

Supporting information:

Can the E_1 state in nitrogenase tell if there is an activation process prior to catalysis ?

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Best E_1 state for Mo-nitrogenase with spin-coupling (2-, 4-, 7-) . # denotes frozen atoms

Mo1	16.0171935373	-6.0245480904	53.3721428915
Fe2	8.2353899341	-7.2618615784	54.8375387089
Fe3	10.7138668236	-5.7214004356	55.3154729009
Fe4	10.3958121841	-6.6549922306	52.7242853853
Fe5	11.0738103689	-8.2942626694	54.8154650215
Fe6	13.7064428047	-7.8895590899	54.2524460523
Fe7	13.4908137351	-5.3888237776	54.9885660999
Fe8	12.9199229823	-6.0588734786	52.2526139766
C9	17.7247667526	-2.4141365354	54.3026180608
H10	18.0435154620	-1.4844377305	53.8273944311
H11	16.6306532754	-2.3815302013	54.3896384378
C12	18.1064326467	-3.6300904202	53.4337109903
C13	19.6371658254	-3.6540288223	53.1629645418
H14	20.1473444845	-3.8216581994	54.1147955639
H15	19.9319210038	-2.6667942034	52.7970527769
C16	20.0233991819	-4.7283546687	52.1457805668
H17	19.6573940269	-4.4573701645	51.1494369471
H18	19.5238772323	-5.6615168589	52.3953219669
C19	17.3938066970	-3.6965082058	52.0559134815
O20	16.8673736129	-4.8581969033	51.7770958545
O21	17.4607812721	-2.7372705000	51.2903271305
O22	17.7155568450	-4.8171954507	54.1567885515
C23	12.0228315070	-6.6938900374	54.0279844763
S24	9.7576751949	-7.4653337349	56.6257437167
S25	15.3213103545	-6.7984160857	55.6208869900
S26	9.0693759510	-5.0187667372	53.8036779760
S27	12.1774530436	-4.3828645482	56.7559795884
S28	12.7517499338	-9.7901747838	55.1012526556
S29	14.2837005668	-4.2045103523	53.2069327702
S30	9.4283204250	-8.7333218278	53.1563508379
S31	14.7005876143	-7.6656048949	52.1170050801
S32	11.2675726400	-6.1999399161	50.6280816097
H33	13.6351749525#	-2.1902100277#	49.0425569888#
C34	13.2979259838#	-2.0241169981#	50.0550230832#
H35	13.8501701127	-2.6922824294	50.7207491897
H36	13.4614809377	-0.9821135599	50.3492431356
N37	11.8630237726	-2.3623490262	50.0416372176
H38	11.3671520556	-2.1947580353	49.1779484310
C39	11.0987917434	-2.8773749155	51.0157812754
N40	11.4974436632	-2.9786454139	52.2711476909
H41	10.9460269169	-3.5796251234	52.8903739253
H42	12.4788884571	-2.8797690296	52.5324476389
N43	9.8074742753	-3.2104082548	50.6911402186
H44	9.7759157220	-3.8424582153	49.8932445510
H45	9.3192600097	-3.6602345616	51.4696705558
H46	7.9324790196	0.3930527763	59.4132657917
C47	8.3300917617	-1.3611972425	60.6866310240
H48	8.1017033398	-1.5893028880	61.7340061917
H49	7.6079300047	-1.9197449229	60.0798717134
C50	9.7175817612	-1.8557838552	60.4182164846
N51	10.7063057995	-1.7293757731	61.3731551624
C52	10.2254178822	-2.4674746712	59.2984157981

