

Supporting Information for the Manuscript:

“Mechanism of Selective Halogenation by SyrB2 - a Computational Study”

Tomasz Borowski, Holger Noack, Mariusz Radoń, Konrad Zych, Per E.M. Siegbahn

1 Complete author list for references 29 and 38

ref 29: Gaussian 03, Revision E.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

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2 Further technical details on CASPT2 calculations

We note that although the σ_L ligand orbital is much more important for the triplet than for the quintet and septet states, we kept it active for all multiplicities to make the calculations fully consistent with each other. However, as a drawback σ_L tended to mix with the inactive orbitals for quintet and septet state of one stereoisomer. To avoid this we constrained the orbitals mostly involved in the unfavorable rotations (i.e., prevented them from mixing with the other orbitals in CASSCF calculations using the SUPSYMMETRY keyword of Molcas). In this way we fixed Fe 3s,3p for the septet [the initial orbitals were taken from the preceding calculations without the σ_L orbital] and σ_L for the quintet (the initial orbitals were taken from the preceding septet calculations on the quintet structure).

3 Kinetic Isotope Effect calculations

Rate constants for hydrogen atom transfer were computed from the Eyring equation:

$$k = \kappa \frac{k_B T}{h} e^{\frac{-\Delta G^\ddagger}{RT}}$$

where κ is a transmission coefficient, usually taken to be 1. $\Delta G^\ddagger$ is an activation free energy, k_B and R are Boltzmann and gas constants.

Correction for tunneling was computed from the Wigner equation relating the transmission coefficient κ with the frequency of the normal mode connected with the reaction coordinate (with imaginary frequency):

$$\kappa(T) = 1 + \frac{1}{24} [\hbar \omega^\ddagger \beta]^2$$

where β is the thermodynamic beta.

The primary kinetic isotope effect (KIE) was calculated as a ratio of the rate constants calculated for protium and deuterium transferred from the substrate to the oxo ligand.

Calculations were performed for a smaller model which comprises the first shell ligands of iron, ethane as a substrate model, and two water molecules forming hydrogen bonds with the chloro ligand. The models were fully optimized and subsequently subjected to frequency calculations at the B3LYP/lacvp level of theory. Free energy was calculated from the not scaled frequencies for room temperature (25 C) and standard pressure of 1 bar.

The two C-H cleavage transition states differ considerably in the magnitude of the imaginary frequency connected with the reactive mode. For protium, the values are i1046 and i279 cm^{-1} , for **TSab** and **TSa'b'**, respectively. As a consequence, KIE are also very different. The Eyring KIE are 6.63 and 2.90 for **TSab** and **TSa'b'**, whereas the KIE calculated with the Wigner correction are 8.29 and 2.93, respectively.

4 Spin density for TSab and TSa'b'

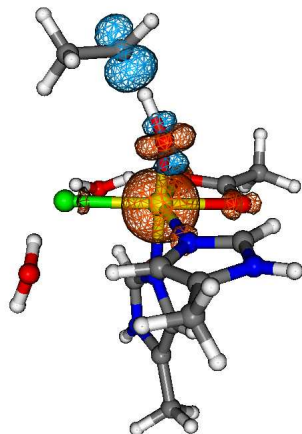


Figure S 1: Spin density plot calculated for a small model of **TSab**. Blue: -0.01 isosurface, red: 0.01 isosurface

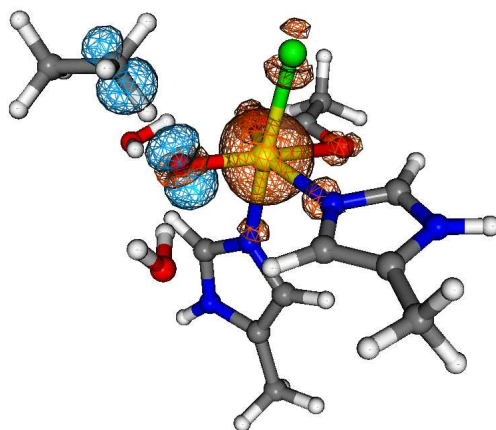


Figure S 2: Spin density plot calculated for a small model of **TSa'b'**. Blue: -0.01 isosurface, red: 0.01 isosurface

Plots of the spin density calculated for the two transition states for the C-H bond cleavage (**TSab** and **TSa'b'**) are presented in Figure S1 and S2. In these calculations the smaller model of the active site, the one used for KIE calculations described above, was employed. From the analysis of the plots it follows that in both transition states the bonding orbital of the cleaving C-H bond is depleted of α spin density, and as a consequence the negative spin density (blue in Figures S1 and S2) dominates. On the oxo group there are α and β spin density contributions, however, their relative size differs for the two transition states. Specifically, for **TSab** the two contributions are of comparable size, and thus the total spin population on the oxo atom is close to zero, i.e. 0.1 (Figure 4A in the main text). On the other hand, for **TSa'b'** the β spin density contribution clearly dominates, which results in the negative spin population of -0.3 (Figure 4B). When the two water molecules are removed from the model, the difference in spin population on the oxo ligand is reduced only slightly, i.e. the values are 0.1 and -0.2 for **TSab** and **TSa'b'**, respectively. Therefore, it is the configuration of the ligands around iron that mostly affects the electronic structure of the C-H cleavage transition state, which manifests in the distribution of the spin density.

5 Relative energies including Zero Point Energy corrections

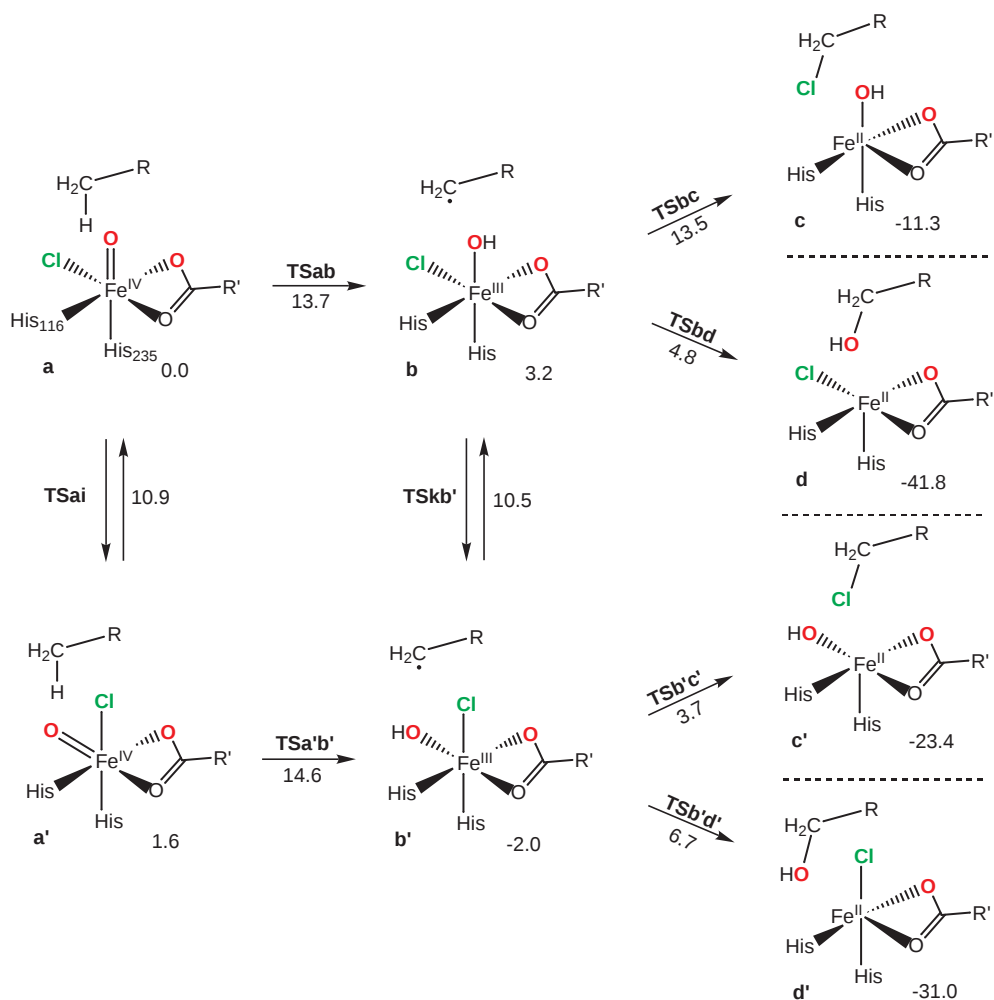


Figure S 3: Suggested reaction mechanism for chlorination and hydroxylation of L-Thr by SyrB2. Relative energies include ZPE and are given in kcal/mol.

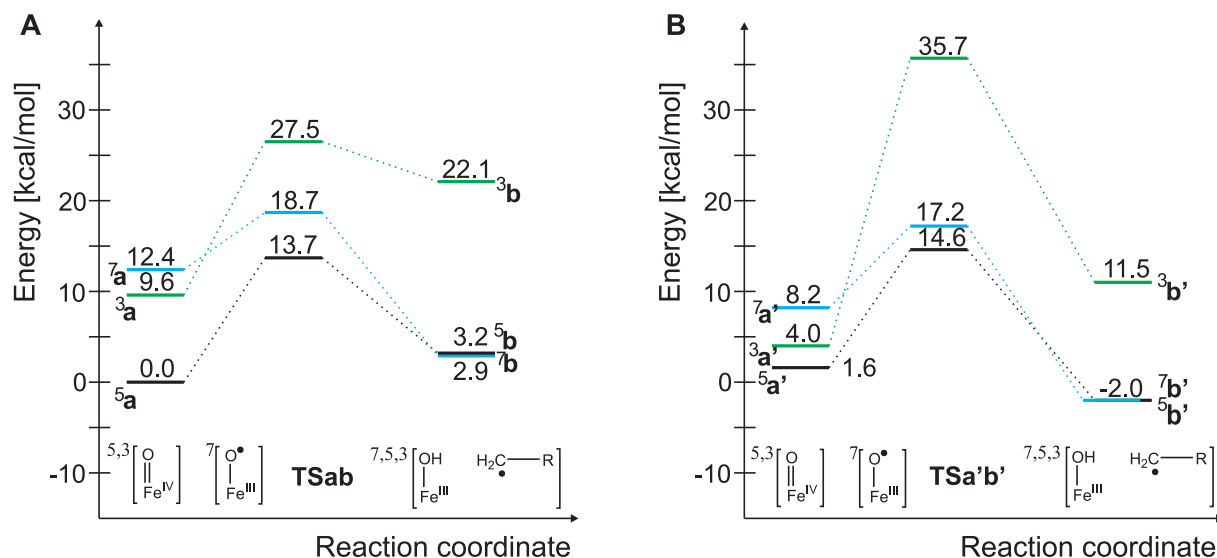


Figure S 4: Calculated energy profiles for the C-H cleavage step in the septet, quintet and triplet spin states for A) the normal (**a**) and B) the alternative (**a'**) configuration of the oxoferryl species. The reported energies combine electronic energy calculated for the bigger basis set, solvent and ZPE corrections.

6 Cartesian coordinates and energies for optimized structures

³ a			
E lacvp = -3210.747545			
H	1.1011999478	31.6992490285	6.1647210261
C	1.5070000361	32.6379999450	5.9509999389
H	2.3930977674	32.4930064291	5.3260986805
H	0.7776901885	33.2264932540	5.3840632982
C	1.9144568432	33.3538990004	7.2591121876
H	1.0416018020	33.7374867241	7.7951512793
H	2.4123116902	32.6299765066	7.9198265702
C	2.9029166386	34.4848898173	7.0292943626
O	3.9366465562	34.2175314810	6.3176765456
O	2.6800328524	35.6528163265	7.5703688888
H	10.1431259819	43.2460479945	12.4666190083
C	9.9049999776	42.7149999374	11.5979999603
H	9.1959996968	43.3493501297	11.0533333909
H	10.8170766934	42.7038781636	10.9851006344
C	9.3360668915	41.3492533669	11.6819279494
N	10.1178534782	40.1899350454	11.6597628084
H	11.1254184728	40.1636335084	11.6823906229
C	9.3023533704	39.1039188332	11.5860919474
H	9.6135923459	38.0753892362	11.5891877444
N	8.0368421800	39.5281421378	11.5587484239
C	8.0325881404	40.9183840446	11.6104940362
H	7.1288071677	41.5056692911	11.6174636709
H	8.8908009972	39.8624230053	17.1734290017
C	7.9660000387	39.3979990082	17.0849990792
H	8.1045303700	38.3626426306	17.4159636864
H	7.2967012198	39.8630204144	17.8197001333

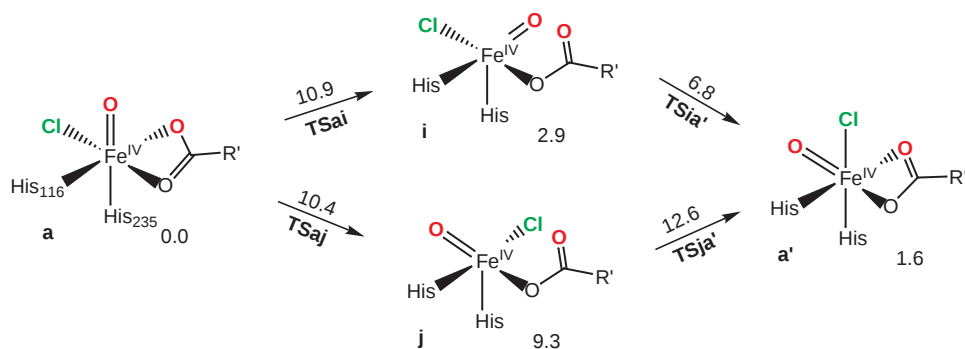


Figure S 5: Mechanism for the configurational change of the Cl-Fe^{IV}=O species. Reported energies include ZPE.

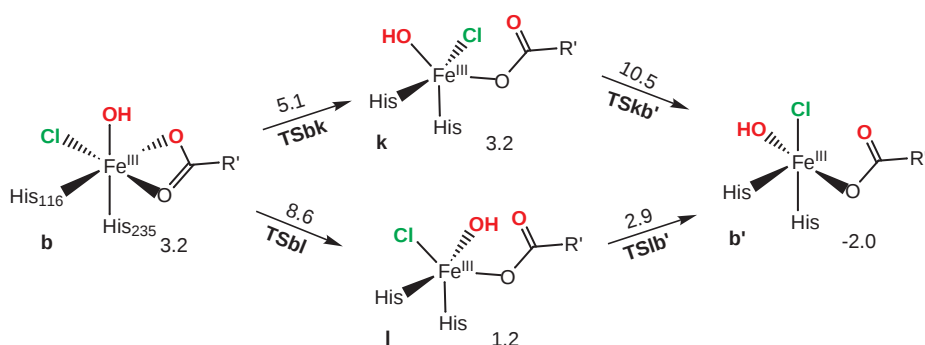


Figure S 6: Mechanism for the configurational change of the Cl-Fe^{III}-OH species. Reported energies include ZPE.

C	7.3342593379	39.4014739461	15.7338211774
N	6.4547516275	40.4021308827	15.3164951525
H	6.2006957569	41.2215341453	15.8462877935
C	5.9862099397	40.1062081176	14.0747657266
H	5.3497280648	40.7651516551	13.5114493105
N	6.5248354056	38.9501916035	13.6618606660
C	7.3624501934	38.5019381911	14.6935760796
H	7.9274656805	37.5928442761	14.5989772081
H	-3.6033639846	36.6101679887	11.2938310068
C	-2.9419999652	37.1860010163	10.7509989865
H	-3.4435311032	37.5157022981	9.8329381454
H	-2.7083818478	38.0848073412	11.3366231345
C	-1.6606140274	36.3894154331	10.4286733042
H	-1.2128363912	36.0223822498	11.3623309379
H	-1.9052104942	35.4942972156	9.8431147557
C	-0.6261601482	37.2337708513	9.6505261520
H	-0.9689147725	37.3908789357	8.6237268114
H	-0.5425623653	38.2328673236	10.1033925951
N	0.7187440067	36.6387681836	9.5663385752
H	1.0737446707	36.2818738101	8.6773460820
C	1.6162887438	36.6852458145	10.5768442221
N	1.2846722372	37.1543487514	11.7902918605
H	0.3412181980	37.4338797974	11.9950271365

