

Supporting Information for

**Methane activation by metal-free Lewis acid centers only — A computational design
and mechanism study**

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Section 1: The method for fitting raw data

We started from the simplest model that ΔG^\ddagger is the first order polynomial function of the six properties (variables) and then gradually added second order and third order terms. Using only first order terms, the least-square fitting results in the R^2 of just 0.78. The mean unsigned error (MUE) of the fitting is 5.2 kcal/mol and the maximum error is 18.2 kcal/mol. This is not satisfactory at all. We might expect that for the purpose of prediction, the MUE of the fitting is better to drop to chemical accuracy, which is usually defined as 2.0 kcal/mol. We then added second order terms. The total number of fitting parameters are 28 including 6 first order terms, 21 second order terms, and one constant. Using all these 28 terms the MUE of the fitting drops to just 1.4 kcal/mol with a maximum error of 5.0 kcal/mol and the R^2 of 0.98. This is quite satisfactory but the fitting parameters are too many that the data may probably be over fitted. Considering simplicity and accuracy of the model, and the law of Occam's razor, variables should not be multiplied unnecessarily and the fitting parameters should be as less as possible. Backward elimination method is commonly used to eliminate terms with small contributions. However, using this method, we could only reduce the number of fitting parameters done to 14 and that is still too many. We tentatively set the maximum number of fitting parameters to 11, including a constant. We tried all possible combinations by selecting 10 out of 27 terms (excluding the constant). The best model (Mod1) we obtained by using the root-mean-square error (RMSE) as the criterion has an R^2 of 0.97, an MUE of 2.0 kcal/mol, and a maximum error of 6.7 kcal/mol. At last, we added all 56 third order terms. Selecting 10 out of 83 terms results in too many combinations. When relating to third second, firstly we used an alternative procedure by replacing two terms in Mod1 (2 out of 10, also excluding the constant) by one of possible combination of two terms in the 56 third order terms and then to get a new model. If the new model is better than the Mod1, we use the new model as the Mod1. If not, we do nothing to the Mod1. Then we continued to replace two terms in Mod1 excluding the constant by one of possible combination of two terms in the 56 third order terms to fit raw data. Repeating the above process until we got the satisfied model that meets our criterion with the MUE below 2.0 kcal/mol. This procedure was repeated for 20 times. The resulting model, which was named Mod2, has an R^2 of 0.98, an MUE of 1.6 kcal/mol, and a maximum error of 6.0 kcal/mol. Although there might still be room for improvement, we decided to stop here since the results are already quite satisfactory. The resulting two models are:

$$\begin{aligned} \Delta G^\ddagger (\text{Mod1}) &= a_0 + a_1 W_{BSi} + a_2 (n_{2p}^B)^2 + a_3 (\varepsilon_{2p}^B)^2 + a_4 q_B q_{Si} + a_5 q_B \varepsilon_{2p}^B + a_6 q_{Si} n_{2p}^B + a_7 q_{Si} \varepsilon_{2p}^B + a_8 W_{BSi} n_{2p}^B + a_9 \varepsilon_{2p}^B \\ &\quad a_{10} n_{2p}^B \varepsilon_{2p}^B \end{aligned} \quad (1)$$

$$\begin{aligned} \Delta G^\ddagger (\text{Mod2}) &= b_0 + b_1 W_{BSi} + b_2 (n_{2p}^B)^3 + b_3 W_{BSi} (\varepsilon_{2p}^B)^2 + b_4 q_B q_{Si} \varepsilon_{BSi} + b_5 q_B \varepsilon_{2p}^B + b_6 (\varepsilon_{BSi})^2 n_{2p}^B + b_7 q_{Si} \varepsilon_{BSi} \varepsilon_{2p}^B + b_8 \\ &\quad n_{2p}^B + b_9 q_{Si} \varepsilon_{BSi} n_{2p}^B + b_{10} n_{2p}^B \varepsilon_{2p}^B \end{aligned} \quad (2)$$

The fitted parameters are -118.6, 143.2, 272.6, -0.005547, 37.43, 0.8733, -47.90, -0.2586, -506.4, -1.524, and 0.8889 for a_0 to a_{10} , respectively, and -97.71, 119.4, 333.7, -0.007002, -0.1022, 0.9200, 0.002767, 0.0007769, -236.5, 0.1529, and 1.092 for b_0 to b_{10} , respectively.

Section 2: the derivatives of ΔG^\ddagger with respect to each property for each silylborane

Table S1. The partial Derivatives of the fitting model with respect to single properties: NBO charges (in a.u.) of B (q_B) and Si (q_{Si}) atoms, Wiberg bond order of the B-Si bond (W_{BSi}), energy of the bonding orbital of the B-Si bond (ε_{BSi} , in kcal/mol), occupancy (n_{2p}^B) and energy (ε_{2p}^B , in kcal/mol) of the empty $2p$ orbital of B.

silylborane	$\frac{\partial \Delta G^\ddagger}{\partial q_B}$	$\frac{\partial \Delta G^\ddagger}{\partial q_{Si}}$	$\frac{\partial \Delta G^\ddagger}{\partial W_{BSi}}$	$\frac{\partial \Delta G^\ddagger}{\partial \varepsilon_{BSi}}$	$\frac{\partial \Delta G^\ddagger}{\partial n_{2p}^B}$	$\frac{\partial \Delta G^\ddagger}{\partial \varepsilon_{2p}^B}$
M1	34.80	4.38	-37.17	-0.59	153.41	0.70
M2	19.11	20.62	12.08	-0.46	107.86	1.01
M3	-52.60	-6.44	-187.29	-1.10	330.94	1.61
M4	33.52	6.98	76.74	-0.17	26.39	0.18
M5	9.51	8.34	36.22	-0.36	71.76	0.61
M6	0.57	6.41	45.17	-0.33	91.16	0.55
M7	14.09	2.04	112.69	-0.04	10.38	0.00
M8	55.23	3.33	40.23	-0.37	64.32	0.15
M9	47.21	7.58	44.78	-0.36	53.54	0.29
M10	46.32	6.58	52.04	-0.32	39.90	0.24
M11	36.89	10.02	42.92	-0.38	47.43	0.42
M12	40.83	8.62	47.11	-0.35	40.72	0.35
M13	46.83	6.80	52.32	-0.32	32.79	0.24
M14	70.03	3.33	51.06	-0.35	50.17	-0.01
M15	25.23	14.28	32.05	-0.43	59.55	0.62
M16	43.04	7.00	51.29	-0.32	35.64	0.28
M17	13.70	14.19	16.12	-0.50	103.33	0.76
M18	3.99	10.13	20.83	-0.41	80.21	0.75
M19	40.01	9.47	42.73	-0.38	48.52	0.39
M20	45.00	7.45	49.85	-0.33	36.00	0.28
M21	42.41	6.67	51.93	-0.32	33.01	0.27
M22	19.41	10.37	33.06	-0.44	116.22	0.57
M23	33.15	11.00	39.21	-0.40	52.54	0.47
M24	21.34	7.66	40.20	-0.35	61.19	0.50
M25	59.99	3.37	49.60	-0.34	50.62	0.08
M26	32.60	1.40	27.07	-0.35	67.12	0.29
M27	23.35	7.33	40.01	-0.35	64.60	0.47
M28	30.13	9.02	39.64	-0.38	59.90	0.45
M29	63.36	-0.26	37.75	-0.30	30.83	-0.01
M30	-45.56	3.90	-11.32	-0.45	107.25	0.89
M31	146.19	-20.67	-143.31	-0.56	261.67	-0.64
M32	32.67	4.93	57.94	-0.24	48.85	0.23

