

Supplementary Information

Theoretical investigation on proton transfer mechanism of extradiol dioxygenase

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Supported Figures and Tables

RMSD for the protein backbone atoms

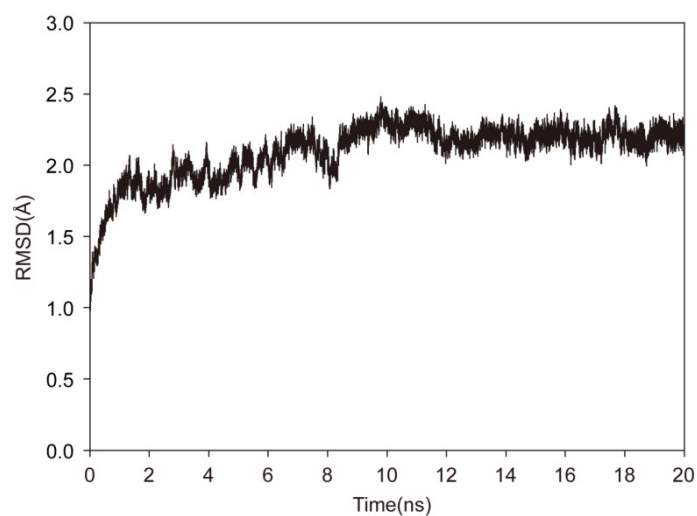


Figure S1 RMSD for the protein backbone atoms along the MD trajectory for HPCD -HPCA

Optimized structures of ⁵1 and ⁵1'

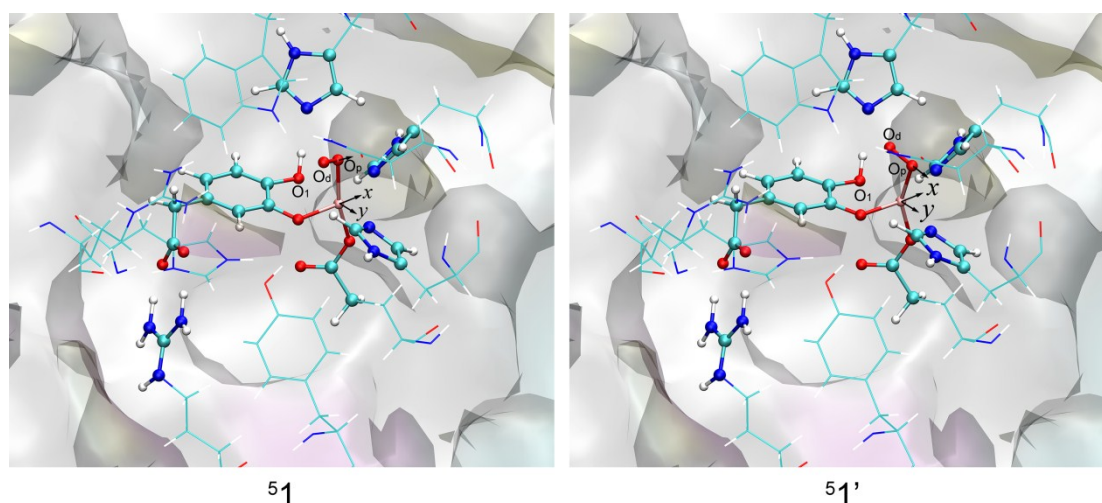


Figure S2 Optimized structures of ⁵1 and ⁵1'

Spin population distribution

Table S1 Spin population distribution of intermediates and transition states at the B3LYP/6-31G(d) level

	Triplet				Quintet				Septet			
	Fe	O1	O2	HPCA	Fe	O1	O2	HPCA	Fe	O1	O2	HPCA
1	3.12	-0.51	-0.73	0.03	4.21	-0.21	-0.59	0.34	4.17	0.55	0.70	0.33
2	2.72	-0.20	-0.66	-0.01	4.10	-0.12	-0.55	0.35	4.15	0.21	0.61	0.78
3	2.81	0.03	-0.03	-0.87	4.18	0.22	0.01	-0.63	4.19	0.27	0.09	1.22
4	2.00	0.01	-0.01	-0.02	3.80	0.01	0.00	0.05	4.23	0.07	0.06	1.35
TS1	2.72	-0.26	-0.65	0.05	4.14	-0.26	-0.66	0.48	4.17	0.32	0.68	0.53
TS2	2.13	-0.01	-0.13	-0.02	3.92	-0.04	-0.30	0.26	4.23	0.08	0.22	1.17
TS3	2.87	-0.06	-0.30	-0.58	4.11	0.27	-0.02	-0.56	4.10	0.39	0.32	0.99
TS4	2.73	-0.03	-0.04	-0.73	4.03	0.07	0.00	-0.32	4.21	0.12	0.06	1.30

Optimized structures in triplet state

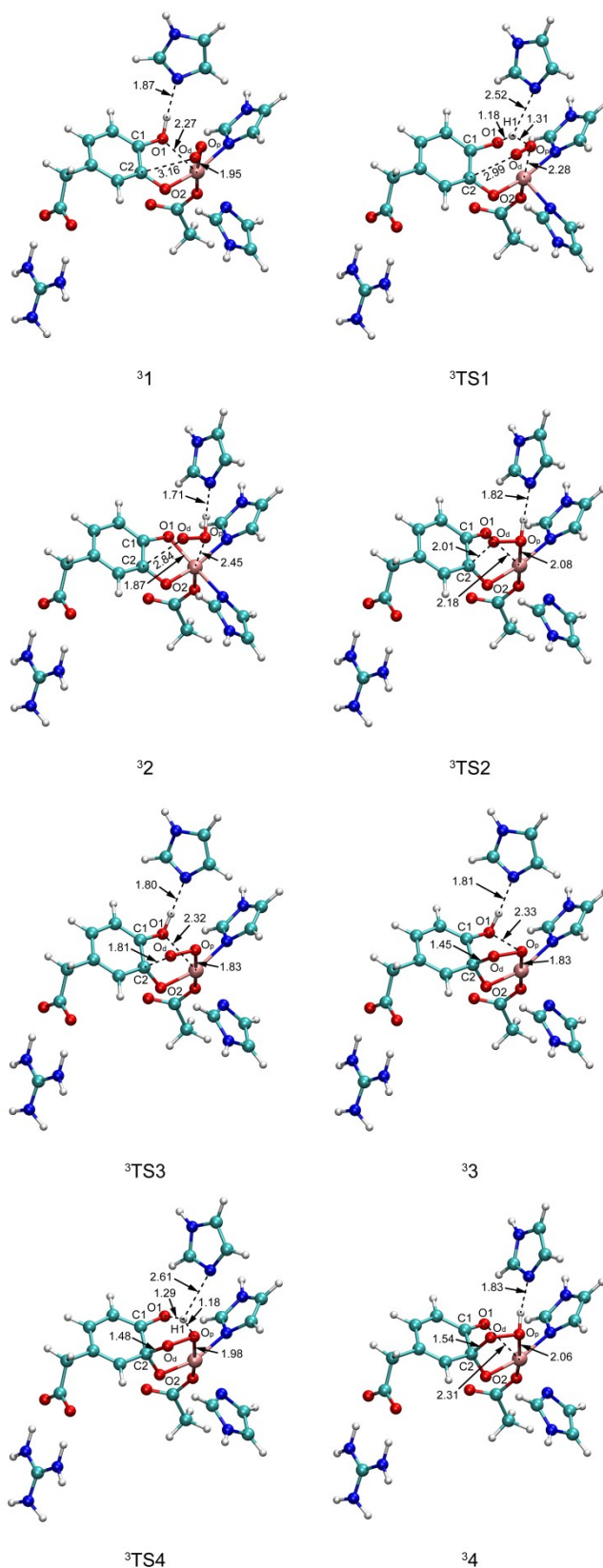


Figure S3 Calculated key structural parameters of intermediates and transition states for QM region in triplet state. Bond lengths (Å) are shown in the frame.

Optimized structures in septet state

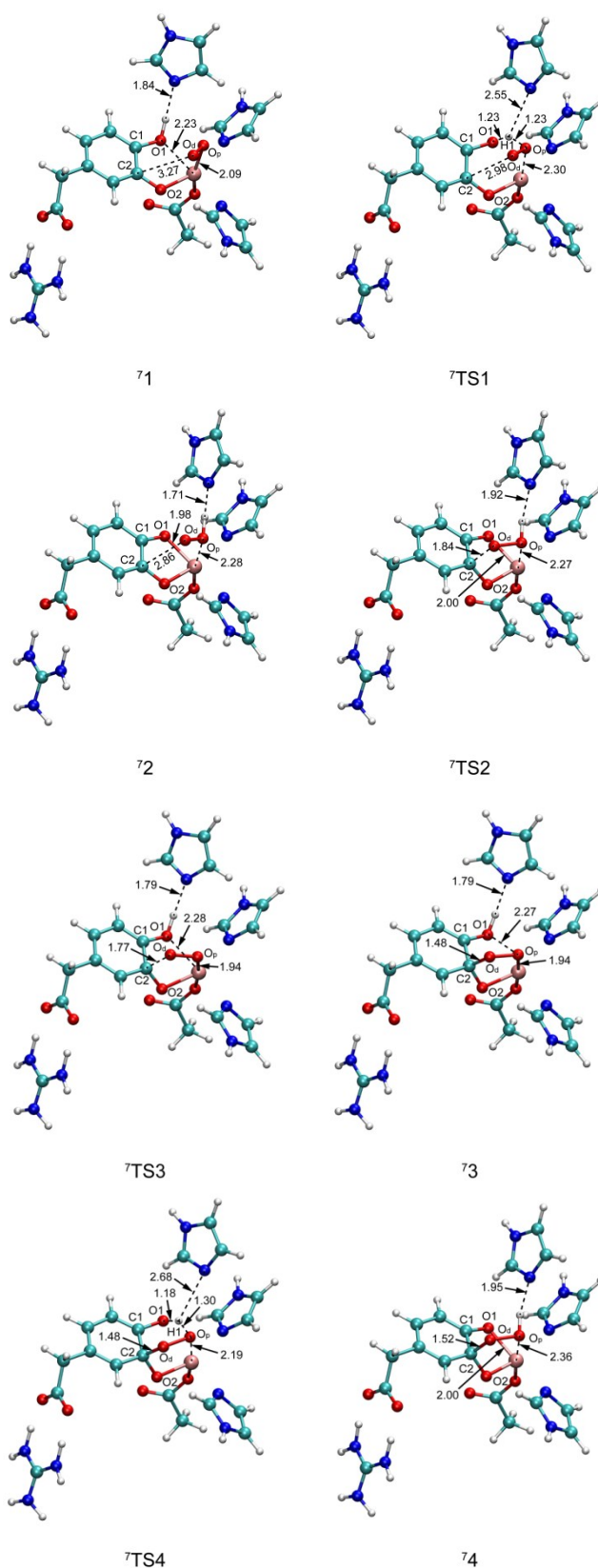


Figure S4 Calculated key structural parameters of intermediates and transition states for QM region in septet state. Bond lengths (Å) are shown in the frame.