H	2.0201012996	37.2717806321	12.5145744512
N	2.8688674615	36.2485329192	10.3460870911
H	3.1162406798	35.9728859455	9.3969389632
H	3.5890112155	36.3230197542	11.0513451712
Fe	6.5916573704	38.2680623406	11.7012995761
Cl	4.7277307563	39.6512487341	11.1645211319
O	5.6336276012	36.3529334740	12.2787565583
C	6.8472504456	35.9116749084	12.3946631123
O	7.7965266897	36.8072703919	12.2974714994
C	7.2193471121	34.4814964886	12.5908377066
H	7.3065798345	34.2476076200	13.6589382528
H	6.4667169816	33.8220912419	12.1548757883
H	8.1947769756	34.3228610577	12.1201749925
O	3.4229145213	37.6128250751	13.3514529783
H	4.1702508259	36.9781633916	13.3529304470
H	3.7473770825	38.4455078611	12.9450772656
O	5.2459685726	42.5715784394	12.2083071128
H	4.8668131046	41.8786281590	11.6227057174
H	4.8374902388	43.4352480835	12.0172612335
O	6.6761912882	37.7538046315	10.1337492001
H	7.0165574720	38.9247974419	7.4778584442
C	5.9719711705	38.9205875852	7.1542947019
C	5.4830177805	37.5076001073	6.8742144723
O	4.1397658307	37.5529453469	6.3358957383
C	6.3757892377	36.7795456892	5.7798110700
C	7.5607080720	36.0372397493	6.3692339898
O	7.4742108203	34.8988563564	6.8475497041
N	5.4642199358	35.8203251738	5.0630265017
S	9.1225752038	37.0035812269	6.3146204551
C	10.1945655391	36.0769415370	7.6059118623
C	11.1072411344	34.9929708635	7.0476659470
N	10.4098542419	33.7290217840	6.8295066125
C	11.1139146856	32.5571043286	6.7707847204
C	10.3076384394	31.2961092709	6.5381220936
H	10.6053983299	30.5415113190	7.2713303869
O	12.3569999945	32.5519980099	6.8970000043
H	4.6758929478	36.3988625911	4.7363065641
H	6.7191323503	37.5233174401	5.0544759036
H	5.5052024598	36.9050143527	7.7900425778
H	3.5302516599	36.9272495707	6.8409285190
H	5.8653655156	39.5375782700	6.2551373514
H	5.3702242106	39.3559679055	7.9553408797
H	4.9418255152	35.0919422548	5.7339802793
H	10.7821440584	36.8888336562	8.0391884677
H	9.5014665029	35.6908397689	8.3575037548
H	11.5972371235	35.3367983916	6.1269892752
H	11.9149707013	34.8027458438	7.7662771374
H	9.4070000005	33.7160000084	6.7599999956
H	9.2272764795	31.4550394283	6.6050103551
H	10.5428075319	30.8943861435	5.5465576882
H	5.9232842800	35.3260783593	4.2959837880

⁷**a**

E lacvp = -3210.739317		
H	1.1011999655	31.6992490115
C	1.5070000123	32.6379999814
H	2.4125479319	32.4897316811
H	0.7914581371	33.2146134271
C	1.8720073606	33.3734875424
H	0.9857437311	33.7840102471
H	2.3278905989	32.6545996839
C	2.8910422628	34.4814360774
O	3.9369465178	34.1784853035
O	2.6848684808	35.6583134771
H	10.1431259601	43.2460480262

C	9.9050000343	42.7149999732	11.5980000081
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N	10.0398862839	40.1848413625	11.7661645918
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C	9.1879755467	39.1231908278	11.6992939385
H	9.4678452657	38.0860622574	11.7433438328
N	7.9365970514	39.5788365239	11.5963260007
C	7.9855266985	40.9730541271	11.5918266255
H	7.0976096644	41.5866962616	11.5339946377
H	8.8908009978	39.8624229998	17.1734290244
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H	8.1285305094	38.3385615734	17.3109858279
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N	6.5288847605	40.6234381365	15.3715754849
H	6.4564234160	41.4917432863	15.8793972686
C	5.9214027893	40.3608614607	14.1784862502
H	5.3636833646	41.0914623009	13.6090109141
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C	7.0494073551	38.5701727579	14.7891070541
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H	-3.6033639981	36.6101680098	11.2938310127
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H	-3.4205992845	37.4759965222	9.8080862816
H	-2.7448628698	38.1059896007	11.3166551843
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H	-1.2446234858	36.0239344553	11.4508757447
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H	-0.4399114553	38.2193931744	10.3268374169
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H	1.0993821308	36.3094687569	8.7628523066
C	1.6784122355	36.5777557565	10.6752269122
N	1.3706459427	36.9573242538	11.9248000686
H	0.4316907420	37.2317743895	12.1576375716
H	2.0957180545	37.0061099050	12.6676995407
N	2.9165183268	36.1318906797	10.3913335111
H	3.1510007641	35.9456118544	9.4175366139
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Fe	6.2405103922	38.3770402119	11.7623586055
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O	5.5402917403	36.3090837643	12.4188763615
C	6.7568630757	35.8769203782	12.2512614423
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C	7.1366578200	34.4360163136	12.3665937755
H	6.9488385549	34.0691489279	13.3817621898
H	6.5284865670	33.8322761113	11.6849568363
H	8.1947769747	34.3228610023	12.1201750038
O	3.3640569259	37.1835262449	13.7788294459
H	4.1600012981	36.6587553493	13.5304133424
H	3.6199739519	38.1249827265	13.7874227617
O	5.1074365277	42.4093249976	11.9461457379
H	4.6334682989	41.6810497437	11.4840883897
H	4.7155511235	43.2697334821	11.7111255514
O	5.9336777918	37.9602745604	9.9381639782
H	7.0143307116	38.9921385899	7.0798789237
C	5.9523570629	38.9463744825	6.8187347395
C	5.4763588109	37.5088636668	6.6689437506
O	4.1094461932	37.4980732505	6.1908700430
C	6.3331408958	36.7167672733	5.5909717512
C	7.5567976266	36.0347119862	6.1772681723
O	7.5105365590	34.9455275219	6.7631075185

N	5.4100426585	35.6987039889	4.9806523270
S	9.1001472824	37.0029027431	5.9352350866
C	10.3065382484	36.1752551794	7.1748880191
C	11.1170884344	35.0027524317	6.6309606671
N	10.4117049932	33.7301145120	6.7489656552
C	11.1079127204	32.5589859055	6.8795222017
C	10.2808112197	31.2947181808	6.9901954197
H	10.6476197119	30.7011707212	7.8320548750
O	12.3569999905	32.5519980061	6.8969999966
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H	5.5459439024	36.9834707677	7.6278098170
H	3.5293288761	36.9085600285	6.7672919388
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H	11.4231052579	35.1964637127	5.5939914597
H	12.0445929249	34.9054514877	7.2086071249
H	9.4070000095	33.7160000169	6.7600000161
H	9.2121935256	31.4873243266	7.1239971203
H	10.4180833147	30.6924964852	6.0855397991
H	5.8473843660	35.1538544688	4.2355164692
³a'			
E lacvp = -3210.758645			
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C	1.5070001022	32.6379999604	5.9510000534
H	2.3565819180	32.4877255635	5.2777598065
H	0.7565308047	33.2387723051	5.4250698941
C	1.9970502651	33.3522451328	7.2309694158
H	1.1614044032	33.7375761038	7.8220782612
H	2.5489712814	32.6361422409	7.8534948534
C	2.9550976952	34.4810431872	6.8893799045
O	3.9993789596	34.1537710970	6.2206739865
O	2.6846507379	35.7022911541	7.2640870968
H	10.1431260421	43.2460479360	12.4666190276
C	9.9049998804	42.7149999718	11.5979999483
H	9.1873213507	43.3456690051	11.0596754532
H	10.8135116633	42.7186557030	10.9798637084
C	9.3533527568	41.3438061952	11.6737372764
N	10.1485497637	40.1951456297	11.6018967382
H	11.1565466714	40.1816338926	11.5879689012
C	9.3471508641	39.0997495169	11.5243190383
H	9.6701485940	38.0757812229	11.4857858832
N	8.0782835748	39.5108365183	11.5487159432
C	8.0542434128	40.8986238077	11.6320695346
H	7.1304434423	41.4577957232	11.6513759438
H	8.8908009639	39.8624230692	17.1734290144
C	7.9660000411	39.3979989058	17.0849989231
H	8.1020791251	38.3662829476	17.4287938049
H	7.2966754842	39.8721875264	17.8135426871
C	7.3436379768	39.3907178255	15.7348071480
N	6.3678997988	40.3069524068	15.3368548562
H	6.0210053165	41.0729074945	15.8934516736
C	5.9468982223	40.0062026252	14.0777821332
H	5.2593175175	40.6070469456	13.5021175005
N	6.6155661036	38.9271715049	13.6557826737
C	7.4834140195	38.5306228348	14.6732295590
H	8.1360165219	37.6855765282	14.5578433487
H	-3.6033640635	36.6101679979	11.2938309203
C	-2.9419997830	37.1860009977	10.7509991006
H	-3.4964234669	37.6333106136	9.9158739090
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C	-1.7429212811	36.3658777075	10.2330388432
H	-1.1679882919	35.9722279158	11.0814172587
H	-2.0910962274	35.4885710815	9.6744043529
C	-0.8202543426	37.2173978703	9.3233170729
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Fe	6.6406188836	38.2668890310	11.7887042101
Cl	6.9600597210	37.4164396864	9.6351469299
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C	6.9545633503	35.9428069978	12.4726214737
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H	7.4082722127	34.2600156563	13.7111966532
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O	4.9725415546	41.8108917215	11.7893593951
H	4.9602009559	40.9140472955	11.3688772394
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C	5.9902474330	38.8780508843	6.3754040951
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C	6.4214009405	36.5699743184	5.3187442914
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O	7.4846413903	34.7887770422	6.5705186822
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C	10.1175789233	36.1107874109	7.4392765523
C	11.0893197242	34.9953226351	7.0810145325
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C	11.1152138395	32.5609170883	6.7574497453
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O	12.3569999863	32.5519979936	6.8969999812
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H	5.5319273347	36.9667112540	7.2841434801
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H	11.7083897532	35.2769296851	6.2196193186
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H	9.4070000504	33.7160000549	6.7600000383
H	9.2308285644	31.4676778366	6.5093513583
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E lacvp = -3210.749853

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C	2.0569743448	33.3404504566	7.2138915335
H	1.2495702714	33.7390755848	7.8344126139
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C	3.0102201548	34.4543427665	6.8162779197
O	4.0686312250	34.0864386169	6.1853726764
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H	10.1431259939	43.2460479966	12.4666190037
C	9.9050000137	42.7150000188	11.5979999943
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C	9.3359566136	41.3525879197	11.6836123544
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H	11.1076161253	40.1622753908	11.9291799463
C	9.2923921773	39.1050285618	11.7001499252
H	9.5934907382	38.0769224373	11.7913686424
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H	8.1246240655	38.3415143442	17.3268219587
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H	5.3795946109	41.0201983061	13.5614788763
N	6.3866813433	39.1140806889	13.7383005161
C	7.2020020837	38.5895029447	14.7409446365
H	7.6771508033	37.6306036123	14.6390427184
H	-3.6033639979	36.6101679934	11.2938309956
C	-2.9419999559	37.1860010094	10.7509989968
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C	-1.9310908850	36.3207399246	9.9722705108
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H	-2.4613083694	35.5989310302	9.3397208602
C	-0.9832304396	37.1841716116	9.0932270952
H	-1.3653566200	37.2546837349	8.0718776340
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Fe	6.3708240523	38.3419439943	11.7783387315
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C	10.3007074681	31.2857733156	6.6238464244
H	10.5808220135	30.5767835135	7.4080712738
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H	4.7587402407	35.8241123247	4.0935130030
H	6.8065239076	37.0105983820	4.2175163896
H	5.5416212303	36.9703403579	6.9972963440
H	3.5759741558	36.7883559138	6.0860847934
H	5.8816588304	39.2199697586	4.9343942064
H	5.3758510449	39.4043976790	6.6265303663
H	5.0067841197	34.7851783537	5.3867823542
H	10.6761590790	37.0389569932	7.5520730626
H	9.3882277484	35.8846165677	7.9802871137
H	11.7123680753	35.2172405659	6.0604458775
H	11.8062095168	34.9306052633	7.7879108142
H	9.4070000113	33.7160000194	6.7600000243
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H	6.0165944150	34.6873994391	3.9351421013
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H	0.7525144192	33.2408266813	5.4328967624
C	2.0126281327	33.3526198572	7.2242251028
H	1.1848672219	33.7385009687	7.8259032004
H	2.5747711897	32.6389186138	7.8398952508
C	2.9615015906	34.4820137565	6.8610317743
O	4.0037894733	34.1477665711	6.1906828207
O	2.6855777845	35.7070118747	7.2145123057
H	10.1431260317	43.2460479370	12.4666190298
C	9.9049999026	42.7149999888	11.5979999537
H	9.1675975359	43.3353542037	11.0749418087
H	10.8064550069	42.7473173750	10.9688656324
C	9.3787910155	41.3376736873	11.6598715727
N	10.1783406655	40.1901237797	11.7058883868
H	11.1821592933	40.1788898419	11.8001821621
C	9.3798217539	39.0926331115	11.5813711205
H	9.7045546246	38.0690191385	11.6235408005
N	8.1137371235	39.4952877686	11.4550968975
C	8.0944350063	40.8857202516	11.4921331288
H	7.1774528595	41.4504982102	11.4195129570
H	8.8908009785	39.8624230416	17.1734290061
C	7.9660000190	39.3979989351	17.0849989174
H	8.1089915016	38.3537690862	17.3833469962
H	7.3054293224	39.8412680094	17.8407887094
C	7.3329479676	39.4403883661	15.7429499356

N	6.4536977224	40.4449681420	15.3264850104
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C	-2.9419998170	37.1860009797	10.7509991059
H	-3.5056318362	37.6783720560	9.9482176626
H	-2.5604050455	37.9794693209	11.4082080142
C	-1.7843824454	36.3471563751	10.1730836727
H	-1.2127917539	35.8900832981	10.9912433210
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C	-0.8408614895	37.2052479014	9.2907568250
H	-1.2384204696	37.2808802109	8.2752278482
H	-0.8024076764	38.2326847272	9.6827307723
N	0.5366232376	36.6975088742	9.1773434528
H	0.8942338210	36.3420575132	8.2917793361
C	1.4452157253	36.8257429257	10.1720180426
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C	6.9654840059	35.9399253577	12.6576939023
O	7.8483393161	36.8496796358	12.3227082630
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H	7.0161778643	38.8944236392	6.6877901787
C	5.9819870947	38.8413338504	6.3356387945
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C	6.4184476015	36.5395797412	5.2625196882
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N	5.5235213809	35.4880079767	4.6674230300
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C	10.1125245671	36.1146746659	7.4043910080
C	11.0886103003	35.0011492466	7.0493899359
N	10.4095705614	33.7294006510	6.8249883339
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H	5.9057069457	39.3371889740	5.3615967871
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H	11.6961860859	35.2763787547	6.1778126584
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H	0.7816135585	33.2168907336	5.3688489427
C	1.9017737111	33.3792350940	7.2482758659
H	1.0247197497	33.7705343429	7.7720775531
H	2.3949760815	32.6701033190	7.9292384992
C	2.8913849805	34.5118413898	7.0158661599
O	3.8973274332	34.2634374313	6.2582560939
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H (*)	10.1431259948	43.2460480024	12.4666190000
C (*)	9.9049999956	42.7149999847	11.5980000004
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H	10.8216438061	42.6760713641	10.9922160056
C	9.3117651507	41.3648705584	11.7302646702
N	10.0387938975	40.2227501552	12.0795009250
H	11.0153835644	40.2031611372	12.3290006705
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H	8.1167182668	38.3516878364	17.3733278523
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N	6.3839297275	40.4409129058	15.3943148425
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C (*)	-2.9419999090	37.1860009939	10.7509989820
H	-3.4188261085	37.4774346917	9.8078610337
H	-2.7415565184	38.1046332998	11.3175264363
C	-1.6384611677	36.3950035955	10.4992224770
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H	-1.8438039281	35.5148071235	9.8768896300
C	-0.5469286927	37.2483801533	9.8179012926
H	-0.8620127523	37.5119003924	8.8037385283
H	-0.4221599385	38.1981042569	10.3584235914
N	0.7699917426	36.5960004964	9.6953690206
H	1.1072267713	36.2950095614	8.7800264480
C	1.6750230403	36.5231648303	10.6996915932
N	1.3636244214	36.8856811360	11.9536058113
H	0.4296155035	37.1769621862	12.1854849604
H	2.0885560292	36.9047590528	12.6966711483
N	2.9104166212	36.0694588232	10.4152610404
H	3.1324007513	35.8634414384	9.4417650238
H	3.6543079855	36.0875874732	11.1014611901
Fe	6.3474197250	38.3848550693	11.7467523535

Cl	4.1933694556	39.4683578200	11.5613875740
O	5.5887229031	36.3409151269	12.2532939142
C	6.8159219208	35.8979003758	12.3348075122
O	7.7590784215	36.7760550296	12.3034502635
C	7.1549775929	34.4450378529	12.4345644670
H	7.0482863580	34.0929817933	13.4675928120
H	6.4898996838	33.8478647216	11.8063901151
H (*)	8.1947769940	34.3228610059	12.1201750000
O	3.4169480833	37.1297664117	13.7384403744
H	4.2180923694	36.6362908596	13.4457478468
H	3.6004008678	38.0802199865	13.5975695870
O	5.5691500139	41.8216695942	9.8699174910
H	4.9265773287	41.1500754185	10.1834623588
H	5.1963289563	42.3224369935	9.1231809158
O	6.3691534512	37.9782072524	10.1488686881
H	7.0803965245	39.0630170524	7.3591429557
C	6.0135493380	39.0448206987	7.1173265167
C	5.5117188020	37.6175752548	6.9462961128
O	4.1514936006	37.6386630524	6.4556732962
C	6.3876518133	36.8333939456	5.8650015826
C	7.5155073184	36.0316925466	6.4872322117
O	7.3685631024	34.8833054831	6.9247412178
N	5.4470108757	35.9271920188	5.1211246227
S	9.1087964833	36.9487949679	6.5556972303
C	10.0573710487	35.9562052479	7.8955773146
C	11.0569640591	34.9380404217	7.3649156860
N	10.4038391633	33.7231834167	6.8870628404
C	11.1264056026	32.5784903634	6.6830753937
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O (*)	12.3569999801	32.5519980669	6.8969999993
H	4.6691909592	36.5358010108	4.8237348418
H	6.7926959917	37.5571350206	5.1511719805
H	5.5651482516	37.0745796615	7.8967260036
H	3.5702989589	36.9725476779	6.9432241360
H	5.8432141616	39.6084906281	6.1928325605
H	5.4818194498	39.5364868895	7.9342988186
H	4.9078872216	35.1706955600	5.7551365977
H	10.5651647210	36.7410923233	8.4588410913
H	9.2928685259	35.4950400012	8.5257584651
H	11.6822466807	35.3787735402	6.5777206037
H	11.7428871677	34.6621455280	8.1773090609
H (*)	9.4069999338	33.7159999487	6.7600000170
H	9.2700221774	31.5045198739	6.2330787256
H	10.6328377098	31.1788237591	5.1372715045
H	5.8896107147	35.4558984088	4.3301459952