M33	23.55	5.60	56.98	-0.26	60.68	0.32
M34	31.67	5.84	-37.98	-0.60	153.11	0.78
M35	-9.74	17.83	77.00	-0.19	62.00	0.72
M36	40.17	-8.95	-77.67	-0.70	208.75	0.47
M37	36.75	-8.29	-86.64	-0.74	225.76	0.56
M38	120.56	-31.31	-186.31	-0.72	346.69	-0.65
M39	33.73	-6.49	-86.34	-0.73	217.76	0.65
M40	-12.21	-23.77	-54.55	-0.62	138.55	0.32
M41	39.84	5.40	61.59	-0.22	47.64	0.16
M42	-92.23	-6.47	-326.87	-1.44	512.51	2.29
M43	-58.42	-8.17	-294.49	-1.34	459.32	1.88
M44	43.77	6.90	64.70	-0.20	55.83	0.14
M45	37.21	2.37	55.59	-0.30	51.04	0.16
M46	47.38	4.96	113.64	-0.05	-42.81	-0.23
M47	45.84	-14.14	-90.00	-0.60	80.90	0.24
M48	51.78	2.57	49.49	-0.27	-1.28	0.10
M49	54.14	2.66	49.35	-0.28	14.90	0.09
M50	56.07	4.01	57.22	-0.27	18.84	0.07

Section 3: Cartesian coordinates for the silylboranes and transition states

M1
0 1
B,-0.0100952442,1.3875153067,0.0038981885
H,-0.2296763267,4.267233441,0.0733359975
H,-2.0356696228,3.1191082521,1.1674718654
H,-1.9224653356,3.1860198607,-1.2370249525
O,0.7701504965,0.9947097,-1.0529100387
O,0.0570886387,0.515021312,1.0588626653
C,1.1276561178,-0.4217539296,0.7808347701
C,1.2315855194,-0.351204091,-0.7766395991
C,2.6370088173,-0.5144317018,-1.331742624
H,3.0444648879,-1.4934427404,-1.0577289895
H,2.6073443433,-0.4480520292,-2.4223532022
H,3.3058998898,0.2634585408,-0.9601131431
C,0.2661394309,-1.3005406028,-1.4839739934
H,0.2460220118,-1.0506693582,-2.5476180471
H,0.5805294929,-2.3425929019,-1.3748405437
H,-0.7485860625,-1.1965734298,-1.0884104298
C,0.7464481306,-1.7845084369,1.335389878
H,1.4981324789,-2.5322747099,1.0608627753
H,0.6963712332,-1.732408356,2.4260257155
H,-0.226881011,-2.1087535939,0.9637119084
C,2.3723231181,0.1119030997,1.4877593859
H,2.1495450001,0.2239080912,2.5517277385
H,3.217766323,-0.5733708199,1.3772727325
H,2.6597174313,1.0908564739,1.0927327051
Si,-1.1171287586,3.0786146234,0.0044082371

M1_TS

0 1

B,-0.9668599884,-0.5478747738,0.1278682384
Si,-2.7155430079,0.8123819388,-0.3209959749
H,-4.0875156594,0.2567257171,-0.492248695
H,-2.7616758042,1.8030182569,0.7812542673
H,-2.3214958359,1.4670028717,-1.5904003831
C,-1.5974395583,-2.1803976479,0.6380782009
H,-0.7816726164,-2.7400876369,0.1792512706
H,-2.5415034145,-2.6286847403,0.3113643536
H,-1.537463171,-2.1757948433,1.7261509652
H,-2.1739252085,-0.9578985195,0.1917640397
O,-0.2195206912,-0.037538102,1.2149845246
O,-0.1907541446,-0.5954597086,-1.0554199063
C,1.1580446631,-0.295441,-0.6559281236
C,0.9436293228,0.5699582392,0.6304925985
C,2.0809798286,0.5020194716,1.6382047774
H,3.0174143585,0.8454789132,1.1856052207
H,1.8535151185,1.1494057834,2.4895814044
H,2.2180172123,-0.5148065189,2.0100592085
C,0.6205929822,2.028979944,0.3017540882
H,0.2384335158,2.5151629303,1.2033766291
H,1.5107442612,2.5676071238,-0.0371650349
H,-0.139864152,2.1036952777,-0.4820701324
C,1.8514884071,0.4290693529,-1.7995043019
H,2.8421054773,0.7800056431,-1.4903680967
H,1.9779208817,-0.2555947993,-2.6427599889
H,1.261453867,1.2820958013,-2.139572515
C,1.8787421012,-1.61126819,-0.3520379187
H,1.7770179995,-2.2728706462,-1.2167860634
H,2.9441640984,-1.4486815147,-0.1613996165
H,1.4448961573,-2.1072646237,0.5213379641

M2

0 1

B,-1.3678371476,-0.296364539,0.0039161876
Si,0.6653876643,-0.2968602355,0.0130474224
H,1.1770698048,-1.5029332071,0.7005307587
H,1.1423083757,-0.2967999453,-1.3904549192
H,1.1654107443,0.9211433151,0.6894945774
F,-2.0776344264,-1.4082699651,0.1497992176
F,-2.0637906651,0.8212611462,-0.1663332182

M2_TS

0 1

B,0.6161892688,0.7841913177,0.0002085277
Si,-1.3530621305,-0.2007235956,-0.0003617801
H,-1.6421460146,-1.0035076262,-1.2115972108
H,-1.6420799658,-1.0047505585,1.2100726927
H,-2.1568042138,1.040845529,0.0003238294
C,2.0064657293,-0.3264098451,0.0001377995
H,2.1769903219,-0.9121896173,-0.9036871713
H,2.1765764716,-0.9137386769,0.903042205
H,2.6820902571,0.5348391888,0.0010829664
H,0.57813842,-0.4798032732,0.0000225263
F,0.6692569695,1.4813225442,1.1767016965
F,0.6698481265,1.4818199432,-1.1759511312

M3

0 1

B,-1.3369595149,-0.3004601978,0.0107813089
Si,0.6872932533,-0.2982359195,0.0193111449
H,1.2113120996,-1.5097215897,0.6890854109
H,1.1472700584,-0.2806625066,-1.3907937641
H,1.185563577,0.9184396408,0.7009988633
Cl,-2.2527245651,-1.7797073835,0.2206965642
Cl,-2.2208405584,1.1915245239,-0.2500794898