H53	9.7830879823	-2.7668486634	58.3645987968
C54	11.7874333109	-2.2561882957	60.8298093077
H55	12.7548830407	-2.3486561153	61.2977783505
N56	11.5514371880	-2.7113436551	59.5753165692
H57	19.1123864475	-4.4013506749	57.5367008976
H58	16.6917106859	-8.9227074401	50.7245526538
C59	18.3072439214	-7.4857207768	50.8287185232
H60	17.7055629384	-6.5755971950	50.7796028086
H61	19.2502696818	-7.2807257047	50.3058184368
C62	18.6260795027	-7.7799457363	52.2693595779
N63	17.7535042776	-7.4907947601	53.3153405892
C64	19.7705703266	-8.3198278121	52.8045120910
H65	20.6965648905	-8.6189050710	52.3395623897
C66	18.3609089879	-7.8390754334	54.4385555544
H67	17.9698305128	-7.7005597150	55.4339959682
N68	19.5800174121	-8.3560119121	54.1747461061
H69	20.2652738440	-8.5627133074	54.8871073704
H70	6.3928520262#	-9.4883349472#	56.5258899215#
C71	5.9306891983	-9.3480020240	55.5427568181
H72	6.4526415981	-9.9762969619	54.8179943195
H73	4.8883486050	-9.6725752336	55.5980433452
S74	5.9545057144	-7.5723644277	55.0180351934
H75	12.2028507100	-3.1600045014	58.9440653846
H76	17.9014609558	-4.5884201676	55.1413660599
C78	18.3027107802	-2.4800718519	55.7411270628
O79	18.3833029770	-3.6671441401	56.2555170370
O80	18.6128348524	-1.4225194822	56.3140352233
C81	21.4740427507	-5.0872833041	51.9800073166
O82	21.8947645932	-6.0199569914	51.3195198115
O83	22.3208179387#	-4.2658019953#	52.6398579885#
H84	15.7024660027#	-0.1996309950#	61.4912299974#
C85	14.8549930045#	-0.0829920069#	60.8320010049#
H86	13.9165020000#	-0.2867340000#	61.3260960000#
H87	14.8254036704	0.9912172126	60.5834307642
C88	15.0599869994#	-0.8751939982#	59.5441969910#
H89	14.3689778807	-0.5133672798	58.7720198241
H90	14.8163060126	-1.9313884121	59.7120549141
C91	16.4978260357	-0.8014587062	59.0164679826
H92	16.8858443035	0.2256775498	59.0954206044
H93	16.5444502107	-1.0469381908	57.9491406967
C94	17.4608503311	-1.7379804864	59.7609224994
O95	17.1633005326	-2.2956315802	60.8242426633
N96	18.6756824072	-1.8819482394	59.1653318050
H97	19.2234244742	-2.6637907399	59.5067313191
H98	18.7640667949	-1.6791009613	58.1594079560
C99	10.6519930120#	0.0100039695#	53.3460010093#
H100	11.1636990020#	0.9592719988#	53.2872699997#
H101	9.5863320020#	0.1850130130#	53.3579369917#
H102	10.9103313608	-0.5672622655	52.4569311514
C103	11.0722432977	-0.7023675643	54.6460152801
H104	10.7248365877	-1.7429004927	54.5967343396
C105	10.3945551156	-0.0550524896	55.8618591641
H106	9.3012186270	-0.1031395850	55.7781166888
H107	10.6783728190	1.0029877288	55.9532525177
H108	10.6797610220	-0.5590131864	56.7916026691
C109	12.5971477817	-0.7071671955	54.8210482887
H110	13.1132445419	-1.1531608512	53.9635550089
H111	12.8935789662	-1.2772732051	55.7085382373
H112	12.9749575140	0.3188119552	54.9367122284
H113	13.4550770923#	-12.2303889584#	53.1883130880#
C114	13.9110028580#	-11.6210550534#	52.4219888816#
H115	14.7494660498	-11.0514632680	52.8401583520
H116	14.2305825506	-12.2337977998	51.5723144833
N117	12.7949954451	-10.7543261555	52.0273001514
H118	12.2527122538	-10.4194443651	52.8376676163
C119	12.6719331323	-10.0579316912	50.9047784537
N120	13.6915668341	-10.0421951024	49.9926796070
H121	13.5148824087	-9.4278037997	49.2056614987
H122	14.5955391014	-9.8439820470	50.4166988610
N123	11.5090271917	-9.4575506504	50.6075081916
H124	10.7785526322	-9.5063264815	51.3263918473
H125	11.5574545850	-8.4983403879	50.2307804188
H126	19.2126453700	-8.2193173922	61.7043361057
C127	19.5978930076#	-7.2298799967#	61.9900510112#
H128	20.6394523076	-7.3571523959	62.3026662879

C129	18.8247807121	-6.7003796722	63.1955915826
O130	19.3703026549	-6.2649398481	64.2068807633
C131	19.4918729811#	-6.2717979766#	60.7990649847#
H132	19.8522547399	-5.2781747029	61.0904429416
H133	18.4379330023	-6.1347600013	60.5315047467
C134	20.2520627026	-6.7605237192	59.5498952403
H135	20.0805159087	-7.8310811707	59.3808240409
H136	21.3381528799	-6.6481132486	59.6947318252
C137	19.8953753254	-6.0690794830	58.2301512991
O138	20.0488580431	-6.6216650934	57.1518581845
O139	19.4342901287	-4.8360776570	58.3978871695
N140	17.4719753714	-6.7379005450	63.0214534345
H141	17.1178180210	-7.0259324024	62.1177549443
C142	16.5368840064#	-6.0058840151#	63.8530429850#
H143	15.8534070909	-6.7096636868	64.3500518968
H144	17.1226644262	-5.5073790786	64.6296175741
C145	15.7154887280	-4.9839548157	63.0305634016
H146	16.3698544024	-4.1711481206	62.6956490740
H147	14.9650901760	-4.5441238808	63.7018544291
C148	15.0446475373	-5.6157431751	61.8216491221
C149	13.9563823542	-6.4909362390	61.9654688700
H150	13.5439286934	-6.6757022669	62.9569985510
C151	15.5461192514	-5.3795735440	60.5298799458
H152	16.3605324044	-4.6710531206	60.4017356104
C153	13.3906080839	-7.1200421097	60.8536355420
H154	12.5435699236	-7.7890103136	60.9814307852
C155	14.9848875525	-6.0139934706	59.4144607170
H156	15.3823830294	-5.8287514353	58.4197427099
C157	13.9093094240	-6.8910353995	59.5740650330
H158	13.4837974568	-7.3949109782	58.7091538265
H159	9.0037569561#	0.7050730609#	60.7752690161#
C160	8.1269791487#	0.1560809904#	60.4649998342#
H161	7.2836720085#	0.4592428886#	61.0677680679#
H269	18.2592770520#	-9.4987539583#	50.1505389810#
C270	17.5839770007#	-8.6559199791#	50.1520231667#
H271	17.2773629644#	-8.4419890150#	49.1387980076#
H273	23.2141828700	-4.6119358102	52.4539928778
H274	12.2918127391	-5.4177015807	57.6180121957