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E lacvp =	-3210.724061		
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H	2.3764380566	32.4967535608	5.3025139159
H	0.7666141672	33.2380765321	5.4113591093
C	1.9486051576	33.3314020728	7.2613859368
H	1.0899339536	33.7056699593	7.8260372489
H	2.4608138109	32.5947597207	7.8967361350
C	2.9313469411	34.4657693476	7.0330875374
O	3.9436308967	34.2130984952	6.2811541093
O	2.7351115597	35.6180048058	7.6105135511
H	10.1431259156	43.2460480779	12.4666189755
C	9.9050000908	42.7149999007	11.5980000683
H	9.2381056492	43.3724362494	11.0276257838
H	10.8318123149	42.6580401358	11.0103321794
C	9.2767453458	41.3776421874	11.6851607081
N	10.0082700075	40.1845309739	11.6963218111

H	11.0128842683	40.1146357131	11.7449923640
C	9.1447851150	39.1347289896	11.6217369072
H	9.4071536957	38.0921503499	11.6566201840
N	7.8986029071	39.6112827418	11.5641664273
C	7.9583754644	41.0022556337	11.5946899508
H	7.0738424127	41.6225976299	11.5757915533
H	8.8908009956	39.8624230009	17.1734290424
C	7.9659999637	39.3979989868	17.0849988376
H	8.1149296872	38.3514006759	17.3721959114
H	7.3105921742	39.8302826087	17.8521457681
C	7.3034092904	39.4435221740	15.7508883532
N	6.4903504489	40.5035224259	15.3374046805
H	6.3087645576	41.3443304135	15.8636756424
C	5.9678513984	40.2298791688	14.1135192353
H	5.3694860070	40.9249071830	13.5460961888
N	6.4082737530	39.0263631070	13.7158602180
C	7.2374770121	38.5271385269	14.7290064644
H	7.7299838228	37.5778941506	14.6279611999
H	-3.6033639913	36.6101679858	11.2938309957
C	-2.9419998363	37.1860010066	10.7509989831
H	-3.4218830326	37.4847426644	9.8116861078
H	-2.7326307154	38.1001708260	11.3212680778
C	-1.6457669035	36.3856864694	10.4904552655
H	-1.2638875102	35.9952542234	11.4439637806
H	-1.8632054411	35.5045016797	9.8734639004
C	-0.5515492196	37.2264241741	9.7973212199
H	-0.8614752066	37.4708316220	8.7767723024
H	-0.4279936862	38.1856361921	10.3208517511
N	0.7663839106	36.5715001903	9.6977333016
H	1.1107528524	36.2570180387	8.7909626786
C	1.6625775611	36.5294654771	10.7136648141
N	1.3330227250	36.9176859886	11.9532968981
H	0.3927188195	37.2021660137	12.1674046715
H	2.0607657976	36.9982742896	12.6952081556
N	2.9064706087	36.0818210608	10.4565248558
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Fe	6.3470365474	38.3367911234	11.8245466404
Cl	4.2212533495	39.5804408335	11.4045433934
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H	7.0687500022	34.0132491694	13.4712712884
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H	4.6606633637	41.7354318891	11.6424992011
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O	6.3288756503	37.7756225765	10.1392891009
H	7.0943832629	38.8943818105	7.4948413789
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C	6.3669661940	36.7589467291	5.6561125804
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O	7.6219861864	34.9104071955	6.5889000958
N	5.4432780075	35.7786703011	4.9870973029
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C	11.0842429491	34.9551419786	6.3151615343
N	10.4081952602	33.7214573781	6.6938999607

C	11.1112275056	32.5795083430	6.9686582355
C	10.2889610535	31.3652379036	7.3479961961
H	10.7234259884	30.9065397766	8.2402368629
O	12.3569999673	32.5519981749	6.8969999591
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H	6.6140656284	37.5421340997	4.9351112009
H	5.5977903908	36.7084938404	7.6980907974
H	3.5696977803	36.8746393651	6.8950947377
H	5.3984934081	39.6102411001	7.1060791320
H	5.9145557102	38.4070069816	9.5084683665
H	4.9041072586	35.0716927011	5.6940224096
H	11.2036782735	36.9839204558	7.0995626094
H	10.0237835139	35.9539177101	7.9472353377
H	11.1183237170	35.0807136174	5.2245052591
H	12.1228407357	34.8450983808	6.6487445629
H	9.4069998853	33.7159998651	6.7600000932
H	9.2370271779	31.5983095839	7.5372528024
H	10.3445301257	30.6239690803	6.5432715633
H	5.9041847801	35.2393183489	4.2511393553

⁷b

E lacvp =	-3210.736976		
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H	0.7680761891	33.2376741724	5.4090051000
C	1.9492677128	33.3336694045	7.2605976494
H	1.0927836990	33.7265054255	7.8156182638
H	2.4471938114	32.5944705118	7.9036442225
C	2.9508222938	34.4486671660	7.0194112167
O	3.9760262272	34.1548357302	6.3012224991
O	2.7531155483	35.6251815407	7.5454064066
H	10.1431259148	43.2460480549	12.4666189899
C	9.9050000937	42.7149999243	11.5980000297
H	9.2198137898	43.3595607382	11.0356543246
H	10.8257111164	42.6690072088	10.9999144893
C	9.2951421215	41.3695309756	11.7070978162
N	10.0338468408	40.1837395455	11.7724041623
H	11.0375616359	40.1219418546	11.8429017840
C	9.1767697025	39.1249074745	11.7126629264
H	9.4514547126	38.0870524512	11.7672297534
N	7.9287577687	39.5863992208	11.6120639219
C	7.9819805875	40.9797895331	11.6022342718
H	7.0969423606	41.5987173007	11.5487392617
H	8.8908009984	39.8624229983	17.1734290277
C	7.9659999721	39.3979989954	17.0849989020
H	8.1245480303	38.3434773934	17.3361237824
H	7.3250798295	39.8026415415	17.8798050182
C	7.2711717291	39.4768458810	15.7696950709
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H	-2.7436485773	38.1057739456	11.3163352028
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C	-0.5564484572	37.2529526729	9.7934403462
H	-0.8840433207	37.5020817225	8.7795231929

H	-0.4315317691	38.2096959438	10.3209731203
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C	1.6819816744	36.5602658773	10.6628399669
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Fe	6.2319277521	38.3634320147	11.7086177797
Cl	4.1045295720	39.6457158043	11.5076793393
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O	6.0939349649	37.9565140709	9.9266842394
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N	5.4429765414	35.6221151053	4.8613766158
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O	12.3569999662	32.5519981697	6.8969999571
H	4.6499993106	36.1402832810	4.4644775879
H	6.5884612472	37.3941657080	4.6755030281
H	5.6283296756	36.7256975746	7.5030497683
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H	5.5098628266	39.5860301970	6.4948026035
H	5.4672982019	38.3810569901	9.3092430101
H	4.9290200992	34.9671088590	5.6266229593
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H	9.2581161647	31.6785883588	7.7272722871
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C	1.8973747683	33.3833724803	7.2464096229

H	1.0219499407	33.7987765823	7.7536152531
H	2.3748786079	32.6757434708	7.9382372273
C	2.9055287193	34.4870000596	6.9752988005
O	3.9432671618	34.1559967752	6.2974561768
O	2.6937084869	35.6898703874	7.4360843356
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H	11.3131649452	40.2554881137	11.9421869677
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C	7.9660000486	39.3979988863	17.0849990123
H	8.1054792476	38.3588601842	17.4020031623
H	7.2999637217	39.8539384742	17.8286935170
C	7.3371386995	39.4136372547	15.7376725847
N	6.5176056775	40.4541391453	15.2799032362
H	6.2869480051	41.2876674409	15.7988216041
C	6.0559687255	40.1608273655	14.0362053084
H	5.4649998710	40.8237438872	13.4157712055
N	6.5512609475	38.9682033944	13.6786704748
C	7.3365266745	38.4860721252	14.7272158774
H	7.8092610809	37.5229479269	14.6657837933
H	-3.6033640546	36.6101679596	11.2938308906
C	-2.9419993940	37.1860010325	10.7509990570
H	-3.4471340426	37.5313771087	9.8409246584
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C	-1.6681102343	36.3816870645	10.4089498649
H	-1.2432259893	35.9620872173	11.3313920942
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C	1.6351910411	36.5651416384	10.5470089487
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H	2.0960877714	37.0929031281	12.4956617313
N	2.8900235616	36.1599175664	10.2561946063
H	3.1121909494	35.9432542149	9.2843712878
H	3.5622481288	35.9324906451	10.9830280135
Fe	6.6209337220	38.1887352746	11.8864049424
Cl	6.8152642585	37.3102848317	9.7835413431
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C	6.3760440448	35.3612749408	12.4922651942
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C	7.2139292470	34.1115645140	12.5513925432
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H	3.9517659488	38.1241239800	12.7355517770
O	5.1041435761	41.5609895521	11.6217230558
H	4.4924418968	42.1580862889	11.1580366011
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O	4.9128489137	38.9395355468	11.4796292719
H	4.5910999517	38.5860915161	10.6232493624

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C	6.3784689077	36.5241688905	5.3456671701
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C	10.1575930307	36.1306580890	7.3633100640
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N	10.4101425713	33.7313401050	6.8071799110
C	11.1106756521	32.5578096570	6.8115382437
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O	12.3569999559	32.5519980225	6.8969999817
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H	3.5334775928	36.8434116839	6.4801134291
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H	5.9564208485	34.8356275341	4.1299905405
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H	0.9782760284	33.8148875720	7.7310360788
H	2.3072950726	32.6720191139	7.9663554139
C	2.8992974164	34.4691724564	7.0141631722
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H	11.6024976002	35.2268999914	5.8821370624
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H	0.7992228318	33.2078983980	5.3395474615
C	1.8554040079	33.3861422187	7.2580326131
H	0.9659894730	33.8186208317	7.7249876627
H	2.2912496148	32.6741839323	7.9724601539
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C	9.5970989014	39.0580048511	11.7668114575
H	10.0082111881	38.0656499982	11.8283494749
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C	2.8261641458	34.5211297602	7.1172121737
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N	0.7102475048	36.3896931443	9.5754682095
H	1.0029697502	36.1924676903	8.6232470889
C	1.6564146224	36.1986058818	10.5230137025
N	1.3574111760	36.3769360075	11.8259626794
H	0.4362792715	36.6577557915	12.1129285739
H	2.1039957488	36.4277270584	12.5042552106
N	2.8803013527	35.8002049269	10.1561139239
H	3.0718999954	35.6997383597	9.1563326009
H	3.6515242426	35.6705704484	10.8053885561
Fe	5.9220363652	38.7460883723	11.9581010708
Cl	4.0622689624	37.6995591569	12.9439862161
O	5.6808313844	35.3960417306	11.2271738824
C	6.6121138224	35.8218854566	11.9350378690
O	6.9248994274	37.1361932791	12.0348830257
C	7.5011570397	34.8980382150	12.7522978536
H	8.0864341468	35.4607397605	13.4812491795
H	6.8683411287	34.1718062053	13.2711763910
H	8.1947769195	34.3228610756	12.1201750011
O	2.1041198736	39.3509228807	10.7529072187
H	2.9156474776	39.5146763508	10.2336796710
H	2.4068428747	39.0851891306	11.6440525743
O	4.8458386811	42.3904310807	12.0459631959
H	4.1861052818	43.0509610092	11.7703395155
H	4.6868096566	41.5231850194	11.5971109143
O	4.9955114975	39.8332654659	11.0916868121
H	7.3543040526	38.3623621861	7.8043492735
C	6.3112110332	38.5471772189	7.5213036490
C	5.6697264550	37.3106577776	6.9036380203
O	4.3198824362	37.6118778159	6.4839230847
C	6.4304309757	36.8387927579	5.6167736904
C	7.7172595144	36.0835354130	5.9336156374
O	7.7374674653	35.0453210746	6.6044067002
N	5.4625553583	35.9762828496	4.8436201156
S	9.1900769269	36.9196300310	5.2205322424
C	10.7151847657	36.0428923693	5.9876368738
C	10.9542779872	34.5824799873	5.5857563687

N	10.3793250760	33.6356823341	6.5289460130
C	11.1367248646	32.6658216065	7.1302402467
C	10.3989831822	31.7375461467	8.0727320262
H	10.9914237474	31.6092082877	8.9823345128
O	12.3569999913	32.5519980419	6.8969999847
H	4.6715948624	36.5992701002	4.6283384444
H	6.6551009457	37.7118526749	4.9978395748
H	5.6691563362	36.4744624595	7.6160377525
H	3.6835030210	36.9136669918	6.8425329133
H	6.2817011411	39.3816017463	6.8124214861
H	5.7563940707	38.8431393246	8.4159424355
H	4.9471327341	35.1466651026	5.4519972479
H	11.5161673579	36.6912089020	5.6223346508
H	10.6358578494	36.1490693300	7.0712866457
H	10.5954045255	34.4005356705	4.5647771947
H	12.0321535596	34.3833126211	5.5920218211
H	9.4069999599	33.7159999926	6.7600000216
H	9.3998763534	32.0968143257	8.3366436279
H	10.3025952342	30.7508936676	7.6061498849
H	5.8676845579	35.5880914368	3.9892938198

k

E lacvp = -3210.747801

H	1.101200	31.699249	6.164721
C	1.507000	32.638000	5.951000
H	2.401423	32.488551	5.339341
H	0.783158	33.214806	5.364627
C	1.896158	33.380692	7.246766
H	1.017053	33.755630	7.778458
H	2.417095	32.685103	7.919045
C	2.850187	34.525993	6.967267
O	3.887347	34.247747	6.263251
O	2.594618	35.714838	7.436075
H	10.143126	43.246048	12.466619
C	9.905000	42.715000	11.598000
H	9.101241	43.275362	11.108177
H	10.775093	42.797150	10.931745
C	9.476287	41.299366	11.723390
N	10.338154	40.216475	11.930096
H	11.333883	40.278795	12.077683
C	9.611976	39.057994	11.872522
H	10.009562	38.066273	11.997340
N	8.333760	39.354145	11.644245
C	8.236136	40.738711	11.538170
H	7.294639	41.220323	11.337526
H	8.890801	39.862423	17.173429
C	7.966000	39.397999	17.084999
H	8.107589	38.350965	17.371751
H	7.304943	39.835355	17.844539
C	7.340259	39.449720	15.740850
N	6.648229	40.557098	15.240995
H	6.491350	41.420914	15.737081
C	6.173748	40.265482	13.996189
H	5.605716	40.927312	13.358441
N	6.535447	39.018178	13.680525
C	7.247507	38.494805	14.759467
H	7.616211	37.483344	14.759491
H	-3.603364	36.610168	11.293831
C	-2.942000	37.186001	10.750999
H	-3.460484	37.490939	9.831539
H	-2.740978	38.103078	11.320641
C	-1.631339	36.457300	10.408983
H	-1.044201	36.287848	11.321265
H	-1.835973	35.463740	9.991341
C	-0.796545	37.272684	9.391002

H	-1.219615	37.161889	8.388287
H	-0.858491	38.344239	9.631747
N	0.617622	36.887265	9.314068
H	0.971539	36.350887	8.520881
C	1.542641	37.283620	10.219413
N	1.203503	38.022098	11.287608
H	0.234219	38.194453	11.495596
H	1.914267	38.455550	11.924335
N	2.825883	36.937208	10.011288
H	3.052470	36.411891	9.169646
H	3.520870	37.034284	10.743220
Fe	6.615492	38.065102	11.819582
Cl	4.908589	36.560782	12.657517
O	6.968933	35.804626	9.455513
C	7.524930	35.617239	10.558412
O	7.787219	36.636402	11.406708
C	7.980819	34.268250	11.053122
H	7.203360	33.524413	10.860808
H	8.883997	33.949854	10.518485
H	8.194777	34.322861	12.120175
O	2.991304	39.204793	12.894427
H	3.581439	38.524975	13.277237
H	3.518583	39.930874	12.464956
O	4.550896	40.949256	11.500254
H	4.948038	40.221903	10.910191
H	4.089314	41.638396	10.991674
O	5.702158	38.923877	10.438164
H	5.903966	38.701605	9.506656
C	5.912419	38.699705	7.071158
C	5.460080	37.326592	6.707542
O	4.147312	37.421240	6.079109
C	6.396336	36.625432	5.656601
C	7.606571	35.914748	6.250080
O	7.624257	34.690038	6.419938
N	5.551240	35.610678	4.936533
S	9.010830	37.035482	6.600139
C	10.108124	36.001110	7.787604
C	11.062726	34.998597	7.145972
N	10.404940	33.726521	6.872210
C	11.115857	32.565068	6.760813
C	10.313074	31.314732	6.461853
H	10.579392	30.537742	7.184127
O	12.357000	32.551998	6.897000
H	4.877573	36.118854	4.357120
H	6.730266	37.372568	4.928655
H	5.401780	36.675132	7.592108
H	3.478393	36.870026	6.600983
H	6.752545	39.184681	6.585869
H	5.208012	39.321312	7.614625
H	4.888549	35.018806	5.636972
H	10.658641	36.789034	8.306234
H	9.413356	35.527861	8.482835
H	11.519635	35.420091	6.240282
H	11.890434	34.799191	7.838897
H	9.407000	33.716000	6.760000
H	9.231747	31.477071	6.492596
H	10.585610	30.940234	5.469367
H	6.113657	34.959035	4.385482
I			
E lacvp = -3210.741685			
H	1.101200	31.699249	6.164721
C	1.507000	32.638000	5.951000
H	2.434048	32.483198	5.391025
H	0.809312	33.189659	5.311001