M3_TS

0 1

B,0.4440617687,0.2007059364,0.000053349
Si,-1.6581648648,-0.1875947645,0.0000819439
H,-2.0990809225,-0.9148977654,-1.212892181
H,-2.09907454,-0.9146745008,1.2131933623
H,-2.1661790649,1.1979010772,-0.0000395678
C,1.5304241939,-1.2245958729,0.0002270859
H,1.5148202074,-1.8342667534,-0.9047201859
H,1.5148201215,-1.8340547203,0.9053173736
H,2.4305355775,-0.6065831569,0.0001529047
H,0.1354990346,-1.0119507401,0.0001957854
Cl,0.750824272,1.0661018485,-1.565158045
Cl,0.7507839766,1.0664675724,1.5650680551

M4

0 1

B,-1.3624538202,-0.3078425729,0.0194324786
Si,0.6712644297,-0.2950731626,0.0176219472
H,1.2864824812,-1.4499639493,0.7224485116
H,1.1530196231,-0.3245299645,-1.3915233543
H,1.2047616725,0.9529144255,0.6266672073
C,-2.166845658,-1.623247939,0.3114713386
H,-1.6903496813,-2.308342381,1.0180699825
H,-3.2086528404,-1.4543394041,0.6040874052
H,-2.1974504204,-2.1613193276,-0.6512142163
C,-2.125953553,1.0247935046,-0.3067238916
H,-2.282966406,1.5045378868,0.6743657366
H,-1.5759920732,1.75034913,-0.9124555026
H,-3.123164724,0.8685344464,-0.732247653

M4_TS

0 1

B,0.2169253497,0.0000226538,0.1474388107
Si,-1.8957676659,-0.0004587427,0.0695628584
H,-2.5520993448,-1.2040683754,0.6439730485
H,-2.552635586,1.2030126407,0.6436498033
H,-2.1110736906,-0.0007036468,-1.3980830727
C,0.9215081266,0.0004123004,1.8182240013
H,0.7663724281,-0.8969280425,2.4214334983
H,0.7659749087,0.8978540562,2.4211801132
H,1.949115822,0.0005874251,1.4492144539
H,-0.3727337557,0.0000463495,1.2712306368
C,0.656357557,-1.3986812702,-0.503386829
H,1.7527814314,-1.4507532179,-0.5563148769
H,0.3176176597,-2.2758053815,0.059577063
H,0.2837162279,-1.503959762,-1.5283206075

C,0.6557322465,1.3987428085,-0.5037739117
H,0.3165920689,2.2758716413,0.0589416157
H,1.752132938,1.4512947785,-0.5567078728
H,0.2830514185,1.5035658552,-1.5287400125

M5

0 1

B,-1.0335629837,0.9002553184,-0.105146335
Si,0.9940400688,1.0600609509,-0.2101369246
H,1.6744719822,0.1868760965,0.7752069718
H,1.4190490176,0.6722458714,-1.5779681753
H,1.4014828504,2.466777457,0.0134465535
C,-1.838192535,2.2473526406,-0.0344808654
C,-1.5011482752,3.2444468966,0.8808978958
C,-2.8680449003,2.559071239,-0.9233096348
C,-2.142590075,4.4740673635,0.9286724003
C,-3.5167231748,3.7837949654,-0.9247634779
C,-3.1519214186,4.7444335689,0.0128663156
C,-1.7780709416,-0.4704263813,-0.1653729045
C,-3.1361073506,-0.6389950752,0.1546105682
C,-1.1014134642,-1.6497603866,-0.5129961488
C,-3.7752977892,-1.8685068028,0.1237505733
C,-1.7097909748,-2.894344325,-0.5673924099
C,-3.0570220152,-3.0005691935,-0.245212097
F,-3.2498602053,1.656464333,-1.8349543108
F,-4.4825682597,4.0469596435,-1.8006144598
F,-3.7705687485,5.9173009601,0.0339634262
F,-1.8046080702,5.3879469575,1.8338622972
F,-0.5469906341,3.0087736845,1.7896047343
F,0.1955636779,-1.6110313741,-0.8231835765
F,-1.0235247359,-3.9783500397,-0.9143697751
F,-3.881043488,0.3986670714,0.5344964332
F,-5.0607367631,-1.9788915698,0.4430533677
F,-3.6556941637,-4.1793746503,-0.2830625017

M5_TS

0 1

B,0.5308361477,0.2146131636,0.0073836839
Si,-1.6139469169,0.1878258121,-0.3597480342
H,-1.7846762027,0.4218707567,-1.8100211893
H,-2.3001800582,-1.0778597766,0.0018183674
H,-2.166245987,1.2991744024,0.4393268482
C,1.1992103156,-1.4148771118,0.4787796783
H,1.085972592,-2.2556509483,-0.2064313893
H,0.8986337745,-1.6914016029,1.4891378153
H,2.2420188792,-1.1004695308,0.4709332311
H,-0.0494336327,-0.8973530658,0.0965692335
C,0.7220136275,1.0703474738,1.3475772347
C,-0.0287718327,0.7951225827,2.4892585617
C,1.6468994492,2.102185785,1.4900440086
C,0.0927587171,1.4850663681,3.6844610997
C,1.8002010494,2.8260129969,2.6682676869
C,1.0184774231,2.517711331,3.771887433
C,1.1363564204,0.7224667224,-1.3868946139
C,1.9564179221,0.0246309073,-2.2691603938
C,0.8133291376,2.0182457425,-1.7959859951
C,2.4380832609,0.5697336595,-3.4560928503

C,1.2734939914,2.6035336745,-2.9628756174
C,2.1001120705,1.8677437101,-3.804054176
F,2.5529336282,2.4007697899,-4.9334029633
F,0.9312079507,3.8480136084,-3.2869477776
F,-0.0002359576,2.7545549911,-1.0202097782
F,3.2206381008,-0.150734205,-4.2576049459
F,2.326800907,-1.2429749237,-2.0191354724
F,2.4538688048,2.441096604,0.4753676823
F,2.6981526678,3.8051106456,2.7466556281
F,1.1584121257,3.1968642575,4.9052130309
F,-0.6590657963,1.1699124869,4.736848837
F,-0.9339491392,-0.204152067,2.4433273161

M6

0 1

B,-0.1878061054,0.1692322461,-0.0218698908
Si,1.6768940057,0.9671602615,-0.0294595147
C,-1.4176911024,1.0773432237,0.0706086352
C,-0.411177913,-1.3445727092,-0.0697249206
N,-2.310615931,1.8142706948,0.1407038162
N,-0.5203059592,-2.4986308657,-0.1097633821
H,2.6535738145,-0.0036237952,-0.5644954644
H,1.6721475775,2.2128207255,-0.8260846728
H,1.9895091534,1.2786595686,1.385943894

M6_TS

0 1

B,-0.9920318205,-0.0301523632,0.2064409215
Si,1.1387062192,-0.0010231597,0.0524821407
C,-1.7366810169,0.0867065507,1.8503570961
H,-1.5766386199,1.0368872115,2.3607004197
H,-1.5416625297,-0.7635978033,2.5044632579
H,-2.7637426947,0.0380899991,1.4912639823
H,-0.4273685148,0.0691274755,1.3112766871
C,-1.3563774867,-1.4420308135,-0.3271479618
C,-1.4090144979,1.2639655452,-0.5433929016
N,-1.5991821609,-2.5090484529,-0.7063448471
N,-1.6916990431,2.2470620489,-1.086423035
H,1.7305893441,-1.1531686115,0.7648710391
H,1.3098105919,-0.1144157964,-1.4069107278
H,1.6834361098,1.2716620396,0.570943879