Cartesian Coordinates for QM Region

Triplet state

31				H	44.4067140	48.6483100	36.9099420
C	40.2700580	38.7321880	37.8579880	C	41.8273340	46.4262890	36.7718110
N	41.1400330	38.7091520	36.7860670	H	40.9798890	47.1023600	36.8359830
H	41.8284430	37.9731380	36.5721150	C	41.5812090	45.0663120	36.5519510
C	41.1221330	39.9350810	36.2072420	O	40.3311440	44.6211800	36.3690060
H	41.7484530	40.1962810	35.3683130	C	42.6876320	44.1856400	36.5305340
N	40.2610400	40.7248690	36.8291960	O	42.3940780	42.8362720	36.3614040
C	39.7182300	39.9859460	37.8599190	H	42.9273930	42.2788850	36.9937380
H	38.9999510	40.4131890	38.5427400	C	43.9792260	44.6746380	36.5999660
C	43.9892430	39.8882720	40.1003560	H	44.8141890	43.9794900	36.5365060
N	45.0515760	40.7650680	40.0334060	C	44.2031650	46.0468720	36.7504400
H	45.8171090	40.8326380	40.6934680	H	45.2217720	46.4205230	36.7799460
C	44.8614970	41.5624140	38.9495500	O	40.3964920	42.8976580	38.3824030
H	45.5247870	42.3791400	38.7140690	O	39.9313470	43.9259490	38.9948950
N	43.7532770	41.2437120	38.3110530	H	40.1236528	37.8974772	38.5380427
C	43.1983610	40.2016350	39.0285490	H	43.8409542	39.1953111	40.9296919
H	42.2744030	39.7386980	38.7287170	H	34.6330104	43.4166575	35.9290923
C	35.6567350	43.4793880	36.2967830	H	39.1430868	51.9625316	32.0828754
N	36.1601260	44.5620960	36.9895140	H	38.0739913	42.5614404	32.6603637
H	35.6423270	45.3840960	37.3061130				
C	37.4719710	44.3244170	37.2440510	3TS1			
H	38.1045860	45.0134600	37.7801040	C	40.0855630	38.9026680	37.6610350
N	37.8424060	43.1541800	36.7529080	N	40.9811050	38.9207170	36.6135590
C	36.7149240	42.6209390	36.1579520	H	41.7154470	38.2228640	36.4334420
H	36.7324160	41.6613810	35.6640230	C	40.9162010	40.1362250	36.0290530
N	40.1116680	52.1120100	32.3894700	H	41.5479390	40.4279590	35.2067280
H	40.7192720	52.3623450	31.6183700	N	39.9849930	40.8784740	36.6113790
C	40.7211460	51.3179370	33.3457900	C	39.4567580	40.1177360	37.6366960
N	40.0863090	51.0195010	34.4777400	H	38.7105860	40.5152600	38.3058400
H	40.5735230	50.4759170	35.2574900	C	43.5843710	39.5683210	40.3173360
H	39.2501620	51.5362210	34.7169150	N	44.4391310	39.9898410	39.3194220
N	41.9617670	50.9117410	33.1478740	H	45.4298570	39.8112930	39.2461870
H	42.4538790	50.3159090	33.9307200	C	43.6749790	40.5851350	38.3585540
H	42.3557380	51.0094840	32.2120520	H	44.0965370	40.9822220	37.4444350
C	39.1256210	42.8056600	32.3644340	N	42.4052780	40.5962740	38.6946240
H	39.5322130	41.9529970	31.8063040	C	42.3371820	39.9696200	39.9185370
H	39.1276930	43.6665200	31.6894270	H	41.3972610	39.8539110	40.4415640
C	40.0965360	43.1063300	33.5222510	C	35.6839360	43.4985600	36.2779200
O	39.8304430	42.4484890	34.6329950	N	36.1743270	44.4788490	37.1187590
O	41.0471570	43.8609170	33.3541840	H	35.6544760	45.2654180	37.5135640
Fe	40.1307500	42.7711950	36.4579190	C	37.4950820	44.2601630	37.3074710
C	43.1277020	46.9304870	36.8587520	H	38.1236480	44.8588130	37.9487280
C	43.3493440	48.4162690	37.0746010	N	37.8817220	43.1890370	36.6291610
C	42.5096470	49.2651230	36.1115950	C	36.7579520	42.7034920	35.9849940
O	42.9926310	49.4127280	34.9531180	H	36.7931400	41.8305230	35.3540270
O	41.4070550	49.7261600	36.5133880	N	40.0986520	52.2094220	32.3538400
H	43.1007460	48.6911660	38.1060720	H	40.7040740	52.4684080	31.5838340

C	40.7076510	51.4022550	33.2985490	C	39.5140800	40.0755160	37.6104670
N	40.0785670	51.0998620	34.4315910	H	38.7127050	40.4525080	38.2272350
H	40.5632610	50.5480540	35.2102960	C	43.3110280	39.6255170	40.3714710
H	39.2496220	51.6251100	34.6774550	N	43.9332900	39.9820860	39.1884410
N	41.9423730	50.9837700	33.0840960	H	44.7963060	39.6093970	38.8133400
H	42.4305160	50.3859080	33.8511500	C	43.0837200	40.7978360	38.5040570
H	42.3304570	51.0831130	32.1449960	H	43.3045280	41.2208040	37.5339620
C	39.0756830	42.9331540	32.1518140	N	41.9760440	41.0002780	39.1915010
H	39.4898850	42.1098900	31.5571610	C	42.1056130	40.2729340	40.3514690
H	39.0386980	43.8148430	31.5055090	H	41.3291080	40.2656400	41.1036820
C	40.0670380	43.2045360	33.2972330	C	35.7339920	43.4776510	36.2497700
O	39.7973430	42.5527990	34.4083150	N	36.2422080	44.4550450	37.0833500
O	41.0449240	43.9234840	33.1286540	H	35.7328990	45.2472700	37.4800390
Fe	39.9083350	42.8812990	36.2777790	C	37.5610380	44.2186550	37.2622240
C	42.9194150	46.9308380	36.8500490	H	38.2062500	44.8364220	37.8662050
C	43.2588860	48.4037200	36.9992390	N	37.9323690	43.1397750	36.5860510
C	42.4524460	49.2918680	36.0457970	C	36.7972210	42.6693220	35.9503070
O	42.9329940	49.4341360	34.8880480	H	36.8199590	41.7987780	35.3152820
O	41.3691500	49.7889080	36.4610590	N	40.1351310	52.0661100	32.3927630
H	43.0744790	48.7258380	38.0309600	H	40.7443250	52.2952110	31.6164250
H	44.3237740	48.5478000	36.7894650	C	40.7347560	51.2740680	33.3573650
C	41.5881920	46.5230360	36.6873560	N	40.0967830	50.9931080	34.4919820
H	40.7964460	47.2641670	36.6351370	H	40.5775780	50.4523460	35.2769020
C	41.2908210	45.1684450	36.5475280	H	39.2625170	51.5159340	34.7243620
O	40.0451620	44.7047970	36.2747110	N	41.9685410	50.8465590	33.1634710
C	42.3066150	44.2186660	36.7166800	H	42.4671780	50.2796550	33.9610060
O	41.8608900	42.9044940	36.7831140	H	42.3782570	50.9606600	32.2361480
H	41.3923200	42.7478600	37.8549140	C	39.0136200	42.9139560	32.0706520
C	43.6266300	44.6003130	36.8589290	H	39.4371380	42.0962110	31.4751420
H	44.4044840	43.8467720	36.9693930	H	38.9768200	43.7993860	31.4293940
C	43.9303420	45.9662310	36.8969910	C	39.9882920	43.1814780	33.2325150
H	44.9665900	46.2778600	36.9982960	O	39.6784640	42.5470840	34.3370300
O	40.2738180	42.8504510	38.5252880	O	40.9748780	43.8957660	33.0728340
O	40.1685490	44.0542050	39.0886530	Fe	39.9838030	42.8666280	36.2139830
H	40.0080116	38.0775726	38.3657916	C	42.9510170	46.8609930	36.9407020
H	43.8995401	39.0383590	41.2102972	C	43.3060420	48.3291440	37.1100650
H	34.6532946	43.4561048	35.9249134	C	42.5053880	49.2200150	36.1499080
H	39.1301023	52.0600871	32.0480962	O	43.0123370	49.3897720	35.0060730
H	38.0398325	42.6527749	32.4713981	O	41.4025070	49.6915710	36.5414720
				H	43.1156980	48.6601540	38.1378600
³²				H	44.3715240	48.4703640	36.9027810
C	40.1656430	38.8734230	37.6839900	C	41.6107290	46.4758190	36.8176800
N	41.1210430	38.9081150	36.6914970	H	40.8224940	47.2222030	36.8334960
H	41.8370390	38.1928090	36.5046860	C	41.2995230	45.1388940	36.5877370
C	41.0516580	40.1147530	36.0817900	O	40.0567630	44.6956550	36.3080240
H	41.7156230	40.4118240	35.2871620	C	42.3014890	44.1468810	36.5726570
N	40.0855730	40.8458350	36.6166430	O	41.8429990	42.8911840	36.3961580