C	1.822582	33.427191	7.243170
H	0.916053	33.830712	7.703102
H	2.286998	32.749994	7.973639
C	2.813759	34.555310	7.000850
O	3.885813	34.240001	6.361002
O	2.565914	35.753622	7.442264
H	10.143126	43.246048	12.466619
C	9.905000	42.715000	11.598000
H	9.285033	43.388573	10.995243
H	10.842499	42.596242	11.038250
C	9.205731	41.408202	11.712492
N	9.866382	40.174809	11.765678
H	10.865816	40.048706	11.809105
C	8.938873	39.174409	11.719817
H	9.148557	38.120989	11.749119
N	7.718099	39.707966	11.642666
C	7.870416	41.096105	11.629926
H	7.024569	41.760127	11.570731
H	8.890801	39.862423	17.173429
C	7.966000	39.397999	17.084999
H	8.141443	38.321693	17.181506
H	7.373793	39.688594	17.963697
C	7.203781	39.644244	15.832455
N	6.601196	40.860411	15.493601
H	6.641690	41.706492	16.040893
C	5.935666	40.725889	14.309121
H	5.432012	41.528394	13.776420
N	6.084877	39.466813	13.879285
C	6.859739	38.783796	14.819614
H	7.108351	37.742817	14.703660
H	-3.603364	36.610168	11.293831
C	-2.942000	37.186001	10.750999
H	-3.518633	37.695973	9.967809
H	-2.548057	37.967918	11.415595
C	-1.802325	36.357671	10.131406
H	-1.153996	35.965025	10.924095
H	-2.210944	35.482269	9.612383
C	-0.948648	37.196564	9.136122
H	-1.274900	37.020765	8.107863
H	-1.104765	38.269728	9.323134
N	0.489953	36.911749	9.182038
H	0.958702	36.440033	8.405686
C	1.279005	37.300658	10.211628
N	0.769866	37.972531	11.256800
H	-0.216270	38.169326	11.292388
H	1.337459	38.250369	12.088527
N	2.586209	36.994788	10.164480
H	2.933950	36.505424	9.346896
H	3.230954	37.289362	10.900880
Fe	5.871113	38.650044	11.963979
Cl	4.768090	40.034700	10.387412
O	5.599485	35.283938	12.072117
C	6.697364	35.744240	11.665836
O	6.987898	37.051816	11.634854
C	7.797985	34.814433	11.227268
H	7.391066	34.034888	10.578087
H	8.601505	35.350378	10.721067
H	8.194777	34.322861	12.120175
O	2.240737	38.557703	13.427030
H	3.134671	38.166126	13.185379
H	2.325229	39.396097	13.908364
O	4.817463	42.614484	12.268871
H	4.590675	41.971607	11.559657
H	4.459356	43.494516	12.055986
O	4.389514	37.567960	12.357153

H	4.611979	36.589531	12.437468
C	5.979255	38.697765	6.997425
C	5.466060	37.344875	6.664105
O	4.147549	37.438214	6.031370
C	6.373454	36.598237	5.616135
C	7.586474	35.928190	6.241100
O	7.579516	34.740968	6.597148
N	5.507703	35.561434	4.955835
S	9.023438	37.050185	6.410469
C	10.210259	36.080470	7.568778
C	11.087092	35.019740	6.907559
N	10.409364	33.732469	6.813269
C	11.111264	32.558324	6.816236
C	10.292135	31.288302	6.709764
H	10.604712	30.594967	7.495578
O	12.357000	32.551998	6.897000
H	4.797622	36.068552	4.417417
H	6.693011	37.319108	4.857045
H	5.389504	36.713689	7.558910
H	3.471820	36.936824	6.588621
H	6.290103	39.361285	6.195866
H	5.804939	39.121282	7.979473
H	4.873488	34.976058	5.697640
H	10.818874	36.894325	7.969280
H	9.597081	35.661113	8.370062
H	11.435844	35.367282	5.925513
H	11.987966	34.865107	7.514623
H	9.407000	33.716000	6.760000
H	9.214747	31.460042	6.790057
H	10.500583	30.803748	5.749843
H	6.037998	34.914067	4.369583

³TSab

E_{laccp} = -3210.718906

$\nu = \text{i1524 cm}^{-1}$

H	1.101200	31.699249	6.164721
C	1.507000	32.638000	5.951000
H	2.390279	32.495872	5.321549
H	0.774909	33.224056	5.384961
C	1.912529	33.355832	7.252937
H	1.037477	33.700846	7.810841
H	2.452857	32.648201	7.898230
C	2.845652	34.526940	7.016200
O	3.864936	34.327357	6.259696
O	2.604351	35.662359	7.610526
H	10.143126	43.246048	12.466619
C	9.905000	42.715000	11.598001
H	9.130372	43.299023	11.089579
H	10.790000	42.761709	10.948514
C	9.422174	41.317191	11.719385
N	10.246960	40.197639	11.873718
H	11.248383	40.218317	11.991323
C	9.476077	39.070860	11.821771
H	9.843336	38.065303	11.928377
N	8.202858	39.426178	11.643678
C	8.151432	40.817085	11.570404
H	7.226220	41.360851	11.444207
H	8.890801	39.862423	17.173429
C	7.966000	39.397999	17.084999
H	8.109113	38.351692	17.374355
H	7.305443	39.835470	17.844861
C	7.329548	39.443460	15.742231
N	6.604477	40.541482	15.264367
H	6.457429	41.407836	15.759197
C	6.105290	40.254259	14.031792

H	5.566086	40.959832	13.417581
N	6.482417	39.011625	13.694206
C	7.234976	38.496306	14.753983
H	7.631594	37.498415	14.710393
H	-3.603364	36.610168	11.293831
C	-2.942000	37.186001	10.750999
H	-3.424079	37.494604	9.816227
H	-2.727106	38.095235	11.327516
C	-1.654029	36.382203	10.483019
H	-1.285661	35.961342	11.428850
H	-1.872317	35.521094	9.838665
C	-0.541305	37.226921	9.829089
H	-0.836587	37.514815	8.815577
H	-0.401183	38.163480	10.388524
N	0.752602	36.536411	9.719502
H	1.086270	36.216314	8.809212
C	1.626706	36.401120	10.745694
N	1.320403	36.803129	11.988307
H	0.398786	37.142298	12.204076
H	2.060691	36.856007	12.720841
N	2.826269	35.848452	10.489347
H	3.059173	35.655834	9.520411
H	3.524845	35.689763	11.208882
Fe	6.554924	38.200583	11.849922
Cl	4.489377	39.270860	11.308682
O	5.103673	35.300891	12.389407
C	6.362094	35.365707	12.521074
O	7.002418	36.508228	12.696468
C	7.215487	34.123426	12.562611
H	7.370769	33.821235	13.605915
H	6.715587	33.304683	12.042670
H	8.194777	34.322861	12.120175
O	3.438182	37.081327	13.632555
H	4.112229	36.412367	13.345136
H	3.770103	37.974190	13.416394
O	5.263934	42.287862	11.807983
H	4.797892	41.518800	11.408566
H	4.796779	43.116318	11.597536
O	6.797049	37.408246	10.261803
H	6.647777	39.071038	7.719629
C	5.863466	38.458384	8.169004
C	5.382528	37.259991	7.381981
O	4.162113	37.589559	6.673291
C	6.390210	36.770264	6.282805
C	7.541329	35.940627	6.824719
O	7.485361	34.705795	6.910724
N	5.583329	35.939971	5.317837
S	8.991217	36.934980	7.319660
C	9.967771	35.677991	8.390910
C	10.997356	34.838125	7.645289
N	10.394379	33.708799	6.945658
C	11.140061	32.607982	6.621768
C	10.408218	31.484449	5.917150
H	10.597966	30.547022	6.447620
O	12.357000	32.551998	6.897000
H	4.923607	36.578652	4.861157
H	6.776936	37.641734	5.745317
H	5.188801	36.415996	8.058475
H	3.432930	36.970892	7.008873
H	5.033127	39.037894	8.568783
H	6.401463	37.979862	9.275779
H	4.896180	35.199065	5.835609
H	10.453004	36.330534	9.119184
H	9.217958	35.067285	8.898871
H	11.580971	35.464075	6.956958

H	11.716013	34.433849	8.370480
H	9.407000	33.716000	6.760000
H	9.328097	31.644918	5.850940
H	10.811110	31.370127	4.905267
H	6.165319	35.447201	4.637724

⁷TSab

E lacvp = -3210.718895

$\nu = \text{i1393 cm}^{-1}$

H	1.101200	31.699249	6.164721
C	1.507000	32.638000	5.951000
H	2.418645	32.491659	5.364682
H	0.795755	33.204700	5.340443
C	1.850274	33.389944	7.251774
H	0.951950	33.760388	7.753732
H	2.349037	32.697857	7.945891
C	2.808139	34.544144	7.024894
O	3.836862	34.316990	6.290757
O	2.574509	35.691731	7.600550
H	10.143126	43.246048	12.466619
C	9.905000	42.715000	11.598000
H	9.173812	43.326418	11.058686
H	10.809114	42.706194	10.973870
C	9.355247	41.349678	11.743441
N	10.126895	40.200247	11.940575
H	11.125158	40.180906	12.080667
C	9.308262	39.108306	11.899618
H	9.611640	38.085955	12.040118
N	8.057689	39.518626	11.686437
C	8.066130	40.905840	11.585479
H	7.166137	41.485080	11.444309
H	8.890801	39.862423	17.173429
C	7.966000	39.397999	17.084999
H	8.122629	38.344018	17.338672
H	7.324336	39.805679	17.877917
C	7.273417	39.468527	15.767209
N	6.562028	40.584051	15.313567
H	6.490361	41.470133	15.789598
C	5.970574	40.287033	14.119539
H	5.428607	41.008957	13.526095
N	6.267790	39.023119	13.778643
C	7.073323	38.509332	14.803400
H	7.462877	37.508762	14.757677
H	-3.603364	36.610168	11.293831
C	-2.942000	37.186001	10.750999
H	-3.400135	37.429813	9.785148
H	-2.787199	38.129854	11.289573
C	-1.609342	36.431611	10.561559
H	-1.229019	36.109365	11.540958
H	-1.774313	35.512210	9.985559
C	-0.540353	37.283297	9.845168
H	-0.868948	37.508344	8.825891
H	-0.426758	38.252428	10.352581
N	0.780773	36.642957	9.732756
H	1.097003	36.287699	8.828379
C	1.697873	36.607404	10.727889
N	1.421437	37.060031	11.959025
H	0.497180	37.384310	12.187547
H	2.165954	37.132129	12.683996
N	2.912580	36.093498	10.452261
H	3.113751	35.844765	9.487934
H	3.658527	36.068824	11.137926
Fe	6.412295	38.250698	11.686041
Cl	4.433795	39.486184	11.124007
O	5.470333	36.126179	12.292357

C	6.709705	35.764908	12.410230
O	7.612055	36.703579	12.440987
C	7.164238	34.345289	12.482110
H	7.144638	33.985218	13.517897
H	6.522319	33.695626	11.883967
H	8.194777	34.322861	12.120175
O	3.470775	37.309087	13.716430
H	4.219431	36.722890	13.457332
H	3.804411	38.225832	13.712891
O	5.173442	42.443468	11.970534
H	4.740736	41.706193	11.483966
H	4.721668	43.285136	11.778909
O	6.809856	37.482061	9.994506
H	6.485239	39.161457	7.424834
C	5.786815	38.499614	7.942390
C	5.335206	37.264774	7.195291
O	4.112432	37.543565	6.467269
C	6.353381	36.746732	6.124113
C	7.530086	35.973042	6.700290
O	7.480978	34.750605	6.899312
N	5.561527	35.840726	5.213295
S	8.994278	37.008248	7.034847
C	10.049205	35.849862	8.144050
C	11.032025	34.941997	7.410839
N	10.401179	33.729097	6.900441
C	11.127313	32.589159	6.682559
C	10.353731	31.393999	6.163577
H	10.596352	30.520076	6.774371
O	12.357000	32.551998	6.897000
H	4.898565	36.435694	4.705805
H	6.714248	37.595143	5.534857
H	5.152920	36.445384	7.903320
H	3.382961	36.968898	6.868305
H	4.946304	39.032465	8.386537
H	6.407118	38.064249	8.968839
H	4.884290	35.145553	5.786567
H	10.579268	36.567569	8.773108
H	9.339546	35.291161	8.758215
H	11.540067	35.493525	6.608274
H	11.818034	34.631577	8.111489
H	9.407000	33.716000	6.760000
H	9.269993	31.543974	6.167323
H	10.675078	31.172477	5.140146
H	6.152236	35.303781	4.575568

TSab

E lacvp = -3210.727109

$\nu = \text{il135 cm}^{-1}$

H	1.101200	31.699249	6.164721
C	1.507000	32.638000	5.951000
H	2.408694	32.490582	5.349634
H	0.788439	33.211425	5.355538
C	1.874701	33.380541	7.251396
H	0.986454	33.753264	7.768913
H	2.382882	32.682347	7.931703
C	2.832822	34.529371	7.005994
O	3.873553	34.279089	6.295467
O	2.586887	35.696327	7.534619
H	10.143126	43.246048	12.466619
C	9.905000	42.715000	11.598000
H	9.167599	43.320930	11.061352
H	10.807024	42.709376	10.970705
C	9.362700	41.349626	11.755213
N	10.133978	40.206239	11.983664
H	11.131121	40.190579	12.131090

C	9.314843	39.113035	11.964424
H	9.616096	38.093977	12.128024
N	8.067377	39.520092	11.734487
C	8.075044	40.903350	11.598328
H	7.176442	41.482356	11.441524
H	8.890801	39.862423	17.173429
C	7.966000	39.397999	17.084999
H	8.122112	38.345221	17.344430
H	7.322645	39.809178	17.874557
C	7.275920	39.464035	15.765751
N	6.538770	40.568790	15.328000
H	6.445710	41.445508	15.817281
C	5.954114	40.274634	14.130923
H	5.393279	40.988070	13.547907
N	6.280770	39.024324	13.771365
C	7.099090	38.514421	14.787504
H	7.511073	37.523298	14.728207
H	-3.603364	36.610168	11.293831
C	-2.942000	37.186001	10.750999
H	-3.418895	37.470135	9.805457
H	-2.751100	38.109290	11.313249
C	-1.632463	36.408680	10.504397
H	-1.236922	36.045607	11.463066
H	-1.830913	35.512438	9.903066
C	-0.564429	37.264618	9.791724
H	-0.896040	37.500156	8.775929
H	-0.448700	38.228368	10.308915
N	0.757982	36.628042	9.669901
H	1.082775	36.299407	8.759278
C	1.669915	36.583226	10.669630
N	1.374749	36.990859	11.911206
H	0.447077	37.304553	12.139971
H	2.115468	37.050406	12.641147
N	2.898276	36.104723	10.389750
H	3.110580	35.882755	9.421543
H	3.646928	36.112879	11.072539
Fe	6.386405	38.308426	11.687414
Cl	4.279099	39.520674	11.318776
O	5.525136	36.234417	12.182121
C	6.755272	35.826139	12.324154
O	7.679579	36.731057	12.354970
C	7.146985	34.389129	12.422955
H	7.050248	34.030979	13.454832
H	6.514993	33.764691	11.787819
H	8.194777	34.322861	12.120175
O	3.435927	37.275097	13.641038
H	4.209916	36.720536	13.391765
H	3.700687	38.208839	13.521535
O	5.253667	42.457006	11.897556
H	4.774360	41.696427	11.494603
H	4.797662	43.291459	11.685483
O	6.613013	37.894856	9.989468
H	6.479182	39.179704	7.222071
C	5.759366	38.555182	7.756529
C	5.332880	37.270166	7.082974
O	4.117072	37.496333	6.327576
C	6.369642	36.705442	6.051637
C	7.537139	35.952538	6.674362
O	7.494478	34.730895	6.882687
N	5.595466	35.761123	5.166938
S	8.979825	37.004391	7.044756
C	10.046451	35.845922	8.145269
C	11.030346	34.946073	7.402952
N	10.401520	33.730191	6.897402
C	11.127374	32.588898	6.683819

C	10.352528	31.391954	6.170946
H	10.595988	30.520419	6.784782
O	12.357000	32.551998	6.897000
H	4.942380	36.329819	4.618710
H	6.741942	37.529086	5.434817
H	5.148821	36.492000	7.835555
H	3.387422	36.936377	6.750633
H	4.899090	39.119410	8.118255
H	6.323510	38.243738	8.848574
H	4.908059	35.089294	5.762023
H	10.573859	36.565295	8.774605
H	9.345417	35.277148	8.760232
H	11.528090	35.502203	6.597152
H	11.823674	34.639613	8.097046
H	9.407000	33.716000	6.760000
H	9.268819	31.542173	6.175897
H	10.672169	31.166191	5.147908
H	6.199251	35.195090	4.567762