M7

0 1

B,-1.3302105724,-0.2929943482,0.0051749503
H,-1.9468068243,0.7248919309,-0.0709496703
H,-1.9473690999,-1.3133955859,0.0057035147
Si,0.6869302458,-0.2927275038,0.0446294735
H,1.2569759746,-1.4705841719,0.7438720304
H,1.1317903405,-0.3503289496,-1.3752877827
H,1.2596042857,0.9363151984,0.6468575142

M7_TS

0 1

B,0.1861813251,0.0000194365,0.1811028529
Si,-1.883556762,-0.0000890185,0.0378970653
H,-2.539984753,-1.1980685219,0.6221181958

H,-2.5401169264,1.1977929857,0.6221697136
H,-2.1243982676,-0.000070328,-1.4238537077
C,0.9609906734,0.0000307032,1.8179977679
H,0.8119464185,-0.8951927897,2.4232738248
H,0.8118259025,0.8952027875,2.4233204029
H,1.979609899,0.0001128382,1.4369058849
H,-0.3457132912,-0.0000284354,1.3130322952
H,0.4884651827,-1.0505263378,-0.294692779
H,0.4883548991,1.0506158502,-0.2946510667

M8

0 1

B,0.1018688292,-1.3606185371,0.2085118396
Si,-0.076044224,-3.4152463825,0.6095117934
C,-1.1463130446,-0.3848573227,0.0511120539
C,-1.9670510789,-0.2284475145,-1.0604280031
C,-1.4453470774,0.4250638824,1.1435340487
C,-3.0453976019,0.6491632541,-1.0756534798
C,-2.5154617851,1.3058773145,1.1723100901
C,-3.3251709154,1.4152687472,0.0480211808
C,1.4763649625,-0.5863808732,-0.0452609637
C,1.6849782232,-0.0032491229,-1.2995107722
C,2.5137944324,-0.3888213657,0.8663261416
C,2.8486936801,0.6602697003,-1.6591945889
C,3.6849596008,0.2909522249,0.5541101882
C,3.8611036988,0.808908558,-0.7209755317
F,-0.6653258292,0.3419216115,2.2352022866
F,-2.7645301941,2.0457221807,2.2494703074
F,-4.3532334,2.2564272623,0.0445809982
F,-3.8038384866,0.7669626226,-2.1622033858
F,-1.7324941492,-0.921548764,-2.1821206809
F,2.4078625243,-0.8205142026,2.127098113
F,4.6325652526,0.4554902217,1.4728968886
F,0.7327393258,-0.0965623676,-2.2372378741
F,2.9930764964,1.1646859784,-2.8810729279
F,4.9775823956,1.4523835719,-1.03514256
C,-1.9566113831,-3.9686394504,0.5339663129
C,0.6278028893,-3.7342468486,2.4037210755
C,0.9458565129,-4.177401349,-0.8700502187
C,-2.7898551039,-3.1530541507,1.5418627148
H,-2.5223406364,-3.3826326492,2.5769037894
H,-2.6970149399,-2.0712826107,1.3964072725
H,-3.8514539782,-3.4084421988,1.4207822001
C,-2.5590683241,-3.7373930767,-0.8636910854
H,-3.6464288078,-3.8824600272,-0.809886794
H,-2.3819653834,-2.7374116332,-1.2586210132
H,-2.178061511,-4.4603187088,-1.5915563691
C,-2.2137843684,-5.4601401765,0.8487703786
H,-2.084663679,-5.7040581127,1.9018502183
H,-3.2581964942,-5.6878222696,0.594898193
H,-1.5869124788,-6.1390817447,0.2666981323
C,0.6994736035,-5.6856747552,-1.032376064
H,0.8901058907,-6.2407725893,-0.1059319716
H,-0.3227868444,-5.8999257639,-1.3566204415
H,1.3742025268,-6.0864554445,-1.8014404968
C,0.5344080516,-3.474081963,-2.1800819495
H,0.8088460597,-2.4135951447,-2.1819762147

H,1.070393505,-3.9368854954,-3.0202020915
H,-0.5319634408,-3.5365166181,-2.3980841961
C,2.4659521519,-3.9653150776,-0.7374974619
H,2.9382292895,-4.2262022717,-1.6943974773
H,2.7335903758,-2.9255947385,-0.5187685503
H,2.9135262277,-4.6000423801,0.0279348142
C,0.1075264422,-5.0354338303,3.0403084167
H,-0.9436492441,-4.9593695567,3.3278221275
H,0.228390657,-5.9089445971,2.3902382092
H,0.6771567726,-5.2266693837,3.9600486553
C,2.1637784152,-3.8359812266,2.4266713944
H,2.5086223295,-3.7564307412,3.4664795876
H,2.4960696221,-4.8072899994,2.0479923983
H,2.6690702634,-3.05658376,1.8552698256
C,0.197878751,-2.5788175222,3.3307625848
H,-0.8874495073,-2.4575974897,3.375408327
H,0.5448199515,-2.7898406199,4.3519740205
H,0.6260585005,-1.620693362,3.0367423452

M8_TS

0 1

B,-0.0794882182,0.7652674302,0.533156364
Si,-0.3128021408,2.5942579795,-0.9733746014
C,-0.0656997062,1.3172272551,2.3133701069
H,-0.8124020753,2.0131262592,2.6961705639
H,0.9370824942,1.6345713613,2.5889839266
H,-0.2752141741,0.3236120588,2.7064119211
H,-0.165408284,1.9198959835,1.0385962216
C,1.3513604664,0.017048475,0.5265840041
C,2.5431282531,0.7314346313,0.6229445901
C,1.5340689616,-1.3693346646,0.5537816052
C,3.8103504248,0.172422244,0.6397096907
C,2.7850413369,-1.980415599,0.5622341853
C,3.9355283309,-1.2087489452,0.593639391
C,-1.3845695268,-0.1484247903,0.3364872815
C,-2.5163354671,-0.19610591,1.1500018408
C,-1.4216382718,-1.0377442157,-0.7383667263
C,-3.5970582113,-1.0409845934,0.9186208514
C,-2.4770253078,-1.8907298244,-1.0145249607
C,-3.5833579915,-1.8922480649,-0.174861433
F,-4.6112721313,-2.699037029,-0.4150804683
F,-2.4351382123,-2.7099098061,-2.0631878718
F,-0.3673001076,-1.1071684883,-1.5680569325
F,-4.6529526642,-1.0196336344,1.7308300638
F,-2.6576326513,0.6305423971,2.2032088589
F,0.4965572051,-2.2163901747,0.613098174
F,2.8799722073,-3.3088027315,0.5712159238
F,5.1349915394,-1.7802812665,0.6123285295
F,4.8945919631,0.9443547819,0.709018599
F,2.4825230694,2.0713045866,0.7177784889
C,0.5249181633,4.2637417244,-0.2699638799
C,0.4946021524,2.09790601,-2.6843620699
C,-2.2444930294,2.8989888529,-1.1902066628
C,0.8091641197,3.3847589988,-3.4771332858
H,1.1483634426,3.09946101,-4.482105639
H,-0.0714675438,4.022893008,-3.6036440914
H,1.6032171218,3.9779476689,-3.0245926007