Best H⁻ E₁ state for Mo-nitrogenase with spin-coupling (2-, 4-, 6-). * denotes frozen atoms

Mo1	15.8985629777	-6.1600694439	53.2055854289
Fe2	8.2413522121	-8.0126553338	54.2377845329
Fe3	10.3014248567	-6.0223083521	55.0293098463
Fe4	10.6199227707	-7.1566391961	52.4269460901
Fe5	11.1354668634	-8.7262111290	54.6598965881
Fe6	13.7553833321	-8.0853419506	54.2612063409
Fe7	12.9000842405	-5.5535404452	54.7970970394
Fe8	13.1073889995	-6.3418574719	52.0801945838
C9	17.5800164527	-2.5732823939	54.1926549982
H10	17.8809447168	-1.6307179758	53.7319762511
H11	16.4845984985	-2.5771060497	54.2651181802
C12	18.0192909877	-3.7709183851	53.3226070444
C13	19.5647567550	-3.7585919712	53.1276950042
H14	20.0260703396	-3.9341736180	54.1044015492
H15	19.8547173522	-2.7555804645	52.7994513837
C16	20.0340607198	-4.8052368741	52.1112183903
H17	19.7316877415	-4.5070624039	51.0984135120
H18	19.5321065976	-5.7513506168	52.3060169887
C19	17.3506008582	-3.8290485380	51.9234710396
O20	16.7577656984	-4.9616447922	51.6500426731
O21	17.4869320212	-2.8890215416	51.1442733457
O22	17.6130202343	-4.9689043774	54.0170124285
C23	12.0468851225	-7.0702165408	53.8975993010
S24	9.5426962114	-7.9435528679	56.2255471618
S25	15.0941761877	-6.6118876932	55.4733141612
S26	8.8779802372	-5.7765335175	53.2037734263
S27	11.4757555367	-4.1384375327	55.7800043244
S28	12.9348912279	-9.9759118684	55.2192801972
S29	14.1239498035	-4.4562110709	53.0444280111
S30	9.8241163116	-9.3735898289	52.8153422724
S31	14.7798279881	-7.9774015422	52.0947832243
S32	11.5392880606	-6.6109585799	50.3622637228
H33	13.6351748707#	-2.1902101419#	49.0425569802#