TSai

E lacvp = -3210.730911

$\nu = i108 \text{ cm}^{-1}$

H	1.101200	31.699249	6.164721
C	1.507000	32.638000	5.951000
H	1.553409	32.766179	4.864553
H	0.856047	33.416667	6.361319
C	2.918680	32.707812	6.580728
H	2.837287	32.543583	7.662952
H	3.556455	31.924764	6.164191
C	3.595408	34.039485	6.353515
O	4.611784	34.059595	5.555959
O	3.123816	35.090982	6.945369
H	10.143126	43.246048	12.466619
C	9.905000	42.715000	11.598001
H	9.317323	43.402837	10.979781
H	10.847646	42.560046	11.055721
C	9.158606	41.428712	11.701876
N	9.780961	40.184309	11.865424
H	10.768814	40.039148	12.007031
C	8.838689	39.202376	11.790761
H	9.022759	38.152592	11.925810
N	7.637575	39.753120	11.582553
C	7.826813	41.137997	11.516878
H	7.006808	41.820359	11.384505
H	8.890801	39.862423	17.173429
C	7.966000	39.397999	17.084999
H	8.146139	38.322497	17.185834
H	7.379049	39.687819	17.968049
C	7.191622	39.630101	15.842354
N	6.564520	40.834901	15.507704
H	6.614883	41.695261	16.031328
C	5.876581	40.675531	14.343836
H	5.365478	41.482744	13.845696
N	6.036157	39.415031	13.911823
C	6.841569	38.757192	14.845356
H	7.118829	37.728547	14.711801
H	-3.603364	36.610168	11.293831
C	-2.942000	37.186001	10.750999
H	-3.409595	37.434169	9.789952
H	-2.778571	38.127440	11.290188
C	-1.609338	36.431547	10.536106
H	-1.160786	36.178136	11.505853
H	-1.806948	35.478761	10.026030
C	-0.587664	37.235328	9.702961
H	-1.037066	37.525916	8.746300

H	-0.314595	38.166793	10.210251
N	0.644752	36.483582	9.381771
H	0.620422	35.883572	8.568709
C	1.813778	36.510463	10.068415
N	1.962497	37.241685	11.182807
H	1.314767	37.975063	11.480229
H	2.917637	37.354909	11.513079
N	2.849378	35.774636	9.624958
H	2.849340	35.360747	8.685291
H	3.734660	35.812909	10.121264
Fe	5.832183	38.706335	11.966978
Cl	4.418486	40.556063	11.391913
O	5.794110	35.482893	11.281369
C	6.659262	35.877486	12.082093
O	6.861978	37.178396	12.420753
C	7.591394	34.923449	12.814833
H	8.257414	35.463854	13.488482
H	6.983332	34.221201	13.395801
H	8.194777	34.322861	12.120175
O	1.121454	39.736675	11.827098
H	1.986495	40.124174	11.572868
H	0.652690	40.321358	12.446816
O	5.340499	43.299549	12.732419
H	4.889431	42.732059	12.071463
H	5.041382	44.222653	12.642973
O	4.747705	37.793138	11.023909
H	6.967628	38.509093	8.062839
C	5.934802	38.550322	7.697894
C	5.553502	37.280101	6.951948
O	4.239666	37.430379	6.368837
C	6.545062	36.971340	5.765782
C	7.789971	36.234356	6.231590
O	7.769560	35.063025	6.625911
N	5.779396	36.138740	4.777330
S	9.299615	37.278672	6.167223
C	10.630479	36.183212	7.002816
C	11.070255	34.934301	6.224425
N	10.406690	33.720488	6.678400
C	11.112521	32.588026	6.983070
C	10.291591	31.388779	7.409613
H	10.744543	30.944702	8.299982
O	12.357000	32.551998	6.897000
H	4.941669	36.695190	4.555407
H	6.823930	37.911702	5.280951
H	5.563207	36.414080	7.626631
H	3.689824	36.610770	6.585324
H	5.827753	39.417793	7.038062
H	5.270075	38.679759	8.554594
H	5.306253	35.144605	5.227833
H	11.452001	36.896840	7.104028
H	10.258981	35.920545	7.995384
H	10.933424	35.087944	5.145985
H	12.139506	34.760756	6.389715
H	9.407000	33.716000	6.760000
H	9.246130	31.633871	7.618738
H	10.321327	30.631352	6.618604
H	6.317521	35.920595	3.937044

TSaj

E_{laccv} = -3210.72922172

$\nu = 197 \text{ cm}^{-1}$

H	1.101198	31.699248	6.164722
C	1.507002	32.638001	5.951000
H	2.188331	32.526059	5.101301
H	0.699006	33.315303	5.652941

C	2.283598	33.195360	7.165907
H	1.600667	33.476380	7.972577
H	2.959339	32.419267	7.545477
C	3.136875	34.390762	6.787230
O	4.099110	34.180664	5.960031
O	2.866574	35.559144	7.296959
H	10.143125	43.246049	12.466620
C	9.905001	42.714999	11.598000
H	9.297065	43.395991	10.991289
H	10.845168	42.588568	11.043836
C	9.188367	41.404536	11.679016
N	9.849944	40.175689	11.829384
H	10.843450	40.061466	11.960977
C	8.945956	39.160141	11.742430
H	9.155262	38.111146	11.852874
N	7.734909	39.683587	11.536232
C	7.865010	41.074302	11.479395
H	7.005754	41.712293	11.337696
H	8.890798	39.862430	17.173434
C	7.966004	39.397991	17.084993
H	8.135635	38.321101	17.182299
H	7.363512	39.694235	17.953482
C	7.255229	39.662532	15.816221
N	6.554746	40.834457	15.515552
H	6.450099	41.629264	16.126978
C	6.005652	40.717253	14.268489
H	5.422612	41.458169	13.738267
N	6.337431	39.524451	13.775831
C	7.103129	38.855644	14.720382
H	7.466919	37.858152	14.549063
H	-3.603365	36.610168	11.293833
C	-2.942000	37.186001	10.750997
H	-3.442484	37.537383	9.841383
H	-2.684259	38.070147	11.347901
C	-1.680457	36.358446	10.411664
H	-1.293555	35.900309	11.333357
H	-1.946953	35.519298	9.756449
C	-0.570496	37.189437	9.730745
H	-0.916483	37.532325	8.751145
H	-0.340022	38.094540	10.309257
N	0.694884	36.457326	9.497880
H	0.960861	36.216089	8.548202
C	1.665134	36.309664	10.430946
N	1.393995	36.550031	11.730056
H	0.471172	36.804353	12.035070
H	2.156029	36.626733	12.389216
N	2.884381	35.910770	10.056651
H	3.056023	35.765118	9.057145
H	3.663071	35.773145	10.700728
Fe	6.010072	38.685933	11.912001
Cl	4.040109	37.910387	12.919129
O	5.515394	35.363290	11.272199
C	6.514443	35.713002	11.932791
O	6.931037	36.993844	12.014617
C	7.352343	34.713088	12.711568
H	7.765328	35.175673	13.611275
H	6.724921	33.862801	12.987246
H	8.194776	34.322862	12.120176
O	2.390782	39.671539	10.587299
H	3.174771	39.432995	10.051520
H	2.570799	39.335987	11.488371
O	4.685729	41.897673	11.744579
H	3.889769	42.442664	11.607863
H	4.611432	41.073940	11.208484
O	5.210263	39.384899	10.615153

H	7.296454	38.468272	7.612361
C	6.236808	38.602315	7.365372
C	5.634723	37.333105	6.778444
O	4.289167	37.584557	6.315035
C	6.437357	36.825330	5.527443
C	7.717312	36.098884	5.913306
O	7.721950	35.013560	6.505977
N	5.500168	35.922368	4.765456
S	9.216139	37.042987	5.431615
C	10.661551	36.138741	6.307644
C	11.007808	34.734806	5.794611
N	10.393136	33.676907	6.582912
C	11.125996	32.634075	7.083448
C	10.348886	31.587305	7.854617
H	10.889813	31.346693	8.773561
O	12.357000	32.551998	6.897000
H	4.702543	36.524323	4.516716
H	6.669277	37.679242	4.884844
H	5.633592	36.521668	7.519156
H	3.657947	36.897390	6.704095
H	6.143709	39.425078	6.648682
H	5.706361	38.875306	8.281364
H	4.994268	35.116702	5.393479
H	11.478308	36.840934	6.121709
H	10.436411	36.127369	7.375968
H	10.755605	34.642236	4.730238
H	12.088283	34.574399	5.883805
H	9.406999	33.716000	6.760000
H	9.331275	31.902293	8.104087
H	10.293802	30.668304	7.260639
H	5.927041	35.508334	3.934489

³TSa'b'

E_{laccp} = -3210.712690

$\nu = \text{i1494 cm}^{-1}$

H	1.101200	31.699251	6.164721
C	1.507000	32.638004	5.951001
H	2.221822	32.533870	5.129132
H	0.707489	33.314980	5.632012
C	2.223923	33.161815	7.216642
H	1.501396	33.366718	8.011871
H	2.909055	32.384063	7.577765
C	3.056270	34.402849	6.975147
O	4.048178	34.312914	6.164044
O	2.746884	35.500292	7.610366
H	10.143126	43.246052	12.466619
C	9.905001	42.715004	11.598001
H	9.023430	43.207263	11.173275
H	10.721630	42.895890	10.885624
C	9.616734	41.261411	11.699630
N	10.586218	40.252502	11.743367
H	11.583801	40.396109	11.779658
C	9.967205	39.037987	11.692895
H	10.466969	38.085827	11.676304
N	8.645282	39.230242	11.635346
C	8.413043	40.606372	11.625346
H	7.420935	41.023013	11.540767
H	8.890801	39.862427	17.173429
C	7.966001	39.398003	17.084999
H	8.078704	38.383851	17.482946
H	7.271039	39.915313	17.757584
C	7.419322	39.330722	15.703668
N	6.571563	40.296462	15.153769
H	6.232932	41.117029	15.631905
C	6.244768	39.944962	13.876745

H	5.636570	40.529518	13.196660
N	6.852737	38.791099	13.590442
C	7.568896	38.386594	14.718956
H	8.105719	37.454360	14.745994
H	-3.603364	36.610172	11.293832
C	-2.941999	37.186005	10.751000
H	-3.400551	37.419412	9.782317
H	-2.791932	38.134878	11.281555
C	-1.610665	36.432374	10.567993
H	-1.189526	36.183590	11.552245
H	-1.787442	35.473635	10.063920
C	-0.574170	37.233047	9.753935
H	-0.942193	37.390798	8.735342
H	-0.437433	38.233732	10.189109
N	0.733554	36.571275	9.641761
H	0.991613	36.108395	8.773604
C	1.695525	36.596718	10.597277
N	1.510792	37.227522	11.771382
H	0.618810	37.617249	12.021263
H	2.348644	37.410043	12.353258
N	2.861497	35.991253	10.343080
H	3.004477	35.604919	9.411252
H	3.600379	35.869007	11.034190
Fe	7.248258	37.858645	11.898614
Cl	8.297199	36.574352	10.256757
O	5.179103	34.939733	11.572113
C	6.236446	35.125039	12.202985
O	6.558971	36.341535	12.716642
C	7.219369	34.035777	12.525586
H	7.320771	33.929143	13.611428
H	6.894866	33.089547	12.092277
H	8.194777	34.322865	12.120176
O	3.973559	37.723011	12.709654
H	4.594787	37.131471	13.178907
H	4.477665	38.075335	11.935600
O	5.277233	41.135949	11.346679
H	5.407827	40.196714	11.038505
H	4.572925	41.587019	10.850201
O	5.937018	38.567656	10.881990
H	7.308405	38.543616	8.388496
C	6.219871	38.508164	8.366619
C	5.611104	37.329606	7.647599
O	4.261328	37.636933	7.249915
C	6.416437	37.028802	6.310609
C	7.682019	36.212727	6.538947
O	7.657469	35.000699	6.776570
N	5.462573	36.297422	5.400026
S	9.193079	37.240032	6.412096
C	10.572703	36.158060	7.191501
C	11.073438	34.976400	6.353691
N	10.406728	33.725196	6.682850
C	11.109728	32.580374	6.945182
C	10.282183	31.356176	7.278528
H	9.225709	31.582267	7.449375
O	12.357001	32.552002	6.897000
H	4.667237	36.936702	5.268152
H	6.663837	37.979181	5.829867
H	5.648085	36.419012	8.260541
H	3.636648	36.857590	7.435488
H	5.735824	39.453516	8.114623
H	5.997592	38.430600	9.709921
H	4.965492	35.380057	5.838617
H	11.358446	36.905969	7.326192
H	10.201552	35.846605	8.170064
H	10.995822	35.204262	5.282369

H	12.135342	34.807909	6.567655
H	9.407001	33.716003	6.760001
H	10.358654	30.633749	6.458515
H	10.697447	30.878746	8.170126
H	5.889137	36.048673	4.504640

⁷TSa'b'

E lacvp = -3210.732381

$\nu = i1120 \text{ cm}^{-1}$

H	1.101200	31.699251	6.164721
C	1.507000	32.638004	5.951001
H	1.232980	32.914574	4.927345
H	1.051260	33.367532	6.629271
C	3.037591	32.622034	6.128578
H	3.287923	32.198583	7.112870
H	3.520615	31.989382	5.380437
C	3.677332	33.988887	6.069651
O	4.802801	34.059722	5.389473
O	3.174373	34.998462	6.665091
H	10.143126	43.246052	12.466619
C	9.905001	42.715004	11.598001
H	9.024223	43.206490	11.171116
H	10.722980	42.894177	10.886131
C	9.615848	41.261197	11.701604
N	10.585587	40.263452	11.861870
H	11.573526	40.419261	11.991715
C	9.982180	39.042307	11.779019
H	10.491849	38.096662	11.839432
N	8.671872	39.213968	11.583803
C	8.431237	40.589587	11.522840
H	7.440454	40.985311	11.348590
H	8.890801	39.862427	17.173429
C	7.966001	39.398003	17.084999
H	8.081695	38.376156	17.460828
H	7.272567	39.902197	17.769273
C	7.418772	39.355153	15.700229
N	6.642378	40.372814	15.134548
H	6.360503	41.220846	15.601371
C	6.299269	40.023547	13.858884
H	5.728883	40.628479	13.163444
N	6.826010	38.826112	13.584393
C	7.508120	38.394146	14.723840
H	7.981012	37.428856	14.764111
H	-3.603364	36.610172	11.293832
C	-2.941999	37.186005	10.751000
H	-3.526539	37.811528	10.064403
H	-2.416119	37.860338	11.439181
C	-1.957150	36.291802	9.984499
H	-1.315539	35.758384	10.697199
H	-2.499382	35.518793	9.426048
C	-1.075108	37.098846	9.007935
H	-1.602897	37.278121	8.067332
H	-0.850863	38.091654	9.422908
N	0.192299	36.430876	8.682547
H	0.291218	35.964288	7.793406
C	1.233605	36.365870	9.548337
N	1.177481	36.968819	10.750430
H	0.353131	37.439998	11.077099
H	2.042475	36.921365	11.321503
N	2.348280	35.703226	9.225191
H	2.500851	35.299214	8.300899
H	3.106275	35.751631	9.918030
Fe	7.141975	37.759888	11.748868
Cl	8.422915	36.422863	10.236543
O	5.112819	34.580914	12.601241

C	6.298956	34.958125	12.741256
O	6.614005	36.260592	12.764976
C	7.462815	34.023942	12.877116
H	7.929736	34.135634	13.862126
H	7.152075	32.989302	12.734466
H	8.194777	34.322865	12.120176
O	3.692434	36.530216	11.449176
H	4.123225	35.833261	12.022852
H	4.345840	37.230033	11.186469
O	5.244647	40.967348	11.239774
H	5.252673	40.010918	10.953083
H	4.569918	41.476303	10.758132
O	5.611174	38.349712	10.708517
H	7.328653	38.397305	8.362569
C	6.244694	38.383518	8.235809
C	5.734393	37.231779	7.401266
O	4.365617	37.487366	7.024219
C	6.607945	37.103147	6.084533
C	7.870893	36.299838	6.370457
O	7.834465	35.099771	6.662099
N	5.786340	36.412211	5.052203
S	9.393637	37.308636	6.254200
C	10.745303	36.152948	6.963044
C	11.063032	34.898238	6.135674
N	10.402504	33.702091	6.636481
C	11.113253	32.591901	6.997143
C	10.301959	31.418259	7.505979
H	10.736541	31.064821	8.445142
O	12.357001	32.552002	6.897000
H	4.919016	36.945184	4.943102
H	6.877697	38.108296	5.740796
H	5.820398	36.277142	7.936869
H	3.867476	36.631739	6.929152
H	5.836627	39.343967	7.909274
H	5.842043	38.287698	9.416192
H	5.289920	35.037843	5.340966
H	11.600910	36.832125	7.000601
H	10.437944	35.902437	7.980467
H	10.830400	35.066052	5.076546
H	12.135564	34.685260	6.203385
H	9.407001	33.716003	6.760001
H	9.247261	31.660622	7.665681
H	10.369069	30.594756	6.786894
H	6.276236	36.350358	4.158205

TSa'b'

E lacvp = -3210.736951

$\nu = \text{i555 cm}^{-1}$

H	1.101200	31.699251	6.164721
C	1.507000	32.638004	5.951001
H	1.241207	32.910016	4.923949
H	1.045134	33.369756	6.622589
C	3.035910	32.623587	6.141168
H	3.278040	32.213042	7.132805
H	3.524619	31.982323	5.404241
C	3.671852	33.990983	6.068487
O	4.789171	34.062587	5.377555
O	3.167224	35.001439	6.662876
H	10.143126	43.246052	12.466619
C	9.905001	42.715004	11.598001
H	9.017812	43.197008	11.174223
H	10.718876	42.896443	10.882328
C	9.628510	41.260484	11.719990
N	10.602797	40.271026	11.901024
H	11.590498	40.433432	12.024183