C,1.7948302988,1.2911950405,-2.5271134856
H,1.6016506284,0.2964106688,-2.1164796487
H,2.2522732318,1.1589382973,-3.5168351821
H,2.5359572357,1.7859037521,-1.8928985367
C,-0.4402827488,1.2666900966,-3.5831582581
H,0.1129041333,0.9939095945,-4.4920117303
H,-0.7701052191,0.3382661268,-3.1177397125
H,-1.3189258874,1.8320941128,-3.9024761579
C,-2.5149363255,3.9470921892,-2.2967783052
H,-2.3232763604,3.5349694933,-3.2915930245
H,-3.5798545037,4.2141195118,-2.2637471925
H,-1.9491952647,4.8701533377,-2.2026056422
C,-3.1079983226,1.6829745477,-1.6012159218
H,-3.3157022655,1.0165078954,-0.7678415404
H,-4.0796485215,2.0627125377,-1.9436338747
H,-2.6866327923,1.0947477662,-2.416369303
C,-2.8329406435,3.412024206,0.1389025251
H,-3.9219209482,3.5153754424,0.0384181343
H,-2.6548713606,2.7102095761,0.9633016175
H,-2.4419215789,4.388494996,0.4332829868
C,2.0308579719,4.4324860268,-0.6298274239
H,2.5470308825,3.5186708716,-0.9115062059
H,2.1542377682,5.1444231997,-1.4497886995
H,2.566440941,4.8477723678,0.2324317269
C,-0.1396399652,5.5620212026,-0.7813787523
H,-1.1769437247,5.6797254818,-0.4616987167
H,0.4226779108,6.4086508413,-0.3652087432
H,-0.092563462,5.6536291716,-1.8700630422
C,0.406704982,4.3156442967,1.2692419217
H,-0.6142501665,4.1472764518,1.6288684903
H,1.0749179697,3.6025129774,1.7541972565
H,0.7066657096,5.3128611734,1.6160263822

M9

0 1

B,0.059448158,0.9478351056,-0.0229782239
Si,0.056058144,-1.0925031465,-0.0057153254
C,1.4049489984,1.7444998903,0.0051115603
C,2.5823509787,1.194278032,0.5258391722
C,1.5295651866,3.0350020607,-0.5261249802
C,3.7977690321,1.8600521031,0.529795664
C,2.7326137812,3.7256601921,-0.5558533133
C,3.8703030976,3.1341165237,-0.020773891
C,-1.3066352489,1.7203119525,-0.0849155407
C,-1.6501860871,2.6357874596,0.909321981
C,-2.2730922096,1.4852965511,-1.0615858766
C,-2.8954562022,3.2429486578,0.9735693836
C,-3.5225756521,2.08889315,-1.0411652417
C,-3.8379439312,2.9626137626,-0.008559146
C,1.4770282977,-1.6422662851,-1.1133205988
C,2.5270935528,-2.5002287068,-0.7999103597
C,1.565461528,-1.0566614158,-2.3738648851
C,3.573543249,-2.7866184353,-1.6666312171
C,2.5743848386,-1.2926153794,-3.2903034674
C,3.5859076158,-2.1776443763,-2.9184824267
H,4.3534215868,-3.4689564386,-1.3500193945
H,2.5585695319,-0.7983049488,-4.2541881068

F,0.4761186033,3.6572133745,-1.0587518264
F,2.8081524989,4.9439617228,-1.0844787857
F,5.0241218577,3.7851524408,-0.0339583397
F,4.8861091341,1.299581179,1.0498985314
F,2.5629390017,-0.0213188129,1.0794417051
F,-0.7613769376,2.9507215119,1.8588677879
F,-3.191725464,4.0952185213,1.9525077146
F,-5.0327799229,3.5415488166,0.0317191716
F,-4.415836832,1.841848535,-1.9971008245
F,-1.995251145,0.684180982,-2.0958157785
C,0.2191141093,-1.7011317504,1.7654374274
C,0.3063829181,-0.8323864792,2.8454610457
C,0.1753982008,-3.0506861461,2.1016521315
C,0.3796521423,-1.2319691213,4.1694631398
C,0.2459451198,-3.5282082217,3.4007832977
C,0.3532819214,-2.5999771312,4.4350021871
H,0.4493723955,-0.4900028853,4.9557332974
H,0.2146611744,-4.5956503583,3.5836696537
C,-1.606467591,-1.7480028742,-0.61021141
C,-1.8454251609,-2.4903349748,-1.7638063287
C,-2.7543056253,-1.4180843186,0.109518473
C,-3.1078372057,-2.8756326431,-2.1911883968
C,-4.0442979132,-1.7628053691,-0.2570163884
C,-4.2099804107,-2.4999454398,-1.4281614873
H,-3.2078327074,-3.4497652313,-3.104615395
H,-4.8809025068,-1.457268894,0.3603342506
F,-0.7958307043,-2.8557078326,-2.524276028
F,-2.5926427947,-0.6931154164,1.2437925504
F,0.0490676635,-3.9394098749,1.0977883114
F,0.3069800773,0.4994020844,2.5822712648
F,2.549596082,-3.0787912883,0.4133746515
F,0.5820613192,-0.185447154,-2.7079426576
H,4.394226526,-2.3897596451,-3.6100261284
H,-5.2068395174,-2.7838828198,-1.747591225
H,0.4100756478,-2.9464428444,5.4613355508

M9_TS

0 1

B,0.6592921333,0.5006973281,-1.2410254136
H,-0.1999740662,-0.2352683451,-1.7836633897
C,0.2982485711,2.0078392907,-0.8049511024
C,-0.7369490558,2.7552968792,-1.3659329035
C,1.052748449,2.6986025745,0.1438173779
C,-1.0192932077,4.0704902423,-1.0201525253
C,0.8156998725,4.0145340168,0.5106935342
C,-0.2336210023,4.709128082,-0.0731914136
C,2.1725591858,-0.0193673139,-1.0813044054
C,2.5539365443,-1.3049322468,-0.7190549953
C,3.2333818719,0.8266063513,-1.4113102501
C,3.8751795619,-1.7282009196,-0.6351204987
C,4.5668141557,0.4517692127,-1.3412366851
C,4.8922392033,-0.8389236863,-0.9442744665
F,6.1641829776,-1.2195553212,-0.875276615
F,5.5332733375,1.3115829842,-1.6585716163
F,2.9850479281,2.0781863583,-1.8275406811
F,4.1661256514,-2.9762412096,-0.2707953753
F,1.6168388589,-2.2245528413,-0.4371382992