C34	13.2979258585#	-2.0241169478#	50.0550232396#
H35	13.9409005007	-2.5834656313	50.7401843439
H36	13.3102956051	-0.9558384700	50.2967674621
N37	11.9267317418	-2.5678327358	50.0494328621
H38	11.4760980374	-2.6428353168	49.1487510869
C39	11.1921436025	-3.0930291280	51.0428186929
N40	11.5106726128	-2.9405102817	52.3183351387
H41	11.1028426302	-3.5523208989	53.0263314914
H42	12.4185683336	-2.5747249290	52.5819333070
N43	10.0309786390	-3.7203916014	50.6853066367
H44	10.2208963350	-4.5144688270	50.0620614406
H45	9.5117976621	-4.0903216172	51.4864988010
H46	7.9265541308	0.3931756053	59.4143079833
C47	8.2974361966	-1.3619548247	60.6826153390
H48	8.3130395829	-1.5524866701	61.7640375779
H49	7.4101648260	-1.8755428253	60.2886973616
C50	9.5292946027	-1.9741904358	60.0921590892
N51	10.7370279131	-1.9417382772	60.7652402718
C52	9.6701590355	-2.6547426265	58.9038961145
H53	8.9777759344	-2.9034545810	58.1135309669
C54	11.5822921753	-2.5973842604	59.9906390681
H55	12.6243549517	-2.7854833572	60.2088464191
N56	10.9878750785	-3.0483072998	58.8543853824
H57	18.9462533326	-4.5324701512	57.4564938257
H58	16.6960919780	-8.9196425413	50.7250358603
C59	18.3451584819	-7.5202819718	50.8453236370
H60	17.7871240922	-6.5841913015	50.7842769221
H61	19.3092604523	-7.3597190742	50.3464581710
C62	18.6125782665	-7.8329691746	52.2946235337
N63	17.6759244684	-7.5933331267	53.2942229305
C64	19.7470452961	-8.3342703751	52.8876169224
H65	20.7093846112	-8.5873869249	52.4717599210
C66	18.2307887291	-7.9299995179	54.4454646220
H67	17.7812530210	-7.8124182735	55.4194943280
N68	19.4826619279	-8.3963303651	54.2456746995
H69	20.1412995834	-8.5572779094	54.9953542528
H70	6.3928521306#	-9.4883347801#	56.5258897734#
C71	6.0446846059	-9.8759956476	55.5626578168
H72	6.6996129252	-10.6975002542	55.2563542829
H73	5.0301240841	-10.2700698368	55.6863297307
S74	5.9968809900	-8.5385305028	54.2793143862
H75	11.4108544777	-3.5604336012	58.0796682349
H76	17.7528440865	-4.7392126055	55.0126614162
C78	18.1468877114	-2.6434982386	55.6352539421
O79	18.2077710979	-3.8332075218	56.1484495330
O80	18.4779105997	-1.5900088646	56.2019298208
C81	21.4981734134	-5.1524124019	52.0299537940
O82	21.9481430453	-6.1314597290	51.4600307873
O83	22.3208179414#	-4.2658020014#	52.6398579915#
H84	15.7024660029#	-0.1996309947#	61.4912299972#
C85	14.8549930092#	-0.0829920021#	60.8320010027#
H86	13.9165020000#	-0.2867340000#	61.3260960000#
H87	14.8255694509	0.9913001267	60.5821405609
C88	15.0599869952#	-0.8751940043#	59.5441969846#
H89	14.3544032818	-0.5287271591	58.7786949940
H90	14.8350517409	-1.9338988737	59.7179818766
C91	16.4915897791	-0.7794023929	58.9981223722
H92	16.8675092658	0.2514740065	59.0865009570
H93	16.5265439347	-1.0122181685	57.9277687966
C94	17.4744201257	-1.7091571521	59.7233024745
O95	17.2361156877	-2.1969433627	60.8330056018
N96	18.6408253695	-1.9292157164	59.0582190472
H97	19.1919693986	-2.7020182872	59.4130488781
H98	18.6798072091	-1.7799572078	58.0401366748
C99	10.6519930332#	0.0100038852#	53.3460009832#
H100	11.1636989625#	0.9592720192#	53.2872699834#
H101	9.5863320017#	0.1850130095#	53.3579370086#
H102	10.9094409980	-0.5776427698	52.4639624809
C103	11.0813406884	-0.6638980433	54.6618297098
H104	10.7538769274	-1.7093536463	54.6551603734
C105	10.4080225787	0.0128458669	55.8640650695
H106	9.3147745551	-0.0313260028	55.7784500557
H107	10.6958381974	1.0715945752	55.9378952393
H108	10.6867394661	-0.4800750090	56.8015494901
C109	12.6071986656	-0.6437311852	54.8258110901

