

Pivotal Role of Water in Terminating Enzymatic Function: A Density Functional Theory Study of the Mechanism-based Inactivation of Cytochromes P450

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Complete list of authors of Gaussian 09

Gaussian 09, revision B.01; Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K.; Burant, J. C.; Millam, J. M.; Iyengay, 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.; Adamo, C.; Jaramillo, J.; Comperts, R.; Startmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenbuerg, 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.; Pople, J. A.; Gaussian, Inc.: Wallingford CT, 2010.

Table S1. Raw energy data obtained at the B3LYP/B1 level**(a) Cpd I + tBPA**

	DE [kcal/mol]	D(E+ZPE) [kcal/mol]	E [Eh]	ZPE [Eh]	E+ZPE [Eh]
2RC	0.3	0.3	-2051.932229	0.510501	-2051.421728
4RC	0.0	0.0	-2051.932760	0.510523	-2051.422237
6RC	9.8	8.4	-2051.917183	0.508277	-2051.408906
2TSco	14.1	13.6	-2051.910311	0.509727	-2051.400584
4TSco	13.9	13.8	-2051.910614	0.510317	-2051.400297
6TSco	18.4	15.9	-2051.903489	0.506523	-2051.396966
2Int1rad	-19.7	-18.8	-2051.964169	0.512039	-2051.452130
2Int	-28.9	-27.4	-2051.978759	0.512917	-2051.465842
4Int	-23.2	-23.3	-2051.969676	0.510322	-2051.459354
6Int	-26.0	-26.7	-2051.974186	0.509432	-2051.464754
2TSmig	-25.9	-26.2	-2051.974109	0.510159	-2051.463950
4TSmig	-22.1	-23.3	-2051.967980	0.508572	-2051.459408
6TSmig	-25.1	-27.0	-2051.972685	0.507355	-2051.465330
2Int2	-77.1	-75.4	-2052.055555	0.513194	-2051.542361
4Int2	-78.8	-77.7	-2052.058390	0.512364	-2051.546026
6Int2	-83.0	-82.6	-2052.064954	0.511157	-2051.553797
2TSco(Cb)	21.6	20.5	-2051.898322	0.508693	-2051.389629
4TSco(Cb)	20.8	20.2	-2051.899640	0.509545	-2051.390095
6TSco(Cb)	23.9	21.0	-2051.894720	0.505946	-2051.388774
4Int1(Cb)	-18.2	-17.2	-2051.961774	0.512120	-2051.449654
6Int1(Cb)	-7.3	-8.7	-2051.944398	0.508363	-2051.436035
4Int1(Cb)'	-1.8	-2.5	-2051.935561	0.509299	-2051.426262
4TScn(Cb)	-2.7	-1.7	-2051.937015	0.512024	-2051.424991
6TScn(Cb)	-2.4	-4.9	-2051.936528	0.506435	-2051.430093
4TScn(Cb)'	-0.5	-1.5	-2051.933534	0.508895	-2051.424639
2Int2(Cb)	-62.1	-58.2	-2052.031677	0.516743	-2051.514934
4Int2(Cb)	-31.8	-30.0	-2051.983383	0.513354	-2051.470029
6Int2(Cb)	-60.2	-58.2	-2052.028770	0.513816	-2051.514954
4Int2(Cb)'	-59.7	-56.8	-2052.027831	0.515007	-2051.512824

(b) Cpd I + tBPA + Thr

	ΔE [kcal/mol]	$\Delta(E+ZPE)$ [kcal/mol]	E [Eh]	ZPE [Eh]	E+ZPE [Eh]
EtOH (thr)			-155.0314288	0.080398	-154.9510308
2RC + thr	0.3	0.3	-2206.963658	0.590899	-2206.372759
4RC + thr	0.0	0.0	-2206.964189	0.590921	-2206.373268
6RC + thr	9.8	8.4	-2206.948611	0.588675	-2206.359936
2TSco + thr	14.1	13.6	-2206.941740	0.590125	-2206.351615
4TSco + thr	13.9	13.8	-2206.942042	0.590715	-2206.351327
6TSco + thr	18.4	15.9	-2206.934918	0.586921	-2206.347997
2Int + thr	-28.9	-27.4	-2207.010188	0.593315	-2206.416873
4Int + thr	-23.2	-23.3	-2207.001105	0.590720	-2206.410385
6Int + thr	-26.0	-26.7	-2207.005615	0.589830	-2206.415785
2TSmig + thr	-25.9	-26.2	-2207.005538	0.590557	-2206.414981
4TSmig + thr	-22.1	-23.3	-2206.999409	0.588970	-2206.410439
6TSmig + thr	-25.1	-27.0	-2207.004114	0.587753	-2206.416361
2Int2 + thr	-77.1	-75.4	-2207.086984	0.593592	-2206.493392
4Int2 + thr	-78.8	-77.7	-2207.089818	0.592762	-2206.497056
6Int2 + thr	-83.0	-82.6	-2207.096383	0.591555	-2206.504828
2TSco(Cb) + thr	21.6	20.5	-2206.929750	0.589091	-2206.340659
4TSco(Cb) + thr	20.8	20.2	-2206.931069	0.589943	-2206.341126
6TSco(Cb) + thr	23.9	21.0	-2206.926148	0.586344	-2206.339804
4Int1(Cb) + thr	-18.2	-17.2	-2206.993203	0.592518	-2206.400685
6Int1(Cb) + thr	-7.3	-8.7	-2206.975827	0.588761	-2206.387066
4Int1(Cb)' + thr	-1.8	-2.5	-2206.966990	0.589697	-2206.377293
4TScn(Cb) + thr	-2.7	-1.7	-2206.968444	0.592422	-2206.376022
6TScn(Cb) + thr	-2.4	-4.9	-2206.967957	0.586833	-2206.381124
4TScn(Cb)' + thr	-0.5	-1.5	-2206.964963	0.589293	-2206.375670
2Int2(Cb) + thr	-62.1	-58.2	-2207.063106	0.597141	-2206.465965
4Int2(Cb) + thr	-31.8	-30.0	-2207.014812	0.593752	-2206.421060
6Int2(Cb) + thr	-60.2	-58.2	-2207.060199	0.594214	-2206.465985
4Int2(Cb)' + thr	-59.7	-56.8	-2207.059260	0.595405	-2206.463855
2TSoc-thr	-46.4	-45.6	-2207.038124	0.592174	-2206.445950
4TSoc-thr	-48.1	-48.1	-2207.040878	0.591022	-2206.449856
6TSoc-thr	-52.7	-53.2	-2207.048116	0.590018	-2206.458098
2Pro-thr	-122.1	-116.2	-2207.158830	0.600387	-2206.558443
4Pro-thr	-121.9	-116.9	-2207.158402	0.598848	-2206.559554
6Pro-thr	-125.2	-121.2	-2207.163757	0.597332	-2206.566425

(c) Cpd I + tBPA + Thr + Water

	ΔE [kcal/mol]	$\Delta(E+ZPE)$ [kcal/mol]	E [Eh]	ZPE [Eh]	E+ZPE [Eh]
EtOH (thr)			-155.0314288	0.080398	-154.9510308
Water (w)			-76.40702432	0.021141	-76.38588332
2RC + thr + w	0.3	0.3	-2283.370682	0.612040	-2282.758642
4RC + thr + w	0.0	0.0	-2283.371213	0.612062	-2282.759151
6RC + thr + w	9.8	8.4	-2283.355636	0.609816	-2282.745820
2TSco + thr + w	14.1	13.6	-2283.348764	0.611266	-2282.737498
4TSco + thr + w	13.9	13.8	-2283.349067	0.611856	-2282.737211
6TSco + thr + w	18.4	15.9	-2283.341942	0.608062	-2282.733880
2Int + thr + w	-28.9	-27.4	-2283.417212	0.614456	-2282.802756
4Int + thr + w	-23.2	-23.3	-2283.408129	0.611861	-2282.796268
6Int + thr + w	-26.0	-26.7	-2283.412640	0.610971	-2282.801669
2TSmig + thr + w	-25.9	-26.2	-2283.412562	0.611698	-2282.800864
4TSmig + thr + w	-22.1	-23.3	-2283.406433	0.610111	-2282.796322
6TSmig + thr + w	-25.1	-27.0	-2283.411138	0.608894	-2282.802244
2Int2 + thr + w	-77.1	-75.4	-2283.494008	0.614733	-2282.879275
4Int2 + thr + w	-78.8	-77.7	-2283.496843	0.613903	-2282.882940
6Int2 + thr + w	-83.0	-82.6	-2283.503407	0.612696	-2282.890711
2TSco(Cb) + thr + w	21.6	20.5	-2283.336775	0.610232	-2282.726543
4TSco(Cb) + thr + w	20.8	20.2	-2283.338094	0.611084	-2282.727010
6TSco(Cb) + thr + w	23.9	21.0	-2283.333173	0.607485	-2282.725688
4Int1(Cb) + thr + w	-18.2	-17.2	-2283.400227	0.613659	-2282.786568
6Int1(Cb) + thr + w	-7.3	-8.7	-2283.382851	0.609902	-2282.772949
4Int1(Cb)' + thr + w	-1.8	-2.5	-2283.374014	0.610838	-2282.763176
4TScn(Cb) + thr + w	-2.7	-1.7	-2283.375468	0.613563	-2282.761905
6TScn(Cb) + thr + w	-2.4	-4.9	-2283.374981	0.607974	-2282.767007
4TScn(Cb)' + thr + w	-0.5	-1.5	-2283.371987	0.610434	-2282.761553
2Int2(Cb) + thr + w	-62.1	-58.2	-2283.470130	0.618282	-2282.851848
4Int2(Cb) + thr + w	-31.8	-30.0	-2283.421836	0.614893	-2282.806943
6Int2(Cb) + thr + w	-60.2	-58.2	-2283.467223	0.615355	-2282.851868
4Int2(Cb)' + thr + w	-59.7	-56.8	-2283.466284	0.616546	-2282.849738
2Int2 + thr--w	-84.5	-81.0	-2283.505840	0.617655	-2282.888185
4Int2 + thr--w	-86.3	-83.3	-2283.508674	0.616825	-2282.891849
6Int2 + thr--w	-90.4	-88.1	-2283.515239	0.615618	-2282.899621
2TS--thr--w	-81.9	-76.3	-2283.501680	0.620978	-2282.880702
4TS--thr--w	-82.2	-78.6	-2283.502205	0.617756	-2282.884449
6TS--thr--w	-87.6	-84.5	-2283.510750	0.616983	-2282.893767
2Pro--thr--w	-127.5	-120.0	-2283.574319	0.623930	-2282.950389
4Pro--thr--w	-128.7	-121.9	-2283.576378	0.622967	-2282.953411
6Pro--thr--w	-136.5	-130.0	-2283.588746	0.622419	-2282.966327

Table S2. Raw energy data obtained at the B3LYP/B2//B3LYP/B1 level

(b) Cpd I + tBPA

	DE [kcal/mol]	D(E+ZPE) [kcal/mol]	E [Eh]	ZPE [Eh]	E+ZPE [Eh]
2RC	0.2	0.2	-3192.167535	0.510501	-3191.657034
4RC	0.0	0.0	-3192.167855	0.510523	-3191.657332
6RC	11.9	10.5	-3192.148835	0.508277	-3191.640558
2TSco	14.5	14.0	-3192.144733	0.509727	-3191.635006
4TSco	14.9	14.8	-3192.144123	0.510317	-3191.633806
6TSco	21.2	18.7	-3192.134072	0.506523	-3191.627549
2Int1rad	-17.8	-16.8	-3192.196155	0.512039	-3191.684116
2Int	-25.7	-24.2	-3192.208864	0.512917	-3191.695947
4Int	-19.6	-19.7	-3192.199110	0.510322	-3191.688788
6Int	-19.9	-20.6	-3192.199571	0.509432	-3191.690139
2TSmig	-23.9	-24.2	-3192.206008	0.510159	-3191.695849
4TSmig	-19.6	-20.8	-3192.199056	0.508572	-3191.690484
6TSmig	-20.1	-22.1	-3192.199836	0.507355	-3191.692481
2Int2	-75.1	-73.4	-3192.287461	0.513194	-3191.774267
4Int2	-76.6	-75.4	-3192.289890	0.512364	-3191.777525
6Int2	-78.3	-77.9	-3192.292639	0.511157	-3191.781482
2TSco(Cb)	22.0	20.8	-3192.132853	0.508693	-3191.624160
4TSco(Cb)	21.5	20.9	-3192.133531	0.509545	-3191.623986
6TSco(Cb)	27.6	24.7	-3192.123865	0.505946	-3191.617919
4Int1(Cb)	-13.3	-12.3	-3192.189123	0.512120	-3191.677003
6Int1(Cb)	-0.6	-2.0	-3192.168858	0.508363	-3191.660495
4Int1(Cb)'	11.6	10.8	-3192.149392	0.509299	-3191.640093
4TScn(Cb)	3.6	4.5	-3192.162126	0.512024	-3191.650102
6TScn(Cb)	3.2	0.7	-3192.162680	0.506435	-3191.656245
4TScn(Cb)'	3.7	2.7	-3192.161987	0.508895	-3191.653092
2Int2(Cb)	-55.7	-51.8	-3192.256586	0.516743	-3191.739843
4Int2(Cb)	-25.9	-24.1	-3192.209111	0.513354	-3191.695757
6Int2(Cb)	-50.5	-48.4	-3192.248304	0.513816	-3191.734488
4Int2(Cb)'	-51.7	-48.8	-3192.250172	0.515007	-3191.735164

(b) Cpd I + tBPA + Thr

	ΔE [kcal/mol]	$\Delta(E+ZPE)$ [kcal/mol]	E [Eh]	ZPE [Eh]	E+ZPE [Eh]
EtOH (thr)			-155.094823	0.080398	-155.014425
2RC + thr	0.2	0.2	-3347.262357	0.590899	-3346.671458
4RC + thr	0.0	0.0	-3347.262678	0.590921	-3346.671757
6RC + thr	11.9	10.5	-3347.243658	0.588675	-3346.654983
2TSco + thr	14.5	14.0	-3347.239556	0.590125	-3346.649431
4TSco + thr	14.9	14.8	-3347.238946	0.590715	-3346.648231
6TSco + thr	21.2	18.7	-3347.228895	0.586921	-3346.641974
2Int + thr	-25.7	-24.2	-3347.303687	0.593315	-3346.710372
4Int + thr	-19.6	-19.7	-3347.293933	0.590720	-3346.703213
6Int + thr	-19.9	-20.6	-3347.294394	0.589830	-3346.704564
2TSmig + thr	-23.9	-24.2	-3347.300831	0.590557	-3346.710274
4TSmig + thr	-19.6	-20.8	-3347.293879	0.588970	-3346.704909
6TSmig + thr	-20.1	-22.1	-3347.294659	0.587753	-3346.706906
2Int2 + thr	-75.1	-73.4	-3347.382284	0.593592	-3346.788692
4Int2 + thr	-76.6	-75.4	-3347.384713	0.592762	-3346.791951
6Int2 + thr	-78.3	-77.9	-3347.387462	0.591555	-3346.795907
2TSco(Cb) + thr	22.0	20.8	-3347.227676	0.589091	-3346.638585
4TSco(Cb) + thr	21.5	20.9	-3347.228354	0.589943	-3346.638411
6TSco(Cb) + thr	27.6	24.7	-3347.218688	0.586344	-3346.632344
4Int1(Cb) + thr	-13.3	-12.3	-3347.283946	0.592518	-3346.691428
6Int1(Cb) + thr	-0.6	-2.0	-3347.263681	0.588761	-3346.674920
4Int1(Cb)' + thr	11.6	10.8	-3347.244215	0.589697	-3346.654518
4TScn(Cb) + thr	3.6	4.5	-3347.256949	0.592422	-3346.664527
6TScn(Cb) + thr	3.2	0.7	-3347.257503	0.586833	-3346.670670
4TScn(Cb)' + thr	3.7	2.7	-3347.256809	0.589293	-3346.667516
2Int2(Cb) + thr	-55.7	-51.8	-3347.351409	0.597141	-3346.754268
4Int2(Cb) + thr	-25.9	-24.1	-3347.303934	0.593752	-3346.710182
6Int2(Cb) + thr	-50.5	-48.4	-3347.343127	0.594214	-3346.748913
4Int2(Cb)' + thr	-51.7	-48.8	-3347.344994	0.595405	-3346.749589
2TSoc-thr	-37.4	-36.6	-3347.322287	0.592174	-3346.730113
4TSoc-thr	-39.0	-38.9	-3347.324773	0.591022	-3346.733751
6TSoc-thr	-41.7	-42.3	-3347.329149	0.590018	-3346.739131
2Pro-thr	-109.1	-103.2	-3347.436592	0.600387	-3346.836205
4Pro-thr	-108.9	-103.9	-3347.436258	0.598848	-3346.837410
6Pro-thr	-110.2	-106.2	-3347.438281	0.597332	-3346.840949

(c) Cpd I + tBPA + Thr + Water

	ΔE [kcal/mol]	$\Delta(E+ZPE)$ [kcal/mol]	E [Eh]	ZPE [Eh]	E+ZPE [Eh]
EtOH (thr)			-155.094823	0.080398	-155.014425
Water (w)			-76.458366	0.021141	-76.437225
2RC + thr + w	0.2	0.2	-3423.720723	0.612040	-3423.108683
4RC + thr + w	0.0	0.0	-3423.721044	0.612062	-3423.108982
6RC + thr + w	11.9	10.5	-3423.702024	0.609816	-3423.092208
2TSco + thr + w	14.5	14.0	-3423.697921	0.611266	-3423.086655
4TSco + thr + w	14.9	14.8	-3423.697311	0.611856	-3423.085455
6TSco + thr + w	21.2	18.7	-3423.687261	0.608062	-3423.079199
2Int + thr + w	-25.7	-24.2	-3423.762053	0.614456	-3423.147597
4Int + thr + w	-19.6	-19.7	-3423.752298	0.611861	-3423.140437
6Int + thr + w	-19.9	-20.6	-3423.752760	0.610971	-3423.141788
2TSmig + thr + w	-23.9	-24.2	-3423.759196	0.611698	-3423.147498
4TSmig + thr + w	-19.6	-20.8	-3423.752245	0.610111	-3423.142134
6TSmig + thr + w	-20.1	-22.1	-3423.753025	0.608894	-3423.144131
2Int2 + thr + w	-75.1	-73.4	-3423.840650	0.614733	-3423.225917
4Int2 + thr + w	-76.6	-75.4	-3423.843078	0.613903	-3423.229175
6Int2 + thr + w	-78.3	-77.9	-3423.845828	0.612696	-3423.233132
2TSco(Cb) + thr + w	22.0	20.8	-3423.686041	0.610232	-3423.075809
4TSco(Cb) + thr + w	21.5	20.9	-3423.686720	0.611084	-3423.075636
6TSco(Cb) + thr + w	27.6	24.7	-3423.677053	0.607485	-3423.069568
4Int1(Cb) + thr + w	-13.3	-12.3	-3423.742311	0.613659	-3423.128652
6Int1(Cb) + thr + w	-0.6	-2.0	-3423.722047	0.609902	-3423.112145
4Int1(Cb)' + thr + w	11.6	10.8	-3423.702581	0.610838	-3423.091742
4TScn(Cb) + thr + w	3.6	4.5	-3423.715314	0.613563	-3423.101751
6TScn(Cb) + thr + w	3.2	0.7	-3423.715868	0.607974	-3423.107894
4TScn(Cb)' + thr + w	3.7	2.7	-3423.715175	0.610434	-3423.104741
2Int2(Cb) + thr + w	-55.7	-51.8	-3423.809775	0.618282	-3423.191493
4Int2(Cb) + thr + w	-25.9	-24.1	-3423.762300	0.614893	-3423.147407
6Int2(Cb) + thr + w	-50.5	-48.4	-3423.801493	0.615355	-3423.186138
4Int2(Cb)' + thr + w	-51.7	-48.8	-3423.803360	0.616546	-3423.186814
2Int2 + thr--w	-78.8	-75.3	-3423.846644	0.617655	-3423.228989
4Int2 + thr--w	-80.3	-77.4	-3423.849073	0.616825	-3423.232248
6Int2 + thr--w	-82.1	-79.8	-3423.851822	0.615618	-3423.236204
2TS--thr--w	-64.5	-58.9	-3423.823771	0.620978	-3423.202793
4TS--thr--w	-65.5	-61.9	-3423.825448	0.617756	-3423.207692
6TS--thr--w	-68.7	-65.6	-3423.830447	0.616983	-3423.213464
2Pro--thr--w	-111.0	-103.5	-3423.897927	0.623930	-3423.273997
4Pro--thr--w	-112.5	-105.7	-3423.900376	0.622967	-3423.277409
6Pro--thr--w	-115.2	-108.7	-3423.904638	0.622419	-3423.282219

