531753867	1.877069773	3.196094037	dmol	1	H	0.000	
	H43	-2.422285640	-0.860511004	3.336528710	dmol	1	H	0.000	
	H44	-2.184280534	1.790135280	3.027655558	dmol	1	H	0.000	
	H45	-3.563981421	-0.138204086	2.460887124	dmol	1	H	0.000	
	H46	-3.162801990	-1.671656949	2.160030638	dmol	1	H	0.000	
	1HNH <sub>2</sub> fe26nh23bhtka 32s_2a.cmmf	43							
		C1	1.373791381	8.290189531	0.785926399	dmol	1	C	0.000
		H2	2.282831092	7.983920698	0.251350542	dmol	1	H	0.000
		H3	1.298346368	9.390156224	0.766862860	dmol	1	H	0.000
		H4	1.448714383	7.957274572	1.829816632	dmol	1	H	0.000
		S5	-0.142965777	7.551376019	-0.031394170	dmol	1	S	0.000
		C6	0.938686157	-3.550324319	-2.920093496	dmol	1	C	0.000
H7		1.847244833	-2.960873181	-2.907055635	dmol	1	H	0.000	
N8		0.013574531	-3.430840752	-1.897075820	dmol	1	N	0.000	
C9		0.492081844	-4.465860300	-3.845551100	dmol	1	C	0.000	
H10		0.915647895	-4.835999107	-4.771359862	dmol	1	H	0.000	
C11		-0.988730806	-4.250167229	-2.181475663	dmol	1	C	0.000	
H12		-1.850769391	-4.394396817	-1.541481686	dmol	1	H	0.000	
N13		-0.742903448	-4.908489322	-3.362959651	dmol	1	N	0.000	
H14		-1.355581536	-5.584510379	-3.802923768	dmol	1	H	0.000	
C15		-0.628265572	-4.868563061	1.405907449	dmol	1	C	0.000	
H16		-1.048279105	-5.845549642	1.082445246	dmol	1	H	0.000	
H17		-0.836760583	-4.782943397	2.496679214	dmol	1	H	0.000	
C18		0.909515694	-4.950928085	1.249974169	dmol	1	C	0.000	
O19		1.520905911	-5.989536312	1.602984582	dmol	1	O	0.000	
O20		1.448562984	-3.882732425	0.739929271	dmol	1	O	0.000	
O21		-1.212327721	-3.806819912	0.696039545	dmol	1	O	0.000	
Fe22		0.135786169	5.331138655	0.188913217	dmol	1	Fe	0.000	
Fe23		-1.449139268	2.783934123	1.051864245	dmol	1	Fe	0.000	
Fe24		1.285244237	2.853593174	0.972974458	dmol	1	Fe	0.000	
Fe25		0.040428163	2.831833823	-1.379083732	dmol	1	Fe	0.000	
Fe26		-0.074965017	0.233703528	-1.327022184	dmol	1	Fe	0.000	
Fe27		-1.688875553	0.351306898	0.817664497	dmol	1	Fe	0.000	
Fe28		1.219381517	0.219488081	1.027034424	dmol	1	Fe	0.000	
Mo29		0.056779357	-2.211073474	0.146996154	dmol	1	Mo	0.000	
S30		-1.618452629	4.337272247	-0.766991827	dmol	1	S	0.000	
S31		-0.049384827	4.289970048	2.158316156	dmol	1	S	0.000	
S32		-0.025688952	1.504422516	-3.180415441	dmol	1	S	0.000	
S33		1.803589167	4.263985615	-0.803082674	dmol	1	S	0.000	
S34		-1.913554475	-1.133388170	-0.813357241	dmol	1	S	0.000	
S35		-3.430413205	1.717013680	0.509729459	dmol	1	S	0.000	
S36		0.497890112	-1.526407545	2.557763250	dmol	1	S	0.000	
S37		1.872255985	-0.956558877	-0.849301449	dmol	1	S	0.000	
S38	2.781841562	1.539552413	1.975988711	dmol	1	S	0.000		

	N39	-0.069866194	1.618615519	0.204711361	dmol	1	N	0.000