C	10.003390	39.045437	11.849527
H	10.516838	38.103216	11.927859
N	8.692671	39.208356	11.655612
C	8.446487	40.580574	11.561960
H	7.455373	40.970957	11.379950
H	8.890801	39.862427	17.173429
C	7.966001	39.398003	17.084999
H	8.085665	38.372195	17.448532
H	7.276945	39.893259	17.780364
C	7.406241	39.366896	15.704802
N	6.639949	40.395643	15.144398
H	6.375096	41.248707	15.612072
C	6.279235	40.049413	13.872701
H	5.713638	40.661179	13.179936
N	6.785016	38.843660	13.595957
C	7.470963	38.402673	14.730147
H	7.927896	37.429789	14.766644
H	-3.603364	36.610172	11.293832
C	-2.941999	37.186005	10.751000
H	-3.526226	37.798422	10.052342
H	-2.428658	37.872752	11.436220
C	-1.941846	36.293241	10.002305
H	-1.295220	35.779980	10.725306
H	-2.471174	35.504100	9.454127
C	-1.068642	37.097305	9.015605
H	-1.601100	37.263357	8.075174
H	-0.850886	38.095816	9.420118
N	0.203109	36.436416	8.691672
H	0.301761	35.960972	7.807128
C	1.250036	36.391514	9.551674
N	1.194610	37.006825	10.747479
H	0.366529	37.471495	11.074100
H	2.061320	36.972017	11.316525
N	2.369719	35.736995	9.228249
H	2.519188	35.321794	8.308260
H	3.130574	35.796808	9.915542
Fe	7.141014	37.775213	11.775676
Cl	8.432170	36.447808	10.245596
O	5.116589	34.625701	12.567224
C	6.308006	34.974630	12.735523
O	6.655411	36.267277	12.799708
C	7.450538	34.013793	12.860751
H	7.908291	34.090248	13.853259
H	7.123086	32.989483	12.685133
H	8.194777	34.322865	12.120176
O	3.712278	36.595280	11.454572
H	4.142722	35.886018	12.015986
H	4.370984	37.287388	11.194730
O	5.255557	40.978151	11.239196
H	5.292368	40.028622	10.939574
H	4.598737	41.484926	10.731275
O	5.719068	38.359667	10.707009
H	7.288314	38.421099	8.288236
C	6.201380	38.379661	8.198174
C	5.700729	37.227093	7.353771
O	4.338185	37.487122	6.957872
C	6.590978	37.096037	6.051311
C	7.852747	36.295732	6.354933
O	7.816337	35.094420	6.641544
N	5.782576	36.399630	5.011722
S	9.373929	37.309415	6.265917
C	10.713775	36.159041	7.005765
C	11.067259	34.914844	6.177556
N	10.403979	33.707952	6.648762
C	11.112539	32.590163	6.989723

C	10.297770	31.405718	7.467287
H	10.728111	31.029733	8.399604
O	12.357001	32.552002	6.897000
H	4.920444	36.936811	4.883451
H	6.863087	38.100143	5.706288
H	5.774712	36.272285	7.889725
H	3.836452	36.631790	6.871830
H	5.770069	39.332438	7.878828
H	5.844966	38.264648	9.352962
H	5.279692	35.043778	5.314147
H	11.561881	36.845110	7.074143
H	10.377512	35.899781	8.011866
H	10.864062	35.090263	5.113432
H	12.139437	34.710837	6.273146
H	9.407001	33.716003	6.760001
H	9.242722	31.645573	7.628509
H	10.366794	30.599297	6.729242
H	6.286466	36.325120	4.126549

TSbc

E lacvp = -3210.724992

$\nu = i220 \text{ cm}^{-1}$

H	1.101198	31.699247	6.164722
C	1.507002	32.638003	5.950999
H	2.398751	32.499017	5.333201
H	0.780718	33.226511	5.380846
C	1.892425	33.340146	7.270366
H	1.007986	33.693236	7.808483
H	2.396723	32.613156	7.924260
C	2.856789	34.497480	7.097484
O	3.869396	34.315262	6.323840
O	2.654790	35.597316	7.764994
H	10.143136	43.246047	12.466619
C	9.904988	42.715000	11.598001
H	9.065944	43.244066	11.134006
H	10.753914	42.830327	10.910596
C	9.533135	41.283766	11.738393
N	10.447575	40.231818	11.861142
H	11.448307	40.329410	11.938028
C	9.763297	39.049610	11.838514
H	10.218600	38.076838	11.897370
N	8.458373	39.299510	11.719199
C	8.300765	40.684613	11.647962
H	7.335694	41.154817	11.532739
H	8.890803	39.862418	17.173431
C	7.965998	39.398005	17.084995
H	8.102111	38.361540	17.411467
H	7.296352	39.862452	17.821063
C	7.338144	39.393833	15.731828
N	6.649386	40.485647	15.191008
H	6.529502	41.381877	15.637344
C	6.137450	40.138217	13.972651
H	5.604803	40.818494	13.320145
N	6.466881	38.867632	13.698525
C	7.202541	38.395559	14.796192
H	7.554109	37.379244	14.825808
H	-3.603365	36.610167	11.293831
C	-2.941998	37.186002	10.750999
H	-3.370592	37.382602	9.761488
H	-2.828287	38.151301	11.260976
C	-1.589892	36.450279	10.641511
H	-1.260224	36.141229	11.643460
H	-1.714655	35.523950	10.066104
C	-0.480494	37.293501	9.979271
H	-0.776572	37.566799	8.961536

H	-0.340802	38.238637	10.523429
N	0.810482	36.596044	9.874364
H	1.102245	36.212254	8.975995
C	1.708948	36.466338	10.880754
N	1.489354	36.973781	12.103752
H	0.601748	37.382863	12.340582
H	2.269036	36.997852	12.797072
N	2.852003	35.806705	10.624880
H	3.046047	35.544298	9.663090
H	3.534126	35.599514	11.347798
Fe	6.906671	37.870459	11.737583
Cl	5.049339	38.803333	10.536930
O	4.981433	34.730470	12.499520
C	6.216493	34.996700	12.584513
O	6.658931	36.226548	12.771025
C	7.267915	33.915866	12.535156
H	7.480840	33.570266	13.554589
H	6.918477	33.059486	11.955752
H	8.194778	34.322860	12.120175
O	3.695047	36.905223	13.649186
H	4.150390	36.053555	13.431737
H	4.361487	37.618131	13.662450
O	5.184789	41.822400	11.590731
H	4.657027	42.586431	11.296917
H	4.930713	41.015965	11.088041
O	7.645153	36.958897	10.227234
H	7.638375	35.988513	10.123094
C	6.069413	38.571716	8.119294
C	5.454471	37.376476	7.485911
O	4.148431	37.655576	6.954490
C	6.339266	36.897435	6.245696
C	7.573810	36.125370	6.673968
O	7.531486	34.951741	7.068730
N	5.433584	36.054960	5.389682
S	9.093924	37.135047	6.568401
C	10.358144	36.109452	7.580175
C	11.103527	35.024756	6.804889
N	10.410240	33.741447	6.792184
C	11.109495	32.563788	6.840878
C	10.282718	31.295196	6.810460
H	10.629540	30.625051	7.601623
O	12.357000	32.551998	6.897000
H	4.681012	36.682643	5.079921
H	6.627666	37.776587	5.663795
H	5.419831	36.535731	8.190469
H	3.488990	36.970847	7.299030
H	5.670336	39.544769	7.862683
H	7.036960	38.466975	8.594204
H	4.842100	35.240214	5.940797
H	11.047450	36.888522	7.913531
H	9.816025	35.721127	8.444785
H	11.324242	35.371559	5.786033
H	12.072861	34.840491	7.283487
H	9.407000	33.716000	6.760000
H	9.210632	31.474284	6.935051
H	10.444165	30.780769	5.856858
H	5.918926	35.640264	4.591080

TSbd

E lacvp = -3210.736824

$\nu = \text{i150 cm}^{-1}$

H	1.101200	31.699249	6.164721
C	1.507000	32.638000	5.951000
H	2.406776	32.492447	5.346013
H	0.787358	33.216138	5.361757

C	1.879706	33.370240	7.258275
H	0.992124	33.748148	7.773489
H	2.372076	32.658554	7.936692
C	2.857275	34.512376	7.047064
O	3.900557	34.268347	6.337117
O	2.626081	35.665267	7.610797
H	10.143126	43.246048	12.466619
C	9.905000	42.715000	11.598000
H	9.179909	43.330166	11.054968
H	10.812455	42.700753	10.977960
C	9.345099	41.353602	11.738211
N	10.095049	40.213037	12.041255
H	11.076976	40.200266	12.269845
C	9.280063	39.119819	11.974813
H	9.563606	38.106746	12.197923
N	8.051062	39.518476	11.637891
C	8.073749	40.902220	11.483838
H	7.188019	41.477474	11.259345
H	8.890801	39.862423	17.173429
C	7.966000	39.397999	17.084999
H	8.119981	38.343109	17.335777
H	7.321669	39.805558	17.875524
C	7.286638	39.478280	15.761452
N	6.590073	40.602634	15.306398
H	6.511245	41.482591	15.792396
C	6.019609	40.320553	14.098857
H	5.488606	41.047022	13.501758
N	6.318243	39.059877	13.751102
C	7.101294	38.530469	14.783869
H	7.487361	37.528753	14.734946
H	-3.603364	36.610168	11.293831
C	-2.942000	37.186001	10.750999
H	-3.410597	37.455439	9.797170
H	-2.762410	38.116637	11.304610
C	-1.625648	36.410946	10.528656
H	-1.241921	36.059443	11.496517
H	-1.814673	35.507390	9.935241
C	-0.548206	37.258626	9.820171
H	-0.870293	37.489734	8.800284
H	-0.432291	38.224841	10.332641
N	0.772505	36.615053	9.712181
H	1.102689	36.279548	8.805820
C	1.680975	36.577507	10.715212
N	1.381469	36.996229	11.952828
H	0.452882	37.310908	12.176186
H	2.119900	37.062076	12.682819
N	2.909406	36.095008	10.444672
H	3.128758	35.868940	9.477996
H	3.655764	36.114775	11.128967
Fe	6.337626	38.296239	11.681106
Cl	4.269013	39.496710	11.267235
O	5.562322	36.277138	12.258593
C	6.793551	35.847997	12.383274
O	7.730681	36.732084	12.412376
C	7.155119	34.400800	12.449459
H	7.078003	34.025722	13.476924
H	6.496639	33.799355	11.819165
H	8.194777	34.322861	12.120175
O	3.448793	37.298754	13.682353
H	4.228363	36.748377	13.438906
H	3.706320	38.234398	13.566746
O	5.247795	42.438841	11.837360
H	4.762119	41.673934	11.450817
H	4.770179	43.267297	11.650381
O	6.617758	37.699715	9.947235

H	7.445743	37.810718	9.439798
C	5.824555	38.761792	7.639800
C	5.385863	37.426611	7.159964
O	4.119945	37.547054	6.434265
C	6.396681	36.759248	6.147978
C	7.525504	35.961668	6.783772
O	7.524303	34.725888	6.832546
N	5.582797	35.844651	5.275830
S	8.913968	36.992571	7.416355
C	10.001343	35.707919	8.353161
C	10.996207	34.919769	7.502004
N	10.396534	33.724427	6.922499
C	11.131803	32.597900	6.664203
C	10.369608	31.426703	6.078596
H	10.585732	30.530749	6.667254
O	12.357000	32.551998	6.897000
H	4.886634	36.441595	4.812356
H	6.822759	37.544945	5.514075
H	5.245003	36.752872	8.013533
H	3.439651	36.947912	6.881433
H	6.589179	39.334701	7.122352
H	5.216398	39.255203	8.385861
H	4.928059	35.129213	5.860513
H	10.521637	36.352366	9.064970
H	9.314731	35.053159	8.894476
H	11.438375	35.565375	6.731026
H	11.826592	34.587635	8.138130
H	9.407000	33.716000	6.760000
H	9.287320	31.583494	6.049613
H	10.725930	31.237695	5.060410
H	6.151512	35.319445	4.609407

TSbk

E lacvp = -3210.735571

$\nu = \text{i23 cm}^{-1}$

H	1.101200	31.699247	6.164722
C	1.507000	32.638002	5.950999
H	2.322558	32.502165	5.234382
H	0.739679	33.264558	5.483964
C	2.058181	33.290690	7.240283
H	1.249373	33.650809	7.882341
H	2.617900	32.534508	7.808264
C	3.023274	34.429768	6.962276
O	4.000164	34.186829	6.165362
O	2.844183	35.583079	7.548208
H	10.143123	43.246046	12.466626
C	9.905005	42.715003	11.597990
H	9.205497	43.340567	11.033902
H	10.822773	42.670295	10.994408
C	9.303482	41.358042	11.728331
N	9.989517	40.221158	12.180854
H	10.939334	40.206748	12.520105
C	9.176000	39.133046	12.061860
H	9.431391	38.130884	12.358432
N	8.000396	39.520050	11.554558
C	8.069170	40.899844	11.330264
H	7.244498	41.405140	10.847238
H	8.890801	39.862432	17.173428
C	7.966000	39.397988	17.085001
H	8.129422	38.336309	17.300012
H	7.336797	39.775361	17.901432
C	7.262815	39.520496	15.783287
N	6.401396	40.573437	15.458537
H	6.201624	41.369407	16.044938
C	5.836967	40.326743	14.242203

H	5.114129	40.955423	13.753883
N	6.303279	39.167590	13.766899
C	7.186673	38.655996	14.719736
H	7.671397	37.707780	14.573153
H	-3.603366	36.610168	11.293831
C	-2.941998	37.186001	10.750999
H	-3.443498	37.546807	9.845857
H	-2.679897	38.064261	11.355323
C	-1.684680	36.355889	10.407735
H	-1.316490	35.865624	11.319168
H	-1.943902	35.543287	9.717496
C	-0.555674	37.206567	9.785448
H	-0.847730	37.540479	8.785452
H	-0.399950	38.116560	10.382763
N	0.738394	36.511991	9.641983
H	1.077181	36.257634	8.717143
C	1.613214	36.330351	10.662832
N	1.273523	36.607699	11.927492
H	0.345706	36.926982	12.148202
H	1.981762	36.589065	12.693767
N	2.844663	35.864091	10.373123
H	3.064409	35.663217	9.395961
H	3.531363	35.666137	11.095040
Fe	6.218427	38.438743	11.758628
Cl	3.859130	39.336214	11.933442
O	5.162019	35.356889	12.289783
C	6.405266	35.527692	12.446639
O	6.965383	36.729777	12.400508
C	7.316246	34.365825	12.773670
H	7.683911	34.474310	13.801450
H	6.757850	33.432585	12.696337
H	8.194776	34.322862	12.120176
O	3.252700	36.730000	13.759962
H	3.990116	36.162159	13.433210
H	3.500639	37.671085	13.643322
O	5.586956	40.901041	9.675226
H	4.720404	40.935749	10.127310
H	5.721450	39.973065	9.379644
O	5.736193	37.978758	10.037288
H	7.020316	38.957960	7.563169
C	6.070947	38.815479	7.062926
C	5.572535	37.450491	6.751182
O	4.208155	37.498633	6.286232
C	6.423222	36.770896	5.577803
C	7.670811	36.081743	6.095212
O	7.659038	34.928587	6.546988
N	5.509481	35.783240	4.905738
S	9.152190	37.155244	6.007545
C	10.472375	36.191591	7.012409
C	11.080640	34.962758	6.329754
N	10.408400	33.725407	6.702937
C	11.111014	32.579948	6.962848
C	10.286553	31.359418	7.316687
H	10.724153	30.876302	8.194315
O	12.357000	32.551998	6.897000
H	4.721184	36.334538	4.543460
H	6.685869	37.539817	4.847250
H	5.660514	36.791305	7.627718
H	3.631657	36.844261	6.801886
H	5.505591	39.670456	6.711598
H	4.805493	37.805688	9.790562
H	4.983939	35.066537	5.598166
H	11.222642	36.972132	7.160239
H	10.023906	35.938419	7.975447
H	11.100370	35.101178	5.240318

H	12.122799	34.845704	6.648786
H	9.407000	33.716000	6.760000
H	9.236289	31.590915	7.517331
H	10.334900	30.638995	6.492720
H	5.972370	35.258189	4.160593

TSbl

E lacvp = -3210.724941

$\nu = \text{i52 cm}^{-1}$

H	1.101199	31.699247	6.164723
C	1.507001	32.638003	5.950998
H	2.270614	32.514649	5.176783
H	0.719053	33.288018	5.555705
C	2.144563	33.237213	7.221743
H	1.378837	33.516800	7.950786
H	2.792906	32.481519	7.683713
C	3.008734	34.441987	6.913876
O	4.023793	34.260906	6.149323
O	2.700792	35.593526	7.445736
H	10.143137	43.246049	12.466627
C	9.904987	42.714999	11.597991
H	9.232323	43.364548	11.025659
H	10.830078	42.655547	11.009520
C	9.281292	41.371003	11.707709
N	9.969294	40.168162	11.500678
H	10.965392	40.079631	11.371438
C	9.070631	39.142918	11.474374
H	9.303617	38.105952	11.315383
N	7.839390	39.633798	11.658535
C	7.961132	41.017749	11.805068
H	7.111525	41.661386	11.941024
H	8.890800	39.862424	17.173426
C	7.966000	39.397998	17.085002
H	8.142724	38.327356	17.234647
H	7.363247	39.725152	17.943867
C	7.206299	39.573365	15.819758
N	6.516832	40.736320	15.459129
H	6.507925	41.604179	15.972688
C	5.851473	40.525775	14.289180
H	5.297722	41.299012	13.777693
N	6.084350	39.270507	13.879602
C	6.912838	38.666485	14.832931
H	7.202223	37.635098	14.743937
H	-3.603364	36.610166	11.293835
C	-2.941999	37.186003	10.750994
H	-3.436490	37.504687	9.825487
H	-2.716245	38.090064	11.331098
C	-1.663250	36.384411	10.452985
H	-1.225590	36.025898	11.394319
H	-1.903399	35.487916	9.867624
C	-0.623270	37.220310	9.685553
H	-0.989276	37.441140	8.678568
H	-0.483499	38.194477	10.178047
N	0.683376	36.565806	9.529755
H	0.987733	36.253463	8.610089
C	1.605355	36.459450	10.514855
N	1.396758	36.937357	11.752083
H	0.554804	37.437046	11.981978
H	2.107415	36.761141	12.492585
N	2.780628	35.867753	10.232495
H	2.939997	35.594338	9.262860
H	3.580102	36.112323	10.817702
Fe	6.059412	38.522668	11.929589
Cl	4.876060	40.554767	10.906259
O	6.172299	36.453802	13.017685