Table S3. Raw energy data obtained at the B3LYP(SCRf)/B2//B3LYP/B1 level**(a) Cpd I + tBPA**

	ΔE [kcal/mol]	$\Delta(E+ZPE)$ [kcal/mol]	E [Eh]	ZPE [Eh]	E+ZPE [Eh]
2RC	0.1	0.1	-3192.183852	0.510501	-3191.673351
4RC	0.0	0.0	-3192.184068	0.510523	-3191.673545
6RC	11.7	10.3	-3192.165440	0.508277	-3191.657163
2TSco	14.6	14.1	-3192.160775	0.509727	-3191.651048
4TSco	15.9	15.8	-3192.158722	0.510317	-3191.648405
6TSco	22.1	19.6	-3192.148875	0.506523	-3191.642352
2Int1rad	-15.7	-14.7	-3192.209015	0.512039	-3191.696976
2Int	-27.5	-26.0	-3192.227917	0.512917	-3191.715000
4Int	-22.9	-23.1	-3192.220639	0.510322	-3191.710317
6Int	-21.4	-22.1	-3192.218248	0.509432	-3191.708816
2TSmig	-23.8	-24.0	-3192.222013	0.510159	-3191.711854
4TSmig	-21.7	-22.9	-3192.218617	0.508572	-3191.710045
6TSmig	-20.4	-22.4	-3192.216576	0.507355	-3191.709221
2Int2	-72.6	-70.9	-3192.299752	0.513194	-3191.786558
4Int2	-76.6	-75.4	-3192.306124	0.512364	-3191.793760
6Int2	-77.0	-76.6	-3192.306704	0.511157	-3191.795547
2TSco(Cb)	23.3	22.2	-3192.146902	0.508693	-3191.638209
4TSco(Cb)	23.8	23.2	-3192.146067	0.509545	-3191.636522
6TSco(Cb)	29.4	26.5	-3192.137287	0.505946	-3191.631341
4Int1(Cb)	-11.3	-10.3	-3192.202063	0.512120	-3191.689943
6Int1(Cb)	1.5	0.1	-3192.181690	0.508363	-3191.673327
4Int1(Cb)'	13.3	12.6	-3192.162834	0.509299	-3191.653535
4TScn(Cb)	5.5	6.4	-3192.175342	0.512024	-3191.663318
6TScn(Cb)	5.3	2.8	-3192.175586	0.506435	-3191.669151
4TScn(Cb)'	4.7	3.7	-3192.176529	0.508895	-3191.667634
2Int2(Cb)	-55.6	-51.7	-3192.272725	0.516743	-3191.755982
4Int2(Cb)	-24.5	-22.7	-3192.223130	0.513354	-3191.709776
6Int2(Cb)	-50.6	-48.6	-3192.264777	0.513816	-3191.750961
4Int2(Cb)'	-51.0	-48.2	-3192.265330	0.515007	-3191.750323

(b) Cpd I + tBPA + Thr

	ΔE [kcal/mol]	$\Delta(E+ZPE)$ [kcal/mol]	E [Eh]	ZPE [Eh]	E+ZPE [Eh]
EtOH (thr)			-155.0991321	0.080398	-155.0187341
2RC + thr	0.1	0.1	-3347.282984	0.590899	-3346.692085
4RC + thr	0.0	0.0	-3347.283201	0.590921	-3346.692280
6RC + thr	11.7	10.3	-3347.264572	0.588675	-3346.675897
2TSco + thr	14.6	14.1	-3347.259907	0.590125	-3346.669782
4TSco + thr	15.9	15.8	-3347.257855	0.590715	-3346.667140
6TSco + thr	22.1	19.6	-3347.248007	0.586921	-3346.661086
2Int + thr	-27.5	-26.0	-3347.327049	0.593315	-3346.733734
4Int + thr	-22.9	-23.1	-3347.319771	0.590720	-3346.729051
6Int + thr	-21.4	-22.1	-3347.317380	0.589830	-3346.727550
2TSmig + thr	-23.8	-24.0	-3347.321145	0.590557	-3346.730588
4TSmig + thr	-21.7	-22.9	-3347.317749	0.588970	-3346.728779
6TSmig + thr	-20.4	-22.4	-3347.315708	0.587753	-3346.727955
2Int2 + thr	-72.6	-70.9	-3347.398885	0.593592	-3346.805293
4Int2 + thr	-76.6	-75.4	-3347.405256	0.592762	-3346.812494
6Int2 + thr	-77.0	-76.6	-3347.405836	0.591555	-3346.814281
2TSco(Cb) + thr	23.3	22.2	-3347.246035	0.589091	-3346.656944
4TSco(Cb) + thr	23.8	23.2	-3347.245199	0.589943	-3346.655256
6TSco(Cb) + thr	29.4	26.5	-3347.236419	0.586344	-3346.650075
4Int1(Cb) + thr	-11.3	-10.3	-3347.301195	0.592518	-3346.708677
6Int1(Cb) + thr	1.5	0.1	-3347.280822	0.588761	-3346.692061
4Int1(Cb)' + thr	13.3	12.6	-3347.261966	0.589697	-3346.672269
4TScn(Cb) + thr	5.5	6.4	-3347.274474	0.592422	-3346.682052
6TScn(Cb) + thr	5.3	2.8	-3347.274718	0.586833	-3346.687885
4TScn(Cb)' + thr	4.7	3.7	-3347.275661	0.589293	-3346.686368
2Int2(Cb) + thr	-55.6	-51.7	-3347.371857	0.597141	-3346.774716
4Int2(Cb) + thr	-24.5	-22.7	-3347.322262	0.593752	-3346.728510
6Int2(Cb) + thr	-50.6	-48.6	-3347.363909	0.594214	-3346.769695
4Int2(Cb)' + thr	-51.0	-48.2	-3347.364463	0.595405	-3346.769058
2TSoc-thr	-33.6	-32.8	-3347.336714	0.592174	-3346.744540
4TSoc-thr	-37.1	-37.0	-3347.342274	0.591022	-3346.751252
6TSoc-thr	-37.8	-38.4	-3347.343487	0.590018	-3346.753469
2Pro-thr	-104.2	-98.3	-3347.449264	0.600387	-3346.848877
4Pro-thr	-106.4	-101.5	-3347.452827	0.598848	-3346.853979
6Pro-thr	-106.5	-102.4	-3347.452876	0.597332	-3346.855544

(c) Cpd I + tBPA + Thr + Water

	ΔE	$\Delta(E+ZPE)$	E	ZPE	E+ZPE
EtOH (thr)			-155.0991321	0.080398	-155.0187341
Water (w)			-76.46446529	0.021141	-76.44332429
2RC + thr + w	0.1	0.1	-3423.747450	0.612040	-3423.135410
4RC + thr + w	0.0	0.0	-3423.747666	0.612062	-3423.135604
6RC + thr + w	11.7	10.3	-3423.729037	0.609816	-3423.119221
2TSco + thr + w	14.6	14.1	-3423.724373	0.611266	-3423.113107
4TSco + thr + w	15.9	15.8	-3423.722320	0.611856	-3423.110464
6TSco + thr + w	22.1	19.6	-3423.712473	0.608062	-3423.104411
2Int + thr + w	-27.5	-26.0	-3423.791514	0.614456	-3423.177058
4Int + thr + w	-22.9	-23.1	-3423.784237	0.611861	-3423.172376
6Int + thr + w	-21.4	-22.1	-3423.781845	0.610971	-3423.170874
2TSmig + thr + w	-23.8	-24.0	-3423.785610	0.611698	-3423.173912
4TSmig + thr + w	-21.7	-22.9	-3423.782214	0.610111	-3423.172103
6TSmig + thr + w	-20.4	-22.4	-3423.780173	0.608894	-3423.171279
2Int2 + thr + w	-72.6	-70.9	-3423.863350	0.614733	-3423.248617
4Int2 + thr + w	-76.6	-75.4	-3423.869721	0.613903	-3423.255818
6Int2 + thr + w	-77.0	-76.6	-3423.870302	0.612696	-3423.257606
2TSco(Cb) + thr + w	23.3	22.2	-3423.710500	0.610232	-3423.100268
4TSco(Cb) + thr + w	23.8	23.2	-3423.709664	0.611084	-3423.098580
6TSco(Cb) + thr + w	29.4	26.5	-3423.700885	0.607485	-3423.093400
4Int1(Cb) + thr + w	-11.3	-10.3	-3423.765660	0.613659	-3423.152001
6Int1(Cb) + thr + w	1.5	0.1	-3423.745287	0.609902	-3423.135385
4Int1(Cb)' + thr + w	13.3	12.6	-3423.726431	0.610838	-3423.115593
4TScn(Cb) + thr + w	5.5	6.4	-3423.738939	0.613563	-3423.125376
6TScn(Cb) + thr + w	5.3	2.8	-3423.739183	0.607974	-3423.131209
4TScn(Cb)' + thr + w	4.7	3.7	-3423.740126	0.610434	-3423.129692
2Int2(Cb) + thr + w	-55.6	-51.7	-3423.836322	0.618282	-3423.218040
4Int2(Cb) + thr + w	-24.5	-22.7	-3423.786727	0.614893	-3423.171834
6Int2(Cb) + thr + w	-50.6	-48.6	-3423.828374	0.615355	-3423.213019
4Int2(Cb)' + thr + w	-51.0	-48.2	-3423.828928	0.616546	-3423.212382
2Int2 + thr--w	-75.7	-72.2	-3423.868307	0.617655	-3423.250652
4Int2 + thr--w	-79.7	-76.7	-3423.874678	0.616825	-3423.257853
6Int2 + thr--w	-80.1	-77.8	-3423.875259	0.615618	-3423.259641
2TS--thr--w	-57.9	-52.3	-3423.839857	0.620978	-3423.218879
4TS--thr--w	-61.4	-57.8	-3423.845545	0.617756	-3423.227789
6TS--thr--w	-62.4	-59.3	-3423.847089	0.616983	-3423.230106
2Pro--thr--w	-106.4	-98.9	-3423.917164	0.623930	-3423.293234
4Pro--thr--w	-109.4	-102.5	-3423.921938	0.622967	-3423.298971
6Pro--thr--w	-109.7	-103.2	-3423.922557	0.622419	-3423.300138

Table S4. Mulliken group spin densities and group charges for optimized geometries

(a) Spin density

	Fe	O	Por	SH	tBPA
2RC	1.33	0.79	-0.57	-0.56	0.00
4RC	1.18	0.85	0.45	0.51	0.00
6RC	3.18	0.62	0.87	0.33	0.00
2TSco	1.57	0.36	-0.40	-0.31	-0.22
4TSco	1.22	0.83	0.22	0.40	0.33
6TSco	3.77	0.19	0.44	0.84	-0.24
2Int _{rad}	1.97	0.12	-0.16	-0.04	-0.89
2Int1	1.05	-0.01	-0.09	0.03	0.01
4Int1	2.64	0.03	-0.06	0.40	0.00
6Int1	4.14	0.03	0.42	0.41	0.00
2TSmig	1.06	0.00	-0.09	0.02	0.00
4TSmig	2.63	0.01	-0.06	0.41	0.00
6TSmig	4.13	0.02	0.44	0.41	0.00
2Int2	1.17	0.00	-0.13	-0.05	0.00
4Int2	2.59	0.00	-0.01	0.42	0.00
6Int2	4.09	0.00	0.51	0.40	0.00
2TSco(Cb)	1.05	0.69	-0.56	-0.43	0.24
4TSco(Cb)	1.22	0.82	0.20	0.40	0.35
6TSco(Cb)	3.89	0.06	0.05	0.84	-0.30
4Int1(Cb)	1.10	0.33	-0.08	0.00	1.65
6Int1(Cb)	4.13	0.25	0.66	0.83	-0.86
4Int1(Cb)'	2.67	0.22	0.16	0.81	-0.86
4TScn(Cb)	1.11	0.24	0.15	0.01	1.48
6TScn(Cb)	4.12	0.26	0.66	0.82	-0.85
4TScn(Cb)'	2.67	0.22	0.15	0.72	-0.76
2Int2(Cb)	0.98	0.01	-0.07	0.07	0.01
4Int2(Cb)	1.01	0.21	1.22	0.06	0.49
6Int2(Cb)	4.12	0.15	0.36	0.34	0.03
4Int2(Cb)'	2.89	0.05	0.04	0.00	0.02

	Fe	O	Por	SH	tBPA	Thr
2TSoc-thr	1.18	0.00	-0.13	-0.05	0.00	0.00
4TSoc-thr	2.58	0.00	-0.01	0.43	0.00	0.00
6TSoc-thr	4.08	0.00	0.52	0.40	0.00	0.00
2Pro-thr	1.11	0.00	-0.10	-0.02	0.00	0.00
4Pro-thr	2.61	0.00	-0.03	0.42	0.00	0.00
6Pro-thr	4.10	0.00	0.49	0.41	0.00	0.00

	Fe	O	Por	SH	tBPA	Thr	wat
2TSoc-thr-w	1.10	0.00	-0.09	0.00	0.00	0.00	0.00
4TSoc-thr-w	2.59	0.00	-0.02	0.43	0.00	0.00	0.00
6TSoc-thr-w	4.08	0.00	0.51	0.41	0.00	0.00	0.00
2Pro-thr-w	1.18	0.00	-0.13	-0.05	0.00	0.00	0.00
4Pro-thr-w	2.58	0.00	-0.01	0.43	0.00	0.00	0.00
6Pro-thr-w	4.08	0.00	0.52	0.41	0.00	0.00	0.00

(b) Charge

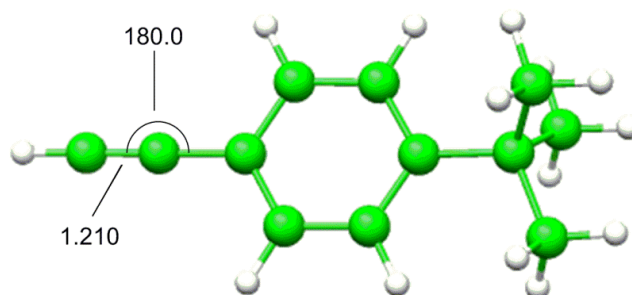
	Fe	O	Porphyrin	SH	tBPA
2RC	0.58	-0.44	-0.07	-0.05	-0.02
4RC	0.56	-0.42	-0.08	-0.05	-0.01
6RC	0.65	-0.45	-0.13	-0.05	-0.01
2TSco	0.51	-0.43	-0.22	-0.08	0.21
4TSco	0.50	-0.41	-0.26	-0.02	0.19
6TSco	0.88	-0.53	-0.46	-0.10	0.21
2Int _{rad}	0.42	-0.46	-0.28	0.06	0.27
2Int1	0.28	-0.40	-0.52	0.01	0.63
4Int1	0.48	-0.39	-0.48	-0.17	0.56
6Int1	0.54	-0.39	-0.65	-0.07	0.58
2TSmig	0.27	-0.41	-0.53	0.05	0.63
4TSmig	0.47	-0.39	-0.45	-0.14	0.51
6TSmig	0.53	-0.39	-0.62	-0.04	0.52
2Int2	0.26	-0.28	-0.40	0.08	0.34
4Int2	0.44	-0.28	-0.37	-0.10	0.32
6Int2	0.50	-0.29	-0.50	-0.03	0.31
2TSco(Cb)	0.51	-0.46	-0.18	-0.04	0.16
4TSco(Cb)	0.50	-0.46	-0.26	0.02	0.19
6TSco(Cb)	3.89	0.06	0.50	0.84	-0.30
4Int1(Cb)	0.27	-0.39	-0.49	0.07	0.53
6Int1(Cb)	0.90	-0.63	-0.41	-0.11	0.24
4Int1(Cb)'	0.76	-0.59	-0.27	-0.10	0.19
4TScn(Cb)	0.29	-0.44	-0.35	0.03	0.47
6TScn(Cb)	0.92	-0.63	-0.41	-0.11	0.24
4TScn(Cb)'	0.67	-0.54	-0.25	-0.14	0.26
2Int2(Cb)	0.30	-0.54	-0.14	-0.05	0.43
4Int2(Cb)	0.30	-0.45	-0.53	0.02	0.66
6Int2(Cb)	0.57	-0.56	-0.28	-0.14	0.41
4Int2(Cb)'	0.41	-0.56	-0.20	-0.08	0.43

	Fe	O	Por	SH	tBPA	Thr
2TSoc-thr	0.26	-0.32	-0.40	0.08	0.28	0.10
4TSoc-thr	0.44	-0.34	-0.38	-0.10	0.28	0.09
6TSoc-thr	0.52	-0.35	-0.51	-0.03	0.27	0.10
2Pro-thr	0.28	-0.38	-0.50	0.08	0.45	0.07
4Pro-thr	0.44	-0.38	-0.41	-0.12	0.44	0.04
6Pro-thr	0.50	-0.39	-0.55	-0.03	0.44	0.02

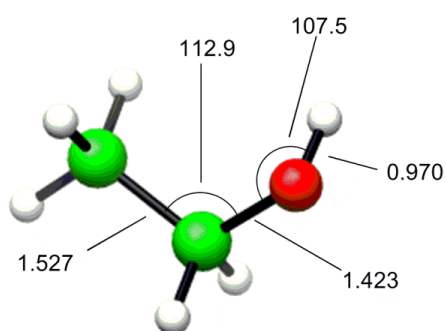
	Fe	O	Por	SH	tBPA	Thr	wat
2TSoc-thr-w	0.28	-0.46	-0.49	0.06	0.28	0.24	0.10
4TSoc-thr-w	0.44	-0.43	-0.36	-0.09	0.20	0.22	0.03
6TSoc-thr-w	0.53	-0.47	-0.48	-0.02	0.20	0.21	0.04
2Pro-thr-w	0.26	-0.40	-0.37	0.09	0.39	0.27	-0.24
4Pro-thr-w	0.45	-0.40	-0.36	-0.10	0.38	0.26	-0.23
6Pro-thr-w	0.42	-0.43	-0.48	-0.02	0.39	0.28	-0.17

Figure S1. Optimized geometries of organic molecules

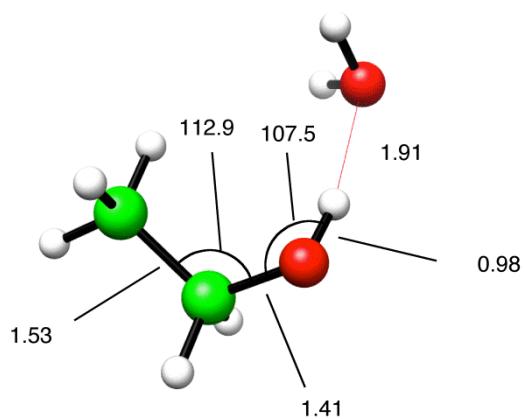
tBPA



Thr model (C₂H₅OH)



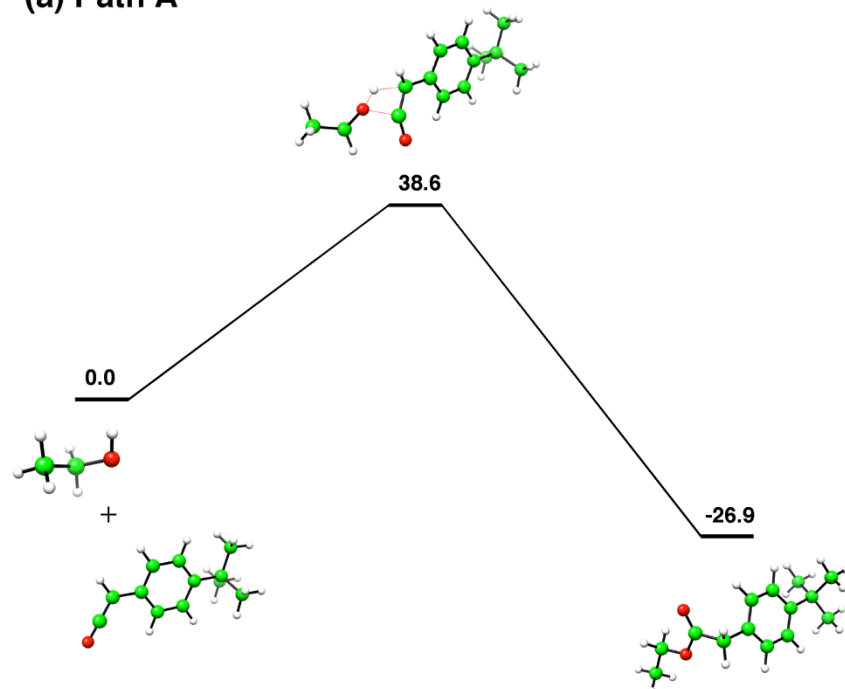
Thr---H₂O model (C₂H₅OH---H₂O)



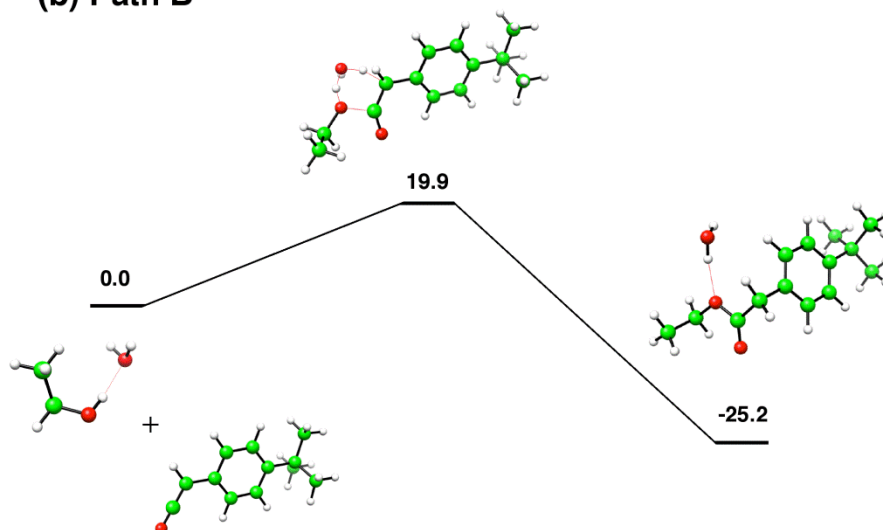
* bond distances are in Å, and bond angles in degrees.