	N40	-1.481681416	1.407101131	2.548446590	dmol	1	N	0.000
	H41	-0.636502458	-0.953756358	3.045886702	dmol	1	H	0.000
	H42	-2.306136049	1.470044514	3.147693961	dmol	1	H	0.000
	H43	-0.631855360	1.363825654	3.118726301	dmol	1	H	0.000
TS: <b>1HNH<sub>2</sub>→ NH<sub>3</sub></b> fe26nh23bhtk 329_1_4152.9 1a.cmmf	43							
	C1	1.322448441	8.199042962	0.775222637	dmol	1	C	0.000
	H2	2.228496192	7.887106328	0.236643939	dmol	1	H	0.000
	H3	1.250647449	9.297921070	0.754817291	dmol	1	H	0.000
	H4	1.403426088	7.866128321	1.819560506	dmol	1	H	0.000
	S5	-0.209743370	7.477787721	-0.027028754	dmol	1	S	0.000
	C6	0.997395140	-3.642925824	-2.945580406	dmol	1	C	0.000
	H7	1.929322390	-3.091811136	-2.932365742	dmol	1	H	0.000
	N8	0.085740925	-3.508146740	-1.913024085	dmol	1	N	0.000
	C9	0.506769471	-4.517695258	-3.888991614	dmol	1	C	0.000
	H10	0.904419294	-4.883146981	-4.828816034	dmol	1	H	0.000
	C11	-0.948348086	-4.282518092	-2.205306914	dmol	1	C	0.000
	H12	-1.815792483	-4.398980453	-1.567220512	dmol	1	H	0.000
	N13	-0.738781683	-4.925685709	-3.401993102	dmol	1	N	0.000
	H14	-1.395585113	-5.540805175	-3.867655594	dmol	1	H	0.000
	C15	-0.684867328	-4.823188339	1.370437676	dmol	1	C	0.000
	H16	-1.154568417	-5.776553031	1.046092029	dmol	1	H	0.000
	H17	-0.867141315	-4.738265078	2.465919838	dmol	1	H	0.000
	C18	0.846750289	-4.959034572	1.196187911	dmol	1	C	0.000
	O19	1.422577714	-6.041175991	1.468254858	dmol	1	O	0.000
	O20	1.423498202	-3.868998023	0.771370295	dmol	1	O	0.000
	O21	-1.240862230	-3.740800234	0.676602547	dmol	1	O	0.000
	Fe22	0.080570938	5.265561609	0.211868633	dmol	1	Fe	0.000
	Fe23	-1.424375538	2.611174798	1.118223475	dmol	1	Fe	0.000
	Fe24	1.366812879	2.858056994	0.968701679	dmol	1	Fe	0.000
	Fe25	0.022645860	2.808170691	-1.341703237	dmol	1	Fe	0.000
	Fe26	0.027254117	0.250278653	-1.312401259	dmol	1	Fe	0.000
	Fe27	-1.583214580	0.096512884	0.910387681	dmol	1	Fe	0.000
	Fe28	1.368572686	0.234821920	0.996692997	dmol	1	Fe	0.000
	Mo29	0.073150143	-2.183207030	0.129225387	dmol	1	Mo	0.000
	S30	-1.685531536	4.206557938	-0.659260585	dmol	1	S	0.000
	S31	-0.026104880	4.219202523	2.181224335	dmol	1	S	0.000
	S32	0.021412828	1.525164255	-3.153622469	dmol	1	S	0.000
S33	1.759507519	4.272409017	-0.837039627	dmol	1	S	0.000	
S34	-1.827761586	-1.121367494	-0.889648043	dmol	1	S	0.000	
S35	-3.373242136	1.443777276	0.651427046	dmol	1	S	0.000	
S36	0.185245675	-1.223232002	2.488497569	dmol	1	S	0.000	
S37	1.945196168	-0.997802717	-0.856232577	dmol	1	S	0.000	
S38	2.948619307	1.571083481	1.890148095	dmol	1	S	0.000	
N39	0.023714642	1.599172169	0.235358740	dmol	1	N	0.000	