C	6.871299	36.009625	12.022315
O	7.321055	36.879789	11.165545
C	7.154558	34.546086	11.855017
H	6.500390	33.956226	12.498492
H	7.013263	34.254535	10.810306
H	8.194777	34.322861	12.120176
O	3.355938	36.298458	13.511193
H	4.286319	36.483876	13.249342
H	3.325839	35.715147	14.287156
O	5.195799	43.061874	12.760574
H	4.916359	42.514463	11.990774
H	4.824228	43.959312	12.690176
O	4.546439	37.681777	11.255651
H	6.692177	38.411934	8.789926
C	5.963436	38.506310	7.995454
C	5.461998	37.311043	7.272159
O	4.218405	37.588852	6.592717
C	6.461351	36.815952	6.127371
C	7.614158	36.001496	6.669831
O	7.558509	34.770382	6.808094
N	5.631709	35.987843	5.182879
S	9.061917	37.020528	7.133978
C	10.071929	35.802495	8.217793
C	11.044159	34.899207	7.469599
N	10.398928	33.711576	6.921038
C	11.129214	32.582882	6.669836
C	10.369845	31.400396	6.105395
H	10.591185	30.513711	6.706158
O	12.357000	32.551998	6.897000
H	4.913298	36.624283	4.814787
H	6.826561	37.693968	5.588704
H	5.335643	36.460480	7.959550
H	3.520862	36.924053	6.904200
H	5.559397	39.478740	7.743609
H	3.954023	38.282518	10.760256
H	5.016567	35.196173	5.697819
H	10.612594	36.488198	8.873609
H	9.346447	35.240054	8.809889
H	11.568619	35.464347	6.687200
H	11.820043	34.555409	8.165763
H	9.407000	33.716000	6.760000
H	9.287031	31.554166	6.078902
H	10.722035	31.197466	5.088438
H	6.183332	35.563970	4.434219

TSkb'

E lacvp = -3210.737755

$\nu = \text{il0 cm}^{-1}$

H	1.101201	31.699249	6.164720
C	1.506999	32.638000	5.951002
H	2.340037	32.502359	5.255020
H	0.746593	33.255191	5.460495
C	2.019710	33.301583	7.246586
H	1.191537	33.623136	7.884588
H	2.609562	32.567911	7.812894
C	2.930583	34.480583	6.972257
O	3.936985	34.279537	6.203427
O	2.671074	35.632647	7.530774
H	10.143127	43.246048	12.466619
C	9.904999	42.714999	11.598002
H	8.992563	43.171472	11.200379
H	10.696957	42.942725	10.869249
C	9.683208	41.255439	11.684738
N	10.657394	40.305410	12.014404
H	11.605190	40.506011	12.295767

C	10.115691	39.062542	11.908128
H	10.610607	38.143899	12.161753
N	8.840465	39.174005	11.509646
C	8.563605	40.534279	11.357276
H	7.588225	40.902627	11.085790
H	8.890799	39.862429	17.173431
C	7.966001	39.397992	17.084996
H	8.077883	38.401220	17.524264
H	7.265695	39.940909	17.733029
C	7.426280	39.259576	15.713808
N	6.629735	40.215005	15.071279
H	6.358308	41.108425	15.453040
C	6.284554	39.760659	13.838584
H	5.734231	40.346071	13.112711
N	6.828991	38.539425	13.662942
C	7.533618	38.220832	14.830951
H	8.109119	37.317045	14.938300
H	-3.603364	36.610166	11.293832
C	-2.942000	37.186004	10.750997
H	-3.419316	37.427407	9.792470
H	-2.793693	38.133411	11.285250
C	-1.599314	36.465624	10.523582
H	-1.107721	36.277416	11.488050
H	-1.766083	35.480893	10.069475
C	-0.658688	37.282519	9.610105
H	-1.067799	37.320936	8.596242
H	-0.605625	38.324835	9.957314
N	0.706490	36.743555	9.501285
H	1.002876	36.256611	8.655281
C	1.670991	36.931519	10.427546
N	1.449667	37.626597	11.559996
H	0.537882	37.974098	11.798805
H	2.266517	37.817333	12.157284
N	2.895694	36.426580	10.209152
H	3.087079	35.968118	9.320143
H	3.608522	36.527545	10.923800
Fe	7.391478	37.721029	11.821339
Cl	6.602085	35.899821	10.444437
O	9.595476	35.824421	14.529092
C	9.209030	35.655625	13.361639
O	8.760159	36.700251	12.611847
C	9.149704	34.340712	12.646761
H	9.945602	34.273803	11.895975
H	9.246300	33.510818	13.346863
H	8.194777	34.322861	12.120176
O	3.982110	37.794649	12.504103
H	4.386204	37.474228	13.328869
H	4.679051	38.263855	11.947358
O	5.439139	41.336373	11.409152
H	5.544901	40.385968	11.099487
H	4.737223	41.803659	10.923900
O	5.950104	38.795997	10.989257
H	5.727744	38.491166	10.082108
C	5.983771	38.639017	7.686196
C	5.485200	37.346791	7.138867
O	4.208531	37.536910	6.499469
C	6.464376	36.743644	6.029452
C	7.599109	35.914953	6.605305
O	7.547546	34.678823	6.658565
N	5.611033	35.875557	5.145876
S	9.020416	36.907084	7.195257
C	9.908452	35.670584	8.370492
C	10.972558	34.796646	7.723319
N	10.391195	33.698442	6.960997
C	11.145182	32.616665	6.601833

C	10.428236	31.519551	5.841713
H	10.529051	30.578294	6.390718
O	12.357000	32.551998	6.897000
H	4.928684	36.492110	4.692191
H	6.862312	37.566110	5.428029
H	5.411976	36.584685	7.930994
H	3.531653	36.887307	6.883930
H	5.415576	39.534540	7.461167
H	6.967964	38.716769	8.133162
H	4.957920	35.157154	5.719079
H	10.353840	36.344565	9.105035
H	9.114389	35.096255	8.853764
H	11.643738	35.397691	7.095940
H	11.602003	34.370433	8.517061
H	9.407000	33.716000	6.760000
H	9.365731	31.725700	5.682970
H	10.912781	31.379821	4.870215
H	6.162464	35.350419	4.463922

TS1b'

E lacvp = -3210.727614

$\nu = i23 \text{ cm}^{-1}$

H	1.101201	31.699247	6.164719
C	1.506999	32.638002	5.951002
H	1.967696	32.583350	4.958686
H	0.706440	33.384063	5.915338
C	2.577663	33.005503	7.009049
H	2.103457	33.276644	7.957291
H	3.227400	32.141589	7.179075
C	3.444286	34.144608	6.514824
O	4.387354	33.830565	5.698294
O	3.176888	35.362891	6.883902
H	10.143126	43.246048	12.466620
C	9.905000	42.715000	11.597999
H	9.200996	43.341977	11.040318
H	10.818470	42.676879	10.989162
C	9.313960	41.352918	11.727480
N	10.068748	40.192090	11.941191
H	11.065511	40.162280	12.091832
C	9.242796	39.106669	11.884440
H	9.553453	38.085720	12.021889
N	7.996868	39.520961	11.645393
C	8.023560	40.913506	11.537598
H	7.116008	41.469292	11.350737
H	8.890802	39.862423	17.173428
C	7.965999	39.397999	17.085000
H	8.120819	38.344795	17.342491
H	7.321448	39.809448	17.873343
C	7.290973	39.472898	15.764204
N	6.589395	40.597265	15.317200
H	6.508932	41.471944	15.812924
C	6.016139	40.319778	14.111132
H	5.469936	41.027340	13.498096
N	6.322168	39.061215	13.765447
C	7.106947	38.524174	14.785786
H	7.465156	37.510267	14.739265
H	-3.603363	36.610169	11.293833
C	-2.942000	37.186000	10.750996
H	-3.404026	37.457578	9.795173
H	-2.754130	38.113838	11.305655
C	-1.630003	36.388048	10.529369
H	-1.275811	35.998027	11.495286
H	-1.842164	35.506712	9.910058
C	-0.499781	37.197530	9.853496
H	-0.877680	37.658098	8.934850

H	-0.148884	38.024410	10.482333
N	0.674226	36.384586	9.456072
H	0.757511	36.141938	8.477845
C	1.780423	36.160656	10.200839
N	1.778056	36.382421	11.534079
H	0.958578	36.708096	12.015427
H	2.646452	36.295776	12.041953
N	2.878958	35.654481	9.635592
H	2.972504	35.587123	8.609694
H	3.690124	35.439939	10.214131
Fe	6.257433	38.337737	11.721931
Cl	6.233025	38.118819	9.374209
O	5.061469	35.278847	11.599638
C	6.295575	35.395982	11.791937
O	6.847462	36.566697	12.151224
C	7.250368	34.241357	11.569728
H	6.751746	33.303570	11.824847
H	7.491287	34.205633	10.498653
H	8.194777	34.322861	12.120175
O	2.575614	38.985315	9.775033
H	3.259585	38.874215	10.484887
H	3.023760	38.921354	8.911608
O	4.852702	41.551058	11.594633
H	4.359961	42.171926	11.029899
H	4.531612	40.618168	11.462921
O	4.423056	38.901879	11.778995
H	4.005970	38.859383	12.662142
C	6.027161	38.764925	5.841209
C	5.634373	37.332091	5.851406
O	4.308474	37.164987	5.280863
C	6.633603	36.446935	4.955899
C	7.731505	35.836765	5.799799
O	7.611476	34.748343	6.379279
N	5.805911	35.378761	4.308636
S	9.217632	36.900582	5.927174
C	10.113661	36.116383	7.428038
C	11.089020	34.991306	7.105993
N	10.408185	33.726025	6.849242
C	11.115398	32.560853	6.759031
C	10.312506	31.304977	6.485703
H	10.525342	30.566010	7.264019
O	12.357000	32.551998	6.897000
H	5.007311	35.874040	3.884605
H	7.060267	37.080811	4.173903
H	5.651494	36.927709	6.869053
H	3.766265	36.564660	5.892114
H	5.800637	39.360139	4.962626
H	6.464771	39.229535	6.715001
H	5.273356	34.680599	5.047567
H	10.641269	36.972429	7.853044
H	9.328456	35.801049	8.119849
H	11.732061	35.262230	6.259124
H	11.762224	34.857694	7.964567
H	9.407000	33.716000	6.760000
H	9.233504	31.480662	6.445295
H	10.636364	30.872164	5.533628
H	6.327823	34.828691	3.624309

TSb'c'

E_{laccp} = -3210.749058

$\nu = \text{i235 cm}^{-1}$

H	1.101200	31.699249	6.164721
C	1.507000	32.638000	5.951000
H	2.357680	32.495824	5.278314
H	0.755331	33.240581	5.429253

C	1.986675	33.336388	7.239786
H	1.146313	33.685298	7.846474
H	2.558031	32.619658	7.845678
C	2.911782	34.498691	6.936655
O	3.903728	34.259157	6.158616
O	2.679628	35.665636	7.473742
H	10.143126	43.246048	12.466619
C	9.904999	42.715000	11.598000
H	9.090329	43.265908	11.116320
H	10.769161	42.807926	10.925283
C	9.491287	41.297494	11.724641
N	10.362743	40.226754	11.953365
H	11.354278	40.301716	12.121143
C	9.653810	39.060954	11.892547
H	10.072805	38.079944	12.032474
N	8.375646	39.344270	11.637883
C	8.258136	40.729683	11.522790
H	7.304036	41.202466	11.326797
H	8.890801	39.862423	17.173429
C	7.966000	39.397999	17.084999
H	8.108011	38.351982	17.376395
H	7.304336	39.837790	17.842553
C	7.340455	39.444835	15.738927
N	6.603333	40.532608	15.258409
H	6.421474	41.385680	15.764028
C	6.138971	40.241984	14.007820
H	5.585572	40.916719	13.366277
N	6.550997	39.015851	13.668064
C	7.285796	38.506396	14.738854
H	7.698130	37.513298	14.706949
H	-3.603364	36.610168	11.293831
C	-2.941999	37.186001	10.750999
H	-3.442633	37.519985	9.834330
H	-2.706301	38.081750	11.340397
C	-1.662489	36.386412	10.427347
H	-1.237260	35.986172	11.358088
H	-1.906511	35.512022	9.810999
C	-0.603020	37.239724	9.694695
H	-0.945323	37.468621	8.681169
H	-0.482059	38.204697	10.208123
N	0.721681	36.605652	9.568293
H	1.040706	36.255714	8.664739
C	1.631676	36.569472	10.569995
N	1.335859	36.987261	11.807785
H	0.392710	37.230140	12.058907
H	2.113803	37.105345	12.505437
N	2.880320	36.131165	10.289552
H	3.079306	35.859919	9.326913
H	3.533509	35.870320	11.025660
Fe	6.684374	38.129778	11.725307
Cl	7.229193	37.287232	9.542560
O	5.037847	35.120131	12.204824
C	6.281283	35.231326	12.391360
O	6.872277	36.407471	12.562330
C	7.202255	34.042795	12.484144
H	7.297075	33.733683	13.532716
H	6.800925	33.201939	11.916120
H	8.194777	34.322861	12.120175
O	3.542933	37.332508	13.214363
H	4.087342	36.513849	13.215267
H	4.033181	38.021122	12.691875
O	5.141188	41.358431	11.422317
H	4.504448	41.949077	10.984618
H	4.905705	40.390019	11.291901
O	4.905780	38.731851	11.289739

H	4.454754	38.314319	10.528446
C	6.001925	38.486582	7.405157
C	5.451797	37.257557	6.775479
O	4.137349	37.514472	6.200855
C	6.344701	36.707976	5.612539
C	7.588345	35.991137	6.119307
O	7.554757	34.831947	6.549748
N	5.466000	35.756881	4.841488
S	9.089295	37.031827	6.031923
C	10.281143	36.165350	7.261213
C	11.107232	35.012863	6.698948
N	10.411088	33.732859	6.769087
C	11.108193	32.560498	6.867293
C	10.281349	31.292421	6.927596
H	10.626791	30.680846	7.765708
O	12.357000	32.551998	6.897000
H	4.728820	36.326219	4.410650
H	6.623495	37.531009	4.948776
H	5.357628	36.452483	7.518384
H	3.469736	36.919538	6.673403
H	5.353709	39.049796	8.063527
H	6.928564	38.943316	7.079785
H	4.880988	35.069979	5.515775
H	10.925543	36.998412	7.550414
H	9.670633	35.873271	8.118810
H	11.432094	35.236563	5.673673
H	12.024743	34.908195	7.291389
H	9.407000	33.716000	6.760000
H	9.209165	31.479993	7.037348
H	10.444972	30.710862	6.013922
H	5.978826	35.217116	4.141679

TSb'd'

E lacvp = -3210.747467

$\nu = i223 \text{ cm}^{-1}$

H	1.101200	31.699249	6.164721
C	1.507000	32.638000	5.951000
H	2.425262	32.496949	5.373917
H	0.800856	33.206721	5.336940
C	1.830394	33.375422	7.266759
H	0.922773	33.744124	7.754408
H	2.298952	32.667218	7.967319
C	2.808193	34.527069	7.117526
O	3.797575	34.382646	6.318106
O	2.631244	35.599623	7.848681
H	10.143126	43.246048	12.466619
C	9.905000	42.715000	11.598000
H	9.061922	43.238280	11.134384
H	10.751386	42.830744	10.908070
C	9.541278	41.279639	11.748473
N	10.468349	40.246097	11.932471
H	11.464944	40.362226	12.034447
C	9.810217	39.051238	11.914990
H	10.279733	38.086374	11.992733
N	8.504610	39.272534	11.741575
C	8.323390	40.654857	11.627957
H	7.344623	41.078937	11.452027
H	8.890801	39.862423	17.173429
C	7.966000	39.397999	17.084999
H	8.101243	38.362630	17.415199
H	7.294849	39.865696	17.817434
C	7.346985	39.387957	15.729838
N	6.653254	40.468780	15.168329
H	6.516495	41.366780	15.606646
C	6.165060	40.106345	13.945492