H	40.8330600	42.2343130	38.8774430	C	39.0571690	42.9038320	32.1254880
C	43.6336520	44.5205220	36.7210960	H	39.4608640	42.0844820	31.5176880
H	44.4196700	43.7666870	36.6937860	H	39.0271940	43.7979090	31.4957630
C	43.9469050	45.8756160	36.8814920	C	40.0447930	43.1355230	33.2863020
H	44.9912600	46.1685500	36.9695400	O	39.8162080	42.3673860	34.3188860
O	40.1034460	42.9142980	38.6623710	O	40.9744720	43.9346440	33.1659160
O	40.5253310	44.1101210	39.1199290	Fe	40.0260390	42.7297790	36.1725310
H	40.0717738	38.0561716	38.3948786	C	42.8012750	46.8695240	37.0591740
H	43.7820056	39.0980336	41.1963246	C	43.1362000	48.3418150	37.2170460
H	34.7002625	43.4531366	35.9043678	C	42.3805510	49.2163010	36.2051890
H	39.1634164	51.9286517	32.0889048	O	42.9531870	49.3846340	35.0961020
H	37.9780395	42.6281007	32.3859377	O	41.2542590	49.6722040	36.5426840
³TS2				H	42.9108520	48.6816560	38.2336560
C	40.1913370	38.8310460	37.6797070	H	44.2092500	48.4831210	37.0526860
N	41.1126040	38.8186430	36.6560640	C	41.5296090	46.4231550	36.8673240
H	41.8284060	38.1013610	36.4835970	H	40.6970460	47.1191290	36.8316560
C	41.0428970	40.0133950	36.0159940	C	41.2515210	45.0149600	36.6263510
H	41.6760780	40.2721860	35.1840430	O	40.1651280	44.6405900	36.0492310
N	40.1112310	40.7798890	36.5631250	C	42.4088090	44.0697370	36.5965660
C	39.5609180	40.0440120	37.5958840	O	42.1922520	42.8890090	36.2274100
H	38.7797400	40.4479470	38.2217380	H	40.9678450	42.3703090	38.5217720
C	43.3453260	39.6349910	40.2793930	C	43.7153410	44.5814200	36.9064140
N	44.0207640	39.9422030	39.1118970	H	44.5525540	43.8867330	36.9139730
H	44.8740830	39.5203570	38.7689620	C	43.8937170	45.9167220	37.0811250
C	43.2197580	40.7636510	38.3769740	H	44.8982700	46.3029280	37.2367530
H	43.4891860	41.1410450	37.3998880	O	40.3118700	43.0614070	38.2050790
N	42.0975280	41.0259980	39.0170340	O	40.9302530	44.3211370	38.4885670
C	42.1631930	40.3237590	40.1999720	H	40.0857387	38.0229402	38.3988856
H	41.3612710	40.3590210	40.9255270	H	43.7752672	39.1094816	41.1296195
C	35.5664600	43.4683460	36.1820780	H	34.5270965	43.4214642	35.8625337
N	36.1103350	44.5182320	36.8944500	H	39.1594767	51.9516336	32.0680904
H	35.6165260	45.3364070	37.2566990	H	38.0195711	42.6270346	32.4455781
C	37.4268810	44.2477580	37.0928980	³TS3			
H	38.0849870	44.9142360	37.6284690	C	40.1774840	38.8266900	37.8005780
N	37.7598730	43.0912580	36.5477800	N	41.0333680	38.8237470	36.7191430
C	36.6042160	42.5994420	35.9743260	H	41.7500400	38.1125860	36.5134510
H	36.5869210	41.6581630	35.4462790	C	40.9471190	40.0343590	36.1157040
N	40.1327660	52.0632150	32.3754580	H	41.5393700	40.3067830	35.2570580
H	40.7529860	52.2887590	31.6069240	N	40.0671050	40.8004840	36.7396370
C	40.7030610	51.2685240	33.3505840	C	39.5766290	40.0585830	37.7947660
N	40.0397130	50.9825210	34.4674180	H	38.8478350	40.4647470	38.4794710
H	40.4950390	50.4326850	35.2622040	C	43.8503910	39.8111450	40.0624480
H	39.1923360	51.4940260	34.6768670	N	44.9621740	40.3798210	39.4742340
N	41.9437190	50.8430290	33.1804690	H	45.9164990	40.3082910	39.7957100
H	42.4257540	50.2923600	33.9750250	C	44.5467620	41.0557390	38.3736690
H	42.3798690	50.9606290	32.2670310	H	45.2257300	41.5411890	37.6897160

N	43.2394960	40.9840070	38.2369410	H	40.0676929	37.9875852	38.4832119
C	42.7905370	40.2131900	39.2936990	H	43.8954826	39.2033392	40.9677985
H	41.7425970	40.0025150	39.4239080	H	34.4696977	43.4419962	35.8635929
C	35.5076720	43.5172000	36.1807520	H	39.1591458	51.9593702	32.0604588
N	36.0238650	44.5698570	36.9105830	H	38.0267884	42.5847962	32.5430629
H	35.5133110	45.3768450	37.2739740				
C	37.3445830	44.3390450	37.1086310	33			
H	37.9920320	45.0087010	37.6559290	C	40.1689850	38.8498070	37.7953570
N	37.7027870	43.1992580	36.5413410	N	41.0300720	38.8479570	36.7181070
C	36.5663280	42.6803590	35.9567680	H	41.7463880	38.1360670	36.5133650
H	36.5782880	41.7470280	35.4150950	C	40.9494320	40.0591000	36.1165700
N	40.1330450	52.0698810	32.3667740	H	41.5543340	40.3293960	35.2661480
H	40.7537910	52.2800650	31.5941500	N	40.0669730	40.8264540	36.7364060
C	40.6981790	51.2701590	33.3437610	C	39.5703900	40.0831680	37.7885130
N	40.0321030	50.9940510	34.4616910	H	38.8374210	40.4875780	38.4699060
H	40.4930290	50.4496430	35.2629070	C	43.8448110	39.7930080	40.1483780
H	39.1948050	51.5216840	34.6708680	N	44.9366110	40.3954700	39.5563330
N	41.9321980	50.8283020	33.1738870	H	45.8928540	40.3573930	39.8785030
H	42.4122560	50.2698760	33.9771340	C	44.4954710	41.0572300	38.4562440
H	42.3694410	50.9470570	32.2608060	H	45.1543980	41.5738090	37.7751630
C	39.0781250	42.8263570	32.2443130	N	43.1914180	40.9374290	38.3213310
H	39.4763670	41.9811660	31.6690130	C	42.7706780	40.1584370	39.3829670
H	39.0846830	43.7007800	31.5869780	H	41.7314100	39.9087890	39.5138650
C	40.0526910	43.0839300	33.4120110	C	35.4907220	43.5143980	36.1615690
O	39.7629200	42.3942160	34.4980340	N	36.0021530	44.5701930	36.8893650
O	41.0232790	43.8165200	33.2552110	H	35.4884240	45.3753190	37.2518200
Fe	39.8763320	42.8462330	36.3302250	C	37.3241110	44.3442890	37.0866980
C	42.8514980	46.9121900	37.0785610	H	37.9632530	45.0200270	37.6345080
C	43.1370080	48.3980240	37.2241760	N	37.6886450	43.2063810	36.5212150
C	42.3772360	49.2437880	36.1961060	C	36.5537020	42.6822360	35.9384010
O	42.9406210	49.3855710	35.0761880	H	36.5694250	41.7483980	35.3977030
O	41.2545830	49.7159960	36.5277550	N	40.1128130	52.1062010	32.3729230
H	42.8806730	48.7375470	38.2330880	H	40.7335270	52.3254990	31.6026340
H	44.2084950	48.5690330	37.0782910	C	40.6802140	51.2954660	33.3400040
C	41.5688620	46.4357000	36.9123700	N	40.0208860	51.0175880	34.4609390
H	40.7302720	47.1237710	36.8688870	H	40.4797420	50.4617110	35.2565660
C	41.2805430	45.0186640	36.7514970	H	39.1908090	51.5530900	34.6791510
O	40.2560230	44.6431050	35.9714680	N	41.9074180	50.8411400	33.1547950
C	42.4633760	44.1431500	36.7340420	H	42.3947370	50.2892840	33.9519350
O	42.1984010	42.8376440	36.4131000	H	42.3388380	50.9656350	32.2381250
H	42.5573750	42.1921520	37.0904240	C	39.0766090	42.8432200	32.2457250
C	43.7334340	44.6306760	36.9247060	H	39.4778150	41.9997740	31.6699290
H	44.5819240	43.9489690	36.8934640	H	39.0802960	43.7175530	31.5881440
C	43.9370910	46.0052500	37.0873670	C	40.0524790	43.1036340	33.4123250
H	44.9496470	46.3827020	37.1885180	O	39.7528400	42.4272180	34.5049420
O	40.1434790	43.2125780	38.1046060	O	41.0307660	43.8231260	33.2490950
O	40.5160450	44.5494130	38.3288770	Fe	39.8978480	42.8796840	36.3298820

C	42.8395970	46.9179380	37.0575350	H	38.0253080	45.1330000	37.6306500
C	43.1250900	48.4049970	37.1964310	N	37.7762820	43.3014090	36.5376570
C	42.3556790	49.2477310	36.1731130	C	36.6438870	42.7445200	35.9773480
O	42.9117780	49.3874700	35.0495620	H	36.6719060	41.8041420	35.4486470
O	41.2372880	49.7222420	36.5156290	N	40.0867140	52.2296520	32.3473530
H	42.8741850	48.7436370	38.2063190	H	40.7049750	52.4616170	31.5790710
H	44.1942100	48.5795350	37.0408460	C	40.6589550	51.4048310	33.3001950
C	41.5591160	46.4284630	37.0955990	N	40.0020010	51.1178230	34.4211540
H	40.7125710	47.1013960	37.1942470	H	40.4638590	50.5603610	35.2135920
C	41.2351640	44.9641180	37.0044980	H	39.1857020	51.6689380	34.6520760
O	40.3172630	44.6397040	36.0056850	N	41.8834950	50.9495640	33.1041310
C	42.4839330	44.1188920	36.7920960	H	42.3535840	50.3553540	33.8854190
O	42.2217410	42.8036110	36.4756770	H	42.2984260	51.0548950	32.1772460
H	42.4957750	42.1715610	37.1991580	C	39.0822590	42.9119990	32.1836520
C	43.7373870	44.6463790	36.7251960	H	39.4889150	42.0783360	31.5980870
H	44.5819020	43.9894160	36.5241400	H	39.0502120	43.7864070	31.5275650
C	43.9369320	46.0324110	36.8845560	C	40.0850250	43.1953970	33.3165660
H	44.9455260	46.4328230	36.8373340	O	39.8417840	42.5014230	34.4184580
O	40.0745920	43.2716410	38.1042700	O	41.0478250	43.9250950	33.1348480
O	40.5956280	44.6411420	38.2649080	Fe	39.9301070	42.8886660	36.2253530
H	40.0593894	38.0102447	38.4783717	C	42.8313080	46.9843340	36.9650830
H	43.9109054	39.1771222	41.0451613	C	43.1062670	48.4720250	37.1018380
H	34.4516886	43.4345823	35.8494178	C	42.3191190	49.3151610	36.0943610
H	39.1408267	51.9896482	32.0631118	O	42.8376170	49.4224110	34.9487140
H	38.0261578	42.5982823	32.5445705	O	41.2263460	49.8236730	36.4686170
				H	42.8649980	48.8014550	38.1172840
³TS4				H	44.1721950	48.6543630	36.9343040
C	40.1120790	38.9039790	37.6724650	C	41.5580160	46.4873870	37.0568380
N	41.0250180	38.9184580	36.6415600	H	40.7079960	47.1536530	37.1727580
H	41.7548980	38.2139830	36.4661140	C	41.2778620	45.0270020	36.9820170
C	40.9631660	40.1278680	36.0420970	O	40.3936060	44.6394810	35.9641850
H	41.5978550	40.4080720	35.2178940	C	42.5270260	44.1696580	36.8828050
N	40.0304200	40.8789630	36.6121860	O	42.2700140	42.8725950	36.9406670
C	39.4917030	40.1232850	37.6368030	H	41.3496910	42.8349330	37.8468670
H	38.7300550	40.5133720	38.2945720	C	43.7792220	44.7239350	36.7143260
C	43.5018920	39.5398700	40.4359710	H	44.6344680	44.0598980	36.6163590
N	44.2951610	40.0080280	39.4091600	C	43.9404320	46.1089520	36.7646380
H	45.2833610	39.8472020	39.2783940	H	44.9357970	46.5349480	36.6748220
C	43.4758090	40.6405640	38.5203660	O	40.2854420	43.2437080	38.1395020
H	43.8351630	41.1146570	37.6179790	O	40.5977290	44.6899040	38.2516380
N	42.2254970	40.6270220	38.9291260	H	40.0260690	38.0825544	38.3807513
C	42.2305130	39.9398220	40.1220410	H	43.8744197	39.0016651	41.2993245
H	41.3239620	39.7883130	40.6945820	H	34.5309841	43.4641578	35.8825434
C	35.5667520	43.5569100	36.2049680	H	39.1172834	52.1030529	32.0350925
N	36.0660640	44.6311700	36.9138160	H	38.0448594	42.6422899	32.5068208
H	35.5400930	45.4284550	37.2780140				
C	37.3945770	44.4393360	37.0944830	34			