N40	-1.402973716	1.412773135	2.799246094	dmol	1	N	0.000	
H41	-0.793896716	-0.100868012	2.789758448	dmol	1	H	0.000	
H42	-2.313187180	1.511805083	3.270508976	dmol	1	H	0.000	
H43	-0.658216463	1.751699066	3.405511871	dmol	1	H	0.000	
NH <sub>3</sub> fe26nh23bhtf9 _4a.cmmf	43							
	C1	1.289862998	8.187970309	0.704440249	dmol	1	C	0.000
	H2	2.180893890	7.886387981	0.137219824	dmol	1	H	0.000
	H3	1.213573755	9.288040258	0.693850987	dmol	1	H	0.000
	H4	1.404024421	7.848398644	1.742863560	dmol	1	H	0.000
	S5	-0.257310377	7.450731715	-0.059067461	dmol	1	S	0.000
	C6	0.977015046	-3.750516841	-3.129155080	dmol	1	C	0.000
	H7	1.898227551	-3.180401262	-3.154516164	dmol	1	H	0.000
	N8	0.125831549	-3.661736775	-2.044035003	dmol	1	N	0.000
	C9	0.447689616	-4.610563675	-4.067106002	dmol	1	C	0.000
	H10	0.795054972	-4.943852030	-5.038248881	dmol	1	H	0.000
	C11	-0.908362344	-4.447133343	-2.294743318	dmol	1	C	0.000
	H12	-1.730197824	-4.585725884	-1.600265681	dmol	1	H	0.000
	N13	-0.758857922	-5.056258317	-3.517086404	dmol	1	N	0.000
	H14	-1.446255558	-5.646884989	-3.969800806	dmol	1	H	0.000
	C15	-0.669915197	-4.843893393	1.334750584	dmol	1	C	0.000
	H16	-1.072107449	-5.860209000	1.141488702	dmol	1	H	0.000
	H17	-0.879972761	-4.612216407	2.404651601	dmol	1	H	0.000
	C18	0.872364505	-4.908784879	1.203163849	dmol	1	C	0.000
	O19	1.506307814	-5.927171182	1.572091570	dmol	1	O	0.000
	O20	1.399568835	-3.827067564	0.702730966	dmol	1	O	0.000
	O21	-1.260558490	-3.894488353	0.484579412	dmol	1	O	0.000
	Fe22	0.102941798	5.230602476	0.179143781	dmol	1	Fe	0.000
	Fe23	-1.305268303	2.608088629	1.320639502	dmol	1	Fe	0.000
	Fe24	1.389156804	2.758852713	0.951001875	dmol	1	Fe	0.000
	Fe25	0.012542685	2.747267764	-1.320764988	dmol	1	Fe	0.000
	Fe26	0.042442216	0.206927764	-1.440190596	dmol	1	Fe	0.000
Fe27	-1.588519176	-0.030688135	0.703438502	dmol	1	Fe	0.000	

	Fe28	1.206279170	0.093622702	0.973720991	dmol	1	Fe	0.000
	Mo29	-0.013821625	-2.243872126	0.001562645	dmol	1	Mo	0.000
	S30	-1.699280128	4.080505187	-0.528937448	dmol	1	S	0.000
	S31	0.167294687	4.274651071	2.183234754	dmol	1	S	0.000
	S32	0.076396408	1.558160589	-3.216628315	dmol	1	S	0.000
	S33	1.772489981	4.193114729	-0.858267326	dmol	1	S	0.000
	S34	-1.813030833	-1.154178777	-1.237000564	dmol	1	S	0.000
	S35	-3.275660255	1.334168960	1.242587556	dmol	1	S	0.000
	S36	-0.264718924	-1.261913606	2.191233588	dmol	1	S	0.000
	S37	1.904633620	-1.040200774	-0.896608308	dmol	1	S	0.000
	S38	2.792480162	1.352162077	1.998470521	dmol	1	S	0.000
	N39	-0.024012651	1.548277710	0.242872649	dmol	1	N	0.000
	N40	-1.144313297	1.818285227	3.335231654	dmol	1	N	0.000
	H41	-0.832390281	0.841313972	3.302640677	dmol	1	H	0.000