H	5.624602	40.743389	13.255570
N	6.513471	38.836327	13.694331
C	7.236308	38.379410	14.804828
H	7.598461	37.367445	14.851012
H	-3.603364	36.610168	11.293831
C	-2.941999	37.186001	10.750999
H	-3.346162	37.337423	9.743635
H	-2.869876	38.170269	11.231424
C	-1.561283	36.487062	10.700397
H	-1.252834	36.215290	11.720088
H	-1.644053	35.542436	10.147777
C	-0.459216	37.347803	10.042750
H	-0.758941	37.616941	9.024931
H	-0.334523	38.292559	10.589818
N	0.855503	36.683186	9.930864
H	1.132529	36.269747	9.037445
C	1.791577	36.630092	10.903266
N	1.575527	37.104888	12.137459
H	0.657148	37.401131	12.423283
H	2.367506	37.137957	12.818287
N	3.006789	36.103256	10.594650
H	3.120819	35.750521	9.642323
H	3.620186	35.732829	11.321019
Fe	6.975148	37.819031	11.798903
Cl	8.299564	36.518178	10.216502
O	4.995159	34.732978	12.423208
C	6.224658	34.988226	12.586910
O	6.631792	36.230552	12.826067
C	7.289776	33.929126	12.593793
H	7.532067	33.669675	13.632724
H	6.942464	33.028974	12.085268
H	8.194777	34.322861	12.120175
O	3.794550	36.965669	13.626516
H	4.200271	36.088324	13.420179
H	4.510826	37.619439	13.739935
O	5.173736	40.960929	11.268144
H	4.664422	41.525624	10.661667
H	5.216847	40.016347	10.940533
O	5.551697	38.374859	10.680838
H	4.754953	37.823612	10.517651
C	6.127979	38.465139	8.229142
C	5.530647	37.302253	7.519429
O	4.192470	37.605239	7.074006
C	6.352353	36.927574	6.210725
C	7.630151	36.146975	6.490526
O	7.616121	34.932377	6.729130
N	5.417843	36.106138	5.352613
S	9.118040	37.200313	6.404181
C	10.497881	36.158193	7.242477
C	11.074094	34.997022	6.427705
N	10.407656	33.730463	6.696778
C	11.109077	32.578827	6.928548
C	10.279519	31.343800	7.216210
H	10.634452	30.884613	8.143339
O	12.357000	32.551998	6.897000
H	4.671430	36.739828	5.046248
H	6.579383	37.847075	5.666088
H	5.541895	36.402669	8.154201
H	3.539332	36.898480	7.391200
H	5.623236	39.419750	8.151812
H	7.133839	38.405628	8.619755
H	4.851380	35.318259	5.899427
H	11.251614	36.931993	7.409268
H	10.092644	35.840347	8.205349
H	11.066954	35.236454	5.355795

H	12.122876	34.846185	6.709850
H	9.407000	33.716000	6.760000
H	9.209505	31.552328	7.306116
H	10.431091	30.613332	6.414590
H	5.893185	35.683033	4.551900

TSia'

E lacvp = -3210.739648

$\nu = i51 \text{ cm}^{-1}$

H	1.101200	31.699249	6.164721
C	1.507000	32.638000	5.951000
H	1.656953	32.707616	4.867994
H	0.804932	33.422508	6.249819
C	2.856119	32.773313	6.699655
H	2.672604	32.833325	7.779060
H	3.477637	31.896365	6.503428
C	3.623823	33.997011	6.254728
O	4.598431	33.805290	5.430693
O	3.252494	35.164932	6.676712
H	10.143126	43.246048	12.466619
C	9.905000	42.715000	11.598001
H	9.207302	43.343969	11.034654
H	10.819999	42.665459	10.993208
C	9.303359	41.355754	11.739577
N	10.049576	40.180091	11.891547
H	11.053479	40.132129	11.975253
C	9.202849	39.106499	11.878361
H	9.502086	38.078475	11.982270
N	7.953516	39.542882	11.726439
C	7.997019	40.936310	11.631140
H	7.093862	41.512702	11.500268
H	8.890801	39.862423	17.173429
C	7.966000	39.397999	17.084999
H	8.128213	38.337662	17.306375
H	7.332834	39.781031	17.895961
C	7.268403	39.513558	15.778078
N	6.474739	40.608828	15.417709
H	6.333431	41.437018	15.975827
C	5.907239	40.378732	14.200771
H	5.300942	41.078571	13.639535
N	6.314657	39.179490	13.771097
C	7.150519	38.624839	14.736689
H	7.574977	37.645575	14.606118
H	-3.603364	36.610168	11.293831
C	-2.942000	37.186001	10.750999
H	-3.406673	37.489174	9.806908
H	-2.739184	38.096530	11.329977
C	-1.629837	36.381762	10.504222
H	-1.368718	35.812693	11.405954
H	-1.807806	35.639496	9.714124
C	-0.412910	37.253401	10.103333
H	-0.712602	37.974734	9.332994
H	-0.053737	37.841241	10.953598
N	0.724013	36.483079	9.537739
H	0.615241	36.180774	8.579091
C	1.900756	36.140971	10.125083
N	2.182826	36.425681	11.405419
H	1.696136	37.139572	11.955629
H	3.118255	36.188282	11.727767
N	2.824979	35.476945	9.406030
H	2.784616	35.354064	8.383699
H	3.714490	35.278448	9.853338
Fe	6.151924	38.491111	11.891706
Cl	6.209675	38.190245	9.618340
O	5.161388	35.317856	11.594207

C	6.295216	35.492234	12.103463
O	6.786750	36.709114	12.381714
C	7.167640	34.314472	12.522815
H	7.258539	34.317941	13.616156
H	6.678523	33.388505	12.216492
H	8.194777	34.322861	12.120175
O	1.852924	38.747932	12.700646
H	2.797300	38.894247	12.440951
H	1.645044	39.172934	13.549544
O	4.701610	41.606274	11.760549
H	4.444129	40.667229	11.582933
H	4.302066	42.209948	11.109962
O	4.505900	38.882669	11.901779
H	6.985872	39.032244	6.406735
C	5.970356	38.865772	6.034181
C	5.636194	37.381989	5.975064
O	4.338110	37.211117	5.371109
C	6.701986	36.590376	5.083407
C	7.750996	35.907261	5.937186
O	7.598176	34.785539	6.435696
N	5.938269	35.582440	4.283206
S	9.250950	36.936082	6.206162
C	10.056203	36.032446	7.689212
C	11.059956	34.944844	7.330057
N	10.404429	33.719864	6.884877
C	11.123751	32.573624	6.697565
C	10.344421	31.355357	6.245636
H	10.490826	30.546323	6.967927
O	12.357000	32.551998	6.897000
H	5.139377	36.096562	3.883700
H	7.181636	37.295336	4.397064
H	5.636943	36.941583	6.979177
H	3.820368	36.498241	5.871073
H	5.874516	39.308244	5.036376
H	5.270775	39.369601	6.704890
H	5.387191	34.753704	4.925048
H	10.546267	36.847704	8.224731
H	9.230183	35.650118	8.294440
H	11.767073	35.298980	6.569670
H	11.662779	34.720198	8.221794
H	9.407000	33.716000	6.760000
H	9.272603	31.543443	6.134408
H	10.745012	31.008318	5.287890
H	6.506314	35.134230	3.562851

TSja'

E lacvp = -3210.728415

$\nu = i39 \text{ cm}^{-1}$

H	1.101201	31.699249	6.164722
C	1.506999	32.638000	5.950999
H	2.391498	32.500149	5.322520
H	0.776665	33.228367	5.387780
C	1.907190	33.339588	7.261651
H	1.028683	33.691978	7.810472
H	2.419243	32.614578	7.912527
C	2.870104	34.498058	7.077985
O	3.849498	34.345726	6.264393
O	2.698465	35.572739	7.800516
H	10.143127	43.246048	12.466619
C	9.904998	42.715000	11.598001
H	9.262894	43.377895	11.007592
H	10.837809	42.618504	11.025307
C	9.227414	41.399731	11.711226
N	9.871253	40.170086	11.913338
H	10.859002	40.046143	12.075820

C	8.948035	39.167751	11.842689
H	9.140458	38.120392	11.982421
N	7.748239	39.703587	11.603659
C	7.909919	41.083321	11.509577
H	7.070640	41.727676	11.319891
H	8.890801	39.862423	17.173429
C	7.966000	39.397999	17.084997
H	8.157828	38.325043	17.204924
H	7.386399	39.690758	17.971243
C	7.153506	39.594193	15.857017
N	6.205500	40.615051	15.697645
H	6.024930	41.356129	16.357311
C	5.538566	40.447159	14.521129
H	4.720734	41.085117	14.169725
N	6.023090	39.347248	13.922646
C	7.013342	38.805126	14.745312
H	7.529867	37.903038	14.473618
H	-3.603368	36.610168	11.293838
C	-2.941996	37.186001	10.750992
H	-3.389576	37.471291	9.794172
H	-2.728704	38.101902	11.315598
C	-1.664212	36.321915	10.561229
H	-1.430947	35.827816	11.515317
H	-1.870403	35.512524	9.849609
C	-0.419667	37.094387	10.080423
H	-0.609810	37.541149	9.100133
H	-0.198571	37.931816	10.758577
N	0.792796	36.259666	9.921992
H	1.156437	36.086342	8.981356
C	1.615144	35.865559	10.916747
N	1.321811	36.135128	12.208509
H	0.520205	36.684944	12.464526
H	1.987934	35.912228	12.930067
N	2.732257	35.185013	10.613399
H	2.958861	35.129738	9.620099
H	3.528630	35.151558	11.249499
Fe	5.904994	38.892464	11.936172
Cl	3.954494	37.993599	11.029540
O	5.561568	35.265320	11.870432
C	6.601068	35.862808	12.222689
O	6.799358	37.188332	12.179671
C	7.786154	35.082333	12.807560
H	8.593012	35.755131	13.105563
H	7.436164	34.537453	13.691955
H	8.194777	34.322861	12.120175
O	2.410525	40.873814	11.355379
H	2.799149	41.445911	10.668260
H	2.836438	39.988560	11.283203
O	3.127002	41.879124	13.726867
H	2.397050	42.298344	14.212421
H	2.806010	41.525475	12.847380
O	5.264279	40.382671	11.578232
H	7.076053	38.744473	8.410498
C	6.068506	38.799110	7.985625
C	5.532885	37.421860	7.611200
O	4.254731	37.583351	6.964111
C	6.499626	36.697231	6.576751
C	7.460913	35.676037	7.163814
O	7.458591	34.488960	6.808192
N	5.640845	36.015705	5.548951
S	8.649470	36.349663	8.391193
C	9.451072	34.745102	9.082545
C	10.697216	34.264317	8.348748
N	10.348797	33.615417	7.091725
C	11.212842	32.771236	6.449115

C	10.697300	32.129765	5.176745
H	10.810057	31.044392	5.253081
O	12.357000	32.551998	6.897000
H	5.004068	36.733631	5.181881
H	7.088860	37.467243	6.063066
H	5.429129	36.793915	8.503696
H	3.590525	36.908348	7.317316
H	6.089009	39.441410	7.097818
H	5.404751	39.252293	8.724559
H	4.927353	35.255188	5.974978
H	9.685758	35.030460	10.109488
H	8.661374	33.989761	9.088718
H	11.399261	35.092644	8.185760
H	11.221430	33.537144	8.984189
H	9.407000	33.716000	6.760000
H	9.649992	32.365017	4.965829
H	11.311658	32.459599	4.332562
H	6.192938	35.565945	4.816501

small model ³a'

H	9.754059	42.339817	11.618723
C	9.353353	41.343807	11.673738
N	10.148550	40.195145	11.601896
H	11.156547	40.181633	11.587969
C	9.347151	39.099751	11.524319
H	9.670149	38.075783	11.485785
N	8.078283	39.510838	11.548716
C	8.054243	40.898624	11.632070
H	7.130444	41.457794	11.651376
H	7.793641	39.395981	16.711073
C	7.343638	39.390717	15.734807
N	6.367900	40.306953	15.336855
H	6.021005	41.072906	15.893452
C	5.946898	40.006203	14.077782
H	5.259317	40.607048	13.502117
N	6.615566	38.927170	13.655783
C	7.483414	38.530624	14.673229
H	8.136017	37.685577	14.557843
Fe	6.640619	38.266888	11.788704
Cl	6.960060	37.416439	9.635147
O	5.759557	36.438156	12.324520
C	6.954563	35.942806	12.472622
O	7.927641	36.806889	12.404463
C	7.256845	34.500557	12.652171
H	7.408272	34.260017	13.711197
H	6.456375	33.874363	12.256748
H	8.194777	34.322861	12.120175
O	5.324322	39.193375	11.390605

small model ⁷a'

H	9.749575	42.342876	11.621384
C	9.335957	41.352589	11.683613
N	10.107677	40.190346	11.801946
H	11.107616	40.162277	11.929180
C	9.292392	39.105030	11.700150
H	9.593491	38.076923	11.791368
N	8.037131	39.525749	11.519243
C	8.045735	40.920269	11.497686
H	7.138317	41.496239	11.379191
H	7.778514	39.424000	16.722910
C	7.285225	39.492405	15.770224
N	6.492903	40.574020	15.373156
H	6.329565	41.410236	15.912569
C	5.963387	40.318043	14.143295
H	5.379595	41.020199	13.561479

N	6.386682	39.114082	13.738300
C	7.202002	38.589504	14.740945
H	7.677151	37.630604	14.639043
Fe	6.370824	38.341946	11.778338
Cl	5.811839	37.909920	9.513253
O	5.644381	36.358730	12.421043
C	6.861480	35.899723	12.397297
O	7.808786	36.767681	12.205138
C	7.203189	34.458572	12.553140
H	7.232345	34.179558	13.613336
H	6.466947	33.823307	12.056302
H	8.194777	34.322861	12.120175
O	4.730220	39.323597	11.575393

small model a'

H	9.762112	42.340996	11.614800
C	9.378791	41.337673	11.659871
N	10.178341	40.190125	11.705889
H	11.182159	40.178890	11.800182
C	9.379822	39.092632	11.581371
H	9.704555	38.069019	11.623541
N	8.113737	39.495289	11.455097
C	8.094435	40.885719	11.492133
H	7.177453	41.450497	11.419513
H	7.791382	39.409691	16.714813
C	7.332948	39.440388	15.742949
N	6.453698	40.444969	15.326485
H	6.191096	41.255836	15.865595
C	5.998463	40.159271	14.076381
H	5.365619	40.808990	13.487931
N	6.554979	39.008743	13.676718
C	7.380947	38.550655	14.700775
H	7.952177	37.646652	14.605783
Fe	6.480700	38.267445	11.784525
Cl	6.342385	37.171017	9.725992
O	5.745422	36.342331	12.757332
C	6.965484	35.939926	12.657694
O	7.848339	36.849678	12.322708
C	7.414273	34.532402	12.858650
H	7.847054	34.404415	13.858251
H	6.579258	33.839901	12.746615
H	8.194777	34.322861	12.120175
O	5.173296	39.259453	11.454922

small model ³a

H	9.748786	42.340004	11.621044
C	9.336067	41.349255	11.681928
N	10.117853	40.189934	11.659762
H	11.125419	40.163635	11.682390
C	9.302353	39.103920	11.586092
H	9.613592	38.075390	11.589188
N	8.036842	39.528141	11.558748
C	8.032588	40.918385	11.610494
H	7.128807	41.505669	11.617464
H	7.789565	39.398968	16.707636
C	7.334260	39.401474	15.733821
N	6.454751	40.402130	15.316495
H	6.200696	41.221535	15.846288
C	5.986210	40.106209	14.074766
H	5.349728	40.765152	13.511449
N	6.524836	38.950191	13.661860
C	7.362450	38.501938	14.693576
H	7.927466	37.592846	14.598977
Fe	6.591657	38.268063	11.701300
Cl	4.727731	39.651249	11.164521

O	5.633627	36.352932	12.278756
C	6.847250	35.911674	12.394663
O	7.796527	36.807270	12.297471
C	7.219347	34.481495	12.590837
H	7.306580	34.247608	13.658938
H	6.466717	33.822090	12.154876
H	8.194777	34.322861	12.120175
O	6.676191	37.753803	10.133749

small model ⁷a

H	9.738128	42.345432	11.626707
C	9.296842	41.368126	11.702624
N	10.039886	40.184841	11.766165
H	11.044177	40.127556	11.834916
C	9.187976	39.123192	11.699294
H	9.467845	38.086063	11.743344
N	7.936597	39.578838	11.596326
C	7.985527	40.973053	11.591826
H	7.097610	41.586697	11.533995
H	7.768441	39.426708	16.721577
C	7.256252	39.501141	15.779374
N	6.528885	40.623440	15.371575
H	6.456423	41.491745	15.879397
C	5.921403	40.360863	14.178486
H	5.363683	41.091461	13.609011
N	6.224521	39.112007	13.796210
C	7.049407	38.570171	14.789107
H	7.435874	37.568707	14.718431
Fe	6.240510	38.377041	11.762359
Cl	4.113859	39.483185	11.295701
O	5.540292	36.309082	12.418877
C	6.756863	35.876919	12.251262
O	7.654827	36.767757	11.957919
C	7.136658	34.436016	12.366593
H	6.948839	34.069149	13.381763
H	6.528487	33.832275	11.684957
H	8.194777	34.322861	12.120175
O	5.933678	37.960274	9.938164

small model a

H	9.742478	42.345123	11.634234
C	9.311765	41.364872	11.730265
N	10.038794	40.222752	12.079501
H	11.015384	40.203159	12.329000
C	9.222978	39.134663	11.997602
H	9.494632	38.120895	12.227427
N	8.010848	39.542088	11.615900
C	8.044977	40.922649	11.428022
H	7.197748	41.468922	11.031114
H	7.777591	39.409824	16.713593
C	7.291452	39.440331	15.755280
N	6.383930	40.440914	15.394315
H	6.135884	41.237839	15.960550
C	5.863636	40.156963	14.169754
H	5.144609	40.761433	13.646749
N	6.395137	39.013954	13.717570
C	7.283042	38.558193	14.699846
H	7.841906	37.650272	14.565322
Fe	6.347420	38.384853	11.746753
Cl	4.193369	39.468357	11.561388
O	5.588723	36.340916	12.253294
C	6.815922	35.897900	12.334807
O	7.759079	36.776054	12.303451
C	7.154978	34.445038	12.434565
H	7.048286	34.092983	13.467593

H	6.489900	33.847866	11.806390
H	8.194777	34.322861	12.120175
O	6.369153	37.978207	10.148869