Figure S2. Reactions between ketene and C₂H₅OH in the absence of the heme-SH unit, as obtained at the B3LYP(SCRF)/B2//B3LYP/B1 level:: (a) Path A; (b) Path B.

(a) Path A



(b) Path B



* Relative energies are given in kcal/mol.

**XYZ coordinates of optimized geometry
(in Å)**

1tBPA

C	11.721303	29.010198	0.703084
C	12.739446	28.611668	0.183922
H	10.824891	29.360980	1.160890
C	13.941171	28.141338	-0.430116
C	14.060172	28.078324	-1.831586
C	15.036453	27.728917	0.346000
C	15.232146	27.619579	-2.420403
H	13.224791	28.392538	-2.449988
C	16.205921	27.270763	-0.258884
H	14.965325	27.769620	1.428746
C	16.336055	27.203284	-1.653730
H	15.285260	27.585815	-3.504953
H	17.025194	26.962856	0.381072
C	17.612359	26.703437	-2.353315
C	17.270113	25.478097	-3.234577
C	18.184617	27.831797	-3.244735
C	18.704599	26.283768	-1.350944
H	16.866201	24.659309	-2.628233
H	16.528526	25.722090	-4.002528
H	18.170065	25.112692	-3.744124
H	18.441364	28.712637	-2.645290
H	19.093740	27.490244	-3.754708
H	17.470075	28.146785	-4.012394
H	19.589145	25.934204	-1.895335
H	19.017898	27.119399	-0.714719
H	18.371772	25.465298	-0.702362

1Thr

O	14.254662	33.389738	1.488819
H	13.600900	34.014094	1.137277
C	14.625608	33.842042	2.785734
H	13.762342	33.830428	3.471734
H	15.339735	33.099141	3.156134
C	15.265913	35.227938	2.770759
H	15.587562	35.523553	3.776744
H	16.137696	35.240110	2.108041
H	14.556078	35.985908	2.413505

1Thr---w

O	14.917677	32.198659	2.115228
H	15.056127	32.029984	1.162554
C	14.039933	33.301223	2.228498
H	13.083391	33.112912	1.709241
H	13.804646	33.397499	3.294827
C	14.653874	34.606841	1.717187
H	13.968878	35.453111	1.852523
H	15.586052	34.823717	2.250317
H	14.887890	34.531336	0.647055
O	15.521203	32.050449	-0.694675
H	14.951025	32.620594	-1.233048
H	16.370545	32.517417	-0.658558

2RC

H	7.721943	34.458910	1.646065
S	7.917860	34.026907	2.912057
Fe	8.889773	31.721971	2.346725
N	9.547477	32.435846	0.577712
N	10.662139	32.174410	3.185238
N	8.139738	31.288453	4.174746
N	7.024067	31.566218	1.570939
C	8.851750	32.493567	-0.600713
C	9.707992	32.946238	-1.669677
C	10.936239	33.157279	-1.122724
C	10.826250	32.833065	0.277914
C	11.789362	32.611791	2.541329
C	12.887305	32.726157	3.469599
C	12.407662	32.352662	4.687168
C	11.019576	32.009519	4.495947
C	8.835083	31.240247	5.358395
C	7.981915	30.768438	6.421748
C	6.766356	30.517296	5.865101
C	6.875149	30.844269	4.463938
C	5.902613	31.085206	2.209406
C	4.802989	30.989987	1.281088
C	5.269139	31.403074	0.072001
C	6.657722	31.747046	0.254900
C	7.505116	32.175154	-0.754280
H	7.084860	32.266087	-1.751350
C	11.871089	32.918241	1.188304
H	12.833883	33.248275	0.810691
C	10.170801	31.581106	5.512208
H	10.593414	31.497496	6.508911
C	5.835412	30.734626	3.548423
H	4.885829	30.358951	3.917163
H	11.842537	33.498004	-1.606386
H	9.393281	33.078703	-2.696866
H	13.885129	33.052353	3.206264
H	12.928584	32.308716	5.634954
H	8.291124	30.649406	7.452238
H	5.867026	30.150843	6.343143
H	3.809135	30.648024	1.539883
H	4.738504	31.468986	-0.869189
O	9.281298	30.178499	2.012372
C	11.716346	29.010727	0.705906
C	12.736089	28.611759	0.184946
H	10.814337	29.366380	1.169945
C	13.938012	28.142685	-0.429099
C	14.060941	28.078830	-1.830889
C	15.035649	27.729130	0.344391
C	15.233225	27.620670	-2.420323
H	13.224743	28.391300	-2.449344
C	16.205912	27.271339	-0.259914
H	14.963356	27.767589	1.427267
C	16.337388	27.204004	-1.654508
H	15.285858	27.586392	-3.505229
H	17.024554	26.962333	0.380800
C	17.613589	26.703421	-2.354139
C	17.272079	25.477678	-3.235009
C	18.187258	27.830344	-3.246333
C	18.705796	26.283751	-1.351675
H	16.867924	24.659557	-2.627940
H	16.529682	25.721521	-4.002244
H	18.171653	25.111508	-3.745142
H	18.445249	28.710946	-2.646873
H	19.095749	27.488317	-3.757555
H	17.471895	28.146252	-4.012915
H	19.590868	25.933946	-1.895399
H	19.018272	27.119453	-0.715054

H 18.372179 25.465808 -0.702879

4RC

H	7.771586	34.536091	1.767326
S	7.922562	34.058198	3.022905
Fe	8.819022	31.747008	2.409383
N	9.560772	32.496271	0.687075
N	10.581773	32.111223	3.320964
N	8.000907	31.270840	4.195542
N	6.981645	31.677106	1.571069
C	8.907680	32.615547	-0.510414
C	9.814243	33.070824	-1.536215
C	11.029751	33.221399	-0.943081
C	10.861692	32.857928	0.442455
C	11.742956	32.529214	2.727164
C	12.814999	32.570806	3.691789
C	12.284544	32.172540	4.880034
C	10.891585	31.887081	4.634349
C	8.655554	31.162451	5.398799
C	7.752692	30.687060	6.418721
C	6.547885	30.496426	5.816576
C	6.713060	30.864034	4.431151
C	5.822441	31.220053	2.158339
C	4.749321	31.202723	1.195206
C	5.268244	31.640201	0.016630
C	6.662806	31.921598	0.252497
C	7.556119	32.351224	-0.715578
H	7.170287	32.491544	-1.720804
C	11.877969	32.878003	1.388428
H	12.863065	33.186712	1.052495
C	9.995642	31.453198	5.607167
H	10.381696	31.321411	6.613471
C	5.700087	30.823570	3.480452
H	4.725950	30.471672	3.806057
H	11.963035	33.544251	-1.385955
H	9.539319	33.246021	-2.568375
H	13.831490	32.869737	3.470726
H	12.773588	32.075840	5.840807
H	8.023922	30.525003	7.454017
H	5.621513	30.147213	6.254178
H	3.735368	30.891875	1.411807
H	4.769806	31.761679	-0.936538
O	9.210046	30.212219	2.033657
C	11.842913	28.990980	0.652770
C	12.858145	28.594583	0.122547
H	10.942459	29.340771	1.123368
C	14.051917	28.124860	-0.506874
C	14.028734	27.627116	-1.824293
C	15.284535	28.141905	0.166940
C	15.192933	27.169007	-2.429246
H	13.086704	27.603212	-2.363874
C	16.445262	27.679707	-0.452281
H	15.325602	28.519108	1.184505
C	16.432072	27.181494	-1.763225
H	15.131718	26.791069	-3.446062
H	17.372240	27.711735	0.109510
C	17.692179	26.658052	-2.475115
C	17.489674	25.170378	-2.851296
C	17.938544	27.480949	-3.762662
C	18.950930	26.762280	-1.593121
H	17.320960	24.559549	-1.957080
H	16.631090	25.031201	-3.516725
H	18.377532	24.782888	-3.366302
H	18.094237	28.540018	-3.527142

H	18.830640	27.113428	-4.284773
H	17.095146	27.414219	-4.457979
H	19.818976	26.380528	-2.142633
H	19.167736	27.799319	-1.312191
H	18.856224	26.171515	-0.674868

6RC

H	7.820555	34.417363	1.678692
S	7.956356	33.986273	2.952511
Fe	8.826082	31.672802	2.434670
N	9.602775	32.429473	0.656008
N	10.606397	32.152219	3.402821
N	7.936073	31.309766	4.282821
N	6.943731	31.591848	1.543366
C	8.961665	32.484680	-0.546890
C	9.892599	32.910542	-1.570494
C	11.095243	33.101586	-0.955556
C	10.904420	32.792953	0.445577
C	11.760295	32.561177	2.800793
C	12.812519	32.655328	3.791584
C	12.261127	32.297553	4.986832
C	10.871094	31.982305	4.728230
C	8.581736	31.265976	5.490161
C	7.650647	30.839115	6.513607
C	6.453895	30.623420	5.896868
C	6.642478	30.923580	4.492855
C	5.786627	31.164846	2.144628
C	4.732849	31.096771	1.154068
C	5.276063	31.478509	-0.036156
C	6.670247	31.780802	0.210924
C	7.604445	32.184725	-0.745098
H	7.237714	32.278659	-1.763758
C	11.891287	32.856233	1.437049
H	12.879375	33.165680	1.107589
C	9.930043	31.578378	5.688428
H	10.294886	31.493886	6.708638
C	5.659320	30.843599	3.498054
H	4.676834	30.510058	3.820943
H	12.030346	33.418249	-1.399509
H	9.648645	33.042314	-2.616976
H	13.831765	32.958619	3.589086
H	12.739650	32.250618	5.956794
H	7.891986	30.723154	7.562586
H	5.522274	30.297829	6.341939
H	3.712836	30.795133	1.355647
H	4.788501	31.549491	-1.000201
O	9.245972	30.123748	2.135422
C	11.878847	28.956840	0.702704
C	12.887315	28.571294	0.152019
H	10.983670	29.295394	1.190864
C	14.074032	28.115361	-0.500465
C	14.102042	27.910491	-1.893668
C	15.248306	27.854517	0.225281
C	15.258742	27.463919	-2.521450
H	13.205268	28.104002	-2.474687
C	16.401972	27.406981	-0.417368
H	15.249281	28.003292	1.301007
C	16.439596	27.199276	-1.803947
H	15.237263	27.317788	-3.598014
H	17.283043	27.218129	0.186175
C	17.694423	26.701381	-2.542885
C	17.382351	25.352856	-3.235297
C	18.112494	27.740221	-3.611175
C	18.887484	26.487098	-1.592193

H	17.094470	24.592964	-2.499818
H	16.564276	25.444541	-3.957531
H	18.264889	24.987328	-3.774981
H	18.347596	28.705588	-3.148309
H	19.003707	27.395182	-4.149884
H	17.321640	27.908440	-4.349786
H	19.755964	26.137701	-2.162027
H	19.176407	27.414971	-1.085308
H	18.669295	25.732850	-0.827629

2TSco

H	9.049872	34.424269	1.873959
S	9.039529	33.641163	2.975538
Fe	9.542897	31.501248	1.886470
N	10.225341	32.531202	0.286376
N	11.385197	31.516618	2.693055
N	8.820544	30.682777	3.579850
N	7.658938	31.645517	1.147545
C	9.505517	32.924651	-0.812610
C	10.378683	33.533686	-1.787351
C	11.635941	33.491200	-1.268795
C	11.530718	32.857765	0.023648
C	12.527192	32.006289	2.114613
C	13.654196	31.819278	2.997178
C	13.175526	31.220148	4.121874
C	11.757299	31.039724	3.923595
C	9.531522	30.317577	4.696783
C	8.651285	29.732435	5.676912
C	7.399935	29.747550	5.139832
C	7.513061	30.346189	3.833028
C	6.517253	31.150414	1.722448
C	5.386686	31.361763	0.847519
C	5.861420	31.987764	-0.261685
C	7.283366	32.157733	-0.067535
C	8.136168	32.759616	-0.980933
H	7.700439	33.124288	-1.906148
C	12.604307	32.617627	0.870082
H	13.584199	32.945171	0.536370
C	10.901109	30.477843	4.860830
H	11.334614	30.145103	5.798952
C	6.443897	30.546540	2.968935
H	5.466341	30.213935	3.304593
H	12.559893	33.848379	-1.705508
H	10.053391	33.932186	-2.739924
H	14.667656	32.127984	2.774042
H	13.713191	30.932021	5.016358
H	8.966165	29.365792	6.645630
H	6.473632	29.396680	5.576694
H	4.370331	31.065745	1.074138
H	5.317667	32.313420	-1.139351
O	9.694999	30.062225	1.061931
C	10.549672	28.304644	1.700853
C	11.621744	28.082164	1.141363
H	9.718539	28.143701	2.350915
C	12.829603	27.939963	0.425893
C	12.855765	27.294619	-0.832451
C	14.048022	28.423874	0.947961
C	14.048570	27.148625	-1.523851
H	11.927856	26.918831	-1.252141
C	15.235254	28.265843	0.239578
H	14.047405	28.929323	1.908643
C	15.271086	27.626497	-1.010435
H	14.028092	26.650803	-2.489016
H	16.147755	28.653849	0.678093

C	16.566464	27.440815	-1.817913
C	16.811480	25.931503	-2.059473
C	16.427767	28.161105	-3.181394
C	17.798356	28.016791	-1.093763
H	16.922243	25.394930	-1.110330
H	15.988624	25.466818	-2.612532
H	17.728944	25.785517	-2.642520
H	16.262669	29.235585	-3.042469
H	17.341677	28.030644	-3.773658
H	15.591191	27.767411	-3.768041
H	18.692083	27.860692	-1.708195
H	17.702974	29.094582	-0.919170
H	17.971976	27.527021	-0.128705

4TSco

H	8.043696	33.910700	1.533618
S	9.170904	33.822970	2.274050
Fe	9.558601	31.449619	2.071063
N	10.089767	31.973958	0.160293
N	11.407514	31.909319	2.704082
N	9.004088	31.047160	3.943667
N	7.648760	31.204945	1.435529
C	9.286618	31.984606	-0.950839
C	10.050448	32.373362	-2.113810
C	11.323696	32.596204	-1.687939
C	11.335853	32.344003	-0.264571
C	12.477394	32.283357	1.925519
C	13.652476	32.447326	2.746886
C	13.282738	32.165373	4.025469
C	11.881602	31.822593	3.987059
C	9.795408	31.068266	5.063143
C	9.031106	30.672535	6.223762
C	7.767166	30.419651	5.793066
C	7.755292	30.662554	4.368785
C	6.585608	30.802945	2.198383
C	5.406184	30.664719	1.379830
C	5.773607	30.980414	0.106689
C	7.177196	31.311164	0.148719
C	7.933049	31.673278	-0.961462
H	7.419207	31.718053	-1.917175
C	12.453271	32.475230	0.551589
H	13.384390	32.769538	0.077000
C	11.133348	31.435886	5.091993
H	11.637875	31.411879	6.053065
C	6.630923	30.549964	3.566550
H	5.706982	30.239767	4.045272
H	12.182474	32.916322	-2.264576
H	9.646619	32.464654	-3.114180
H	14.625537	32.741472	2.374614
H	13.888472	32.177768	4.922610
H	9.428433	30.608785	7.228754
H	6.906808	30.104605	6.369726
H	4.433255	30.363120	1.746593
H	5.165002	30.991367	-0.788687
O	9.934334	29.820426	1.798714
C	10.025126	28.762426	0.095864
C	11.169351	28.480428	-0.268119
H	8.959270	28.735044	0.035205
C	12.527891	28.229723	-0.553870
C	13.241457	29.031037	-1.476087
C	13.212886	27.157552	0.057063
C	14.572523	28.762821	-1.759414
H	12.731189	29.859708	-1.957047
C	14.547970	26.904445	-0.240337

H	12.684227	26.531943	0.769517
C	15.264565	27.695260	-1.153747
H	15.087183	29.401228	-2.472216
H	15.032808	26.071386	0.256019
C	16.740714	27.440982	-1.502184
C	16.874896	27.182190	-3.022560
C	17.579222	28.684888	-1.119297
C	17.318914	26.223711	-0.755545
H	16.296461	26.301253	-3.323417
H	16.521040	28.032413	-3.615016
H	17.924927	27.006051	-3.286253
H	17.512102	28.886574	-0.044144
H	18.634793	28.523885	-1.370423
H	17.243537	29.582244	-1.649759
H	18.367004	26.080214	-1.041406
H	17.289285	26.359250	0.331585
H	16.780681	25.301147	-1.001087

6TSco

H	8.297402	34.619082	1.772788
S	8.316914	34.044441	2.997359
Fe	9.629115	31.222622	1.748014
N	10.211484	32.571731	0.246691
N	11.451075	31.633775	2.695561
N	8.875297	30.674007	3.628724
N	7.638620	31.643685	1.201151
C	9.451938	32.961874	-0.825291
C	10.286550	33.633575	-1.796641
C	11.553506	33.638787	-1.292553
C	11.498939	32.970001	-0.011657
C	12.562961	32.170945	2.100616
C	13.701593	32.033333	2.981346
C	13.256386	31.407797	4.108160
C	11.844143	31.160115	3.919737
C	9.630934	30.327224	4.721398
C	8.785494	29.716317	5.722905
C	7.519774	29.699443	5.216676
C	7.584300	30.302914	3.904134
C	6.515358	31.125923	1.807855
C	5.366819	31.335884	0.958553
C	5.809479	31.972845	-0.163322
C	7.233815	32.156530	-0.011615
C	8.074011	32.761056	-0.945398
H	7.606868	33.122392	-1.857408
C	12.584648	32.779358	0.843857
H	13.544420	33.157944	0.503248
C	11.002006	30.548560	4.851492
H	11.460656	30.223471	5.781261
C	6.495321	30.499818	3.052331
H	5.530226	30.146714	3.404693
H	12.447896	34.060735	-1.733665
H	9.936443	34.050967	-2.732495
H	14.702159	32.383632	2.760766
H	13.819555	31.143218	4.994371
H	9.125460	29.360253	6.687345
H	6.616374	29.328334	5.684263
H	4.355145	31.035828	1.201304
H	5.231845	32.295538	-1.020529
O	9.898074	29.732304	1.024999
C	10.054503	27.782430	0.201110
C	10.978181	27.734243	-0.602257
H	9.224130	27.503599	0.808185
C	12.062902	27.792132	-1.510357
C	11.861322	28.162223	-2.858293

C	13.371449	27.468547	-1.100925
C	12.928419	28.203897	-3.744067
H	10.860403	28.417791	-3.191927
C	14.430399	27.514999	-2.003388
H	13.546867	27.183117	-0.068287
C	14.240305	27.881314	-3.345282
H	12.734313	28.495648	-4.772262
H	15.420579	27.258836	-1.643932
C	15.388968	27.940985	-4.366753
C	15.091859	26.967016	-5.532467
C	15.508987	29.381623	-4.920382
C	16.745061	27.549618	-3.749142
H	15.009396	25.935761	-5.170768
H	14.157826	27.216590	-6.046689
H	15.900347	27.004182	-6.272741
H	15.729579	30.093062	-4.116386
H	16.319130	29.438879	-5.657629
H	14.586893	29.708422	-5.412251
H	17.527374	27.603955	-4.514551
H	17.033415	28.223857	-2.934588
H	16.735669	26.525288	-3.359476