H110	13.1276563832	-1.0838442053	53.9655385509
H111	12.9183723085	-1.2084837928	55.7102001923
H112	12.9690447432	0.3895424826	54.9280764510
H113	13.4550770972#	-12.2303889389#	53.1883131066#
C114	13.9110028472#	-11.6210550770#	52.4219888505#
H115	14.6090595423	-10.9196873359	52.8847853544
H116	14.4163558094	-12.2478672606	51.6801058254
N117	12.7880876666	-10.9244491831	51.7889133002
H118	12.0076066880	-10.6782974540	52.4035412551
C119	12.7955058612	-10.3345096375	50.6019478879
N120	13.9442323359	-10.2841793476	49.8708069154
H121	13.8573177960	-9.7485315561	49.0147907797
H122	14.7651903961	-10.0139273977	50.4063375160
N123	11.6554655690	-9.8601428977	50.0568474199
H124	10.8451805295	-9.9199879819	50.6798739339
H125	11.7239727258	-8.8918499541	49.7061417441
H126	19.1944405447	-8.2138903628	61.7109193902
C127	19.5978929948#	-7.2298799970#	61.9900510110#
H128	20.6400335903	-7.3713126041	62.2940446577
C129	18.8369723013	-6.6821775555	63.1970414594
O130	19.3919910999	-6.1977567228	64.1803739302
C131	19.4918729947#	-6.2717979790#	60.7990649904#
H132	19.9266293984	-5.3008392700	61.0614069370
H133	18.4369161018	-6.0736420652	60.5832830458
C134	20.1532782716	-6.8230654799	59.5193763273
H135	19.9364565615	-7.8917195002	59.4032670818
H136	21.2482551187	-6.7486219103	59.5905522089
C137	19.7432206145	-6.1771743024	58.1903071014
O138	19.8534364972	-6.7745884434	57.1275220826
O139	19.2906953174	-4.9362956156	58.3249461714
N140	17.4818625693	-6.7648667033	63.0528281329
H141	17.1233709724	-7.0915190008	62.1638945712
C142	16.5368840094#	-6.0058840138#	63.8530429874#
H143	15.8494725611	-6.6977838125	64.3606643095
H144	17.1135470121	-5.4858194610	64.6216843088
C145	15.7270065165	-5.0131968583	62.9862698326
H146	16.3737339130	-4.1867704219	62.6720204793
H147	14.9360650585	-4.5832017144	63.6163020850
C148	15.1251574420	-5.6688192419	61.7539963254
C149	14.0911411682	-6.6142139339	61.8586118835
H150	13.6809652587	-6.8556741541	62.8381142259
C151	15.6236779012	-5.3627765577	60.4771757274
H152	16.3982051751	-4.6059051118	60.3805278370
C153	13.5685575457	-7.2341858444	60.7211478022
H154	12.7594168763	-7.9535350411	60.8185152680
C155	15.1022195513	-5.9837917653	59.3362592409
H156	15.4891560844	-5.7330883002	58.3525713404
C157	14.0739810730	-6.9228850084	59.4545044442
H158	13.6674642720	-7.3988728741	58.5667716744
H159	9.0037569399#	0.7050730470#	60.7752690866#
C160	8.1269792709#	0.1560810487#	60.4649996347#
H161	7.2836720149#	0.4592427893#	61.0677681268#
H269	18.2592770429#	-9.4987539657#	50.1505389506#
C270	17.5839770153#	-8.6559199397#	50.1520233041#
H271	17.2773629666#	-8.4419890163#	49.1387980066#
H273	23.2219852597	-4.6153691668	52.5054599738
H274	12.4326316646	-6.6194883238	55.8075893016

Best A₂ state for V-nitrogenase with spin-coupling (2-, 4-, 5-).

V	99.5463159391	62.3314898241	7.2185815755
Fe	105.2671594896	59.7647815601	2.2139160720
Fe	102.8278352367	61.3946375213	2.8125921171
Fe	105.0991269246	61.0449860189	5.0580012232
Fe	102.8511259488	59.0756101167	3.8466392742
Fe	100.3450949423	59.8649905040	5.4672166581
Fe	100.5523703709	62.2794691685	4.1899877771
Fe	102.4145140098	61.6740154325	6.0586573658
C	101.8283120831	60.7265021269	4.4337325865
S	105.0367007319	58.7315596189	4.5748748550
S	104.5390182664	61.8344703134	7.1409311618
S	105.0346096787	62.1487749755	3.0075335951
S	102.9950851273	59.4232384531	1.5074221604
S	101.2446703846	63.1638545184	2.0608940370
S	98.5197432413	61.4827902395	5.1865384995