C	40.1677340	38.8387420	37.6683330	C	41.5385140	46.3731940	37.1539450
N	41.0743640	38.8391320	36.6311370	H	40.6848350	47.0252080	37.3171020
H	41.7984100	38.1320390	36.4524960	C	41.2225840	44.9151240	36.9358450
C	40.9759150	40.0348650	35.9913230	O	40.1928420	44.6822830	36.1269110
H	41.5888900	40.3035250	35.1472390	C	42.4535150	44.0546500	36.5722800
N	40.0418330	40.7898970	36.5530520	O	42.2576580	42.8697120	36.2619560
C	39.5200130	40.0426950	37.5937480	H	40.9997150	42.4643340	38.5226670
H	38.7393460	40.4307920	38.2305630	C	43.7686270	44.6480900	36.5937410
C	43.3105760	39.6456190	40.2435970	H	44.6194020	44.0030110	36.3937450
N	43.9836290	39.9421450	39.0719410	C	43.9107980	45.9730910	36.8289030
H	44.8230080	39.5003890	38.7191720	H	44.9091060	46.4075860	36.8158660
C	43.1964510	40.7824740	38.3448870	O	40.2979550	43.1132580	38.2051000
H	43.4686150	41.1519150	37.3657480	O	40.8982360	44.4484360	38.3621180
N	42.0837870	41.0689080	38.9929470	H	40.0759221	38.0274193	38.3859523
C	42.1415210	40.3584280	40.1729070	H	43.7432014	39.1236552	41.0956137
H	41.3450610	40.4066390	40.9035260	H	34.4961689	43.4033930	35.8580318
C	35.5334570	43.4722570	36.1798940	H	39.1506274	51.9431103	32.0725689
N	36.0628510	44.5601700	36.8441350	H	38.0440256	42.6327151	32.4615260
H	35.5557150	45.3776020	37.1880430				
C	37.3852140	44.3235740	37.0433060				
H	38.0326020	45.0306520	37.5366340				
N	37.7361050	43.1511740	36.5450020				
C	36.5855000	42.6139600	36.0020180				
H	36.5832370	41.6512540	35.5141290				
N	40.1222300	52.0603520	32.3820090				
H	40.7445360	52.2885500	31.6160710				
C	40.6919970	51.2736330	33.3634630				
N	40.0223350	50.9825190	34.4747450				
H	40.4748740	50.4319660	35.2721190				
H	39.1647550	51.4807500	34.6740050				
N	41.9437360	50.8727860	33.2084310				
H	42.4047980	50.2875680	33.9935630				
H	42.3741590	50.9592230	32.2908280				
C	39.0746930	42.9290740	32.1350570				
H	39.4830980	42.1273370	31.5067650				
H	39.0238610	43.8320250	31.5189650				
C	40.0814400	43.1597470	33.2838310				
O	39.8574970	42.4150170	34.3298980				
O	41.0275920	43.9338790	33.1267260				
Fe	39.9470700	42.7463190	36.2040230				
C	42.7909460	46.8740840	37.0871670				
C	43.0971870	48.3543340	37.2460170				
C	42.3447900	49.2120310	36.2156080				
O	42.9206680	49.3638490	35.1053710				
O	41.2220580	49.6770840	36.5501530				
H	42.8369760	48.6934750	38.2524920				
H	44.1693650	48.5206660	37.1042160				

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51				H	43.2296840	48.7587700	38.0535890
				H	44.4879550	48.6657120	36.8084720
C	40.3410600	38.6752610	37.8653160	C	41.8658230	46.5032350	36.7553590
N	41.2169830	38.6387360	36.7981890	H	41.0354120	47.2019940	36.7782570
H	41.8964500	37.8940900	36.5864860	C	41.5991040	45.1445290	36.5765330
C	41.2183000	39.8659280	36.2196230	O	40.3697350	44.6845770	36.3544620
H	41.8488940	40.1139130	35.3796610	C	42.6738660	44.2289510	36.6052880
N	40.3736650	40.6701670	36.8405230	O	42.3037750	42.8968530	36.4610770
C	39.8154820	39.9397660	37.8689960	H	42.8131830	42.3129380	37.0957840
H	39.1137180	40.3844190	38.5580190	C	43.9785260	44.6778280	36.6754300
C	43.9702310	39.9038260	40.1152260	H	44.7995640	43.9645520	36.6403890
N	45.0431900	40.7655680	40.0164090	C	44.2292170	46.0520250	36.7841680
H	45.8293340	40.8206950	40.6526720	H	45.2561120	46.4014230	36.8121910
C	44.8239450	41.5770220	38.9488430	O	40.2084370	42.8197590	38.4635100
H	45.4892970	42.3863980	38.6953240	O	39.8469690	43.9353980	39.0575370
N	43.6870200	41.2816730	38.3503850	H	40.1721065	37.8448494	38.5445143
C	43.1432020	40.2411330	39.0787100	H	43.8393379	39.2074672	40.9451331
H	42.1943380	39.8064720	38.8190980	H	34.6566110	43.4586355	35.9211053
C	35.6838450	43.5179970	36.2793550	H	39.1407946	51.9797850	32.0821145
N	36.1703630	44.5450060	37.0652580	H	38.0448643	42.5522568	32.6053486
H	35.6468160	45.3458670	37.4239380				
C	37.4870170	44.3246510	37.2877280	5TS1			
H	38.1187650	44.9531580	37.8966490	C	40.1878480	38.7940790	37.6866580
N	37.8735300	43.2103740	36.6845660	N	41.0988330	38.7897540	36.6524000
C	36.7565340	42.7007430	36.0495860	H	41.8269240	38.0831330	36.4826370
H	36.7963950	41.7903340	35.4725440	C	41.0393490	39.9947090	36.0417150
N	40.1083340	52.1406800	32.3862150	H	41.6839440	40.2631860	35.2203840
H	40.7089320	52.4053270	31.6143960	N	40.1082170	40.7519750	36.5983560
C	40.7342450	51.3489130	33.3334550	C	39.5692280	40.0121780	37.6315290
N	40.1136640	51.0406340	34.4706310	H	38.8125500	40.4212470	38.2828010
H	40.6155670	50.5039530	35.2444300	C	43.5920090	39.5829030	40.3545940
H	39.2761930	51.5500390	34.7208500	N	44.4490430	40.0435920	39.3757670
N	41.9775500	50.9567330	33.1223750	H	45.4465080	39.8993180	39.3193730
H	42.4712620	50.3437290	33.8882660	C	43.6827250	40.6425540	38.4180660
H	42.3562920	51.0496950	32.1797900	H	44.1033360	41.0735040	37.5191810
C	39.0993490	42.7882060	32.3162010	N	42.4092580	40.6152310	38.7378830
H	39.4998160	41.9367440	31.7520000	C	42.3410810	39.9616400	39.9470280
H	39.1136910	43.6559530	31.6502730	H	41.3977070	39.8103790	40.4548920
C	40.0624740	43.0576630	33.4876520	C	35.5849380	43.5035560	36.2134070
O	39.7792500	42.4070350	34.5958060	N	36.0974740	44.4695540	37.0577350
O	41.0315260	43.7956490	33.3300880	H	35.5930920	45.2613390	37.4623640
Fe	40.0303960	42.8414960	36.4660790	C	37.4158460	44.2264390	37.2335950
C	43.1785980	46.9705110	36.8502290	H	38.0605550	44.8125960	37.8716600
C	43.4342630	48.4565400	37.0195660	N	37.7792840	43.1536450	36.5448170
C	42.5662520	49.2923390	36.0685040	C	36.6425600	42.6950940	35.9038310
O	43.0055080	49.4102940	34.8895350	H	36.6541130	41.8230470	35.2687840
O	41.4803340	49.7674980	36.4986090	N	40.1026280	52.2154350	32.3476610

H	40.7072140	52.4720340	31.5761920	N	40.1912190	40.6745420	36.6057560
C	40.7121760	51.4097240	33.2933890	C	39.6183110	39.9419300	37.6241760
N	40.0832420	51.1087300	34.4270780	H	38.8192490	40.3438110	38.2290000
H	40.5719050	50.5636630	35.2085230	C	43.3387140	39.6344600	40.3357190
H	39.2558730	51.6364360	34.6730490	N	43.9929110	39.9831020	39.1675130
N	41.9466780	50.9907210	33.0791360	H	44.8638080	39.6055600	38.8169600
H	42.4364150	50.3956040	33.8484900	C	43.1604190	40.7930900	38.4549930
H	42.3347740	51.0906420	32.1401150	H	43.4093760	41.2052700	37.4866470
C	39.0565670	42.9436750	32.0780500	N	42.0357040	41.0027930	39.1103880
H	39.4604270	42.1192950	31.4784710	C	42.1349030	40.2843280	40.2795420
H	39.0145460	43.8278450	31.4361650	H	41.3385630	40.2822510	41.0117020
C	40.0613360	43.1994870	33.2092940	C	35.6288590	43.4947970	36.1855000
O	39.8214380	42.5063660	34.3075910	N	36.1635650	44.4862760	36.9847700
O	41.0262070	43.9361170	33.0555220	H	35.6680590	45.2860480	37.3837480
Fe	39.8886520	42.8574020	36.1585650	C	37.4835160	44.2292910	37.1490600
C	42.9549720	46.9839680	36.8793930	H	38.1459430	44.8514270	37.7312550
C	43.2875390	48.4592410	37.0137990	N	37.8278160	43.1287150	36.4988260
C	42.4710410	49.3273020	36.0506770	C	36.6763730	42.6648900	35.8915400
O	42.9436770	49.4529200	34.8875910	H	36.6716190	41.7732100	35.2836280
O	41.3854200	49.8225270	36.4622550	N	40.1485990	52.0628160	32.3703920
H	43.1053230	48.7924550	38.0424910	H	40.7619710	52.2772120	31.5932590
H	44.3510110	48.6067700	36.7986860	C	40.7310310	51.2734620	33.3457180
C	41.6344540	46.5669250	36.6916830	N	40.0802320	51.0008310	34.4740830
H	40.8389580	47.3014980	36.6108870	H	40.5527780	50.4671000	35.2708490
C	41.3398310	45.2067750	36.5529870	H	39.2426430	51.5245620	34.6919150
O	40.1345030	44.7390990	36.2168150	N	41.9649280	50.8369300	33.1646490
C	42.3616280	44.2458090	36.7553320	H	42.4586300	50.2890440	33.9671090
O	41.9477520	42.9406810	36.7827200	H	42.3913550	50.9564550	32.2460520
H	41.3559890	42.7608390	37.8410370	C	39.0103810	42.9089030	32.0344430
C	43.6746660	44.6523250	36.9213720	H	39.4147280	42.0838750	31.4358970
H	44.4602800	43.9088650	37.0443700	H	38.9798000	43.7973730	31.3978460
C	43.9676690	46.0198160	36.9536920	C	39.9976010	43.1457030	33.1863500
H	45.0010210	46.3370790	37.0641000	O	39.7521360	42.4067930	34.2467940
O	40.2505140	42.8374770	38.4149070	O	40.9416770	43.9211220	33.0669160
O	40.1417670	44.0198790	39.0210320	Fe	40.0234820	42.8038010	36.0952430
H	40.0757658	37.9771700	38.3946974	C	42.8974980	46.9245150	37.0336370
H	43.9066902	39.0388694	41.2386058	C	43.2422290	48.3948210	37.1915720
H	34.5470983	43.4617096	35.8863111	C	42.4658570	49.2610750	36.1893770
H	39.1334824	52.0665181	32.0435633	O	43.0011940	49.4044880	35.0566450
H	38.0252835	42.6651099	32.4128306	O	41.3517020	49.7342480	36.5460190
				H	43.0247040	48.7410900	38.2082710
52				H	44.3128530	48.5355020	37.0118880
C	40.2527310	38.7344110	37.7321850	C	41.5876280	46.5184640	36.8426050
N	41.2078850	38.7277090	36.7393240	H	40.7855070	47.2492320	36.8099650
H	41.9194900	38.0041610	36.5702960	C	41.2937770	45.1647350	36.5681310
C	41.1449870	39.9169450	36.0924430	O	40.1329470	44.7482140	36.1343510
H	41.8064110	40.1719370	35.2799460	C	42.3505370	44.1741410	36.6001760