	H42	-2.108350062	1.823317209	3.679037153	dmol	1	H	0.000
	H43	-0.524169026	2.356909628	3.945775192	dmol	1	H	0.000
TS: NH <sub>3</sub> → FeMo-co + NH <sub>3</sub> fe2nh3ti329_1 _4189.45a.cm mf	43							
	C1	1.165604001	8.108278123	0.871973068	dmol	1	C	0.000
	H2	2.171610660	7.902834934	0.479456395	dmol	1	H	0.000
	H3	1.028844426	9.199247578	0.953768395	dmol	1	H	0.000
	H4	1.081091155	7.659369063	1.869642166	dmol	1	H	0.000
	S5	-0.165805544	7.412831526	-0.254087686	dmol	1	S	0.000
	C6	1.063982177	-3.666081366	-3.139035348	dmol	1	C	0.000
	H7	1.988838647	-3.102137510	-3.113955640	dmol	1	H	0.000
	N8	0.175797978	-3.598878452	-2.081988823	dmol	1	N	0.000
	C9	0.561417267	-4.493006060	-4.120434212	dmol	1	C	0.000
	H10	0.940734057	-4.800398349	-5.087958352	dmol	1	H	0.000
	C11	-0.856740110	-4.363731766	-2.394777382	dmol	1	C	0.000
	H12	-1.712765430	-4.514804309	-1.746492998	dmol	1	H	0.000
	N13	-0.669500680	-4.939916433	-3.629662426	dmol	1	N	0.000
	H14	-1.338957994	-5.520246494	-4.121832073	dmol	1	H	0.000
	C15	-0.504527752	-4.994763723	1.135799073	dmol	1	C	0.000
	H16	-0.827890296	-5.976622093	0.727492187	dmol	1	H	0.000
	H17	-0.748517600	-5.011676899	2.223511905	dmol	1	H	0.000
	C18	1.039941031	-4.936593613	1.043087416	dmol	1	C	0.000
	O19	1.731807187	-5.945991164	1.320144054	dmol	1	O	0.000
	O20	1.502059397	-3.774794202	0.679074574	dmol	1	O	0.000
	O21	-1.157234493	-3.936991745	0.480137437	dmol	1	O	0.000
	Fe22	0.017746367	5.197607603	0.039581760	dmol	1	Fe	0.000
	Fe23	-1.415850198	2.644270906	1.128973301	dmol	1	Fe	0.000
	Fe24	1.281263209	2.794534491	0.902962720	dmol	1	Fe	0.000
	Fe25	-0.092861085	2.713012778	-1.402661844	dmol	1	Fe	0.000
	Fe26	-0.022300658	0.179093613	-1.464066469	dmol	1	Fe	0.000
	Fe27	-1.552972194	-0.006781717	0.768918145	dmol	1	Fe	0.000
	Fe28	1.187809103	0.153179974	0.981160428	dmol	1	Fe	0.000
	Mo29	0.025210830	-2.228525284	0.045972936	dmol	1	Mo	0.000
	S30	-1.806091132	4.076489770	-0.664775183	dmol	1	S	0.000
	S31	-0.023729479	4.272756263	4.2067524389	dmol	1	S	0.000
S32	-0.094861023	1.485709067	-3.268833321	dmol	1	S	0.000	
S33	1.684386520	4.138364631	-0.961763728	dmol	1	S	0.000	
S34	-1.842268991	-1.191810132	-1.136029839	dmol	1	S	0.000	
S35	-3.268321427	1.341604093	1.309498260	dmol	1	S	0.000	
S36	-0.202216056	-1.235133535	2.224897035	dmol	1	S	0.000	
S37	1.891726349	-0.975841462	-0.892510691	dmol	1	S	0.000	
S38	2.736886608	1.474865046	1.982357406	dmol	1	S	0.000	
N39	-0.098149177	1.554839380	0.183210514	dmol	1	N	0.000	
N40	-1.202289990	1.841578110	3.797971478	dmol	1	N	0.000	
H41	-0.795180201	0.904852321	3.738173333	dmol	1	H	0.000	