S	101.0355026920	60.5600472235	7.6644125958
C	100.5385924029	57.1834090492	4.4943105874
O	101.7869014409	57.3576709627	4.3818968898
O	99.7135136551	57.9340822076	5.0944731120
O	100.0092145351	56.0654948489	3.9562622250
C	97.7776438109	66.3238253723	5.5326090930
C	98.7504717063	66.2645692152	6.7425744062
C	98.4185489469	65.1725284960	7.8012519789
C	97.2001426828	65.6097052299	8.6457422101
C	96.7615786095	64.5532458318	9.6947385245
C	95.2679301680	64.4454875840	9.8432462521
C	99.6246683185	64.8651985042	8.7210165322
O	97.2748285573	65.1707372513	5.1819961368
O	97.5842889503	67.3879264195	4.9437342161
O	94.6808878247	63.9787462532	8.6806171398
O	94.5882422560	64.7040329291	10.8078410508
O	99.9973142431	63.6177883197	8.7272947424
O	100.1537594358	65.7574119346	9.3891107351
O	98.1055529514	63.9373388741	7.1255599105
H	97.8499093642	64.2766010820	6.1672208901
H	99.7400574485	66.0487400777	6.3222574664
H	98.7996525325	67.2461773413	7.2183253685
H	97.4464102338	66.5488751587	9.1494788241
H	96.3808162056	65.8196761033	7.9488052039
H	97.1280026489	63.5701201567	9.3829479387
H	97.1796605587	64.7768810998	10.6780628687
C	106.6482281454	57.1295661929	1.2834356929
H	105.8336506337	56.8872677493	0.5947588460
H	106.3423076087	56.8798909039	2.3035657292
S	107.1067235443	58.9182011483	1.1551332359
C	93.8170899606	61.0269089666	1.8605913139
C	93.6139174978	61.1769433574	3.3666946095
C	94.6216104296	62.2043536112	3.8921787213
C	94.4621942945	62.5271321916	5.3698632518
N	95.6877538402	63.2067362146	5.8763720156
C	93.0790262844	59.8959601323	1.1410744300
H	94.8896685561	60.9033646170	1.6676319820
H	93.5459019241	61.9795631204	1.3838761824
H	93.7734543679	60.2145807919	3.8754694257
H	92.5813633360	61.4856029339	3.5905410349
H	95.6324151609	61.8114873569	3.7247505904
H	94.5531490721	63.1312920077	3.3076956093
H	94.3351655538	61.6147362056	5.9633425601
H	93.6070953888	63.1805435633	5.5691114157
H	95.6393001308	63.4046954600	6.8840106245
H	96.5308263713	62.6139771066	5.7055536164
H	95.9434273656	64.1151841875	5.4065054213
H	91.9890650009	59.9610520799	1.2454051768
H	93.4048998609	58.9145809163	1.4526838819
C	100.0989993028	60.0520006371	10.8889971916
C	99.1977560724	61.2906604260	10.6858459744
C	98.0090161633	61.0401244972	9.8192631444
N	98.0015916745	61.2588238056	8.4506943566
C	96.8077546326	60.4843920382	10.1871436128
C	96.8391441429	60.8138333855	8.0042348574
N	96.0756172702	60.3504658244	9.0230230467
H	100.7720111841	59.8784110929	10.1700238452
H	99.4796615403	59.1535236998	11.0189460268
H	100.5712427280	60.2159537877	11.7550861890
H	98.8328907367	61.5997527285	11.6746415761
H	99.7766977857	62.1239778541	10.2844854433
H	96.4253459411	60.1745368133	11.1473482686
H	95.1769666898	59.9007929216	8.9277617451
H	96.5578046812	60.7561576474	6.9652037229
C	101.6500025950	56.1420052972	7.7050018218
N	102.8165550730	56.9752042338	7.3911463469
C	103.3454047090	57.9237523809	8.1730590535
N	102.8098339054	58.1432984381	9.4074763978
N	104.4481801045	58.5770160613	7.8050953008
H	101.7218508293	55.2516469973	7.0724437718
H	100.7886343724	56.5995588075	7.4843449788
H	101.6262276849	55.8261440169	8.6535096651
H	103.0531575969	57.0430435614	6.4032450481
H	103.2174580579	58.9319503003	9.8964046440
H	101.7965149746	58.1682699960	9.4313692669