O	42.0040130	42.9541060	36.2921580	H	42.4032330	50.9540330	32.2771310
H	40.8655050	42.2408300	38.6686630	C	39.0214560	42.9574680	31.9985650
C	43.6674850	44.6013700	36.8585880	H	39.4198430	42.1479300	31.3752840
H	44.4740810	43.8699950	36.8615180	H	38.9700370	43.8589700	31.3817510
C	43.9272830	45.9481690	37.0353200	C	40.0320720	43.1706650	33.1363520
H	44.9557630	46.2740130	37.1739650	O	39.8451510	42.3764600	34.1607320
O	40.1763920	42.9264120	38.3881050	O	40.9496430	43.9828680	33.0233170
O	40.6435540	44.1405780	38.8397320	Fe	39.9548660	42.7514490	36.0431570
H	40.1191371	37.9264912	38.4449536	C	42.8139170	46.9138380	37.1120610
H	43.7873489	39.1035511	41.1715511	C	43.1830460	48.3800710	37.2481200
H	34.5876728	43.4599940	35.8683467	C	42.4248800	49.2469870	36.2304150
H	39.1738666	51.9434009	32.0691364	O	42.9913710	49.4036110	35.1164540
H	37.9753840	42.6352270	32.3617857	O	41.2972460	49.7044060	36.5636720
				H	42.9761930	48.7390980	38.2626580
⁵TS2				H	44.2561210	48.4991540	37.0672270
C	40.2433440	38.7315490	37.7459100	C	41.5240320	46.5119640	36.9103420
N	41.1935150	38.7309700	36.7478290	H	40.7203550	47.2394030	36.8549810
H	41.9107230	38.0140410	36.5781090	C	41.2129910	45.1328660	36.6240310
C	41.1161940	39.9201690	36.1007990	O	40.1159830	44.7791430	36.0746740
H	41.7661970	40.1806910	35.2808160	C	42.3099080	44.1340820	36.6641620
N	40.1575220	40.6693740	36.6159930	O	42.0336490	42.9482010	36.3070130
C	39.5972110	39.9329650	37.6377110	H	40.8756890	42.3864040	38.5902690
H	38.7947680	40.3261440	38.2438390	C	43.6295720	44.5913900	36.9757450
C	43.3312320	39.6449030	40.3202870	H	44.4422040	43.8671380	36.9937260
N	44.0015080	39.9891490	39.1602820	C	43.8639920	45.9244490	37.1473930
H	44.8715880	39.6022570	38.8184480	H	44.8829710	46.2681130	37.3084220
C	43.1801470	40.8027440	38.4377330	O	40.2173270	43.0903530	38.3167760
H	43.4435080	41.2046190	37.4690280	O	40.8422560	44.3132270	38.6200760
N	42.0491700	41.0237300	39.0775260	H	40.1146639	37.9205346	38.4558959
C	42.1317090	40.3036660	40.2483340	H	43.7714763	39.1130060	41.1608591
H	41.3268210	40.3054990	40.9715070	H	34.5178959	43.4359373	35.8364855
C	35.5639850	43.4796680	36.1335140	H	39.1742172	51.9318933	32.0694814
N	36.1118440	44.4927150	36.8945070	H	37.9952752	42.6675857	32.3412541
H	35.6202210	45.2940110	37.2954830				
C	37.4364550	44.2402750	37.0385970	⁵TS3			
H	38.1025820	44.8836250	37.5917510	C	40.1863340	38.7685960	37.8343700
N	37.7713470	43.1235460	36.4121210	N	41.0600700	38.7854670	36.7672890
C	36.6071590	42.6423520	35.8439200	H	41.7790970	38.0778970	36.5572170
H	36.5898120	41.7343390	35.2601760	C	40.9689370	40.0012470	36.1741730
N	40.1493270	52.0408980	32.3730700	H	41.5699790	40.2874680	35.3254360
H	40.7677460	52.2569800	31.6003640	N	40.0699510	40.7508510	36.7888850
C	40.7217980	51.2552920	33.3546570	C	39.5698490	39.9917980	37.8257860
N	40.0603060	50.9756280	34.4744850	H	38.8212770	40.3810030	38.4991400
H	40.5235510	50.4405950	35.2749940	C	43.8334820	39.8232380	40.0576850
H	39.2113290	51.4855260	34.6812130	N	44.9380620	40.3766590	39.4417270
N	41.9629620	50.8304280	33.1876800	H	45.9003800	40.2836760	39.7320060
H	42.4506460	50.2929700	33.9902290	C	44.5046560	41.0684010	38.3582900

H	45.1737670	41.5475870	37.6598610	O	40.6001240	44.5774880	38.3807130
N	43.1926690	41.0205470	38.2581070	H	40.0703942	37.9258552	38.5098237
C	42.7596250	40.2490110	39.3213950	H	43.8907978	39.2167120	40.9635111
H	41.7123720	40.0516740	39.4786330	H	34.3503036	43.4039612	35.8025181
C	35.3941450	43.4860600	36.0928340	H	39.1548905	51.9589745	32.0672323
N	35.9104360	44.5279440	36.8363320	H	38.0246872	42.6183913	32.4884808
H	35.4021960	45.3315310	37.2099690				
C	37.2291530	44.2981270	37.0291530	53			
H	37.8723640	44.9599830	37.5872900	C	40.1939570	38.7648560	37.8361070
N	37.5894420	43.1665070	36.4426930	N	41.0817150	38.7794130	36.7806770
C	36.4521160	42.6542460	35.8514800	H	41.7972260	38.0670130	36.5750010
H	36.4623620	41.7287670	35.2961880	C	41.0036890	39.9962530	36.1882760
N	40.1278150	52.0766140	32.3741300	H	41.6208210	40.2800590	35.3502090
H	40.7461670	52.2957100	31.6020740	N	40.1001210	40.7494880	36.7915830
C	40.7025980	51.2778610	33.3466770	C	39.5835020	39.9916160	37.8214280
N	40.0427870	50.9951950	34.4671800	H	38.8297280	40.3836350	38.4874140
H	40.5097840	50.4524700	35.2642590	C	43.8317630	39.8230010	40.1488110
H	39.2045600	51.5188630	34.6824700	N	44.9272820	40.4558370	39.5963440
N	41.9386580	50.8450330	33.1711180	H	45.8769970	40.4210330	39.9381430
H	42.4239640	50.2851390	33.9731350	C	44.4977370	41.1527930	38.5137900
H	42.3689420	50.9641460	32.2547210	H	45.1600600	41.7077140	37.8685970
C	39.0673530	42.8707300	32.1696220	N	43.1971630	41.0256340	38.3520670
H	39.4656460	42.0275620	31.5913430	C	42.7672970	40.2013630	39.3756590
H	39.0524790	43.7428210	31.5093320	H	41.7285290	39.9373380	39.4811990
C	40.0558640	43.1355730	33.3220760	C	35.4462450	43.5041810	36.1173270
O	39.8023160	42.4629250	34.4196310	N	35.9591940	44.5402890	36.8717460
O	41.0166770	43.8821220	33.1512400	H	35.4477000	45.3391320	37.2512770
Fe	39.7570820	42.8858880	36.3115440	C	37.2801290	44.3166560	37.0578780
C	42.8647910	46.9282750	37.0743100	H	37.9219840	44.9749450	37.6221440
C	43.1883000	48.4085600	37.2009760	N	37.6448490	43.1948180	36.4559650
C	42.4106600	49.2564630	36.1872640	C	36.5088370	42.6818540	35.8628610
O	42.9601040	49.4062100	35.0612580	H	36.5232910	41.7623780	35.2978150
O	41.2886610	49.7198740	36.5321570	N	40.1150100	52.0999380	32.3798100
H	42.9671420	48.7609230	38.2142160	H	40.7331410	52.3270640	31.6098790
H	44.2574340	48.5587310	37.0209170	C	40.6929380	51.2952170	33.3460570
C	41.5629330	46.4872760	36.9872980	N	40.0358300	51.0079420	34.4670910
H	40.7389510	47.1935650	36.9858170	H	40.5021120	50.4580180	35.2592820
C	41.2317360	45.0735330	36.8092530	H	39.2006400	51.5340660	34.6881850
O	40.2218970	44.7503850	36.0100710	N	41.9281900	50.8631090	33.1646900
C	42.4008400	44.1639540	36.7498350	H	42.4098840	50.2878920	33.9597740
O	42.0470360	42.8639620	36.4997730	H	42.3511030	50.9766700	32.2439990
H	42.4653470	42.2098370	37.1335870	C	39.0761710	42.8709590	32.1718550
C	43.6865540	44.6140380	36.8688320	H	39.4749520	42.0293330	31.5918180
H	44.5199360	43.9150490	36.8117970	H	39.0595980	43.7435390	31.5123390
C	43.9271480	45.9932390	37.0177140	C	40.0690540	43.1371060	33.3189830
H	44.9531060	46.3467220	37.0650880	O	39.8078000	42.4808490	34.4286010
O	39.8252270	43.4581440	38.1374630	O	41.0393210	43.8663690	33.1399370