2Int1rad

H	-0.778509	3.479486	1.933144
S	-2.024684	3.011168	1.701130
Fe	-1.403395	1.042615	0.646546
N	-0.777436	2.105581	-0.953961
N	0.428894	1.146923	1.436719
N	-2.034799	-0.027181	2.237099
N	-3.278424	1.021123	-0.102458
C	-1.546828	2.543138	-2.000783
C	-0.727090	3.257172	-2.949933
C	0.543319	3.242786	-2.462824
C	0.500648	2.527200	-1.210563
C	1.547754	1.699337	0.854792
C	2.682096	1.542047	1.727305
C	2.240496	0.890605	2.840327
C	0.836118	0.638366	2.649074
C	-1.301311	-0.352693	3.352277
C	-2.122309	-1.079280	4.287431
C	-3.359984	-1.182245	3.729251
C	-3.302799	-0.509688	2.455681
C	-4.371247	0.381038	0.426422
C	-5.518208	0.578588	-0.424499
C	-5.105550	1.346183	-1.470252
C	-3.703364	1.612700	-1.266211
C	-2.909097	2.329486	-2.149279
H	-3.387269	2.737990	-3.033798
C	1.593519	2.332369	-0.378965
H	2.552134	2.720903	-0.707347
C	0.035681	-0.045094	3.553243
H	0.495100	-0.377070	4.478715
C	-4.389574	-0.343197	1.610152
H	-5.332653	-0.787474	1.911877
H	1.437921	3.674520	-2.893190
H	-1.094862	3.701211	-3.866168
H	3.680943	1.893920	1.502531
H	2.802347	0.594439	3.717070
H	-1.779130	-1.454224	5.243230
H	-4.245798	-1.655748	4.133079
H	-6.503530	0.174650	-0.229912
H	-5.680485	1.701601	-2.315852
O	-0.992109	-0.503572	-0.304744
C	-0.424235	-1.627960	0.186472

C	0.740762	-2.075256	-0.233689
H	-1.001639	-2.155357	0.952071
C	1.915726	-2.368757	-0.896293
C	1.919710	-3.101487	-2.125715
C	3.187811	-1.990125	-0.369496
C	3.105536	-3.414138	-2.762375
H	0.968948	-3.405077	-2.553143
C	4.362487	-2.312299	-1.032537
H	3.219146	-1.432116	0.561422
C	4.363535	-3.032625	-2.242534
H	3.057856	-3.969494	-3.695292
H	5.301047	-1.994131	-0.591545
C	5.649874	-3.407626	-2.994795
C	5.742883	-4.948009	-3.121033
C	5.620481	-2.780614	-4.410183
C	6.918115	-2.908452	-2.276285
H	5.770306	-5.421311	-2.132865
H	4.889982	-5.364369	-3.667222
H	6.655188	-5.232097	-3.660112
H	5.566553	-1.687454	-4.352618
H	6.528336	-3.048278	-4.965019
H	4.760240	-3.127129	-4.992358
H	7.805310	-3.199413	-2.850117
H	6.930388	-1.816601	-2.180886
H	7.016861	-3.340904	-1.274000

2Int1

H	8.450644	33.745307	3.710217
S	7.896412	32.683510	3.081373
Fe	9.665565	32.062700	1.847123
N	10.031123	33.947395	1.241998
N	10.953923	32.338822	3.378017
N	9.422883	30.124055	2.376064
N	8.485900	31.738238	0.244556
C	9.455727	34.571833	0.164925
C	9.917542	35.938218	0.075599
C	10.777417	36.131015	1.112165
C	10.837469	34.883336	1.837696
C	11.621944	33.494438	3.717090
C	12.348510	33.306308	4.948152
C	12.100428	32.031897	5.361762
C	11.226080	31.435075	4.381783
C	9.930868	29.521620	3.498481
C	9.494534	28.145729	3.566601
C	8.712802	27.927537	2.473072
C	8.667192	29.171259	1.740915
C	7.850478	30.577643	-0.111549
C	7.063396	30.783227	-1.306262
C	7.231034	32.084706	-1.663794
C	8.124290	32.671658	-0.689898
C	8.566533	33.988518	-0.729063
H	8.193542	34.613077	-1.535497
C	11.586318	34.678217	2.990760
H	12.169259	35.514128	3.365850
C	10.759074	30.127911	4.437302
H	11.070288	29.526482	5.286604
C	7.937354	29.373419	0.575908
H	7.374930	28.530949	0.184248
H	11.326011	37.025917	1.378044
H	9.613433	36.642055	-0.689004
H	12.958794	34.062936	5.425342
H	12.466473	31.528294	6.247881
H	9.756630	27.454439	4.358081

H	8.198138	27.020607	2.180731
H	6.467110	30.020276	-1.790933
H	6.803036	32.614977	-2.505327
O	11.222156	31.411640	0.597240
C	12.401000	31.185334	0.987990
C	13.456987	30.784953	0.201387
H	12.683301	31.434829	2.031849
C	13.952216	29.526587	-0.163585
C	13.324084	28.304257	0.227560
C	15.115282	29.435659	-0.976800
C	13.833168	27.087456	-0.180322
H	12.430751	28.350817	0.843775
C	15.619319	28.207435	-1.374352
H	15.596134	30.360385	-1.280247
C	14.991871	27.005696	-0.988866
H	13.330091	26.176860	0.128766
H	16.507190	28.180441	-1.994138
C	15.517091	25.628520	-1.415857
C	15.855838	24.801671	-0.149890
C	14.417487	24.899593	-2.229161
C	16.783836	25.719903	-2.288090
H	16.631082	25.294499	0.447362
H	14.980947	24.651569	0.490307
H	16.229173	23.813290	-0.441627
H	14.156150	25.462280	-3.132267
H	14.778779	23.911667	-2.537085
H	13.502178	24.753183	-1.647017
H	17.110914	24.710815	-2.560591
H	16.602409	26.268726	-3.218953
H	17.613207	26.201872	-1.758239

4Int1

H	-3.386109	0.494471	3.390650
S	-3.379993	-0.400636	2.377201
Fe	-1.349884	0.407856	1.325421
N	-2.268876	1.136050	-0.324942
N	-1.407014	2.238118	2.159261
N	-0.123265	-0.220741	2.818717
N	-1.059773	-1.351372	0.370918
C	-2.587662	0.443976	-1.465149
C	-3.341850	1.285889	-2.364203
C	-3.480454	2.491276	-1.748883
C	-2.807812	2.387609	-0.475311
C	-2.058832	3.343698	1.669029
C	-1.932828	4.443095	2.592797
C	-1.188397	3.993767	3.641301
C	-0.861686	2.617597	3.361965
C	0.230316	0.484359	3.943290
C	0.979943	-0.357971	4.842545
C	1.061808	-1.585201	4.257160
C	0.366494	-1.493703	2.996851
C	-0.427627	-2.464937	0.872964
C	-0.514015	-3.548824	-0.072023
C	-1.205189	-3.078493	-1.150743
C	-1.544695	-1.708093	-0.864246
C	-2.254085	-0.877789	-1.724902
H	-2.579834	-1.300127	-2.670622
C	-2.721441	3.417976	0.450563
H	-3.196063	4.360802	0.197047
C	-0.102184	1.808546	4.198093
H	0.250945	2.243591	5.128000
C	0.229125	-2.540930	2.096172
H	0.673039	-3.494364	2.365848
H	-3.986040	3.378882	-2.107609

H	-3.712130	0.975909	-3.333296
H	-2.357114	5.427277	2.439448
H	-0.876488	4.532499	4.527193
H	1.378029	-0.038744	5.797516
H	1.541928	-2.480327	4.632175
H	-0.100200	-4.537142	0.085017
H	-1.476773	-3.603376	-2.058279
O	0.642479	1.141650	0.175017
C	1.777750	0.651630	0.372583
C	2.857733	0.788309	-0.496916
H	2.020120	0.171275	1.346092
C	3.219655	-0.010792	-1.596301
C	2.476449	-1.158171	-2.009770
C	4.373281	0.329018	-2.353637
C	2.872136	-1.898389	-3.106914
H	1.585999	-1.437539	-1.454268
C	4.762536	-0.424060	-3.450701
H	4.940863	1.201905	-2.046240
C	4.022348	-1.552932	-3.854698
H	2.281934	-2.762636	-3.395204
H	5.648036	-0.130578	-4.001576
C	4.420453	-2.405912	-5.066665
C	4.685383	-3.858627	-4.597506
C	3.259500	-2.399357	-6.092845
C	5.689223	-1.884460	-5.768434
H	5.505240	-3.895538	-3.871457
H	3.802612	-4.308301	-4.132168
H	4.963540	-4.480745	-5.456007
H	3.046770	-1.382715	-6.441623
H	3.530688	-3.007497	-6.963599
H	2.336321	-2.811227	-5.673188
H	5.924250	-2.528947	-6.622217
H	5.556792	-0.866619	-6.152194
H	6.559340	-1.891951	-5.102330

6Int1

H	10.248866	34.136045	3.744893
S	8.975608	33.718975	3.563483
Fe	9.523875	31.967654	2.071514
N	10.116673	33.140615	0.455184
N	11.536914	31.744385	2.595253
N	9.069569	30.358595	3.338928
N	7.623853	31.810642	1.255200
C	9.277784	33.679760	-0.480527
C	10.035540	34.554562	-1.352551
C	11.329344	34.520946	-0.922822
C	11.372163	33.626114	0.216387
C	12.592311	32.429886	2.049475
C	13.798342	32.097044	2.774148
C	13.446092	31.208431	3.752630
C	12.022530	30.988699	3.632003
C	9.901491	29.828689	4.293409
C	9.149616	28.914293	5.125954
C	7.865995	28.916066	4.662195
C	7.819887	29.833806	3.544093
C	6.588996	31.054918	1.735671
C	5.398427	31.330960	0.960603
C	5.744153	32.250407	0.012817
C	7.148659	32.543857	0.200094
C	7.908924	33.412729	-0.590137
H	7.380466	33.922265	-1.391116
C	12.513795	33.302112	0.956212
H	13.442535	33.774102	0.647083
C	11.263366	30.117579	4.424171

H	11.793259	29.603512	5.221485
C	6.678763	30.148856	2.798544
H	5.762029	29.636577	3.076983
H	12.183082	35.046385	-1.332727
H	9.622057	35.111991	-2.183828
H	14.781752	32.498576	2.561443
H	14.086288	30.741168	4.490982
H	9.558427	28.350396	5.955306
H	7.019853	28.355280	5.039607
H	4.431449	30.871189	1.122762
H	5.115261	32.689393	-0.751692
O	10.060152	30.265618	0.470733
C	10.407480	29.102424	0.774496
C	10.970413	28.161700	-0.081706
H	10.157054	28.691266	1.778333
C	12.324870	27.922536	-0.375195
C	12.671744	26.871271	-1.271264
C	13.388188	28.701592	0.166654
C	13.990320	26.619901	-1.599953
H	11.865932	26.276099	-1.689439
C	14.706009	28.444456	-0.176279
H	13.150758	29.512597	0.849180
C	15.039796	27.401306	-1.064414
H	14.219960	25.810807	-2.285772
H	15.485654	29.062487	0.252585
C	16.489479	27.095420	-1.465927
C	16.833692	25.642318	-1.052984
C	16.628287	27.242119	-3.002279
C	17.503519	28.042687	-0.796776
H	16.746091	25.508938	0.031099
H	16.179178	24.910163	-1.536472
H	17.865097	25.409092	-1.341231
H	16.388438	28.261617	-3.324205
H	17.659383	27.024719	-3.304167
H	15.970693	26.554414	-3.543316
H	18.516211	27.779237	-1.120119
H	17.331943	29.088642	-1.074562
H	17.477386	27.966791	0.296045

2TSmig

H	7.374531	31.276280	4.553583
S	8.118564	30.169303	4.328365
Fe	9.364885	30.951833	2.648387
N	7.799278	31.798792	1.720563
N	9.728762	32.698564	3.577607
N	11.055661	30.148718	3.444108
N	9.116029	29.243102	1.594542
C	6.958352	31.181530	0.831049
C	5.916588	32.093034	0.414851
C	6.142000	33.268410	1.061576
C	7.320174	33.074371	1.874504
C	9.004693	33.861046	3.489674
C	9.566243	34.867999	4.359361
C	10.634805	34.297438	4.978447
C	10.728664	32.942357	4.484506
C	11.842232	30.735096	4.412809
C	12.841442	29.803323	4.869842
C	12.643497	28.639445	4.187430
C	11.520837	28.854156	3.311618
C	9.858555	28.090491	1.658766
C	9.296509	27.084365	0.787857
C	8.198547	27.640414	0.206100
C	8.090593	28.985955	0.719662
C	7.086954	29.878820	0.365209

H	6.340121	29.529765	-0.341794
C	7.880152	34.045029	2.695649
H	7.398342	35.017671	2.724790
C	11.704330	32.035133	4.881584
H	12.416325	32.369427	5.630440
C	10.980434	27.899983	2.459022
H	11.453914	26.922979	2.435298
H	5.577804	34.190759	1.004120
H	5.128011	31.848006	-0.285558
H	9.179254	35.873300	4.468775
H	11.309322	34.736632	5.702749
H	13.588163	30.022323	5.622889
H	13.193975	27.710359	4.267360
H	9.696315	26.086045	0.659965
H	7.511412	27.194692	-0.502252
O	10.531638	31.705062	0.987384
C	11.660658	31.246585	0.766960
C	12.808335	31.152190	0.154079
H	12.229200	30.651097	1.620225
C	13.688108	30.305115	-0.571573
C	13.255616	29.083667	-1.145760
C	15.026032	30.700196	-0.779280
C	14.131475	28.308675	-1.887060
H	12.230887	28.760551	-0.986776
C	15.891225	29.918890	-1.537905
H	15.365706	31.634605	-0.343547
C	15.468473	28.705877	-2.106875
H	13.771622	27.375699	-2.309811
H	16.908875	30.261642	-1.681664
C	16.399563	27.812239	-2.941515
C	16.535631	26.434908	-2.246594
C	15.792831	27.618920	-4.353054
C	17.808509	28.414790	-3.100902
H	16.969461	26.539763	-1.245744
H	15.569308	25.930781	-2.142823
H	17.191306	25.781545	-2.834116
H	15.683677	28.578896	-4.870048
H	16.447611	26.980319	-4.957407
H	14.807325	27.143510	-4.316371
H	18.427880	27.741999	-3.703794
H	17.783660	29.384729	-3.610581
H	18.310277	28.545761	-2.135496

4TSmig

H	7.795034	30.723087	5.194952
S	7.799596	29.802609	4.204712
Fe	9.400072	30.935641	2.808074
N	8.065397	31.730519	1.512679
N	9.428941	32.670227	3.823039
N	11.046898	30.328606	3.835103
N	9.601508	29.334750	1.593726
C	7.521321	31.119164	0.410938
C	6.504713	31.959664	-0.175834
C	6.434421	33.081941	0.589445
C	7.410140	32.928705	1.642119
C	8.589489	33.744249	3.642518
C	8.854954	34.754660	4.634112
C	9.872751	34.288005	5.410081
C	10.228735	32.990347	4.895449
C	11.617774	30.956359	4.916638
C	12.649678	30.127261	5.487362
C	12.686890	28.981499	4.751931
C	11.679675	29.110047	3.728623
C	10.433034	28.254618	1.782920

C	10.191446	27.260873	0.769280
C	9.207283	27.751531	-0.038589
C	8.844232	29.043064	0.483252
C	7.875952	29.869160	-0.073923
H	7.354522	29.505703	-0.953909
C	7.641093	33.868141	2.636256
H	7.045926	34.775764	2.618174
C	11.245480	32.198271	5.412128
H	11.787362	32.578279	6.272533
C	11.397352	28.140114	2.777161
H	11.976822	27.222567	2.808946
H	5.790287	33.943595	0.468377
H	5.929103	31.705324	-1.056825
H	8.328969	35.698126	4.706600
H	10.354576	34.768939	6.251941
H	13.253396	30.398458	6.344236
H	13.327607	28.118147	4.879913
H	10.712423	26.314150	0.699255
H	8.755723	27.290031	-0.907817
O	11.112282	32.081282	1.193505
C	12.205251	31.550270	1.015676
C	13.353554	31.453441	0.326153
H	12.700574	30.913848	1.861704
C	13.970777	30.475716	-0.499714
C	13.276610	29.352774	-1.023962
C	15.322374	30.647595	-0.875683
C	13.913639	28.463879	-1.871700
H	12.238794	29.194731	-0.744726
C	15.946891	29.756547	-1.741100
H	15.860911	31.503039	-0.479771
C	15.261527	28.642710	-2.255896
H	13.355327	27.612917	-2.249887
H	16.981433	29.931176	-2.011902
C	15.921296	27.628534	-3.202797
C	15.908971	26.230942	-2.535069
C	15.123079	27.572624	-4.528588
C	17.381141	27.992489	-3.534482
H	16.474007	26.238062	-1.596078
H	14.892264	25.891040	-2.312835
H	16.369119	25.493015	-3.202692
H	15.113378	28.549939	-5.023927
H	15.583944	26.849849	-5.211970
H	14.084318	27.265300	-4.370986
H	17.800423	27.240538	-4.211681
H	17.456593	28.964536	-4.034944
H	18.012111	28.015962	-2.638826

6TSmig

H	7.574346	30.911029	5.138805
S	7.734028	29.837110	4.333106
Fe	9.307522	30.851489	2.917059
N	8.036647	31.692496	1.494638
N	9.484181	32.719054	3.806999
N	11.075709	30.274601	3.899078
N	9.565213	29.209116	1.654715
C	7.493655	31.047702	0.416418
C	6.517622	31.909595	-0.217890
C	6.491483	33.070996	0.495177
C	7.451604	32.927108	1.569906
C	8.697105	33.812383	3.548541
C	9.029836	34.870614	4.475022
C	10.030941	34.400620	5.275359
C	10.318060	33.051289	4.844086
C	11.654443	30.940036	4.950486

C	12.670232	30.102348	5.548235
C	12.680824	28.928345	4.852541
C	11.672594	29.038880	3.822082
C	10.392457	28.135588	1.873639
C	10.135238	27.123299	0.875790
C	9.150864	27.607426	0.059931
C	8.797105	28.917502	0.554732
C	7.838388	29.763767	-0.011720
H	7.313547	29.385045	-0.884277
C	7.748044	33.901826	2.525961
H	7.200872	34.837458	2.452724
C	11.308578	32.223729	5.381008
H	11.873650	32.623809	6.218124
C	11.357241	28.052641	2.883648
H	11.925012	27.128040	2.939200
H	5.888090	33.952261	0.316735
H	5.939518	31.650852	-1.096232
H	8.562145	35.847084	4.494436
H	10.542942	34.917340	6.077538
H	13.287531	30.383507	6.392403
H	13.308787	28.061183	5.015189
H	10.644976	26.169669	0.813847
H	8.698904	27.126140	-0.798607
O	11.012591	31.936472	1.246710
C	12.113729	31.412942	1.091705
C	13.285235	31.359031	0.432056
H	12.561699	30.739651	1.929100
C	13.916957	30.422343	-0.429280
C	13.223785	29.348856	-1.050174
C	15.285157	30.589715	-0.742737
C	13.875535	28.505467	-1.932581
H	12.173814	29.194379	-0.818015
C	15.927519	29.740864	-1.636695
H	15.822775	31.407543	-0.272954
C	15.241263	28.678985	-2.251031
H	13.316081	27.694284	-2.388567
H	16.975973	29.908535	-1.853094
C	15.916903	27.720638	-3.243823
C	15.798574	26.269598	-2.715987
C	15.204278	27.830027	-4.614749
C	17.410544	28.037988	-3.447757
H	16.290402	26.163061	-1.742560
H	14.755800	25.956459	-2.602416
H	16.279148	25.576771	-3.416606
H	15.279626	28.846479	-5.017262
H	15.668021	27.144519	-5.333784
H	14.142067	27.574023	-4.546596
H	17.842126	27.325090	-4.158613
H	17.564725	29.043053	-3.856193
H	17.976905	27.955205	-2.513127

2Int2

H	7.408136	33.438946	2.487244
S	7.599437	32.102152	2.399889
Fe	9.784772	32.119861	2.025452
N	9.762000	33.603251	0.675932
N	10.232157	33.466349	3.441444
N	10.190640	30.626578	3.309049
N	9.716669	30.762816	0.542271
C	9.484781	33.479335	-0.667399
C	9.431315	34.776829	-1.293571
C	9.681361	35.694102	-0.320057
C	9.878890	34.957416	0.902442
C	10.286685	34.837999	3.320658