F,2.0539132107,2.0809776719,0.7871977251
F,1.570158132,4.6051750116,1.4370653058
F,-0.4841805205,5.9682789277,0.2724766565
F,-2.028986985,4.7210694747,-1.5992851315
F,-1.5295182882,2.214836703,-2.3064875093
C,0.1174778364,-0.7866315145,1.7336259496
C,0.6248599007,-1.9523519646,2.3177987889
C,0.2692977434,0.3531727472,2.5253660788
C,1.2665532689,-1.9897008027,3.5474979603
C,0.8960533371,0.3865265051,3.7583618523
C,1.4073457749,-0.8054630079,4.263535981
H,1.6324594462,-2.9390338941,3.9200530554
H,0.9694887226,1.3260277232,4.2926931262
Si,-0.7258489396,-0.7161574322,0.0469619145
C,0.4179646797,0.3583942636,-3.0140069255
C,-2.3957700601,0.1641679402,0.1186340474
C,-3.10894989,0.2870317442,-1.0732493102
C,-3.0894700284,0.6085830625,1.2449075877
C,-4.3586070323,0.8647894455,-1.2009395978
C,-4.3433246781,1.2023006537,1.1942322274
C,-4.968702291,1.3395605754,-0.0417116109
H,-4.8250197923,0.9334328978,-2.1762151663
H,-4.8093906606,1.530824439,2.1155887049
C,-1.2352289402,-2.4507878947,-0.5007382551
C,-2.070428386,-3.1952142949,0.3305730719
C,-0.9147882588,-3.0747587688,-1.6985082811
C,-2.5522785966,-4.4579347045,0.0314026526
C,-1.357218049,-4.3346507933,-2.0703048109
C,-2.1830553005,-5.025096741,-1.1871018453
H,-3.1911776951,-4.9713212377,0.7399535575
H,-1.0564733544,-4.7483227325,-3.0253930819
H,0.9859994215,-0.4929557789,-3.3797072084
H,-0.5884632458,0.356806444,-3.4309647108
H,0.9089903546,1.2960615687,-3.2805985522
F,-2.5474852008,0.4272011877,2.4602389139
F,-2.5276944015,-0.2216431438,-2.1892445388
F,-0.123696567,-2.4059014168,-2.5693406714
F,-2.4181648918,-2.6412803391,1.5112893599
F,0.4754224019,-3.1260754358,1.6812523032
F,-0.2484452789,1.5090081523,2.0653272536
H,-5.946948989,1.8042636486,-0.1004827618
H,-2.5432193526,-6.0136447865,-1.4506251875
H,1.9077168932,-0.8133260399,5.2258140762

M10

0 1

B,-0.6128402091,-0.3092322341,0.4264072963
Si,0.4054913579,-1.9146800666,1.162915405
C,0.1053267639,1.0565750165,0.1302110237
C,1.2878605926,1.4405791617,0.7718233906
C,-0.356934146,1.9448402024,-0.8498657057
C,1.9676822426,2.6135821917,0.4776723482
C,0.30594155,3.1146931679,-1.1877495382
C,1.4743586717,3.4513740073,-0.514074897
C,-2.1809146373,-0.359163045,0.2874517686
C,-2.9882131196,0.5790420988,0.933696449
C,-2.8564594911,-1.3430603183,-0.4323938519

C,-4.3738225692,0.5395253106,0.895209368
C,-4.2406737731,-1.4018370951,-0.5180537632
C,-5.0026275114,-0.4574499382,0.1581430429
C,2.1365634311,-1.9248776114,0.3796902373
C,3.3409929712,-2.0431352257,1.1111356754
C,2.2230059142,-1.78052204,-1.0227043776
C,4.5687139516,-1.9874904571,0.4526489951
C,3.4727625011,-1.7308105846,-1.6514267973
C,4.6585764614,-1.8235272418,-0.9309131449
H,5.4841077805,-2.079893233,1.0345241195
H,3.5151504525,-1.6231245088,-2.7335916089
F,-1.466272759,1.6670680297,-1.544026686
F,-0.1612762117,3.9153887672,-2.1419213206
F,2.1139237717,4.5718841595,-0.8160947983
F,3.0773837655,2.9434397835,1.1320835992
F,1.7941445238,0.6888966068,1.7526577817
F,-2.4220905758,1.5614771899,1.6480275913
F,-5.1031861209,1.4434846566,1.544217038
F,-6.327358255,-0.505884272,0.1003083036
F,-4.8405984304,-2.3475570063,-1.2364963187
F,-2.1634833113,-2.257750847,-1.1224162554
C,6.0018344912,-1.7687504141,-1.6118365225
H,6.5634286818,-2.6927850814,-1.4426344626
H,5.8940184617,-1.6303399949,-2.6901192811
H,6.6043953056,-0.9427739847,-1.2214934895
C,3.3495200424,-2.2393719431,2.6090707957
H,4.3678331608,-2.4031842677,2.9685415738
H,2.9469685133,-1.3661113353,3.1304826976
H,2.7503802704,-3.1070692001,2.9019377545
C,0.9992210221,-1.673954653,-1.9091164714
H,0.193203014,-2.3441926173,-1.602401621
H,0.5970356699,-0.6525496864,-1.9231227336
H,1.252895244,-1.9230355829,-2.9424652318
C,0.2435119867,-1.6451516862,3.0354525995
H,-0.8283367518,-1.5692984715,3.2572517766
H,0.6288502035,-2.4983686836,3.6003819723
H,0.7270432659,-0.7373711877,3.4004926873
C,-0.4404114118,-3.5780673864,0.8666836471
H,-1.4901758605,-3.5497419003,1.1784529274
H,-0.4009367172,-3.9150934335,-0.1710218383
H,0.0693349958,-4.3276317549,1.4825658603

M10_TS

0 1

B,-0.1094861474,-0.1320712995,-1.3111150064
H,-0.8669078564,-0.5936952687,-3.5954004897
H,0.8980526712,-0.26439181,-3.6902703649
H,0.3181007663,-1.7045464654,-2.8386845492
H,0.0258557442,0.53375568,-2.3623715086
C,1.1703809076,-0.5733113588,-0.4510447772
C,2.4425248969,-0.8641066177,-0.9429886549
C,1.0619970419,-0.6342673157,0.9430516692
C,3.5242832185,-1.1956661345,-0.1344657077
C,2.1157344523,-0.9543566006,1.7854273672
C,3.3619956757,-1.2374478557,1.2416192942
C,-1.5557274636,-0.7475983717,-0.9978067334
C,-2.7202372737,-0.2147468532,-1.5493924617