Fe	39.8107490	42.9113470	36.3068570	C	37.3324610	44.4387960	37.0641010
C	42.8725950	46.9272550	37.0632660	H	37.9717550	45.1103660	37.6183570
C	43.1920580	48.4101620	37.1737690	N	37.7097780	43.3237280	36.4583240
C	42.4002900	49.2514350	36.1656670	C	36.5740230	42.7820430	35.8888270
O	42.9381430	49.3969840	35.0329250	H	36.5980870	41.8609930	35.3257340
O	41.2840670	49.7179350	36.5228950	N	40.0885160	52.2545700	32.3319940
H	42.9815510	48.7662800	38.1876650	H	40.7055060	52.4886870	31.5633780
H	44.2579680	48.5636420	36.9792510	C	40.6609610	51.4293470	33.2832380
C	41.5782820	46.4731440	37.1254010	N	40.0045640	51.1400260	34.4034710
H	40.7512040	47.1695500	37.2226830	H	40.4661080	50.5842060	35.1965870
C	41.2159600	45.0272200	37.0134830	H	39.1861370	51.6883070	34.6336770
O	40.2940610	44.7384170	36.0326950	N	41.8870710	50.9770610	33.0856040
C	42.4293370	44.1446990	36.8130170	H	42.3543860	50.3803790	33.8601650
O	42.0931890	42.8365730	36.5401720	H	42.2991790	51.0776100	32.1571170
H	42.4552380	42.1882710	37.2141930	C	39.0978570	42.9471950	32.0639020
C	43.7018460	44.6235410	36.7474980	H	39.4852030	42.1202330	31.4565090
H	44.5287170	43.9414020	36.5544530	H	39.0447830	43.8297510	31.4202400
C	43.9399180	46.0089350	36.8877210	C	40.1375550	43.2014420	33.1684170
H	44.9599280	46.3790800	36.8293220	O	39.9343340	42.5128380	34.2728080
O	39.9049240	43.4227420	38.1654300	O	41.0946170	43.9394610	32.9706170
O	40.5817830	44.6899460	38.3147760	Fe	39.7921160	42.9198730	36.1243510
H	40.0726279	37.9234145	38.5127768	C	42.8065210	47.0290240	36.9821630
H	43.8878215	39.1936350	41.0374708	C	43.1059290	48.5129570	37.0988350
H	34.4032592	43.4235575	35.8211954	C	42.3185040	49.3466400	36.0827860
H	39.1436882	51.9766459	32.0704238	O	42.8326990	49.4359130	34.9345570
H	38.0341972	42.6174078	32.4913660	O	41.2280510	49.8591630	36.4572310
				H	42.8780680	48.8584330	38.1115780
⁵TS4				H	44.1726260	48.6790850	36.9198540
C	40.1561370	38.8583710	37.7294040	C	41.5445410	46.5372130	37.1382830
N	41.0701270	38.8709580	36.6992880	H	40.7044480	47.2078460	37.2956390
H	41.7960670	38.1636070	36.5198490	C	41.2333490	45.0769140	37.0467930
C	41.0171930	40.0865220	36.1097820	O	40.3974760	44.7376310	36.0026880
H	41.6535830	40.3635960	35.2847270	C	42.4841180	44.2214050	36.9534430
N	40.0864160	40.8394280	36.6762840	O	42.2725520	42.9330630	37.0774040
C	39.5423200	40.0813270	37.6945720	H	41.3882190	42.8625770	37.7907500
H	38.7793890	40.4721930	38.3509620	C	43.7398710	44.7625790	36.6962220
C	43.5678140	39.5511930	40.4569870	H	44.5852520	44.0915200	36.5685370
N	44.4045500	40.0497490	39.4804630	C	43.8997760	46.1355960	36.7235670
H	45.4060290	39.9387790	39.4203030	H	44.8909340	46.5582770	36.5785020
C	43.6165390	40.6505290	38.5425160	O	40.2039540	43.3098240	38.2048480
H	44.0170700	41.1284080	37.6596130	O	40.5477010	44.7337580	38.2987510
N	42.3460850	40.5880600	38.8731660	H	40.0509774	38.0302686	38.4266126
C	42.3043510	39.9036300	40.0662080	H	43.9053447	38.9980594	41.3246339
H	41.3709620	39.7184180	40.5817330	H	34.4580613	43.4846868	35.8583923
C	35.4986380	43.5807240	36.1607580	H	39.1184707	52.1291774	32.0217417
N	36.0021680	44.6293270	36.9046920	H	38.0714084	42.6730203	32.4185786
H	35.4798380	45.4178520	37.2920280				

54				H	44.2123300	48.4925180	37.1544040
C	40.1883970	38.7819150	37.7633840	C	41.5174940	46.4302040	37.2836340
N	41.1273940	38.8094440	36.7554400	H	40.6943180	47.1144730	37.4665650
H	41.8514090	38.1029110	36.5677810	C	41.1397210	44.9894970	37.0679660
C	41.0262060	40.0089750	36.1275960	O	40.0802040	44.7989560	36.2948120
H	41.6642000	40.2900690	35.3044680	C	42.3212060	44.0900170	36.6515040
N	40.0612110	40.7369460	36.6622210	O	42.0485400	42.9241430	36.3079910
C	39.5236130	39.9759040	37.6782140	H	40.8954000	42.5685100	38.6435700
H	38.7195130	40.3441060	38.2977180	C	43.6613320	44.6164750	36.6609490
C	43.3006150	39.6597980	40.3020200	H	44.4824340	43.9447220	36.4237600
N	43.9868310	40.0255300	39.1581800	C	43.8604000	45.9378060	36.8967350
H	44.8622670	39.6452840	38.8230230	H	44.8745940	46.3325890	36.8566160
C	43.1751910	40.8516510	38.4393560	O	40.1890550	43.2428250	38.4272950
H	43.4516440	41.2661370	37.4796530	O	40.8532270	44.5281240	38.4986290
N	42.0346600	41.0639530	39.0658730	H	40.0783823	37.9593264	38.4638588
C	42.0999180	40.3174040	40.2229690	H	43.7380629	39.1267935	41.1442411
H	41.2844540	40.3036300	40.9340620	H	34.4089490	43.4038266	35.7998935
C	35.4553030	43.4785780	36.0859660	H	39.1556382	51.8905405	32.0935746
N	35.9873330	44.5379080	36.7918440	H	38.0119009	42.6662766	32.3472774
H	35.4814380	45.3393160	37.1738760				
C	37.3186540	44.3233510	36.9324630				
H	37.9823010	45.0164970	37.4235110				
N	37.6733310	43.1854510	36.3559010				
C	36.5138000	42.6502820	35.8276190				
H	36.5107970	41.7151320	35.2876700				
N	40.1310820	51.9882330	32.4015030				
H	40.7538940	52.1885510	31.6277760				
C	40.6900910	51.1929200	33.3831960				
N	40.0329430	50.9373010	34.5098110				
H	40.4817830	50.3818940	35.3056670				
H	39.1935750	51.4626380	34.7167280				
N	41.9104650	50.7146540	33.2013420				
H	42.4297530	50.2574180	34.0222550				
H	42.3685510	50.8828330	32.3028750				
C	39.0318650	42.9639740	31.9925450				
H	39.4261800	42.1598370	31.3598880				
H	38.9660270	43.8672320	31.3795070				
C	40.0631700	43.1792430	33.1125160				
O	39.8934680	42.3957350	34.1464740				
O	40.9853960	43.9812830	32.9706250				
Fe	39.8348970	42.8021980	36.0244130				
C	42.7863630	46.8824870	37.1821190				
C	43.1393720	48.3546910	37.3173150				
C	42.3866180	49.2090220	36.2825280				
O	42.9870730	49.3985950	35.1921790				
O	41.2372390	49.6278250	36.5903980				
H	42.9052640	48.7129130	38.3244830				

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71				H	43.2044440	48.7538790	38.0492070
				H	44.4688130	48.6459250	36.8105660
C	40.3445830	38.6479950	37.8390860	C	41.8281030	46.5015250	36.7548480
N	41.2382820	38.6134900	36.7884180	H	41.0019840	47.2056640	36.7727750
H	41.9248820	37.8720170	36.5872810	C	41.5560200	45.1419660	36.5822240
C	41.2313520	39.8331320	36.1955980	O	40.3306790	44.6760670	36.3557220
H	41.8723930	40.0775590	35.3626850	C	42.6293660	44.2273150	36.6179140
N	40.3641680	40.6330760	36.7920880	O	42.2532180	42.8928350	36.4922170
C	39.7997600	39.9040600	37.8189470	H	42.7409020	42.3210350	37.1507590
H	39.0819140	40.3435820	38.4942120	C	43.9374080	44.6657630	36.6930810
C	43.9347840	39.9025930	40.1454140	H	44.7551030	43.9482270	36.6628500
N	45.0281670	40.7306560	39.9989010	C	44.1915570	46.0395890	36.7891560
H	45.8370380	40.7675930	40.6072340	H	45.2202670	46.3853840	36.8220490
C	44.7968640	41.5335400	38.9280680	O	40.2260570	42.6713670	38.5072460
H	45.4775120	42.3166350	38.6383370	O	39.9211730	43.8069260	39.0826250
N	43.6306480	41.2668110	38.3749570	H	40.1754051	37.8242540	38.5256195
C	43.0772390	40.2571790	39.1394310	H	43.8262988	39.2057564	40.9769114
H	42.1023740	39.8568290	38.9214070	H	34.6647629	43.4502126	35.9292669
C	35.6918710	43.4949690	36.2899800	H	39.1399519	51.9949817	32.0780822
N	36.1896380	44.5116340	37.0824120	H	38.0362279	42.5601429	32.5916022
H	35.6753180	45.3191760	37.4401040				
C	37.4996560	44.2675530	37.3147760	7TS1			
H	38.1401760	44.8912880	37.9192480	C	40.1955440	38.7892850	37.6877740
N	37.8722450	43.1479010	36.7128780	N	41.1092300	38.7804410	36.6561500
C	36.7520440	42.6603490	36.0657040	H	41.8368950	38.0725710	36.4899810
H	36.7799480	41.7508190	35.4864270	C	41.0516280	39.9824230	36.0400420
N	40.1082510	52.1554720	32.3805540	H	41.6987140	40.2470110	35.2193900
H	40.7065480	52.4188900	31.6065490	N	40.1184240	40.7418620	36.5901870
C	40.7347590	51.3582960	33.3230160	C	39.5765810	40.0069300	37.6252380
N	40.1239300	51.0579270	34.4659890	H	38.8151120	40.4172940	38.2702310
H	40.6223650	50.5115500	35.2382770	C	43.5980360	39.5863290	40.3506280
H	39.2926630	51.5754730	34.7203760	N	44.4605030	40.0466620	39.3764610
N	41.9681810	50.9440110	33.0951800	H	45.4585850	39.9043350	39.3269740
H	42.4783100	50.3645270	33.8572150	C	43.6995750	40.6444540	38.4138530
H	42.3464350	51.0493200	32.1513800	H	44.1256690	41.0733510	37.5165120
C	39.0882970	42.8009450	32.2971160	N	42.4242350	40.6169950	38.7261870
H	39.4850600	41.9582300	31.7176800	C	42.3493870	39.9646310	39.9356820
H	39.0977470	43.6789240	31.6447050	H	41.4032090	39.8139600	40.4383330
C	40.0606850	43.0481380	33.4650600	C	35.5925190	43.5003440	36.2118420
O	39.7833260	42.3764130	34.5614460	N	36.1172270	44.4519030	37.0657670
O	41.0330650	43.7834980	33.3150310	H	35.6209410	45.2451410	37.4776070
Fe	40.0249690	42.8158290	36.4305750	C	37.4343190	44.1949260	37.2340800
C	43.1439370	46.9620300	36.8512050	H	38.0925270	44.7629610	37.8766180
C	43.4127400	48.4461020	37.0179710	N	37.7840370	43.1260670	36.5311320
C	42.5570270	49.2889930	36.0611430	C	36.6409670	42.6857100	35.8887760
O	43.0024630	49.4061030	34.8861580	H	36.6410010	41.8203660	35.2442170
O	41.4713860	49.7706360	36.4883760	N	40.1090530	52.2073340	32.3433850