C	10.509043	35.450754	4.605560
C	10.578060	34.440193	5.514423
C	10.407005	33.209615	4.783333
C	10.367566	30.750393	4.669065
C	10.485936	29.451550	5.283510
C	10.378126	28.533174	4.285372
C	10.184595	29.270799	3.062794
C	9.767237	29.389797	0.646183
C	9.533689	28.776247	-0.636462
C	9.323953	29.788645	-1.522144
C	9.437668	31.020364	-0.781627
C	9.317487	32.281474	-1.345664
H	9.100697	32.335055	-2.408263
C	10.130917	35.539870	2.135139
H	10.194773	36.622834	2.177779
C	10.455891	31.949382	5.360120
H	10.599613	31.897199	6.435126
C	9.996825	28.687498	1.819417
H	10.014369	27.603685	1.762674
H	9.732411	36.772281	-0.403790
H	9.236269	34.944278	-2.345299
H	10.598539	36.516828	4.771629
H	10.738384	34.502858	6.583352
H	10.637808	29.283718	6.342291
H	10.421383	27.453520	4.351749
H	9.532045	27.708715	-0.815915
H	9.114266	29.726159	-2.582553
O	12.783537	32.087519	1.475661
C	13.486234	31.154165	1.575475
C	14.293809	30.113176	1.688462
H	14.940653	30.122458	2.561698
C	14.368605	28.991111	0.742748
C	13.503791	28.863110	-0.359627
C	15.334904	27.992921	0.927940
C	13.616121	27.786193	-1.230123
H	12.731790	29.608123	-0.536856
C	15.436280	26.914081	0.048277
H	16.019239	28.059074	1.770593
C	14.583623	26.779370	-1.054877
H	12.923335	27.733119	-2.065741
H	16.203027	26.171316	0.240264
C	14.669386	25.606601	-2.047078
C	13.325032	24.840041	-2.061131
C	14.960472	26.151447	-3.465930
C	15.784622	24.609519	-1.678082
H	13.097508	24.430120	-1.070319
H	12.491065	25.486227	-2.354928
H	13.367244	24.006568	-2.773196
H	15.916976	26.685979	-3.491229
H	15.010802	25.328219	-4.189467
H	14.182435	26.844546	-3.802993
H	15.808008	23.793037	-2.408883
H	16.772805	25.083603	-1.681630
H	15.622525	24.163691	-0.689936

4Int2

H	7.098366	32.956587	1.208635
S	7.277850	32.116004	2.252379
Fe	9.651553	32.052053	2.104740
N	9.931543	33.455394	0.689310
N	10.091458	33.438495	3.514568
N	9.867882	30.618003	3.501291
N	9.826696	30.627905	0.669401
C	9.899414	33.275911	-0.677979

C	9.969328	34.545170	-1.350442
C	10.053061	35.501020	-0.382832
C	10.035583	34.816846	0.881829
C	10.176537	34.799755	3.333594
C	10.304395	35.469478	4.603197
C	10.286650	34.502523	5.560206
C	10.146959	33.242271	4.875289
C	9.944059	30.794640	4.865877
C	9.899545	29.523907	5.538155
C	9.798561	28.569096	4.571472
C	9.782101	29.255589	3.307735
C	9.747280	29.265285	0.851727
C	9.693574	28.590782	-0.419823
C	9.730874	29.556806	-1.379576
C	9.804880	30.821424	-0.693667
C	9.834352	32.053133	-1.329016
H	9.811620	32.061755	-2.414110
C	10.141532	35.450568	2.110905
H	10.215180	36.533393	2.113472
C	10.071077	32.014642	5.513284
H	10.120273	32.005786	6.597453
C	9.718869	28.619289	2.077469
H	9.654233	27.535982	2.074592
H	10.131268	36.574424	-0.499435
H	9.964376	34.671681	-2.425588
H	10.395016	36.541174	4.726267
H	10.358758	34.613175	6.634670
H	9.947391	29.394979	6.611920
H	9.747189	27.494007	4.687078
H	9.631203	27.517069	-0.542996
H	9.704673	29.442144	-2.455808
O	13.234103	32.017867	1.964212
C	14.041241	31.192089	1.765556
C	14.962278	30.267679	1.546673
H	15.878560	30.381460	2.119648
C	14.826649	29.141217	0.613396
C	13.664240	28.914715	-0.146279
C	15.888267	28.239249	0.457911
C	13.582619	27.833876	-1.015017
H	12.814102	29.587385	-0.058031
C	15.794074	27.156234	-0.417477
H	16.802279	28.383877	1.029364
C	14.641285	26.921209	-1.177491
H	12.661975	27.703281	-1.576945
H	16.646583	26.490446	-0.496690
C	14.497795	25.736054	-2.148615
C	13.304871	24.852341	-1.711394
C	14.241681	26.266998	-3.579414
C	15.759309	24.852456	-2.184661
H	13.462969	24.452783	-0.703067
H	12.364200	25.413407	-1.704667
H	13.183401	24.005613	-2.398429
H	15.076185	26.890130	-3.920819
H	14.129412	25.432616	-4.283011
H	13.330330	26.872147	-3.632045
H	15.609623	24.023348	-2.885686
H	16.640105	25.412589	-2.519013
H	15.981928	24.418645	-1.203008

6Int2

H	7.048546	33.387236	2.018782
S	7.145304	32.056627	2.241216
Fe	9.452132	31.999886	2.009712
N	9.866678	33.502325	0.609619

N	10.131350	33.339933	3.473059
N	9.988885	30.452980	3.316526
N	9.756820	30.615667	0.452227
C	9.768315	33.377201	-0.757104
C	9.835174	34.680972	-1.371766
C	9.983775	35.588691	-0.364221
C	10.006050	34.845148	0.872380
C	10.236277	34.703761	3.344650
C	10.442634	35.302029	4.642907
C	10.461358	34.284388	5.550253
C	10.269188	33.058551	4.811272
C	10.141994	30.575994	4.678272
C	10.201589	29.266774	5.282237
C	10.088347	28.357001	4.272206
C	9.956981	29.104931	3.045099
C	9.747377	29.246349	0.571776
C	9.648989	28.642477	-0.736219
C	9.598977	29.662119	-1.641835
C	9.665521	30.893982	-0.891763
C	9.659207	32.171775	-1.449044
H	9.587136	32.233751	-2.531000
C	10.165587	35.402744	2.140635
H	10.263112	36.483190	2.192965
C	10.257819	31.781314	5.369455
H	10.376578	31.717066	6.447158
C	9.833581	28.545778	1.774148
H	9.819619	27.461651	1.713493
H	10.081067	36.664347	-0.441051
H	9.787681	34.865387	-2.437621
H	10.564226	36.362744	4.823177
H	10.602259	34.344881	6.622077
H	10.325006	29.079336	6.341444
H	10.100390	27.276458	4.339430
H	9.622818	27.576472	-0.924503
H	9.526566	29.597677	-2.720261
O	13.310716	32.352955	1.699802
C	14.076190	31.471738	1.604227
C	14.953105	30.485655	1.500306
H	15.847102	30.594266	2.108318
C	14.798027	29.301947	0.644734
C	13.653570	29.072415	-0.141024
C	15.821597	28.345632	0.593171
C	13.553886	27.938380	-0.937162
H	12.831361	29.784406	-0.128388
C	15.709269	27.209024	-0.209089
H	16.720159	28.490312	1.188624
C	14.575499	26.972432	-0.996743
H	12.648794	27.808829	-1.523977
H	16.532832	26.503212	-0.209543
C	14.415542	25.733670	-1.895749
C	13.166530	24.932551	-1.455981
C	14.241655	26.181877	-3.366651
C	15.635399	24.795561	-1.822708
H	13.264719	24.592829	-0.418518
H	12.253251	25.533251	-1.525935
H	13.034248	24.049146	-2.093003
H	15.118742	26.741679	-3.711000
H	14.115609	25.309973	-4.020772
H	13.364400	26.824728	-3.495237
H	15.476127	23.930595	-2.476662
H	16.553478	25.294658	-2.153321
H	15.798505	24.416538	-0.807261

2TSco(Cb)

H	8.712417	34.076918	1.372897
S	8.904882	33.491291	2.576123
Fe	9.700347	31.307702	1.797652
N	10.389562	32.138400	0.081131
N	11.495208	31.533781	2.658065
N	8.959473	30.655105	3.548930
N	7.837926	31.249474	0.972676
C	9.695409	32.365615	-1.077486
C	10.574056	32.893198	-2.095047
C	11.812373	32.975817	-1.535518
C	11.684190	32.500253	-0.178047
C	12.636233	31.995430	2.052898
C	13.733029	32.010410	2.991843
C	13.236399	31.568773	4.178807
C	11.839962	31.277857	3.958390
C	9.627000	30.513885	4.741906
C	8.745275	29.976182	5.749039
C	7.536523	29.788199	5.150218
C	7.675276	30.226480	3.781639
C	6.712688	30.725283	1.555374
C	5.605229	30.759979	0.627046
C	6.077042	31.304026	-0.526217
C	7.475432	31.594844	-0.306580
C	8.335858	32.121705	-1.258999
H	7.917958	32.348883	-2.235435
C	12.730054	32.431852	0.736664
H	13.706546	32.763470	0.396139
C	10.968286	30.812964	4.938067
H	11.373634	30.659054	5.933722
C	6.640479	30.236120	2.852968
H	5.679605	29.852234	3.183220
H	12.734106	33.325144	-1.983145
H	10.266759	33.159950	-3.098273
H	14.740590	32.329396	2.757571
H	13.750301	31.447848	5.123849
H	9.028913	29.775314	6.774334
H	6.621726	29.404971	5.584263
H	4.604848	30.410285	0.848226
H	5.545918	31.492313	-1.450576
O	9.961110	29.739892	1.126732
C	10.445066	27.895669	2.836399
C	11.054082	28.319929	1.840618
H	9.709240	27.776571	3.600825
C	12.189561	28.214403	0.945688
C	12.184915	28.726858	-0.361441
C	13.336346	27.532274	1.385061
C	13.290697	28.554879	-1.188031
H	11.307739	29.256314	-0.711447
C	14.438688	27.371906	0.547687
H	13.356406	27.127418	2.392555
C	14.445818	27.876545	-0.761336
H	13.245293	28.963053	-2.194217
H	15.301347	26.840210	0.934038
C	15.642248	27.712664	-1.715600
C	15.193625	26.929702	-2.973214
C	16.158051	29.108286	-2.141164
C	16.810867	26.946951	-1.066636
H	14.830763	25.931192	-2.703957
H	14.388061	27.444287	-3.507157
H	16.033603	26.810739	-3.668950
H	16.492771	29.683724	-1.270265
H	17.006355	29.008609	-2.829791
H	15.382580	29.690940	-2.649508
H	17.634713	26.854261	-1.783500
H	17.198351	27.466453	-0.182732
H	16.518172	25.934118	-0.767331

4TSco(Cb)

H	7.843520	33.306140	2.887338
S	9.175138	33.493047	2.748273
Fe	9.680299	31.429993	1.662598
N	10.308349	32.308155	-0.014744
N	11.502742	31.713181	2.507331
N	9.018061	30.635984	3.431361
N	7.820711	31.312230	0.922794
C	9.560012	32.593935	-1.128686
C	10.388207	33.202366	-2.143728
C	11.644054	33.282458	-1.629177
C	11.585215	32.730963	-0.295263
C	12.613762	32.218395	1.890381
C	13.735672	32.212735	2.798186
C	13.285222	31.694726	3.973284
C	11.890053	31.379017	3.782444
C	9.744455	30.455606	4.581453
C	8.926458	29.824783	5.589629
C	7.699020	29.625455	5.032546
C	7.765525	30.143806	3.685895
C	6.731036	30.719392	1.516462
C	5.595023	30.769834	0.627713
C	6.009175	31.397841	-0.506122
C	7.401929	31.723760	-0.316031
C	8.204011	32.336953	-1.270598
H	7.737487	32.616318	-2.210306
C	12.659856	32.684300	0.579927
H	13.612111	33.061261	0.219493
C	11.079109	30.800224	4.749259
H	11.529336	30.591681	5.715016
C	6.701781	30.167995	2.790249
H	5.761070	29.739598	3.123129
H	12.538354	33.683879	-2.088692
H	10.034204	33.521747	-3.115668
H	14.729447	32.563921	2.551315
H	13.832477	31.530540	4.892786
H	9.262442	29.576075	6.588345
H	6.817788	29.184221	5.480980
H	4.615129	30.372361	0.859928
H	5.441535	31.621312	-1.400427
O	10.099114	29.886669	1.045959
C	10.273457	27.851691	2.671428
C	10.968926	28.307884	1.745839
H	9.491640	27.744357	3.391373
C	12.149679	28.179833	0.916127
C	12.202897	28.632619	-0.412532
C	13.277534	27.528701	1.441474
C	13.345231	28.426589	-1.178390
H	11.343887	29.145755	-0.827100
C	14.417071	27.333630	0.662969
H	13.253066	27.174132	2.467530
C	14.480982	27.773353	-0.667302
H	13.346048	28.785884	-2.203904
H	15.263619	26.827514	1.113513
C	15.717791	27.566284	-1.559664
C	15.323426	26.720846	-2.794834
C	16.250280	28.940727	-2.031037
C	16.857653	26.836982	-0.823183
H	14.949792	25.735854	-2.492506
H	14.541316	27.206819	-3.387311
H	16.192617	26.570134	-3.446990
H	16.544078	29.560554	-1.176089
H	17.129125	28.809387	-2.674580
H	15.498178	29.494359	-2.602825
H	17.711429	26.709351	-1.498422

H	17.207291	27.401897	0.048571
H	16.552098	25.840255	-0.485132

6TSco(Cb)

H	7.926977	34.333802	1.290396
S	8.035707	33.905490	2.569183
Fe	9.626952	31.089891	1.680642
N	10.240895	32.325056	0.104020
N	11.325176	31.737677	2.730098
N	8.752545	30.670637	3.550819
N	7.663567	31.308061	0.945822
C	9.546342	32.559497	-1.055732
C	10.410125	33.207105	-2.016423
C	11.625877	33.361596	-1.416114
C	11.512562	32.807962	-0.086092
C	12.441770	32.306984	2.175454
C	13.502576	32.357278	3.157044
C	13.004946	31.814351	4.304341
C	11.638550	31.429297	4.027816
C	9.427828	30.509221	4.735341
C	8.539149	29.949640	5.729524
C	7.327489	29.779787	5.127426
C	7.468510	30.238802	3.763287
C	6.531208	30.768316	1.514716
C	5.445619	30.810113	0.563365
C	5.936093	31.368828	-0.579798
C	7.327535	31.671529	-0.339276
C	8.200160	32.245706	-1.261936
H	7.788508	32.485332	-2.238212
C	12.530181	32.790684	0.868788
H	13.484142	33.216468	0.570595
C	10.762995	30.851896	4.950686
H	11.158006	30.667557	5.945895
C	6.446721	30.265397	2.811361
H	5.479955	29.879057	3.121777
H	12.519239	33.819727	-1.821892
H	10.111161	33.513720	-3.010893
H	14.489670	32.766865	2.983155
H	13.503115	31.690521	5.257746
H	8.813988	29.730994	6.753850
H	6.412253	29.396268	5.560931
H	4.439726	30.459582	0.757568
H	5.411541	31.564295	-1.506604
O	10.085041	29.564712	1.059399
C	10.181038	27.110879	1.533154
C	10.745098	27.707677	0.610616
H	9.609069	26.833496	2.390424
C	11.586691	27.822636	-0.553287
C	11.663335	28.987289	-1.333182
C	12.354778	26.710000	-0.937355
C	12.482770	29.024002	-2.455973
H	11.078683	29.849864	-1.041736
C	13.171724	26.763689	-2.064420
H	12.307656	25.801184	-0.344729
C	13.257805	27.920511	-2.853845
H	12.515625	29.944175	-3.032673
H	13.747124	25.881118	-2.320715
C	14.148188	28.015558	-4.105300
C	13.266581	28.318911	-5.340690
C	15.178134	29.155541	-3.919239
C	14.921280	26.710643	-4.376284
H	12.535426	27.519426	-5.506676
H	12.714291	29.257441	-5.225887
H	13.887960	28.404248	-6.240787

H	15.822569	28.963161	-3.053882
H	15.816455	29.240578	-4.807362
H	14.691032	30.123853	-3.764336
H	15.536367	26.826219	-5.275939
H	15.592324	26.454155	-3.548473
H	14.245969	25.864107	-4.545160

4Int1(Cb)

H	7.611885	33.712978	1.573925
S	8.346008	33.490744	2.688390
Fe	9.563823	31.780662	1.940810
N	9.931882	32.674741	0.173980
N	11.250372	32.565867	2.722288
N	9.286509	30.756895	3.656381
N	7.972849	30.865709	1.113538
C	9.213534	32.567059	-0.990317
C	9.783647	33.414511	-2.010709
C	10.851690	34.041108	-1.445940
C	10.939332	33.570296	-0.083102
C	12.071628	33.479075	2.111757
C	13.143243	33.860458	3.002951
C	12.960637	33.163620	4.157171
C	11.772762	32.362865	3.973872
C	10.057796	30.796777	4.793502
C	9.452891	30.002602	5.835761
C	8.295861	29.499900	5.324845
C	8.197435	29.978358	3.965956
C	7.065760	30.067850	1.769261
C	6.004839	29.677189	0.871550
C	6.277076	30.250441	-0.332979
C	7.499256	30.999761	-0.170846
C	8.084009	31.776153	-1.162715
H	7.604310	31.790846	-2.136758
C	11.928304	33.954296	0.814354
H	12.661135	34.676335	0.466326
C	11.229997	31.526285	4.941329
H	11.741455	31.465690	5.897169
C	7.161481	29.658358	3.095160
H	6.364892	29.028185	3.479539
H	11.530513	34.754941	-1.895599
H	9.401429	33.507345	-3.019532
H	13.925244	34.568295	2.758079
H	13.559383	33.180662	5.059120
H	9.868113	29.867352	6.826515
H	7.565010	28.863841	5.808371
H	5.168837	29.045370	1.144479
H	5.709742	30.188934	-1.253203
O	10.930511	30.233976	1.171387
C	10.065223	28.118720	1.538993
C	11.072198	28.991431	1.041215
H	9.127307	28.312836	2.046518
C	12.272747	28.436896	0.376731
C	13.259335	29.301063	-0.124844
C	12.450495	27.055040	0.233677
C	14.386207	28.784994	-0.749335
H	13.124604	30.372519	-0.016451
C	13.585986	26.547027	-0.394731
H	11.695511	26.373095	0.616695
C	14.580890	27.397041	-0.901576
H	15.132465	29.477442	-1.127686
H	13.687736	25.471861	-0.485924
C	15.846556	26.874040	-1.601553
C	15.897341	27.427762	-3.046319
C	17.096114	27.352459	-0.822968

C	15.885282	25.335699	-1.675337
H	15.026063	27.098530	-3.623843
H	15.917211	28.522271	-3.064847
H	16.799092	27.068882	-3.556928
H	17.090480	26.967635	0.203206
H	18.008245	26.994399	-1.315364
H	17.152688	28.444561	-0.770197
H	16.803147	25.015743	-2.180881
H	15.881027	24.877685	-0.679686
H	15.038965	24.932269	-2.242990

6Int1(Cb)

H	7.649490	33.939189	1.218198
S	7.711062	33.540916	2.509875
Fe	9.845414	31.167075	1.855508
N	10.353127	32.467285	0.287245
N	11.231326	32.190938	3.038760
N	8.881138	30.598225	3.627540
N	7.995129	30.900646	0.888587
C	9.757064	32.525753	-0.946791
C	10.551862	33.343772	-1.833275
C	11.626361	33.779180	-1.114030
C	11.493700	33.229277	0.214931
C	12.243311	32.998614	2.583257
C	13.130832	33.328030	3.673991
C	12.633207	32.718397	4.787911
C	11.440512	32.011672	4.382461
C	9.422404	30.636069	4.890402
C	8.567105	29.917586	5.805578
C	7.509650	29.451627	5.079858
C	7.708470	29.888339	3.717755
C	6.950358	30.134920	1.357186
C	5.994336	29.921238	0.297323
C	6.473295	30.559206	-0.808869
C	7.729259	31.165926	-0.436674
C	8.548541	31.909848	-1.284019
H	8.204539	32.037864	-2.306370
C	12.373075	33.462130	1.273096
H	13.232106	34.092763	1.062757
C	10.610153	31.280428	5.234817
H	10.909773	31.225606	6.277416
C	6.829722	29.653288	2.659008
H	5.944936	29.063686	2.880784
H	12.434124	34.422073	-1.440359
H	10.304957	33.559592	-2.865160
H	14.009439	33.954953	3.589760
H	13.023570	32.746230	5.797329
H	8.755562	29.798555	6.865101
H	6.659842	28.878455	5.428410
H	5.074805	29.358891	0.398934
H	6.023959	30.620921	-1.792006
O	10.750269	29.639509	1.365412
C	11.175521	27.891738	2.856201
C	11.555199	28.646868	1.826065
H	10.325010	27.826608	3.518937
C	12.828314	28.453665	1.085074
C	13.121910	29.218204	-0.052466
C	13.768717	27.499178	1.495172
C	14.313603	29.027039	-0.748118
H	12.405837	29.959639	-0.390469
C	14.957432	27.313680	0.793495
H	13.563172	26.896587	2.376259
C	15.262926	28.072077	-0.348296
H	14.501870	29.640004	-1.625893