C,-1.7539013718,-1.9162683863,-0.2608868942
C,-3.9904091478,-0.7311127913,-1.3436548016
C,-3.0088862677,-2.4664249312,-0.0211487603
C,-4.1378402422,-1.8664616634,-0.5582314091
F,-5.3433267705,-2.3842441178,-0.3444402156
F,-3.1310187557,-3.5783283187,0.7014117443
F,-0.7138911935,-2.6022466645,0.2325699293
F,-5.0588897122,-0.1532173373,-1.8918097708
F,-2.6317172725,0.8689125473,-2.3430142661
F,-0.114398792,-0.3824614999,1.5277459843
F,1.9452184064,-0.9892243944,3.1051130622
F,4.3875049017,-1.5413534135,2.0314102792
F,4.7150942895,-1.4574645517,-0.6737803926
F,2.6990326605,-0.8146842535,-2.2636033561
C,0.2746862316,2.4204937893,0.73907384
C,-0.9248760879,2.5303544786,1.4788053997
C,1.4992643971,2.5525820921,1.4437935796
C,-0.8893985224,2.7867802281,2.8523767806
C,1.4914552282,2.7984929991,2.8171246795
C,0.3079808879,2.9231454186,3.5440434928
H,-1.8289211251,2.86012694,3.3963371936
H,2.4423452621,2.8875230265,3.3388061562
Si,0.1782909229,2.0716431468,-1.1243894762
C,0.0891718555,-0.6669361939,-3.0791062012
C,1.7605179777,2.38436409,-2.1209720647
H,2.586959711,1.69673196,-1.9364091726
H,1.500685218,2.3189619143,-3.1847818275
H,2.117865951,3.4043601941,-1.9482782461
C,-1.0374796724,3.2181664943,-2.003835812
H,-1.0169096819,3.009918399,-3.0790948734
H,-2.0721917371,3.1609559204,-1.6741088099
H,-0.6800687721,4.2446761468,-1.858565239
C,0.3382348917,3.1591070301,5.0310514745
H,0.6501824028,2.251154669,5.5575528147
H,1.0479931845,3.9500281599,5.2894483003
H,-0.6468323988,3.4447538498,5.4070248266
C,2.857357325,2.4350700192,0.78902673
H,2.9538242024,1.5171818841,0.2048425925
H,3.0604847908,3.2746457305,0.1183104222
H,3.6404010403,2.4250318074,1.5505517815
C,-2.2967683824,2.366949791,0.8647302799
H,-2.6782317984,3.3207366893,0.4848679788
H,-2.3021074338,1.6530034825,0.0405423171
H,-3.003074854,2.0038147707,1.6151999924

M11

0 1

B,0.244828,0.959886,-0.248845
Si,0.135524,-1.065001,0.073284
C,1.550197,1.793478,-0.325818
C,2.814683,1.186533,-0.233225
C,1.567274,3.186255,-0.525625
C,4.005724,1.887876,-0.324174
C,2.739707,3.919548,-0.621464
C,3.962597,3.264233,-0.519691
C,-1.178461,1.623553,-0.323759
C,-1.695427,2.383856,0.718137

C,-2.067941,1.271513,-1.33239
C,-3.030463,2.75958,0.777005
C,-3.404309,1.636488,-1.322822
C,-3.887226,2.38074,-0.250754
C,1.05147,-2.08268,-1.219381
C,1.938902,-3.099456,-0.846291
C,0.853198,-1.808594,-2.581265
C,2.594581,-3.818214,-1.835912
H,2.14059,-3.336208,0.193784
C,1.537402,-2.55818,-3.527354
H,0.179356,-1.028107,-2.923465
C,2.417679,-3.574949,-3.189524
F,0.432941,3.870847,-0.638002
F,2.711011,5.233588,-0.8109
F,5.086739,3.951917,-0.608442
F,5.176628,1.269272,-0.228622
F,2.911136,-0.129017,-0.042116
F,-0.89203,2.734635,1.733483
F,-3.494518,3.474248,1.797464
F,-5.164236,2.739437,-0.215648
F,-4.221385,1.283665,-2.310453
F,-1.611296,0.538562,-2.362841
C,0.729994,-1.456477,1.8229
C,1.423001,-0.525479,2.606122
C,0.423384,-2.712259,2.369422
C,1.801093,-0.869678,3.896919
H,1.676052,0.466823,2.245266
C,0.830911,-3.007256,3.661576
H,-0.135594,-3.460356,1.813642
C,1.524142,-2.105956,4.457369
C,-1.704966,-1.502326,0.048142
C,-2.316415,-2.124138,-1.045476
C,-2.502754,-1.054764,1.114004
C,-3.698885,-2.264245,-1.059492
H,-1.746133,-2.488897,-1.894194
C,-3.877485,-1.212045,1.04547
H,-2.07533,-0.578564,1.993367
C,-4.513633,-1.81106,-0.033906
F,1.345565,-2.290199,-4.829839
F,3.444561,-4.793097,-1.47363
F,0.540901,-4.213217,4.175517
F,2.463092,0.033291,4.639231
F,-4.278477,-2.860326,-2.11412
F,-4.636042,-0.762851,2.060546
H,2.942649,-4.147578,-3.944271
H,1.828152,-2.354914,5.46672
H,-5.590375,-1.923812,-0.06971

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B,-0.1985853316,-0.7040567304,-1.4677900059
H,-0.0929111729,0.4895058518,-1.8474650167
C,1.1417616763,-1.5348259638,-1.1799384609
C,2.3846046903,-1.1238245797,-1.6622195235
C,1.1961413419,-2.6308968608,-0.3193981711
C,3.586419309,-1.731817231,-1.3318941353
C,2.3729457528,-3.283112755,0.0266182239

C,3.581606258,-2.8271738038,-0.4789274391
C,-1.6431034886,-1.3873065781,-1.392703804
C,-2.8125230395,-0.6961559594,-1.0880208573
C,-1.8283436154,-2.7277722464,-1.7311862015
C,-4.0658100334,-1.2871315296,-1.0233352796
C,-3.0622086545,-3.3637161273,-1.6783395135
C,-4.1886288996,-2.6401794922,-1.3101061886
F,-5.3774609701,-3.2293394031,-1.2624960203
F,-3.1763967643,-4.6496628963,-1.9993031071
F,-0.7920404319,-3.4612868438,-2.1594918195
F,-5.1418153555,-0.5701376816,-0.7080234586
F,-2.7567960686,0.6317102082,-0.8692221802
F,0.0788142785,-3.0943212956,0.2669712657
F,2.3484428721,-4.3235954147,0.8548973435
F,4.7204847651,-3.4221031562,-0.1444139023
F,4.737006254,-1.2617269818,-1.8082990262
F,2.4637970732,-0.036914043,-2.4519220721
C,-1.1769614079,0.5365814741,1.485071787
C,-1.8186561902,1.6036786007,2.1288173656
C,-1.4083189294,-0.7724435498,1.9290376926
C,-2.6638022327,1.3372153268,3.1960965515
C,-2.2667903249,-0.9786858648,3.0000934393
C,-2.9134830674,0.0548621644,3.6600600276
Si,-0.0010353738,0.9226212821,0.0661037195
C,-0.185925715,-0.0745278069,-3.1791886685
C,1.7806070081,0.81685337,0.6749033447
C,2.7988262368,1.5393553742,0.0368241121
C,2.1173700198,-0.0825805509,1.6962075011
C,4.117335543,1.331893413,0.4164444215
C,3.4525862578,-0.255605132,2.0315632488
C,4.4828672058,0.4335107898,1.4082285113
C,-0.2779291672,2.6952006493,-0.5332195002
C,0.3364007492,3.7439983979,0.170381659
C,-1.0884475157,3.003389331,-1.6342357207
C,0.1242160931,5.0527806539,-0.2374602273
C,-1.2599638602,4.3303268683,-2.004115031
C,-0.6681032511,5.384170785,-1.3268719938
H,-1.2082046758,0.1760154437,-3.4590049562
H,0.5030044685,0.7113276763,-3.4932370627
H,0.1209560558,-1.0118708611,-3.6456566258
H,-1.6137573553,2.2436990629,-2.2029086011
H,0.9793678366,3.564195126,1.0270961651
H,-1.6884513769,2.6339152665,1.8134196392
H,-0.9551052715,-1.6377316929,1.457528973
H,1.3669093306,-0.6572625488,2.2317587127
H,2.5939287729,2.24435362,-0.7630446788
F,5.0861283001,2.0229283768,-0.2035924211
F,3.7686215731,-1.1341097544,2.9965486969
F,0.7121112172,6.0472541408,0.4449406626
F,-2.0350907011,4.6090359739,-3.0642988236
F,-2.4892454247,-2.2356736799,3.4162368805
F,-3.2756208976,2.3642066477,3.8079174401
H,-0.8162333277,6.4129831164,-1.6315820852
H,-3.5827027248,-0.1303303534,4.4913225076
H,5.5193064775,0.2796573271,1.6833858072