H42	-0.688349049	2.404540472	4.479071911	dmol	1	H	0.000	
H43	-2.189376411	1.754866563	4.046505725	dmol	1	H	0.000	
FeMo-co + NH <sub>3</sub> fe2nh3th329_ 2_4192.84a.c mmf	43							
	C1	1.159530472	8.112622768	0.894026211	dmol	1	C	0.000
	H2	2.098319472	7.870596175	0.375942166	dmol	1	H	0.000
	H3	1.042738183	9.207069977	0.926334543	dmol	1	H	0.000
	H4	1.211480198	7.734356864	1.924951215	dmol	1	H	0.000
	S5	-0.310047016	7.393405355	-0.022052847	dmol	1	S	0.000
	C6	0.996329932	-3.608189277	-3.192545976	dmol	1	C	0.000
	H7	1.902516659	-3.014765445	-3.182250564	dmol	1	H	0.000
	N8	0.124919386	-3.571410020	-2.120090087	dmol	1	N	0.000
	C9	0.500670135	-4.448478741	-4.165247747	dmol	1	C	0.000
	H10	0.872955535	-4.745242226	-5.138521915	dmol	1	H	0.000
	C11	-0.891648689	-4.364424227	-2.414974253	dmol	1	C	0.000
	H12	-1.728932479	-4.534627310	-1.746575422	dmol	1	H	0.000
	N13	-0.709653590	-4.929330852	-3.654621683	dmol	1	N	0.000
	H14	-1.369576721	-5.531592782	-4.131505949	dmol	1	H	0.000
	C15	-0.548077282	-5.008792455	1.115788891	dmol	1	C	0.000
H16	-0.874242023	-6.006925163	0.746236748	dmol	1	H	0.000	

H17	-0.788306705	-4.989959906	2.203604018	dmol	1	H	0.000
C18	0.994836750	-4.955330681	1.016785015	dmol	1	C	0.000
O19	1.689266831	-5.951062520	1.333163081	dmol	1	O	0.000
O20	1.455202771	-3.808055813	0.606351861	dmol	1	O	0.000
O21	-1.195788292	-3.964034090	0.431966500	dmol	1	O	0.000
Fe22	-0.010347567	5.160883958	0.074081304	dmol	1	Fe	0.000
Fe23	-1.432674466	2.672096336	0.931438310	dmol	1	Fe	0.000
Fe24	1.285014030	2.805725411	0.854894270	dmol	1	Fe	0.000
Fe25	0.017157392	2.752714186	-1.478003786	dmol	1	Fe	0.000
Fe26	-0.082580803	0.192874532	-1.512959298	dmol	1	Fe	0.000
Fe27	-1.515752543	0.008680395	0.759474578	dmol	1	Fe	0.000
Fe28	1.212282091	0.171764636	0.887999035	dmol	1	Fe	0.000
Mo29	-0.010276614	-2.246899361	-0.025719696	dmol	1	Mo	0.000
S30	-1.741219021	4.078673453	-0.825258292	dmol	1	S	0.000
S31	-0.117061441	4.170402975	2.023789041	dmol	1	S	0.000
S32	-0.021547145	1.500233110	-3.319510058	dmol	1	S	0.000
S33	1.718061079	4.231251412	-0.919327979	dmol	1	S	0.000
S34	-1.906680553	-1.186278117	-1.143491865	dmol	1	S	0.000
S35	-3.170947913	1.386893622	1.467315522	dmol	1	S	0.000
S36	-0.155146908	-1.225688675	2.171722025	dmol	1	S	0.000
S37	1.832688475	-0.988595390	-0.994852237	dmol	1	S	0.000
S38	2.746320564	1.483658006	1.901652611	dmol	1	S	0.000
N39	-0.067555012	1.573846127	0.061963101	dmol	1	N	0.000
N40	-0.981845833	1.828680615	4.176439694	dmol	1	N	0.000
H41	-0.585983146	0.939850415	3.853197410	dmol	1	H	0.000
H42	-0.643128672	2.065156673	5.113105232	dmol	1	H	0.000
H43	-2.001269518	1.738246052	4.135286782	dmol	1	H	0.000