H	15.652144	26.562005	1.152536
C	16.564280	27.894129	-1.150878
C	16.221034	27.504571	-2.608730
C	17.357284	29.223030	-1.150071
C	17.471024	26.796140	-0.562827
H	15.661269	26.562751	-2.640150
H	15.612777	28.270089	-3.101892
H	17.138022	27.375633	-3.197493
H	17.624765	29.517733	-0.128713
H	18.284172	29.116616	-1.727709
H	16.779769	30.041255	-1.592995
H	18.381971	26.706758	-1.165896
H	17.776095	27.026571	0.464362
H	16.977683	25.817506	-0.561577

4Int1(Cb)'

H	7.923172	34.140881	1.380142
S	8.057231	33.660157	2.637865
Fe	9.744968	31.213666	1.747651
N	10.273956	32.329684	0.138944
N	11.409173	31.836613	2.696709
N	9.019914	30.539614	3.510881
N	7.881346	31.037058	0.958354
C	9.567873	32.484156	-1.029586
C	10.349500	33.214809	-1.994182
C	11.539333	33.504457	-1.397414
C	11.484677	32.948486	-0.070025
C	12.467660	32.521473	2.146825
C	13.531069	32.654282	3.108192
C	13.106445	32.046629	4.250427
C	11.783529	31.543271	3.986272
C	9.709875	30.421622	4.695092
C	8.905301	29.742850	5.677509
C	7.721775	29.439571	5.075538
C	7.800251	29.939362	3.727033
C	6.815442	30.359139	1.511887
C	5.734771	30.271939	0.565135
C	6.153981	30.891159	-0.572856
C	7.494055	31.356204	-0.326659
C	8.276204	32.023708	-1.255756
H	7.843226	32.209502	-2.233681
C	12.511554	33.036082	0.858904
H	13.416131	33.555261	0.558432
C	10.999500	30.879228	4.920003
H	11.425524	30.713873	5.904455
C	6.778124	29.835257	2.793992
H	5.871255	29.323194	3.099749
H	12.384070	34.046111	-1.803409
H	10.014550	33.469732	-2.991548
H	14.472358	33.153880	2.918624
H	13.626249	31.944582	5.194363
H	9.219965	29.533293	6.691824
H	6.861601	28.933213	5.494443
H	4.782682	29.796140	0.762226
H	5.617589	31.026932	-1.503283
O	10.401620	29.550865	1.084549
C	10.731100	27.699729	2.471613
C	11.194073	28.570030	1.569481
H	9.803369	27.548942	3.005625
C	12.565966	28.478687	0.998847
C	12.926326	29.233171	-0.126402
C	13.532303	27.627401	1.551547
C	14.203775	29.131373	-0.673042
H	12.190180	29.893119	-0.572721

C	14.807770	27.530208	0.999448
H	13.276685	27.036658	2.427605
C	15.179172	28.279185	-0.128808
H	14.439276	29.730766	-1.549218
H	15.518944	26.857610	1.467036
C	16.577442	28.195744	-0.767186
C	16.447911	27.719257	-2.233902
C	17.242457	29.592751	-0.741630
C	17.503502	27.212417	-0.025924
H	15.990436	26.724456	-2.281891
H	15.829332	28.398995	-2.829287
H	17.436168	27.663723	-2.707791
H	17.358133	29.951594	0.287750
H	18.237646	29.552877	-1.202535
H	16.650637	30.334021	-1.288998
H	18.483777	27.186125	-0.515937
H	17.662850	27.509620	1.016957
H	17.102846	26.192354	-0.032685

4TScn(Cb)

H	7.878804	33.623055	2.511749
S	8.930298	33.069336	3.157476
Fe	9.575804	31.624167	1.564030
N	9.642933	32.999854	0.133260
N	11.503980	31.937401	2.041433
N	9.552247	29.989039	2.898324
N	7.678389	31.180295	1.052868
C	8.666675	33.308445	-0.777681
C	9.111178	34.379591	-1.638357
C	10.367108	34.711946	-1.231996
C	10.695438	33.833896	-0.132202
C	12.308291	32.909825	1.501108
C	13.621264	32.859850	2.102742
C	13.596109	31.848053	3.012086
C	12.266347	31.284218	2.969681
C	10.543677	29.763208	3.887286
C	9.984653	29.000209	4.960092
C	8.643725	28.867176	4.723608
C	8.348539	29.522326	3.487451
C	6.822981	30.341481	1.716249
C	5.534558	30.325017	1.064534
C	5.623018	31.165799	-0.003649
C	6.958559	31.711104	0.010069
C	7.422127	32.693034	-0.856769
H	6.744452	33.034911	-1.633401
C	11.930764	33.804719	0.509169
H	12.674279	34.526118	0.183420
C	11.819370	30.281829	3.838053
H	12.516361	29.952143	4.603269
C	7.114484	29.623349	2.884074
H	6.283978	29.115102	3.365996
H	11.028634	35.467985	-1.635683
H	8.525823	34.808548	-2.441753
H	14.440883	33.520823	1.850840
H	14.390240	31.505340	3.663206
H	10.543033	28.657213	5.822102
H	7.904443	28.387448	5.352817
H	4.685240	29.739062	1.392674
H	4.859768	31.418033	-0.728875
O	10.346230	30.315660	0.091198
C	9.890364	28.642716	1.555307
C	10.775618	29.215457	0.597932
H	8.858245	28.369661	1.369402
C	12.083828	28.661920	0.259533

C	12.915952	29.322643	-0.665392
C	12.536156	27.451702	0.812881
C	14.148907	28.786688	-1.009530
H	12.575285	30.256755	-1.099969
C	13.779423	26.929889	0.467382
H	11.903695	26.921859	1.520667
C	14.617694	27.579043	-0.454367
H	14.764638	29.322832	-1.726617
H	14.090944	25.996852	0.923520
C	15.991273	27.024212	-0.868732
C	15.997255	26.754499	-2.393034
C	17.089943	28.060095	-0.528334
C	16.334670	25.706634	-0.147895
H	15.232736	26.017137	-2.663228
H	15.801629	27.664922	-2.969047
H	16.973148	26.363555	-2.706627
H	17.114347	28.266426	0.547829
H	18.075581	27.680668	-0.824917
H	16.929354	29.010949	-1.046966
H	17.319831	25.353879	-0.473535
H	16.372718	25.834228	0.940042
H	15.610070	24.916409	-0.375149

6TScn(Cb)

H	6.587551	32.222206	2.587686
S	7.457446	33.205756	2.913387
Fe	10.049727	31.548846	1.953633
N	10.341379	32.943610	0.426203
N	10.795977	32.982031	3.293091
N	9.060337	30.685314	3.589152
N	8.614332	30.628227	0.728705
C	9.963588	32.797885	-0.884622
C	10.544950	33.855991	-1.677573
C	11.266111	34.640006	-0.825032
C	11.129033	34.064043	0.492428
C	11.530049	34.092929	2.955946
C	12.091929	34.683435	4.149363
C	11.685685	33.916348	5.200797
C	10.870108	32.854659	4.656492
C	9.379917	30.875111	4.918416
C	8.687397	29.899498	5.722986
C	7.952794	29.124281	4.872480
C	8.190680	29.615435	3.537747
C	7.808348	29.574354	1.072971
C	7.153612	29.056182	-0.106683
C	7.572913	29.816556	-1.158453
C	8.486330	30.802132	-0.627119
C	9.119354	31.797613	-1.372237
H	8.913767	31.812184	-2.438793
C	11.690397	34.585407	1.661154
H	12.296799	35.480035	1.552073
C	10.229204	31.865711	5.405480
H	10.384312	31.889564	6.480208
C	7.624420	29.098043	2.374069
H	6.956190	28.249948	2.493077
H	11.832212	35.533919	-1.054582
H	10.403195	33.980846	-2.743671
H	12.707910	35.573594	4.168884
H	11.901576	34.053918	6.252753
H	8.751992	29.830375	6.801612
H	7.301135	28.295360	5.118949
H	6.458959	28.225743	-0.115942
H	7.289608	29.732515	-2.200049
O	11.504147	30.438084	1.724319

C	11.667600	28.646713	3.238366
C	12.049016	29.258716	2.133846
H	11.409024	28.123693	4.131521
C	13.117472	28.739213	1.225811
C	13.541124	29.486168	0.118044
C	13.727545	27.499078	1.451296
C	14.539066	29.002647	-0.725096
H	13.082115	30.449549	-0.074778
C	14.724584	27.021717	0.603303
H	13.413168	26.899052	2.301650
C	15.157962	27.760255	-0.509104
H	14.838806	29.615530	-1.571460
H	15.163885	26.054275	0.821338
C	16.255778	27.265071	-1.467612
C	15.682891	27.165103	-2.901696
C	17.437259	28.264438	-1.457379
C	16.798560	25.878188	-1.072173
H	14.848258	26.455679	-2.940712
H	15.315545	28.131844	-3.261578
H	16.455944	26.820249	-3.599875
H	17.871185	28.346325	-0.454166
H	18.226375	27.932383	-2.143761
H	17.124297	29.266803	-1.767598
H	17.573961	25.568421	-1.782359
H	17.249707	25.886100	-0.073322
H	16.013082	25.113847	-1.086251

4TScn(Cb)'

H	6.706930	32.349641	2.784004
S	7.702520	33.187764	3.152374
Fe	9.808782	31.734869	1.864856
N	10.148998	33.054677	0.382231
N	10.948609	32.856402	3.110456
N	9.215745	30.622236	3.443501
N	8.427317	30.814529	0.721870
C	9.670294	32.987890	-0.902346
C	10.227535	34.051582	-1.697593
C	11.049171	34.765644	-0.877821
C	10.997729	34.133678	0.415468
C	11.697021	33.956888	2.773545
C	12.471418	34.398763	3.906961
C	12.189286	33.547097	4.930841
C	11.236397	32.589974	4.425106
C	9.707524	30.683563	4.737396
C	9.044325	29.712262	5.561325
C	8.139052	29.065481	4.772039
C	8.249162	29.626147	3.454886
C	7.608748	29.772171	1.081835
C	6.840578	29.327276	-0.053332
C	7.204210	30.109887	-1.106960
C	8.187106	31.040867	-0.614586
C	8.767178	32.043485	-1.376853
H	8.477199	32.109547	-2.420846
C	11.717867	34.560990	1.524339
H	12.354772	35.431234	1.400299
C	10.671732	31.571700	5.184147
H	10.979773	31.492913	6.221997
C	7.505205	29.228228	2.357626
H	6.793429	28.421420	2.501062
H	11.642384	35.640258	-1.112418
H	10.005429	34.220108	-2.743600
H	13.138440	35.251324	3.902456
H	12.574240	33.556418	5.942510
H	9.246591	29.560370	6.613903

H	7.453091	28.274188	5.046434
H	6.120903	28.518958	-0.030145
H	6.842722	30.078989	-2.126883
O	11.322241	30.604883	1.337507
C	10.920929	28.552394	2.471502
C	11.632701	29.363931	1.678523
H	11.058783	27.617980	2.993239
C	12.857308	28.809356	1.004378
C	13.186865	29.229279	-0.293392
C	13.697516	27.879274	1.627421
C	14.306954	28.718258	-0.940567
H	12.555649	29.964077	-0.782550
C	14.821359	27.373773	0.972019
H	13.483362	27.560683	2.643839
C	15.153819	27.775254	-0.329211
H	14.525987	29.066630	-1.946760
H	15.445572	26.661329	1.500449
C	16.382431	27.237084	-1.084306
C	15.919377	26.523510	-2.376987
C	17.318403	28.411914	-1.456338
C	17.191725	26.229436	-0.245440
H	15.261562	25.678481	-2.143242
H	15.369842	27.199856	-3.040049
H	16.783784	26.138908	-2.932939
H	17.666208	28.934600	-0.557950
H	18.198399	28.042868	-1.997929
H	16.817070	29.145874	-2.095896
H	18.053267	25.875862	-0.823441
H	17.575040	26.681727	0.676414
H	16.594024	25.352102	0.027208

2Int1(Cb)

H	7.493577	33.408723	2.099727
S	8.390069	33.061796	3.049861
Fe	9.817583	31.839902	1.761261
N	9.893886	33.171565	0.286950
N	11.402352	32.666137	2.694677
N	9.920314	30.222606	3.221273
N	8.287107	30.893665	0.835958
C	9.102684	33.233557	-0.825272
C	9.490583	34.352760	-1.653265
C	10.542120	34.950460	-1.029198
C	10.790737	34.195016	0.178458
C	12.112881	33.743493	2.226673
C	13.173507	34.081831	3.150575
C	13.070696	33.216191	4.193321
C	11.957005	32.340652	3.896786
C	10.422994	30.520667	4.556222
C	9.674465	29.788018	5.501708
C	8.639305	29.148253	4.850747
C	8.699955	29.466182	3.476855
C	7.617240	29.788807	1.268306
C	6.607976	29.401965	0.303501
C	6.682416	30.294467	-0.718791
C	7.731718	31.228268	-0.372916
C	8.094378	32.325135	-1.140374
H	7.553945	32.484493	-2.068787
C	11.829373	34.455501	1.071195
H	12.473246	35.299793	0.842761
C	11.459764	31.388601	4.798192
H	11.875128	31.397761	5.801863
C	7.766758	29.162342	2.514356
H	7.005873	28.435243	2.784734
H	11.112161	35.814691	-1.345482

H	9.017929	34.622531	-2.589005
H	13.881095	34.888859	3.009327
H	13.677407	33.160079	5.088071
H	9.857285	29.807920	6.568847
H	7.846826	28.567334	5.305980
H	5.941052	28.556531	0.415268
H	6.090212	30.337374	-1.623966
O	10.997636	30.744728	0.709172
C	10.903998	29.319137	2.556823
C	11.373943	29.646433	1.328166
H	11.197813	28.453944	3.136183
C	12.354550	28.785656	0.608378
C	13.166710	29.356889	-0.382832
C	12.503064	27.417322	0.866634
C	14.102422	28.588443	-1.067569
H	13.049906	30.411769	-0.607263
C	13.445033	26.653165	0.176707
H	11.862428	26.931351	1.597078
C	14.271097	27.217307	-0.805999
H	14.713249	29.071952	-1.825607
H	13.518732	25.596653	0.410866
C	15.314709	26.404554	-1.592956
C	14.969945	26.447856	-3.100968
C	16.719078	27.015928	-1.372251
C	15.362311	24.928284	-1.154263
H	13.983535	26.008657	-3.289462
H	14.956391	27.473160	-3.485035
H	15.711147	25.882726	-3.679993
H	16.994658	26.991238	-0.311689
H	17.474268	26.451775	-1.933803
H	16.766237	28.058164	-1.704630
H	16.120775	24.393622	-1.737638
H	15.626866	24.826167	-0.095473
H	14.403890	24.422189	-1.317322

4Int1(Cb)

H	7.182193	32.981733	2.113857
S	8.216802	32.959296	2.983857
Fe	9.714830	31.872970	1.736134
N	9.844512	33.220475	0.307134
N	11.213271	32.731911	2.788809
N	9.840613	30.158719	3.098279
N	8.276440	30.887465	0.692346
C	9.149524	33.255185	-0.878650
C	9.575939	34.402887	-1.662215
C	10.526254	35.044149	-0.941985
C	10.703505	34.296871	0.292850
C	11.856876	33.886147	2.445603
C	12.807475	34.253465	3.457226
C	12.715380	33.306888	4.444526
C	11.723607	32.368199	4.021674
C	10.365778	30.332505	4.460051
C	9.700800	29.385479	5.313222
C	8.690552	28.788380	4.623207
C	8.649037	29.310548	3.281968
C	7.557495	29.784424	1.094274
C	6.586938	29.434076	0.106124
C	6.723434	30.337512	-0.918715
C	7.767205	31.238821	-0.531107
C	8.187764	32.351760	-1.280039
H	7.710749	32.515802	-2.241274
C	11.618926	34.623985	1.269270
H	12.217558	35.516376	1.116594
C	11.293537	31.278880	4.798631

H	11.693130	31.221524	5.808195
C	7.706474	29.101438	2.321400
H	6.952477	28.350346	2.544218
H	11.081338	35.937489	-1.199272
H	9.180413	34.657123	-2.637622
H	13.445828	35.126792	3.418394
H	13.270657	33.244985	5.371970
H	9.931229	29.262652	6.364369
H	7.955617	28.097112	5.017075
H	5.899843	28.600503	0.180891
H	6.162018	30.399214	-1.842205
O	11.090831	30.769191	0.738028
C	10.824477	29.276558	2.480822
C	11.437945	29.667882	1.279856
H	11.010956	28.338525	2.988067
C	12.461880	28.828526	0.612273
C	12.848152	29.148863	-0.700165
C	13.073879	27.729304	1.231801
C	13.801871	28.387684	-1.362499
H	12.385284	30.000319	-1.187293
C	14.031053	26.971960	0.558555
H	12.825916	27.461801	2.254404
C	14.418159	27.277110	-0.754717
H	14.071015	28.665595	-2.377493
H	14.479336	26.133077	1.078559
C	15.470579	26.463001	-1.525557
C	14.844811	25.917700	-2.832165
C	16.668482	27.379376	-1.874282
C	15.999108	25.266388	-0.711593
H	13.993274	25.262073	-2.617218
H	14.490818	26.722721	-3.484333
H	15.587533	25.337644	-3.392977
H	17.139261	27.772280	-0.965928
H	17.425548	26.816737	-2.434037
H	16.363589	28.232613	-2.488989
H	16.735919	24.714171	-1.305558
H	16.494647	25.586069	0.212168
H	15.197648	24.566986	-0.447142

6Int1(Cb)

H	6.994371	32.532566	2.589224
S	8.116873	32.933201	3.226998
Fe	9.707415	31.877120	1.782686
N	9.942811	33.273626	0.311543
N	11.266160	32.697099	2.907318
N	9.825021	30.011055	3.171688
N	8.279521	30.847470	0.662485
C	9.264667	33.312131	-0.869970
C	9.737026	34.443375	-1.644243
C	10.710768	35.052486	-0.905504
C	10.841666	34.298257	0.325851
C	11.968028	33.810338	2.530885
C	12.949998	34.115538	3.554732
C	12.804387	33.179550	4.535965
C	11.742914	32.285534	4.110944
C	10.220989	30.321230	4.527263
C	9.361252	29.616730	5.403700
C	8.366612	29.007325	4.660927
C	8.567944	29.307214	3.292004
C	7.605849	29.715353	0.998999
C	6.692681	29.366374	-0.073189
C	6.852667	30.304181	-1.051063
C	7.852404	31.242629	-0.577487
C	8.294927	32.377696	-1.268811

H	7.842722	32.547059	-2.242440
C	11.762794	34.545880	1.356962
H	12.409671	35.408011	1.218697
C	11.212689	31.225866	4.878944
H	11.536395	31.190069	5.916374
C	7.696552	29.051979	2.242002
H	6.912441	28.326638	2.445981
H	11.297106	35.924194	-1.167286
H	9.374322	34.721670	-2.625703
H	13.647305	34.943150	3.521442
H	13.363032	33.088581	5.458969
H	9.423688	29.657275	6.484088
H	7.504825	28.479656	5.050494
H	6.030638	28.509589	-0.073279
H	6.341923	30.367170	-2.003760
O	11.106272	30.780249	0.826357
C	10.839510	29.175024	2.495995
C	11.432467	29.629517	1.361340
H	11.020157	28.210359	2.953037
C	12.465698	28.822346	0.649689
C	12.689197	29.052212	-0.716124
C	13.238917	27.840443	1.281443
C	13.630944	28.308790	-1.419858
H	12.111095	29.823510	-1.214059
C	14.182167	27.098304	0.569350
H	13.125262	27.664078	2.347294
C	14.400806	27.308923	-0.799717
H	13.768209	28.516324	-2.477949
H	14.758588	26.352221	1.105685
C	15.432304	26.511697	-1.617908
C	14.714148	25.776032	-2.774677
C	16.485472	27.481543	-2.205519
C	16.170662	25.460041	-0.767790
H	13.968670	25.071619	-2.387967
H	14.197845	26.473671	-3.442432
H	15.437175	25.210880	-3.376110
H	17.018873	28.009974	-1.407002
H	17.223458	26.930623	-2.801919
H	16.026908	28.234805	-2.854589
H	16.889990	24.918040	-1.392460
H	16.729608	25.919736	0.055362
H	15.480530	24.722410	-0.342244

4Int1(Cb)'