H	40.7148480	52.4578110	31.5708600	N	40.2013030	40.6619310	36.5855920
C	40.7139480	51.4021150	33.2924440	C	39.6161720	39.9285030	37.5968640
N	40.0818160	51.1056590	34.4253980	H	38.8104890	40.3306120	38.1924230
H	40.5673480	50.5607770	35.2093660	C	43.3428320	39.6146120	40.3539970
H	39.2544310	51.6350110	34.6676750	N	44.0004340	39.9897600	39.1961700
N	41.9474860	50.9782650	33.0815590	H	44.8902120	39.6463400	38.8585440
H	42.4362520	50.3875200	33.8543190	C	43.1564870	40.7828970	38.4797440
H	42.3398570	51.0794050	32.1445190	H	43.4043360	41.2164850	37.5201710
C	39.0597850	42.9536330	32.0550010	N	42.0183010	40.9529390	39.1243080
H	39.4607690	42.1337440	31.4475290	C	42.1217410	40.2289710	40.2893270
H	39.0120480	43.8417840	31.4191200	H	41.3177460	40.2023770	41.0124410
C	40.0736440	43.2021600	33.1791530	C	35.6404870	43.4877790	36.1992440
O	39.8408450	42.5032390	34.2762120	N	36.1727400	44.4609210	37.0225390
O	41.0385860	43.9373720	33.0232630	H	35.6787570	45.2606750	37.4234750
Fe	39.8892320	42.8418510	36.1275120	C	37.4902160	44.1968970	37.1924700
C	42.9349310	46.9764850	36.8907250	H	38.1529520	44.8017640	37.7924120
C	43.2673210	48.4515670	37.0285970	N	37.8352750	43.1073740	36.5227460
C	42.4605400	49.3221800	36.0597150	C	36.6866660	42.6596880	35.8968780
O	42.9428700	49.4481630	34.9007800	H	36.6823000	41.7798720	35.2719570
O	41.3733390	49.8199560	36.4640100	N	40.1428210	52.0620900	32.3836480
H	43.0776480	48.7840410	38.0560540	H	40.7537000	52.2832850	31.6063890
H	44.3326970	48.5980210	36.8222200	C	40.7354950	51.2734730	33.3546870
C	41.6174710	46.5592530	36.6878210	N	40.0912120	50.9964770	34.4863550
H	40.8230710	47.2940150	36.5989270	H	40.5697680	50.4620180	35.2781700
C	41.3232580	45.1978070	36.5451870	H	39.2546480	51.5189810	34.7110980
O	40.1258330	44.7294100	36.1856410	N	41.9702390	50.8438350	33.1682190
C	42.3479180	44.2410240	36.7541350	H	42.4675910	50.2873370	33.9700540
O	41.9400780	42.9345190	36.7678070	H	42.3876020	50.9601160	32.2447430
H	41.3743910	42.7656140	37.8521370	C	39.0192030	42.9289130	32.0223040
C	43.6594660	44.6486580	36.9404710	H	39.4306700	42.1091850	31.4214580
H	44.4440650	43.9049200	37.0688110	H	38.9736740	43.8155200	31.3840580
C	43.9502950	46.0143090	36.9767620	C	40.0140760	43.1855700	33.1630140
H	44.9814930	46.3341590	37.0981610	O	39.7586240	42.4889750	34.2506120
O	40.2748340	42.8870820	38.3919630	O	40.9721700	43.9361720	33.0176980
O	40.1413450	44.0560210	39.0265890	Fe	40.0302040	42.8009580	36.1022480
H	40.0799495	37.9741322	38.3971736	C	42.9594770	46.9087000	36.9816640
H	43.9079996	39.0411791	41.2357524	C	43.2905950	48.3802440	37.1575870
H	34.5532120	43.4691489	35.8882070	C	42.4957600	49.2525720	36.1752520
H	39.1389145	52.0627478	32.0402228	O	43.0143170	49.4062750	35.0348360
H	38.0312168	42.6714405	32.3954757	O	41.3857800	49.7219350	36.5486150
				H	43.0749330	48.7092550	38.1806950
72				H	44.3580040	48.5362220	36.9717130
C	40.2518030	38.7225610	37.7126510	C	41.6368200	46.4996660	36.8388800
N	41.2193420	38.7176910	36.7320330	H	40.8334300	47.2297850	36.8512110
H	41.9317050	37.9938220	36.5679450	C	41.3359040	45.1545900	36.5815340
C	41.1635960	39.9062690	36.0843360	O	40.1310370	44.7269020	36.2489010
H	41.8384830	40.1645940	35.2840540	C	42.3825280	44.1690350	36.5564970

O	42.0023500	42.9313870	36.2971460	H	42.4048680	50.8974350	32.3181580
H	40.8880300	42.1624740	38.7115500	C	39.0188610	42.9351310	32.0029550
C	43.7064220	44.5899460	36.7394070	H	39.4331470	42.1117390	31.4091020
H	44.5092130	43.8549790	36.7060100	H	38.9619950	43.8144190	31.3560380
C	43.9835390	45.9405160	36.9235530	C	40.0206850	43.2146580	33.1281960
H	45.0185820	46.2595710	37.0233980	O	39.7933130	42.5142800	34.2255320
O	40.1982160	42.8327120	38.3788790	O	40.9641890	43.9778830	32.9752660
O	40.4045250	44.0061370	39.0305310	Fe	39.9995300	42.8036230	36.0693040
H	40.1164588	37.9190888	38.4301342	C	42.8628870	46.8508010	37.1181590
H	43.7949538	39.0858480	41.1883169	C	43.1973950	48.3271710	37.2664290
H	34.6006906	43.4614353	35.8761266	C	42.4321700	49.1913620	36.2528090
H	39.1697550	51.9312632	32.0813288	O	43.0026990	49.3712970	35.1411270
H	37.9894122	42.6436578	32.3562920	O	41.2994980	49.6401360	36.5823470
				H	42.9695050	48.6776260	38.2789490
7TS2				H	44.2684460	48.4728730	37.0955630
C	40.2227040	38.7628240	37.7314280	C	41.5531670	46.4251270	37.0672820
N	41.1874880	38.7662500	36.7477370	H	40.7352950	47.1364080	37.1201340
H	41.9080630	38.0503830	36.5861800	C	41.2332500	45.0317830	36.8471360
C	41.1217120	39.9529610	36.1015300	O	40.1240230	44.7063070	36.1704430
H	41.7962550	40.2226190	35.3050190	C	42.3593820	44.0989980	36.6067410
N	40.1511860	40.6994400	36.6038240	O	41.9888480	42.8857090	36.2569680
C	39.5764220	39.9635870	37.6193870	H	40.8761230	42.4927550	38.6028520
H	38.7699270	40.3585340	38.2183240	C	43.6656740	44.5535180	36.7209970
C	43.3171890	39.6563660	40.3151230	H	44.4881310	43.8563010	36.5698680
N	44.0009210	40.0444280	39.1771720	C	43.9150790	45.9072740	36.9648070
H	44.8991890	39.7062640	38.8579010	H	44.9438210	46.2565030	37.0059000
C	43.1709640	40.8471900	38.4521400	O	40.1633450	43.1284020	38.3145270
H	43.4426520	41.2817240	37.4995910	O	40.7217800	44.4497310	38.5140650
N	42.0173780	41.0167330	39.0679890	H	40.0972980	37.9537019	38.4446570
C	42.0976940	40.2761470	40.2271000	H	43.7582506	39.1233398	41.1548467
H	41.2786730	40.2407970	40.9338960	H	34.5609362	43.4429255	35.8551484
C	35.6049000	43.4771870	36.1619740	H	39.1780754	51.8774237	32.0971405
N	36.1520220	44.4805050	36.9379510	H	37.9941135	42.6452385	32.3472569
H	35.6606630	45.2833370	37.3370900				
C	37.4718080	44.2238890	37.0939030	7TS3			
H	38.1421720	44.8575210	37.6534670	C	40.1868080	38.7620570	37.8403990
N	37.8053350	43.1100160	36.4574840	N	41.0611730	38.7810620	36.7739510
C	36.6455540	42.6384200	35.8708590	H	41.7792220	38.0731810	36.5617490
H	36.6289680	41.7362690	35.2785010	C	40.9713320	39.9982980	36.1837990
N	40.1527700	51.9878120	32.4034970	H	41.5720340	40.2861250	35.3352680
H	40.7735230	52.1949880	31.6301170	N	40.0731040	40.7472980	36.8004320
C	40.7229990	51.2006090	33.3884490	C	39.5711980	39.9856470	37.8345780
N	40.0584010	50.9268020	34.5086530	H	38.8215840	40.3732300	38.5076010
H	40.5218280	50.3874080	35.3089230	C	43.8341840	39.8254650	40.0506810
H	39.2153050	51.4458520	34.7164350	N	44.9402260	40.3766850	39.4354090
N	41.9602580	50.7668330	33.2261700	H	45.9022730	40.2812160	39.7257450
H	42.4505850	50.2290280	34.0437240	C	44.5090710	41.0696960	38.3520230