H	104.8024798562	58.3914852068	6.8575415405
H	104.5032864078	59.5914489905	8.0002718724
C	104.8710010619	65.5940002356	-4.0429952461
C	104.6046810789	64.0835285435	-3.8381936883
C	104.2634369233	63.6273457325	-2.4529767799
N	103.1839996541	62.7943088516	-2.2355443870
C	104.9500460890	63.8233434137	-1.2743282189
C	103.2225901899	62.4915194850	-0.9531262089
N	104.2687829958	63.0938679841	-0.3232256419
H	105.4142233210	65.9758307944	-3.2952586385
H	103.9386900531	66.1635868477	-4.1248840144
H	105.3923871722	65.6470938310	-4.8946699669
H	105.5021582303	63.5419818824	-4.1766010584
H	103.7947684989	63.7551655136	-4.4985999580
H	105.8431827295	64.3790223812	-1.0297864924
H	104.5286532877	62.9728326319	0.6513174377
H	102.5299244372	61.8490370345	-0.4311784555
C	95.6299757402	57.4820326636	6.4910616030
C	97.0398329661	57.2952434612	7.0675559837
O	97.7661948711	56.3310942774	6.3184538142
C	96.9901805012	56.8024437376	8.5148465666
H	95.0594485546	58.2205714647	7.0754734146
H	98.0037215793	56.7201625432	8.9210101176
H	96.5259996186	55.8096606669	8.5554310239
H	96.4169391172	57.4809374760	9.1574670847
H	95.0845625942	56.5313120315	6.5453204361
H	98.2988718870	56.8193593650	5.6627156252
H	97.5711243746	58.2576783356	7.0398048609
C	98.4859996707	66.3580013383	-1.7130007001
C	98.8062104818	65.6203965910	-0.3948537491
C	98.2379509215	66.2405035707	0.8885096012
C	96.7491283960	65.9945835697	1.1372533626
O	96.0353874397	65.3088966119	0.4026524743
N	96.2468785945	66.6187375676	2.2477272691
H	98.7144620115	67.3289719327	-1.6420951176
H	97.4203953663	66.2653818237	-1.9530097264
H	99.0290071105	65.9401255110	-2.4413702110
H	98.4660839786	64.5820782968	-0.4640756037
H	99.8967053092	65.5737914832	-0.2805447336
H	98.7766251531	65.8306650752	1.7549883307
H	98.4180756732	67.3249195667	0.9161785990
H	96.8335939093	66.9206070845	3.0288194773
H	95.3052431751	66.3449369386	2.4964348041
C	103.6859926055	68.3259921635	12.1929976188
C	104.4274335777	68.6163291339	10.8659730655
C	103.8506935802	67.9085635664	9.6307858100
C	103.7580544663	66.3767973793	9.7204265645
C	103.2523466271	65.8153231553	8.3939981372
N	102.8677252042	64.3747925156	8.4547330410
H	104.1085750925	67.5601823910	12.6777192456
H	102.6338333119	68.0769211509	12.0010886835
H	103.6948494749	69.1366815188	12.7784182437
H	104.4064635976	69.6951173511	10.6641489435
H	105.4893116609	68.3548444657	10.9769041399
H	102.8403692485	68.2976665822	9.4411540084
H	104.4548366376	68.1811023823	8.7535842211
H	104.7356479620	65.9419795676	9.9726345874
H	103.0557211155	66.0967123221	10.5158929248
H	102.3486963942	66.3427345926	8.0820393639
H	103.9994979889	65.9049840162	7.6005023638
H	103.6591512066	63.7129880094	8.5265043989
H	102.1512375792	64.1972701870	9.1711457793
H	102.3925068055	64.1077144914	7.5447244774
H	93.7213155930	63.9804262761	8.8589643193
H	95.6198511387	57.7972834465	5.4686067806
H	93.3471300583	60.0483401522	0.1060380432
H	107.5224145779	56.5249257940	1.0242612116
H	100.7327212094	55.6133071215	3.4873711257
S	101.2250197713	63.7461977479	5.9049971393
H	102.0197844611	64.1152716487	2.6304945974
H	94.8291930935	59.8672867016	-1.0815080617
C	95.2420429599	60.2379262897	-2.0081038470
H	95.8060990000	59.4731290000	-2.5212650000
C	96.1753965801	61.4353101561	-1.7394216349
C	97.1819602594	61.1075821703	-0.6569409322

C	98.0738672904	60.0313509602	-0.7918158831
C	97.1925461474	61.8402682587	0.5362783086
C	98.9346783303	59.6777737267	0.2482045383
C	98.0411439057	61.4789310236	1.5845890160
C	98.9063832762	60.3906600423	1.4501408014
H	94.4107635054	60.5263834352	-2.6653814129
H	96.6848684491	61.7095203660	-2.6737124984
H	95.5966094247	62.3148488362	-1.4354086429
H	96.5509226748	62.7134295452	0.6321411735
H	98.1011030095	59.4665502308	-1.7215045260
H	98.0402407513	62.0575091898	2.5018065058
H	99.5766198548	60.1192491039	2.2603993247
H	99.6362776329	58.8577925898	0.1220545953

Best H⁻ A₂ state for V-nitrogenase with spin-coupling (2-, 3-, 5-). * denotes frozen atoms