H	7.227158	32.705407	2.579362
S	8.392715	33.058586	3.164050
Fe	9.820001	31.867119	1.764579
N	9.959622	33.234527	0.171358
N	11.343895	32.730380	2.703343
N	9.960714	30.066364	3.331792
N	8.329708	30.910080	0.868248
C	9.202254	33.235509	-0.951903
C	9.623550	34.319787	-1.825566
C	10.653109	34.949508	-1.191073
C	10.855121	34.246099	0.066199
C	12.043417	33.818118	2.231221
C	13.077375	34.163844	3.179561
C	12.977683	33.287791	4.218251
C	11.891146	32.384613	3.911297
C	10.431998	30.467043	4.620274
C	9.607327	29.862891	5.602422
C	8.560217	29.226395	4.961454
C	8.707185	29.418388	3.564381
C	7.655737	29.802911	1.315585

C	6.664625	29.419856	0.335159
C	6.766743	30.296210	-0.703250
C	7.811298	31.235783	-0.365821
C	8.192187	32.297906	-1.192214
H	7.647110	32.388047	-2.127833
C	11.822481	34.516474	1.039958
H	12.487851	35.355064	0.853807
C	11.438678	31.398764	4.811321
H	11.850778	31.464158	5.815174
C	7.777846	29.168286	2.568262
H	6.972106	28.483554	2.821411
H	11.227060	35.801415	-1.533823
H	9.189767	34.554873	-2.789539
H	13.778241	34.979727	3.055895
H	13.582277	33.239712	5.115037
H	9.722382	30.000503	6.670288
H	7.697756	28.770352	5.431424
H	5.991236	28.578368	0.438218
H	6.192116	30.318056	-1.620601
O	11.060753	30.729970	0.832867
C	10.924507	29.217432	2.616354
C	11.400961	29.591604	1.404334
H	11.226836	28.317955	3.138684
C	12.368960	28.748654	0.647252
C	13.197785	29.349332	-0.312438
C	12.489042	27.366828	0.841659
C	14.122589	28.595256	-1.027354
H	13.104321	30.415702	-0.488267
C	13.420851	26.617637	0.122376
H	11.834215	26.859773	1.544445
C	14.263927	27.210627	-0.828415
H	14.746698	29.101417	-1.759277
H	13.472680	25.550178	0.307573
C	15.295881	26.414667	-1.647164
C	14.950273	26.521863	-3.151831
C	16.709010	26.996879	-1.404739
C	15.323341	24.922049	-1.265885
H	13.957751	26.103667	-3.355412
H	14.950386	27.561635	-3.495144
H	15.682936	25.969722	-3.753836
H	16.984864	26.928180	-0.346203
H	17.455432	26.443204	-1.987941
H	16.771851	28.049976	-1.698011
H	16.076187	24.400716	-1.868238
H	15.584389	24.776155	-0.211327
H	14.359097	24.434692	-1.450120

2TSoc-thr

H	7.642736	33.503317	1.581705
S	7.658202	32.172255	1.826414
Fe	9.855453	31.876315	1.855787
N	10.237345	32.962607	0.210969
N	10.274400	33.493462	2.969452
N	9.872609	30.733542	3.504016
N	9.824065	30.204449	0.744661
C	10.136919	32.528841	-1.093439
C	10.339449	33.624333	-2.007163
C	10.561093	34.733524	-1.249778
C	10.485616	34.316908	0.127025
C	10.510946	34.782490	2.539009
C	10.614831	35.679806	3.661288
C	10.425251	34.929383	4.781146
C	10.213804	33.572802	4.343621
C	9.875411	31.179839	4.805933

C	9.748263	30.072548	5.721384
C	9.668341	28.945423	4.964748
C	9.737346	29.365667	3.587542
C	9.683340	28.904337	1.177501
C	9.549462	28.008407	0.056673
C	9.596756	28.776735	-1.066083
C	9.769208	30.140370	-0.629891
C	9.903245	31.220357	-1.488348
H	9.847319	31.022413	-2.554374
C	10.620810	35.170543	1.211996
H	10.802996	36.221238	1.007124
C	10.016333	32.500908	5.200846
H	9.998087	32.709449	6.266205
C	9.653967	28.505151	2.504587
H	9.540809	27.445230	2.709924
H	10.755527	35.747242	-1.576563
H	10.317672	33.536708	-3.086039
H	10.805490	36.742825	3.584401
H	10.431676	35.247410	5.816036
H	9.733788	30.165226	6.799937
H	9.572091	27.917416	5.290014
H	9.432541	26.935246	0.137928
H	9.527440	28.466630	-2.101079
O	13.164349	30.931491	2.095594
C	14.278802	31.020792	1.699609
C	15.270224	30.447113	0.861735
H	16.271572	30.518459	1.291642
C	15.017527	29.249434	0.038689
C	13.726506	28.831099	-0.332061
C	16.099415	28.499190	-0.445798
C	13.543601	27.719154	-1.147384
H	12.856774	29.373647	0.026369
C	15.906675	27.389164	-1.268505
H	17.113186	28.791866	-0.179471
C	14.623733	26.966845	-1.642175
H	12.524600	27.437200	-1.398529
H	16.782540	26.850125	-1.613627
C	14.368284	25.746080	-2.543752
C	13.516782	24.705977	-1.776871
C	13.604967	26.192323	-3.813921
C	15.675141	25.061608	-2.987072
H	14.038798	24.361618	-0.876736
H	12.552777	25.121448	-1.464593
H	13.315628	23.832228	-2.409585
H	14.189573	26.922424	-4.385462
H	13.405125	25.331488	-4.464387
H	12.643196	26.654775	-3.567685
H	15.445114	24.203224	-3.628767
H	16.316226	25.740917	-3.560641
H	16.250717	24.689408	-2.131723
O	15.023405	32.518694	1.787781
H	15.367173	31.935812	0.760738
C	14.108617	33.625714	1.662968
H	13.671760	33.628064	0.655139
H	13.298434	33.454531	2.377652
C	14.848271	34.921552	1.952195
H	14.150511	35.764490	1.892351
H	15.283223	34.901512	2.956389
H	15.653803	35.089242	1.229290

4TSoc-thr

H	7.499182	33.566699	1.462982
S	7.418594	32.242508	1.725222
Fe	9.771842	31.902361	1.801667

N	10.274589	32.929167	0.134169
N	10.272345	33.523730	2.898579
N	9.825439	30.789410	3.484815
N	9.818298	30.196509	0.720530
C	10.243668	32.460760	-1.162163
C	10.475411	33.536163	-2.089621
C	10.644598	34.666540	-1.348668
C	10.514369	34.282674	0.032467
C	10.506838	34.800382	2.434973
C	10.633021	35.718072	3.536803
C	10.469695	34.990076	4.676909
C	10.244946	33.627623	4.272889
C	9.866002	31.254938	4.779928
C	9.705094	30.167555	5.710299
C	9.565458	29.034427	4.969669
C	9.638851	29.429812	3.586704
C	9.619934	28.915923	1.185911
C	9.517137	27.992456	0.086081
C	9.651112	28.723519	-1.055713
C	9.838387	30.092921	-0.653034
C	10.030774	31.143293	-1.536259
H	10.027460	30.915731	-2.597353
C	10.617423	35.162298	1.100257
H	10.799465	36.208524	0.875308
C	10.049459	32.576244	5.154826
H	10.054008	32.802473	6.216278
C	9.533077	28.550625	2.520475
H	9.378040	27.500568	2.746388
H	10.840773	35.674846	-1.690649
H	10.505331	33.423309	-3.165806
H	10.821055	36.779450	3.434848
H	10.499145	35.329261	5.704504
H	9.707408	30.275224	6.787398
H	9.428395	28.016352	5.310952
H	9.361623	26.926364	0.191831
H	9.630211	28.383050	-2.083067
O	13.404002	30.738273	2.369225
C	14.445565	30.920097	1.832971
C	15.353545	30.447974	0.849440
H	16.396261	30.582663	1.144590
C	15.077727	29.256762	0.024079
C	13.785182	28.734301	-0.164474
C	16.131577	28.620331	-0.648641
C	13.573912	27.632465	-0.986869
H	12.938647	29.186489	0.343668
C	15.909247	27.520319	-1.477212
H	17.145675	28.996085	-0.527367
C	14.624717	26.993941	-1.669047
H	12.556008	27.267075	-1.093990
H	16.763981	27.071924	-1.972343
C	14.338509	25.776933	-2.566282
C	13.723877	24.641553	-1.712815
C	13.339558	26.175750	-3.678822
C	15.612597	25.233676	-3.241047
H	14.414237	24.331169	-0.920103
H	12.788841	24.954387	-1.236033
H	13.505458	23.765641	-2.336790
H	13.752440	26.972962	-4.307708
H	13.117371	25.314923	-4.322000
H	12.391782	26.535045	-3.264025
H	15.359527	24.374997	-3.873545
H	16.087341	25.987176	-3.880014
H	16.351082	24.895417	-2.505152
O	15.088545	32.470376	1.875726
H	15.328010	31.940233	0.791182
C	14.090985	33.509349	1.919241
H	13.561271	33.548759	0.957930

H	13.365613	33.226390	2.688095
C	14.759514	34.835982	2.240654
H	13.999322	35.622243	2.310275
H	15.289172	34.779039	3.196848
H	15.478116	35.117528	1.463531

6TSoc-thr

H	6.925809	33.377929	0.975000
S	7.063307	32.673397	2.121305
Fe	9.377214	32.672018	2.067942
N	9.889974	33.633507	0.276175
N	9.923654	34.464078	3.036416
N	9.841836	31.702266	3.861929
N	9.884637	30.871479	1.101345
C	9.933578	33.051159	-0.971847
C	10.012109	34.074221	-1.984322
C	10.024813	35.276019	-1.337036
C	9.954496	34.994887	0.075203
C	9.980100	35.710221	2.457163
C	10.046306	36.724696	3.482515
C	10.023523	36.077669	4.682421
C	9.943862	34.664371	4.396760
C	9.872046	32.283227	5.110559
C	9.902299	31.258228	6.124304
C	9.898264	30.057008	5.476865
C	9.863358	30.340181	4.063526
C	9.905486	29.626323	1.683145
C	9.969922	28.608667	0.660409
C	9.986953	29.253767	-0.540779
C	9.931667	30.669056	-0.257706
C	9.940659	31.678637	-1.218089
H	9.980579	31.367342	-2.257791
C	9.983668	35.955837	1.085347
H	10.032823	36.994667	0.772194
C	9.907271	33.654894	5.356756
H	9.926930	33.966690	6.396922
C	9.882306	29.380310	3.053991
H	9.908810	28.341052	3.366751
H	10.088665	36.267374	-1.767738
H	10.063672	33.887256	-3.049532
H	10.106916	37.789590	3.296386
H	10.061753	36.506404	5.675901
H	9.934855	31.443750	7.190483
H	9.928177	29.064046	5.907076
H	10.004884	27.543560	0.850767
H	10.039916	28.823350	-1.532649
O	13.479169	29.194291	2.418892
C	14.402364	29.676462	1.852030
C	15.299683	29.544916	0.756784
H	16.316645	29.848288	1.014759
C	15.196366	28.441447	-0.216166
C	13.991144	27.763566	-0.477047
C	16.321105	28.057273	-0.961344
C	13.931952	26.753117	-1.430981
H	13.093562	28.027277	0.074604
C	16.250845	27.047212	-1.921279
H	17.271110	28.559318	-0.789130
C	15.055902	26.363020	-2.181097
H	12.978721	26.255974	-1.592868
H	17.155096	26.794537	-2.464695
C	14.939401	25.235010	-3.221237
C	14.477493	23.933570	-2.522654
C	13.901916	25.630486	-4.299383
C	16.278600	24.949425	-3.927318

H	15.198883	23.622741	-1.758268
H	13.506221	24.058330	-2.032409
H	14.381438	23.119314	-3.251910
H	14.208273	26.545326	-4.819715
H	13.799181	24.832216	-5.045249
H	12.912593	25.809623	-3.864919
H	16.149283	24.138383	-4.653202
H	16.647116	25.825665	-4.473055
H	17.053845	24.637578	-3.218079
O	14.706238	31.299779	2.086419
H	14.969077	30.995135	0.927557
C	13.519062	32.086868	2.322388
H	12.900927	32.093694	1.414622
H	12.951931	31.580103	3.108958
C	13.918559	33.493821	2.732621
H	13.016574	34.084901	2.926047
H	14.528323	33.473854	3.641574
H	14.491979	33.988388	1.941188

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H	8.101654	33.814589	2.905222
S	7.929353	32.500408	2.633614
Fe	9.930359	32.087602	1.752894
N	9.922876	33.767411	0.645209
N	10.924736	33.078503	3.194893
N	10.113181	30.365916	2.786066
N	9.139489	31.044920	0.222745
C	9.354016	33.916042	-0.594801
C	9.487327	35.281411	-1.046064
C	10.149684	35.956173	-0.066972
C	10.413487	35.004223	0.986025
C	11.284021	34.406040	3.210456
C	11.901587	34.743765	4.469628
C	11.898734	33.610366	5.223727
C	11.286763	32.577462	4.422747
C	10.571928	30.239870	4.076077
C	10.443234	28.872872	4.521187
C	9.896450	28.172860	3.489308
C	9.685245	29.113343	2.415279
C	8.852371	29.703289	0.175090
C	8.208338	29.370623	-1.073481
C	8.095755	30.530356	-1.775297
C	8.677261	31.570068	-0.958341
C	8.766236	32.901852	-1.339876
H	8.356318	33.170111	-2.309023
C	11.060994	35.307128	2.177300
H	11.393728	36.330551	2.322861
C	11.117131	31.263588	4.840295
H	11.448140	31.013909	5.843932
C	9.112470	28.793219	1.190845
H	8.818194	27.760694	1.028376
H	10.436978	36.999914	-0.040831
H	9.119940	35.655020	-1.993696
H	12.275977	35.726276	4.728421
H	12.272668	33.468277	6.229974
H	10.738971	28.512966	5.498630
H	9.646539	27.120258	3.445119
H	7.886953	28.375825	-1.355186
H	7.664604	30.687062	-2.756087
O	12.006001	31.778916	0.731967
C	13.177004	31.478774	0.906127
C	13.682062	30.349114	1.785098
H	12.884493	30.091780	2.483945
C	14.079284	29.144289	0.944374

C	13.165447	28.112876	0.696075
C	15.352747	29.046161	0.377616
C	13.522712	27.022469	-0.093817
H	12.167865	28.162853	1.124787
C	15.705319	27.949951	-0.412291
H	16.079588	29.835989	0.550438
C	14.799671	26.911277	-0.669926
H	12.784289	26.243109	-0.261533
H	16.706723	27.916424	-0.827075
C	15.150228	25.689306	-1.538429
C	15.012383	24.399630	-0.694376
C	14.180567	25.618559	-2.742420
C	16.589045	25.751927	-2.086083
H	15.696410	24.416363	0.161899
H	13.996061	24.272900	-0.306899
H	15.249913	23.518097	-1.302658
H	14.263585	26.516258	-3.365724
H	14.411974	24.747212	-3.367418
H	13.137308	25.531086	-2.421603
H	16.789377	24.865208	-2.698175
H	16.746672	26.632526	-2.719386
H	17.332419	25.771610	-1.280875
O	14.178194	32.112280	0.285086
H	14.545465	30.714471	2.351353
C	13.811259	33.175272	-0.634140
H	13.170982	32.751471	-1.413651
H	13.227478	33.921835	-0.088398
C	15.098252	33.747277	-1.197241
H	14.865292	34.552943	-1.901887
H	15.726614	34.158158	-0.400343
H	15.669859	32.979271	-1.728139

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H	7.802593	33.994021	2.959943
S	7.542776	32.675139	2.813075
Fe	9.655784	32.147470	1.823866
N	9.755941	33.725185	0.572073
N	10.814214	33.154435	3.138562
N	9.972378	30.456097	2.885049
N	8.924356	31.024143	0.314993
C	9.188877	33.819086	-0.677726
C	9.348032	35.151876	-1.200437
C	10.024267	35.865770	-0.258374
C	10.273397	34.970366	0.842931
C	11.185917	34.477766	3.073423
C	11.865357	34.866665	4.282425
C	11.896381	33.768452	5.087536
C	11.241710	32.706342	4.368406
C	10.513055	30.368000	4.148437
C	10.417090	29.017787	4.640220
C	9.812973	28.285177	3.663472
C	9.534558	29.188981	2.576767
C	8.627045	29.682448	0.345636
C	7.970195	29.286449	-0.874495
C	7.866247	30.403583	-1.644954
C	8.464360	31.480855	-0.897899
C	8.573066	32.782458	-1.362664
H	8.163962	33.001602	-2.343851
C	10.940482	35.329758	2.005772
H	11.288715	36.354575	2.089736
C	11.095280	31.413840	4.849622
H	11.479460	31.200784	5.842245
C	8.907627	28.819903	1.394843
H	8.608152	27.782124	1.287176
H	10.333132	36.903058	-0.289795
H	8.988395	35.479831	-2.167453
H	12.259452	35.856472	4.475440
H	12.323096	33.669000	6.077526

H	10.774037	28.688774	5.607862
H	9.568307	27.230535	3.664631
H	7.638499	28.279873	-1.095483
H	7.433381	30.505881	-2.631879
O	12.299351	31.606245	0.513046
C	13.440436	31.406808	0.877996
C	13.888444	30.233123	1.735423
H	13.064430	29.990388	2.411077
C	14.234176	29.036274	0.864469
C	13.286711	28.039368	0.602196
C	15.496327	28.914829	0.277151
C	13.601989	26.956551	-0.215343
H	12.295137	28.111850	1.042513
C	15.807069	27.827166	-0.541744
H	16.247479	29.679969	0.458682
C	14.868793	26.820459	-0.808884
H	12.839414	26.202572	-0.391255
H	16.801607	27.774758	-0.970908
C	15.175115	25.604857	-1.702737
C	15.018584	24.305656	-0.876592
C	14.186368	25.575858	-2.892768
C	16.606651	25.641225	-2.271407
H	15.717451	24.291096	-0.032303
H	14.006089	24.199327	-0.473175
H	15.222579	23.427978	-1.502481
H	14.281655	26.480974	-3.503391
H	14.387926	24.709051	-3.534182
H	13.146083	25.507847	-2.557806
H	16.776076	24.760075	-2.900670
H	16.776431	26.528282	-2.892431
H	17.362082	25.629436	-1.477394
O	14.479970	32.190782	0.531138
H	14.756531	30.536131	2.328826
C	14.174117	33.304296	-0.342970
H	13.725225	32.914278	-1.262027
H	13.430758	33.940720	0.146863
C	15.473132	34.041695	-0.609996
H	15.285568	34.895801	-1.270045
H	15.909913	34.415879	0.321729
H	16.204019	33.386248	-1.094714

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H	7.665689	34.035653	3.045430
S	7.379671	32.723003	2.889801
Fe	9.432661	32.203628	1.929006
N	9.695040	33.754249	0.551119
N	10.790701	33.214006	3.166127
N	9.956560	30.447025	2.948233
N	8.864452	30.981781	0.331346
C	9.152563	33.801680	-0.709603
C	9.332922	35.122191	-1.266667
C	9.997712	35.860399	-0.332042
C	10.224353	34.995536	0.803160
C	11.160158	34.533651	3.064526
C	11.874650	34.931593	4.254761
C	11.928579	33.839169	5.070308
C	11.251693	32.765816	4.381483
C	10.535782	30.386387	4.193768
C	10.482578	29.030917	4.689118
C	9.870468	28.280319	3.728058
C	9.542522	29.173666	2.641311
C	8.605954	29.634874	0.380930
C	7.985322	29.211937	-0.853521
C	7.878544	30.318385	-1.642905
C	8.435802	31.422806	-0.896508
C	8.553515	32.729102	-1.370010
H	8.169020	32.923280	-2.367135
C	10.893657	35.360449	1.972179
H	11.249825	36.384834	2.034388

C	11.120449	31.462638	4.861791
H	11.538202	31.259532	5.843724
C	8.910580	28.798434	1.454763
H	8.637677	27.751865	1.354490
H	10.316361	36.893308	-0.397244
H	9.000596	35.429449	-2.250309
H	12.281845	35.919332	4.431470
H	12.390409	33.754540	6.046034
H	10.873465	28.704992	5.644838
H	9.658610	27.218524	3.742443
H	7.682712	28.196920	-1.078431
H	7.472630	30.390229	-2.644072
O	12.361518	31.609166	0.366940
C	13.466475	31.409791	0.825051
C	13.851270	30.216084	1.687125
H	12.993857	29.987298	2.325359
C	14.200582	29.019284	0.818383
C	13.245684	28.037940	0.526588
C	15.474829	28.882462	0.261079
C	13.565183	26.954888	-0.288930
H	12.244468	28.123448	0.941921
C	15.789702	27.795264	-0.557006
H	16.232303	29.635610	0.465654
C	14.843751	26.803829	-0.852752
H	12.796434	26.212791	-0.487428
H	16.793355	27.731029	-0.962917
C	15.153859	25.588346	-1.745567
C	14.968502	24.288112	-0.926989
C	14.187217	25.573396	-2.953825
C	16.595786	25.611881	-2.287917
H	15.652301	24.262699	-0.070669
H	13.948032	24.192517	-0.541290
H	15.173097	23.410008	-1.552186
H	14.302274	26.480299	-3.558305
H	14.392729	24.707514	-3.595286
H	13.140344	25.513577	-2.638579
H	16.767369	24.731841	-2.918223
H	16.785831	26.500079	-2.901400
H	17.336584	25.588576	-1.480518
O	14.527469	32.212492	0.593738
H	14.700734	30.490400	2.319874
C	14.282832	33.350564	-0.265657
H	13.903291	32.989928	-1.227090
H	13.503160	33.971069	0.187309
C	15.594977	34.098471	-0.414299
H	15.453377	34.972242	-1.059989
H	15.961227	34.444219	0.557966
H	16.361898	33.459191	-0.863788