H	45.1796360	41.5466180	37.6535050	O	40.5904630	44.6129030	38.3856770
N	43.1969680	41.0250780	38.2512060	H	40.0702493	37.9183925	38.5144085
C	42.7616220	40.2539500	39.3140190	H	43.8895794	39.2194052	40.9570992
H	41.7139380	40.0585040	39.4707470	H	34.3579864	43.4020546	35.8045690
C	35.4014000	43.4823690	36.0971760	H	39.1565478	51.9562072	32.0670911
N	35.9182810	44.5257570	36.8381700	H	38.0243206	42.6165425	32.4908855
H	35.4106380	45.3312490	37.2084560				
C	37.2358670	44.2930860	37.0357740	73			
H	37.8791680	44.9560430	37.5922160	C	40.1922650	38.7602530	37.8423430
N	37.5951740	43.1581050	36.4552350	N	41.0810130	38.7761290	36.7878100
C	36.4580820	42.6470250	35.8621910	H	41.7953030	38.0630030	36.5805130
H	36.4676220	41.7197040	35.3099650	C	41.0067120	39.9947670	36.1992770
N	40.1296390	52.0743130	32.3733090	H	41.6249000	40.2798380	35.3623480
H	40.7474290	52.2931630	31.6007410	N	40.1047600	40.7484320	36.8046930
C	40.7056260	51.2775870	33.3466460	C	39.5846300	39.9884190	37.8311990
N	40.0467840	50.9954080	34.4677950	H	38.8311200	40.3801690	38.4975280
H	40.5148610	50.4545420	35.2652070	C	43.8355250	39.8264610	40.1393180
H	39.2073790	51.5173740	34.6826210	N	44.9341820	40.4605240	39.5946050
N	41.9423150	50.8463360	33.1711170	H	45.8812010	40.4280370	39.9440760
H	42.4288350	50.2887490	33.9732510	C	44.5115870	41.1563730	38.5087120
H	42.3723010	50.9653220	32.2545900	H	45.1777070	41.7111550	37.8677190
C	39.0672340	42.8686170	32.1724010	N	43.2125150	41.0276930	38.3370990
H	39.4645400	42.0264220	31.5919650	C	42.7763260	40.2032030	39.3581500
H	39.0530570	43.7423040	31.5141510	H	41.7373000	39.9377460	39.4568530
C	40.0558750	43.1291940	33.3261660	C	35.4529980	43.5004190	36.1223060
O	39.8035430	42.4517090	34.4196520	N	35.9675810	44.5368580	36.8751920
O	41.0161820	43.8778830	33.1570560	H	35.4574500	45.3376780	37.2524100
Fe	39.7629290	42.8729270	36.3165520	C	37.2874240	44.3095550	37.0646890
C	42.8641900	46.9335680	37.0775680	H	37.9306070	44.9683540	37.6267840
C	43.1959120	48.4123070	37.2026270	N	37.6500010	43.1848440	36.4667530
C	42.4180570	49.2612070	36.1897050	C	36.5136130	42.6741350	35.8723490
O	42.9667880	49.4105910	35.0634880	H	36.5265010	41.7533020	35.3094670
O	41.2958310	49.7240150	36.5346420	N	40.1185930	52.0945120	32.3790850
H	42.9803000	48.7663420	38.2165490	H	40.7362040	52.3203530	31.6083580
H	44.2650330	48.5572650	37.0182230	C	40.6973390	51.2916640	33.3463810
C	41.5633910	46.5027980	36.9711850	N	40.0409920	51.0055650	34.4681250
H	40.7441600	47.2143140	36.9566620	H	40.5083790	50.4574400	35.2609230
C	41.2224500	45.0864700	36.7970320	H	39.2050530	51.5307240	34.6886550
O	40.2127110	44.7594180	36.0133280	N	41.9328340	50.8600540	33.1652780
C	42.3906290	44.1686490	36.7587670	H	42.4150610	50.2858890	33.9608470
O	42.0311810	42.8709880	36.5114790	H	42.3556850	50.9732680	32.2445270
H	42.4633780	42.2122360	37.1319910	C	39.0770420	42.8657660	32.1793880
C	43.6781660	44.6133920	36.8831910	H	39.4738960	42.0240220	31.5981790
H	44.5090160	43.9105400	36.8351920	H	39.0631400	43.7394820	31.5213110
C	43.9242520	45.9908410	37.0320980	C	40.0700050	43.1271860	33.3274640
H	44.9512180	46.3397160	37.0880830	O	39.8084900	42.4672580	34.4349060
O	39.8265920	43.4848680	38.1551420	O	41.0405330	43.8568240	33.1507320

Fe	39.8196070	42.9018420	36.3140120	C	37.3810630	44.3872720	37.0672860
C	42.8725240	46.9276350	37.0687780	H	38.0300290	45.0565470	37.6125350
C	43.1995630	48.4095370	37.1754670	N	37.7492840	43.2712660	36.4535050
C	42.4079520	49.2514110	36.1677650	C	36.6068840	42.7367810	35.8891160
O	42.9445430	49.3955330	35.0342520	H	36.6225800	41.8188430	35.3215410
O	41.2921940	49.7191670	36.5251410	N	40.0953630	52.2062570	32.3525930
H	42.9946230	48.7688080	38.1895070	H	40.7115060	52.4367830	31.5821800
H	44.2654480	48.5577570	36.9766450	C	40.6725620	51.3855800	33.3065230
C	41.5766690	46.4835390	37.1061990	N	40.0194820	51.1004110	34.4307280
H	40.7523040	47.1853000	37.1858170	H	40.4875420	50.5494350	35.2230010
C	41.2050760	45.0352800	36.9980770	H	39.2038350	51.6514800	34.6639780
O	40.2800450	44.7397310	36.0275480	N	41.8966590	50.9310020	33.1086620
C	42.4205580	44.1468740	36.8125120	H	42.3757660	50.3482450	33.8973960
O	42.0815640	42.8400550	36.5326400	H	42.3120730	51.0431610	32.1827870
H	42.4645350	42.1883370	37.1920620	C	39.0773260	42.9414170	32.0833630
C	43.6975120	44.6180070	36.7752350	H	39.4765760	42.1093020	31.4910110
H	44.5248830	43.9317560	36.5983060	H	39.0301410	43.8168250	31.4299820
C	43.9403800	46.0015770	36.9153870	C	40.0966560	43.2158200	33.1967810
H	44.9626260	46.3668500	36.8705380	O	39.8711320	42.5428500	34.3153980
O	39.9203460	43.4308620	38.1732140	O	41.0581660	43.9472700	33.0150900
O	40.5793530	44.7121670	38.3039950	Fe	39.8586090	42.9339110	36.1539780
H	40.0701860	37.9178712	38.5175332	C	42.8415920	47.0027060	37.0022510
H	43.8862614	39.1972853	41.0286163	C	43.1608600	48.4846310	37.1115930
H	34.4103177	43.4223066	35.8243596	C	42.3644660	49.3241370	36.1080860
H	39.1469617	51.9711373	32.0705880	O	42.8777170	49.4370900	34.9601940
H	38.0342270	42.6143922	32.4977429	O	41.2659930	49.8205970	36.4822200
				H	42.9510840	48.8360300	38.1272080
7TS4				H	44.2261210	48.6383380	36.9144990
C	40.1260820	38.8635530	37.7429360	C	41.5453320	46.5583410	37.0825750
N	41.0562020	38.8891110	36.7276700	H	40.7230950	47.2600290	37.1834360
H	41.7865930	38.1854670	36.5512130	C	41.2014890	45.1097600	37.0063130
C	41.0060630	40.1064220	36.1455950	O	40.2637260	44.7616400	36.0334510
H	41.6650620	40.3980100	35.3437570	C	42.4124620	44.2131730	36.8563430
N	40.0591350	40.8493650	36.7007160	O	42.0660410	42.9005670	36.8566300
C	39.5023600	40.0815650	37.7050130	H	41.3418870	42.8736340	37.7881080
H	38.7267110	40.4633070	38.3513870	C	43.6847460	44.6939860	36.7583500
C	43.5356410	39.5668340	40.4432800	H	44.5144200	43.9968480	36.6604740
N	44.3532740	40.0704330	39.4528360	C	43.9119660	46.0851720	36.8219860
H	45.3523300	39.9529280	39.3671120	H	44.9270880	46.4633150	36.7417760
C	43.5475440	40.6866750	38.5391470	O	40.2301410	43.3508510	38.2664450
H	43.9290010	41.1688210	37.6495860	O	40.5708500	44.7826280	38.3008920
N	42.2842850	40.6274800	38.8977670	H	40.0254698	38.0334186	38.4382191
C	42.2657050	39.9309170	40.0845120	H	43.8882886	39.0165098	41.3075116
H	41.3430800	39.7458570	40.6194860	H	34.4971848	43.4636368	35.8630705
C	35.5385230	43.5426070	36.1691020	H	39.1251839	52.0786644	32.0424170
N	36.0526430	44.5841930	36.9161380	H	38.0481744	42.6675572	32.4280862
H	35.5365330	45.3754840	37.3067420				

74				C	39.0051250	42.9212620	32.0136290
C	40.1918170	38.7936320	37.7420620	H	39.4214000	42.0904730	31.4317290
N	41.1604930	38.8161960	36.7624970	H	38.9518470	43.7927140	31.3559380
H	41.8830010	38.1039030	36.5897560	C	40.0017150	43.2152160	33.1393180
C	41.0889120	40.0108840	36.1309490	O	39.7643990	42.5304550	34.2460080
H	41.7686830	40.2936780	35.3430910	O	40.9477600	43.9728810	32.9796310
N	40.1126370	40.7456330	36.6392240	Fe	39.9855310	42.8624220	36.0788310
C	39.5390350	39.9926520	37.6427760	C	42.8702370	46.8483550	37.1727560
H	38.7272810	40.3713670	38.2452160	C	43.1992490	48.3279470	37.3099580
C	43.2757710	39.6805840	40.3302320	C	42.4290570	49.1824880	36.2910270
N	43.9634140	40.1153610	39.2117540	O	43.0150310	49.3858970	35.1921940
H	44.8765730	39.8122850	38.9000480	O	41.2804000	49.6039150	36.6052430
C	43.1270750	40.9247880	38.5020500	H	42.9666400	48.6803460	38.3207850
H	43.3960150	41.3951780	37.5657160	H	44.2686060	48.4807150	37.1376320
N	41.9628370	41.0547090	39.1093350	C	41.5673090	46.4199900	37.2296230
C	42.0442150	40.2776170	40.2454050	H	40.7513280	47.1247850	37.3510250
H	41.2183070	40.2038930	40.9410910	C	41.2091370	44.9907020	37.0641070
C	35.5703760	43.4756280	36.1479880	O	40.1318900	44.7329120	36.2426410
N	36.0996520	44.5166520	36.8842840	C	42.3624510	44.0849900	36.6777660
H	35.5949080	45.3228880	37.2591230	O	41.9683510	42.8733140	36.3242430
C	37.4218500	44.2864830	37.0536850	H	40.8660030	42.6104780	38.6648160
H	38.0759560	44.9619110	37.5807580	C	43.6575870	44.5543640	36.6865780
N	37.7756970	43.1524960	36.4657410	H	44.4710290	43.8739680	36.4417310
C	36.6245610	42.6406070	35.8952910	C	43.9184600	45.9152850	36.9370830
H	36.6245840	41.7161440	35.3383540	H	44.9442430	46.2727220	36.9026740
N	40.1422040	51.9460110	32.4203660	O	40.1454610	43.2532810	38.4026100
H	40.7643890	52.1360280	31.6433860	O	40.7655180	44.5888160	38.4611880
C	40.7039940	51.1498690	33.4037020	H	40.0739090	37.9778762	38.4495223
N	40.0501580	50.9004470	34.5346880	H	43.7241720	39.1419824	41.1630288
H	40.5104820	50.3524790	35.3336230	H	34.5285651	43.4212453	35.8377232
H	39.2193760	51.4371710	34.7469670	H	39.1662225	51.8466122	32.1123270
N	41.9190770	50.6620320	33.2210060	H	37.9789268	42.6359604	32.3566692
H	42.4432940	50.2073070	34.0577040				
H	42.3789580	50.8412840	32.3250650				