V1	99.6529231078	62.4292255985	7.2109542281
Fe2	105.3854668445	59.9214066903	2.3458387983
Fe3	102.9921610056	61.6919612456	2.8950545529
Fe4	105.2667120144	61.2207308687	5.0440787800
Fe5	103.0271613134	59.1575329604	3.8792382337
Fe6	100.5525569890	59.9087825306	5.4216484688
Fe7	100.7549981367	62.3550169234	4.2061013652
Fe8	102.5585115828	61.8897644755	6.1624731278
C9	102.1519474589	60.9497707272	4.4519870909
S10	105.2907870129	58.9276416210	4.5812624483
S11	104.6733762824	62.0414614214	7.0795855284
S12	105.3382410925	62.2479593905	2.9412412474
S13	103.0937440481	59.6750842232	1.6190776283
S15	101.5755143600	63.5785032791	2.2773030176
S16	98.7249037690	61.6230605173	5.1413797167
S17	101.2093768158	60.7049336843	7.6664998088
C18	100.7813963313	57.2572978897	4.8276304502
O19	102.0211274106	57.7922590821	4.7342606761
O20	99.8572180239	58.1195582895	5.2389059342
O21	100.5666350625	56.0720933595	4.6325646800
C22	97.8311894908	66.4192739892	5.6242292256
C23	98.7908009141	66.3469211230	6.8446583238
C24	98.4595503393	65.2248535572	7.8737310560
C25	97.2244521681	65.6298375897	8.7101984433
C26	96.7665830474	64.5455848929	9.7218088699
C27	95.2679301335#	64.4454875833#	9.8432462654#
C28	99.6636193629	64.9158466906	8.7924501434
O29	97.3347467946	65.2668404147	5.2606805092
O30	97.6402466776	67.4862885944	5.0432639347
O31	94.7022512957	64.0073827577	8.6601920678
O32	94.5748512690	64.6918266962	10.8011193309
O33	100.0706008300	63.6787524372	8.7552971492
O34	100.1777892951	65.7949976059	9.4888967859
O35	98.1754741165	64.0015487759	7.1650974878
H36	97.9016266908	64.3723029441	6.2140658506
H37	99.7886293757	66.1575592067	6.4313868005
H38	98.8192463675	67.3177735493	7.3436319763
H39	97.4561718750	66.5571184647	9.2422624223
H40	96.4179132472	65.8543380972	8.0031454148
H41	97.1319519389	63.5691509227	9.3878580273
H42	97.1704463950	64.7390268664	10.7175066435
C43	106.6793943638	57.1011521039	1.4224994676
H44	105.7598556300	56.7610164948	0.9380028475
H45	106.6060572555	56.9255316928	2.4988695106
S46	106.9718092089	58.8916823184	1.0719863286
C47	93.8560390090	61.0178620823	1.8409979455
C48	93.6940051024	61.1782748243	3.3509498549
C49	94.7324811554	62.1874143610	3.8547804215
C50	94.5753705073	62.5326900777	5.3276409546
N51	95.7908847956	63.2377937071	5.8274206277
C52	93.0790262951#	59.8959601485#	1.1410744386#
H53	94.9220511456	60.8699110700	1.6220484617
H54	93.5939993769	61.9741210749	1.3667457761
H55	93.8427437899	60.2146898095	3.8601845307
H56	92.6736992898	61.5109723631	3.5954301586

H57	95.7338659790	61.7675296590	3.6928152500
H58	94.6862587992	63.1064080864	3.2553989955
H59	94.4600265352	61.6290181925	5.9360062800
H60	93.7133241823	63.1794592341	5.5177275512
H61	95.7499176575	63.4187775929	6.8387052444
H62	96.6489572007	62.6752096332	5.6398139365
H63	96.0118051030	64.1616010083	5.3758636413
H64	91.9927371627	59.9795820391	1.2599237006
H65	93.4048998636#	58.9145809179#	1.4526838844#
C66	100.0989992610#	60.0520006530#	10.8889971563#
C67	99.2057601750	61.2926311801	10.6640732235
C68	98.0656489873	61.0404260976	9.7346364352
N69	98.1198788555	61.2807613950	8.3697841053
C70	96.8671826177	60.4390199706	10.0320647493
C71	96.9977217399	60.8000956046	7.8589123823
N72	96.1997076070	60.3002859294	8.8313532064
H73	100.7720112696#	59.8784110559#	10.1700238713#
H74	99.4745246498	59.1573942921	11.0172627292
H75	100.5712427270#	60.2159537750#	11.7550861919#
H76	98.7931085917	61.5892555413	11.6376369391
H77	99.8014625712	62.1313486299	10.2995993118
H78	96.4505451628	60.0961089967	10.9663785762
H79	95.3397788046	59.7936124688	8.6785379830
H80	96.7725823328	60.7419672578	6.8061697332
C81	101.6500026134#	56.1420054254#	7.7050017999#
N82	102.7981726558	56.9907043130	7.3742604970
C83	103.3313220030	57.9166494104	8.1640081082
N84	102.8728205468	58.0710442256	9.4389498440
N85	104.3969257167	58.6267651044	7.7673824405
H86	101.7101724232	55.2646356914	7.0568549059
H87	100.7886343228#	56.5995587291#	7.4843450096#
H88	101.6262276732#	55.8261440211#	8.6535096662#
H89	102.9107957400	57.1428172374	6.3651700044
H90	103.2834015868	58.8428306641	9.9491902415
H91	101.8688025240	58.0112565548	9.5555632168
H92	104.7439041805	58.4762238568	6.8146935405
H93	104.4507402394	59.6170354676	8.0220350152
C94	104.8710010733#	65.5940002370#	-4.0429952382#
C95	104.6215927497	64.0788208205	-3.8431559873
C96	104.2306870956	63.6313339369	-2.4703394542
N97	103.0168513625	63.0168347410	-2.2368478012
C98	104.9694179007	63.6708585826	-1.3084552920
C99	103.0254179174	62.6899181503	-0.9599543147
N100	104.1830036186	63.0699841797	-0.3508828243
H101	105.4142233361#	65.9758308102#	-3.2952586576#
H102	103.9334971895	66.1543973259	-4.1247471649
H103	105.3923871597#	65.6470938288#	-4.8946699747#
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O111	97.7467035928	56.3825130269	6.1381215639
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