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H	8.162157	33.572911	1.156881
S	8.110640	32.238533	1.373296
Fe	10.311753	31.833215	1.503784
N	10.710271	32.943631	-0.135541
N	10.606275	33.476461	2.639158
N	10.066023	30.701218	3.148001
N	10.073339	30.182840	0.371926
C	10.708826	32.488335	-1.432413
C	11.010411	33.568212	-2.334917
C	11.165685	34.696780	-1.566118
C	10.956804	34.293314	-0.196292
C	10.826375	34.766857	2.217272
C	10.864535	35.664331	3.349065

C	10.664624	34.901617	4.458087
C	10.498348	33.539246	4.004265
C	10.080629	31.144312	4.444292
C	9.834764	30.044699	5.353546
C	9.655626	28.937284	4.587936
C	9.793539	29.358959	3.210905
C	9.748118	28.921116	0.789300
C	9.563674	28.045311	-0.346863
C	9.792927	28.794633	-1.457141
C	10.110920	30.129264	-0.999437
C	10.430528	31.184228	-1.838603
H	10.449464	30.983773	-2.905570
C	11.007250	35.154869	0.898359
H	11.185242	36.208008	0.701284
C	10.277774	32.457182	4.849610
H	10.239832	32.659569	5.915729
C	9.633089	28.522057	2.116549
H	9.390745	27.481631	2.309724
H	11.353572	35.712156	-1.894146
H	11.065256	33.478877	-3.412850
H	11.021775	36.733813	3.284270
H	10.624465	35.214695	5.493857
H	9.801960	30.133758	6.432082
H	9.444942	27.923228	4.903083
H	9.298934	26.997604	-0.280917
H	9.761668	28.490981	-2.495693
O	12.470139	31.240734	1.634267
C	13.533990	31.616690	1.105018
C	14.425320	31.033780	0.214192
H	15.394862	31.524354	0.147223
C	14.376212	29.670804	-0.324092
C	13.364532	28.736631	-0.028842
C	15.408499	29.240331	-1.177628
C	13.396373	27.455576	-0.571001
H	12.560226	29.021170	0.638431
C	15.430992	27.954671	-1.715731
H	16.214509	29.929858	-1.424327
C	14.422669	27.023795	-1.429135
H	12.590772	26.773836	-0.311154
H	16.256075	27.685463	-2.367029
C	14.403312	25.595752	-2.001826
C	14.425988	24.570644	-0.843003
C	13.116307	25.391732	-2.836887
C	15.613082	25.312247	-2.912776
H	15.333325	24.685296	-0.238936
H	13.565285	24.691579	-0.176737
H	14.404391	23.545771	-1.235061
H	13.080738	26.094970	-3.677191
H	13.077334	24.372983	-3.243541
H	12.214468	25.546931	-2.235231
H	15.556100	24.287126	-3.297203
H	15.641116	25.987515	-3.775879
H	16.561524	25.410423	-2.372128
O	13.952924	33.013945	1.366201
H	13.941248	33.621302	0.126789
C	13.953778	33.481987	2.735455
H	13.753432	34.554675	2.685587
H	13.120750	32.999940	3.247674
C	15.288221	33.181481	3.400576
H	15.278829	33.546490	4.434338
H	15.477846	32.103242	3.421538
H	16.114655	33.667690	2.870923
O	13.970336	33.581440	-0.971720
H	14.020352	32.556494	-1.001045
H	13.080935	33.855785	-1.330289

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H	7.414262	33.198452	2.254712
S	7.565127	32.305035	1.251039
Fe	9.880357	31.908620	1.632627
N	10.608123	32.830310	-0.027258
N	10.292351	33.573004	2.689111
N	9.730899	30.885252	3.368727
N	9.913324	30.164254	0.637449
C	10.739184	32.283099	-1.282642
C	11.131456	33.293792	-2.229210
C	11.214830	34.471933	-1.536595
C	10.878218	34.171679	-0.168079
C	10.578367	34.824654	2.181817
C	10.621271	35.795335	3.242947
C	10.372212	35.124194	4.402520
C	10.169139	33.743919	4.051004
C	9.706226	31.405000	4.641504
C	9.416344	30.369282	5.603012
C	9.250195	29.217471	4.900023
C	9.444044	29.547307	3.509372
C	9.579353	28.926931	1.137505
C	9.551177	27.949003	0.080860
C	9.888404	28.599349	-1.066515
C	10.114475	29.976809	-0.712836
C	10.505925	30.954517	-1.611744
H	10.642492	30.660042	-2.647126
C	10.847030	35.112191	0.853387
H	11.065207	36.143833	0.595539
C	9.902551	32.736865	4.968320
H	9.841447	33.014242	6.015808
C	9.350736	28.632727	2.473995
H	9.104515	27.606818	2.727905
H	11.455621	35.458665	-1.912576
H	11.297177	33.120055	-3.285028
H	10.827041	36.849156	3.104307
H	10.329977	35.513725	5.411699
H	9.350831	30.524408	6.672330
H	9.021041	28.226392	5.269937
H	9.316792	26.901461	0.219720
H	9.993569	28.197025	-2.065598
O	13.355341	31.012760	1.834578
C	14.239208	31.430848	1.115396
C	14.944904	30.975185	-0.012288
H	15.918416	31.443420	-0.153663
C	14.807567	29.615600	-0.554977
C	13.766579	28.729758	-0.209211
C	15.739633	29.152857	-1.501415
C	13.676570	27.467396	-0.788656
H	13.035750	29.033320	0.531923
C	15.640940	27.885974	-2.075328
H	16.561724	29.803085	-1.796174
C	14.604629	27.004329	-1.737299
H	12.852767	26.826681	-0.482749
H	16.396011	27.591285	-2.796893
C	14.459471	25.598402	-2.345665
C	14.510901	24.536503	-1.221341
C	13.103914	25.490421	-3.084609
C	15.578918	25.277525	-3.354621
H	15.465964	24.582671	-0.685616
H	13.711573	24.682973	-0.487081
H	14.401820	23.526926	-1.638132
H	13.046622	26.218542	-3.902376
H	12.974470	24.487709	-3.511973
H	12.260728	25.677836	-2.410883
H	15.434718	24.269834	-3.761840
H	15.581295	25.977950	-4.197840
H	16.568983	25.306201	-2.885395

O	14.645445	32.910997	1.331921
H	14.383541	33.416010	0.179147
C	14.138609	33.546205	2.528061
H	14.005980	34.601476	2.270047
H	13.165242	33.111670	2.764581
C	15.120391	33.369332	3.675004
H	14.749474	33.888120	4.566804
H	15.233614	32.308594	3.919416
H	16.103739	33.776887	3.418540
O	14.244024	33.404711	-0.976158
H	14.379374	32.341408	-0.964577
H	13.308228	33.585701	-1.218455

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H	6.657651	32.528663	0.948140
S	7.221047	31.932853	2.023742
Fe	9.128529	33.240898	2.002181
N	8.823731	34.622780	0.455938
N	8.703730	34.814821	3.331845
N	10.237919	32.382245	3.552576
N	10.427087	32.234555	0.674881
C	9.045001	34.405549	-0.887171
C	8.435269	35.461446	-1.657946
C	7.855043	36.319243	-0.769702
C	8.106849	35.793706	0.549996
C	8.002324	35.957064	3.029634
C	7.620504	36.634457	4.248136
C	8.096184	35.886620	5.282754
C	8.771158	34.747456	4.702956
C	10.095374	32.650391	4.894189
C	10.798650	31.656751	5.668479
C	11.372372	30.792740	4.781799
C	11.021540	31.252478	3.459966
C	11.177006	31.125319	0.984007
C	11.669761	30.514778	-0.229190
C	11.205051	31.276058	-1.270841
C	10.425669	32.346135	-0.694050
C	9.777391	33.347127	-1.419158
H	9.866950	33.306514	-2.500752
C	7.714656	36.403648	1.741910
H	7.150339	37.327550	1.656434
C	9.405034	33.740230	5.426369
H	9.376290	33.820319	6.509014
C	11.448973	30.662678	2.272590
H	12.093309	29.792982	2.352374
H	7.315037	37.234194	-0.978186
H	8.464439	35.534841	-2.737778
H	7.066436	37.563571	4.291776
H	8.010026	36.079585	6.344593
H	10.848681	31.637576	6.749830
H	11.985413	29.924850	4.988761
H	12.263519	29.609045	-0.268224
H	11.349216	31.114909	-2.332396
O	14.444378	29.263964	1.896859
C	15.159656	29.760483	1.045434
C	15.630591	29.391891	-0.224046
H	16.526736	29.916146	-0.553416
C	15.395786	28.068038	-0.819712
C	14.480838	27.124350	-0.308008
C	16.082233	27.706423	-1.992899
C	14.271482	25.906290	-0.948525
H	13.950125	27.344740	0.611716
C	15.866939	26.482611	-2.625076

H	16.800608	28.402962	-2.421939
C	14.952235	25.545532	-2.123855
H	13.556526	25.215498	-0.507619
H	16.432686	26.267163	-3.525811
C	14.683439	24.184715	-2.789663
C	15.026438	23.045378	-1.800172
C	13.189576	24.085493	-3.181545
C	15.526039	23.979852	-4.063355
H	16.084408	23.080749	-1.515728
H	14.433188	23.112344	-0.882092
H	14.827979	22.066909	-2.256076
H	12.920736	24.871227	-3.897222
H	12.976220	23.114210	-3.645896
H	12.533740	24.190369	-2.310748
H	15.301840	23.000970	-4.503191
H	15.309522	24.740848	-4.822001
H	16.600533	24.007518	-3.848836
O	15.537347	31.240537	1.262721
H	14.953513	31.781189	0.238614
C	15.265693	31.781734	2.577573
H	15.138562	32.858101	2.425842
H	14.327807	31.357985	2.944082
C	16.417156	31.483415	3.523443
H	16.223378	31.938911	4.501522
H	16.525825	30.403829	3.664013
H	17.358222	31.884237	3.133397
O	14.513551	31.806464	-0.833960
H	14.794825	30.784413	-0.950612
H	13.530137	31.783665	-0.777319

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H	7.846470	33.562367	1.605766
S	7.804216	32.210477	1.654143
Fe	9.985053	31.820351	1.700230
N	10.469172	33.084794	0.217549
N	10.429596	33.268120	3.020319
N	9.920419	30.479448	3.189977
N	9.910181	30.304344	0.387005
C	10.406682	32.817962	-1.133112
C	10.702956	34.003313	-1.895853
C	10.935547	35.003382	-0.997067
C	10.775118	34.426785	0.313254
C	10.715700	34.593579	2.762503
C	10.814099	35.338827	3.991455
C	10.575013	34.458928	5.002381
C	10.336846	33.175689	4.391531
C	9.911336	30.756886	4.538462
C	9.718972	29.549005	5.303174
C	9.606536	28.531807	4.408194
C	9.722117	29.119367	3.096852
C	9.691927	28.970715	0.647770
C	9.539145	28.230895	-0.579970
C	9.659377	29.128879	-1.595231
C	9.894280	30.415377	-0.985773
C	10.121333	31.582722	-1.697099
H	10.096061	31.522623	-2.780827
C	10.890430	35.137174	1.499408
H	11.120455	36.196057	1.431951
C	10.087953	32.010521	5.101265
H	10.051612	32.082702	6.183935
C	9.616145	28.408558	1.912614
H	9.447392	27.338400	1.979981
H	11.184317	36.039307	-1.189799
H	10.725806	34.050530	-2.977219
H	11.036315	36.396606	4.053896

H	10.563546	34.643331	6.069120
H	9.685037	29.505104	6.384312
H	9.459098	27.476407	4.598228
H	9.361517	27.164526	-0.637105
H	9.603864	28.954945	-2.662380
O	13.754318	30.847042	1.546401
C	14.492689	31.497301	0.843373
C	15.141908	31.061859	-0.464743
H	16.209864	31.300022	-0.395671
C	14.933378	29.608408	-0.811427
C	13.679694	29.132712	-1.216922
C	15.986871	28.695252	-0.747978
C	13.495764	27.792249	-1.539935
H	12.836770	29.816187	-1.277882
C	15.800392	27.349012	-1.075190
H	16.973880	29.034232	-0.439743
C	14.550276	26.863596	-1.477687
H	12.503989	27.468928	-1.842937
H	16.652858	26.681688	-1.010817
C	14.298653	25.389722	-1.843224
C	13.221437	24.803383	-0.899445
C	13.801617	25.297729	-3.305788
C	15.569040	24.527810	-1.713477
H	13.548713	24.852872	0.145365
H	12.273993	25.347047	-0.977685
H	13.026393	23.752414	-1.147104
H	14.550023	25.697422	-3.999702
H	13.607327	24.253056	-3.579126
H	12.873965	25.860168	-3.456108
H	15.341075	23.490042	-1.982829
H	16.366776	24.874230	-2.380532
H	15.957325	24.525816	-0.688559
O	14.850575	32.781158	1.127767
H	14.517392	33.918600	-0.524365
C	14.318908	33.345526	2.354671
H	13.231441	33.243139	2.349594
H	14.708624	32.765546	3.197236
C	14.753880	34.798458	2.407044
H	14.348815	35.271049	3.308300
H	15.844974	34.885955	2.428366
H	14.381389	35.345342	1.534035
O	14.245201	34.240219	-1.400230
H	14.747282	31.732506	-1.241689
H	13.275106	34.236135	-1.369610

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H	7.548028	33.046278	2.672204
S	7.550874	32.114367	1.692821
Fe	9.908851	31.821884	1.643507
N	10.340089	33.052614	0.085612
N	10.434036	33.300111	2.903508
N	10.104954	30.504094	3.167116
N	9.843461	30.279267	0.357809
C	10.256347	32.746495	-1.253653
C	10.457174	33.928141	-2.052767
C	10.642886	34.963593	-1.183883
C	10.557065	34.410779	0.144200
C	10.608553	34.633310	2.590259
C	10.783274	35.408583	3.788461
C	10.726098	34.537181	4.835551
C	10.513521	33.228719	4.279120
C	10.255943	30.796597	4.502575
C	10.178065	29.593988	5.294193
C	9.962863	28.568108	4.427819
C	9.911089	29.143428	3.106954

C	9.648135	28.952706	0.673127
C	9.447598	28.178263	-0.522505
C	9.535187	29.042845	-1.572408
C	9.788296	30.346521	-1.017696
C	9.987206	31.490468	-1.776037
H	9.930270	31.395392	-2.855628
C	10.666071	35.157482	1.307640
H	10.818573	36.227468	1.207380
C	10.433964	32.065102	5.030431
H	10.522965	32.155562	6.108332
C	9.679036	28.415904	1.951505
H	9.523792	27.346555	2.051578
H	10.812474	36.009281	-1.407198
H	10.443267	33.949983	-3.135047
H	10.938847	36.479760	3.810074
H	10.824798	34.746319	5.893153
H	10.275841	29.560102	6.371734
H	9.847250	27.513708	4.643432
H	9.270137	27.110553	-0.539941
H	9.444484	28.832375	-2.630420
O	13.851422	31.068709	1.487201
C	14.461238	31.738692	0.686413
C	15.049498	31.273784	-0.639470
H	16.114019	31.538719	-0.630898
C	14.860638	29.802868	-0.917029
C	13.611894	29.295599	-1.298332
C	15.922924	28.904107	-0.810448
C	13.439650	27.939053	-1.553926
H	12.763331	29.968391	-1.394120
C	15.748883	27.541671	-1.070762
H	16.906902	29.267137	-0.520476
C	14.502978	27.024846	-1.446823
H	12.450928	27.591235	-1.839413
H	16.607617	26.886078	-0.975499
C	14.265271	25.532051	-1.737281
C	13.196676	24.983103	-0.761743
C	13.765670	25.360843	-3.191775
C	15.544771	24.690702	-1.568459
H	13.527493	25.086364	0.278014
H	12.244270	25.514329	-0.862440
H	13.010119	23.919638	-0.957113
H	14.507765	25.733462	-3.907164
H	13.583024	24.301514	-3.411393
H	12.830975	25.903799	-3.368248
H	15.327240	23.638317	-1.784234
H	16.336771	25.011616	-2.254787
H	15.936183	24.744047	-0.546080
O	14.714355	33.069746	0.861607
H	14.264121	34.067280	-0.873704
C	14.273577	33.661114	2.113193
H	14.150917	34.721391	1.879793
H	13.305159	33.236252	2.382584
C	15.301859	33.446541	3.213025
H	14.979697	33.963531	4.124366
H	15.404178	32.381918	3.442178
H	16.279368	33.842873	2.918806
O	13.966137	34.236925	-1.783704
H	14.601989	31.904340	-1.420504
H	12.997498	34.237435	-1.722092

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H	6.974234	32.880522	1.786467
S	7.514768	31.642692	1.859443

Fe	9.663544	32.351088	1.371833
N	9.400876	34.021979	0.141681
N	10.102837	33.702194	2.916866
N	10.835815	30.954754	2.405364
N	10.182605	31.289733	-0.374972
C	9.147247	33.991727	-1.210342
C	8.735969	35.299777	-1.659092
C	8.755566	36.118622	-0.568546
C	9.173699	35.314305	0.554320
C	9.765088	35.034607	2.953543
C	9.927056	35.542379	4.295287
C	10.358783	34.502120	5.064671
C	10.469459	33.354340	4.196054
C	11.109139	30.989623	3.754614
C	11.668017	29.726428	4.171981
C	11.736986	28.935052	3.062754
C	11.209707	29.705157	1.963238
C	10.608812	29.980258	-0.432318
C	10.481128	29.485354	-1.780210
C	9.965560	30.501294	-2.531882
C	9.779295	31.626155	-1.650099
C	9.298850	32.876605	-2.033131
H	9.043040	33.002814	-3.080894
C	9.331673	35.780648	1.858738
H	9.104874	36.827794	2.036240
C	10.919715	32.093723	4.585540
H	11.176147	31.966965	5.633355
C	11.096522	29.250478	0.650217
H	11.431271	28.237924	0.449111
H	8.519947	37.174210	-0.519428
H	8.483409	35.551520	-2.681286
H	9.736118	36.564490	4.597221
H	10.592562	34.502950	6.121886
H	11.978687	29.490199	5.181832
H	12.119232	27.925715	2.982795
H	10.757185	28.488270	-2.097879
H	9.736602	30.501351	-3.590023
O	15.691130	30.035544	2.525725
C	15.303456	30.758361	1.634616
C	15.410677	30.488043	0.140621
H	16.442814	30.762552	-0.128270
C	15.132353	29.059200	-0.285353
C	14.254517	28.818261	-1.350153
C	15.752798	27.956588	0.311467
C	14.009948	27.522018	-1.800585
H	13.757256	29.655724	-1.833846
C	15.495769	26.659219	-0.138317
H	16.428326	28.109899	1.145932
C	14.622190	26.406304	-1.205549
H	13.330633	27.384747	-2.638179
H	15.999012	25.837634	0.359828
C	14.328524	24.990263	-1.734483
C	12.812636	24.699628	-1.624993
C	14.759939	24.895083	-3.217704
C	15.081642	23.901684	-0.946029
H	12.477862	24.752051	-0.582420
H	12.217372	25.413236	-2.204883
H	12.587457	23.695010	-2.003732
H	15.834375	25.082431	-3.325404
H	14.547028	23.894567	-3.614205
H	14.230548	25.621662	-3.843095
H	14.840862	22.914618	-1.357146
H	16.168014	24.030051	-1.010884
H	14.800634	23.896261	0.113373
O	14.760170	31.982573	1.864891
H	13.412656	32.725069	0.491891
C	14.722786	32.418948	3.248956

H	14.019961	31.781104	3.792332	O	12.968818	32.882245	-0.358593
H	15.716788	32.273486	3.681751	H	14.756217	31.181952	-0.393347
C	14.298284	33.875686	3.260512	H	12.143418	32.372569	-0.301545
H	14.265504	34.239628	4.293420				
H	15.006605	34.494227	2.699791				
H	13.302647	34.003833	2.824025				