M12

0 1

B,-0.0686243755,0.2650208155,-0.5069468609
Si,0.7765387361,1.9130877579,-1.3945672637
C,0.6714257678,-1.0459990746,-0.1194060835
C,2.0493097703,-1.2039087613,-0.3460319475
C,0.0403051715,-2.1354993696,0.507879968
C,2.7550988197,-2.3421877445,0.0104005796
C,0.7152640046,-3.2879618431,0.879405118
C,2.0794116322,-3.388552888,0.6277936137
C,-1.6218825857,0.4227565038,-0.3088888192
C,-2.5387306528,-0.254501547,-1.1031142457
C,-2.136460864,1.4193717864,0.5123988799
C,-3.8928913835,0.0491902038,-1.1066081995
C,-3.4825752174,1.7448405507,0.5545163195
C,-4.3643870907,1.0557676618,-0.2714873872
C,2.1955188533,2.6315211603,-0.3920905407
C,3.4517352522,2.8761141261,-0.9661006455
C,2.0254239704,2.9215503661,0.9718788154
C,4.502418738,3.4041226832,-0.2184425601
H,3.6236084224,2.6421633294,-2.0138329003
C,3.0614663899,3.4494851897,1.7396607279
H,1.067640742,2.7359350384,1.4535956823
C,4.2811344801,3.6812485977,1.1217951378
H,5.4774682174,3.5962892669,-0.6523055622
H,2.9399195087,3.6775290329,2.7927921275
F,-1.2610992929,-2.1026649765,0.7833971729
F,0.0791249996,-4.2929166472,1.4718750546
F,2.7344108908,-4.4830374728,0.9747873212
F,4.0578733369,-2.4457365338,-0.2287165346
F,2.7454084541,-0.2358980148,-0.9392208674
F,-2.1024860516,-1.2159763513,-1.932257582
F,-4.7396153163,-0.6096850753,-1.8943656956
F,-5.6587188508,1.3514941727,-0.254987102
F,-3.9352577209,2.6989273604,1.3627864166
F,-1.2911085701,2.0987913908,1.3064327004
C,1.301253024,1.4728784764,-3.1506382097
C,1.3607409195,0.1587708031,-3.6355208871
C,1.6036043615,2.5148283148,-4.0439560126
C,1.7194977978,-0.120039229,-4.9535012661
H,1.1192955353,-0.6779438595,-2.9836110067
C,1.9753284208,2.2633787769,-5.3617793306
H,1.5410164776,3.5484291783,-3.7089189892
C,2.0251929729,0.9435258802,-5.7873174754
H,1.7626020308,-1.1332744506,-5.3370492652
H,2.2149511502,3.0614412441,-6.0556779043
C,-0.6116752286,3.181230604,-1.5674314686
C,-0.7356208683,4.3075364868,-0.7438963738
C,-1.6448167212,2.9229872676,-2.4856892808
C,-1.8532849314,5.1404941998,-0.8090920116
H,0.0464135499,4.5439468767,-0.0268252239
C,-2.7723180507,3.7348522579,-2.5684596134
H,-1.5732381791,2.0657592972,-3.1540669622
C,-2.8525091629,4.8291404392,-1.7169972044
H,-1.9597370724,6.0114715858,-0.1719962646
H,-3.574837921,3.5399993774,-3.2717340743
F,-3.9385522908,5.6209920035,-1.7841981348
F,5.2900499554,4.190261891,1.8532863994

F,2.377098075,0.6877963939,-7.0604297383

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B,0.6889576535,0.4226584361,-1.2558315467
H,0.0302217929,-0.5087047341,-1.7867316069
C,0.0091369157,1.8699423822,-1.1453638503
C,-1.1293300354,2.2100645851,-1.8760294562
C,0.3963719504,2.8335547413,-0.2147530007
C,-1.8299559193,3.3968818122,-1.7213727916
C,-0.2648413547,4.0413525905,-0.0334657408
C,-1.3905316588,4.3278660153,-0.7907470548
C,2.2275176644,0.1879084618,-0.885003037
C,2.7380346043,-1.0402652218,-0.470882264
C,3.1824665491,1.1930173656,-1.0400173581
C,4.0668580804,-1.2518126363,-0.1338915231
C,4.5223274871,1.0295358976,-0.7109193613
C,4.9661072031,-0.1995263638,-0.2421494402
F,6.2457454801,-0.3767805822,0.0680871879
F,5.3859005915,2.0308935823,-0.8653375906
F,2.8339522658,2.3794053191,-1.5572113394
F,4.4857381066,-2.4492483785,0.2702956714
F,1.9250857289,-2.1116172351,-0.4215284963
F,1.4371966615,2.6109869923,0.6075882328
F,0.1603992949,4.9121340119,0.8805077385
F,-2.0462447173,5.4704493832,-0.6192595958
F,-2.9214813299,3.6389536894,-2.4443720966
F,-1.6403180196,1.3288220411,-2.7563959146
C,0.2685547419,-1.1005620694,1.6682671327
C,0.1597706137,-2.3562825131,2.2864058762
C,1.0682433904,-0.1273364914,2.2871520865
C,0.8125936636,-2.6349414168,3.4847368116
C,1.7306762839,-0.3844110412,3.4857586249
C,1.5856968252,-1.6380455104,4.0599363158
H,0.7377124573,-3.6027653976,3.9678014515
H,2.352481898,0.3613143542,3.9685792408
Si,-0.658466044,-0.7808716952,0.0660555028
C,0.6628719179,-0.1332346087,-3.008913363
C,-2.15281539,0.3189906745,0.3777877084
C,-3.2614243534,0.3004402674,-0.4841456369
C,-2.143424211,1.2638262995,1.4160947686
C,-4.3173185486,1.1965078214,-0.3346639477
C,-3.1871807296,2.170984757,1.5862570874
C,-4.2527986713,2.1192086395,0.6992464374
H,-5.1718867865,1.1955478761,-1.0020351101
H,-3.1870862473,2.9054318806,2.3843915625
C,-1.3022382959,-2.4021783276,-0.6553681079
C,-2.5134673643,-2.923258084,-0.1647035855
C,-0.6262605307,-3.144361651,-1.6363396629
C,-3.0327838448,-4.1297553572,-0.6262587824
C,-1.129449989,-4.3501548465,-2.1209840123
C,-2.326539301,-4.8173886299,-1.6023223684
H,-3.9642894045,-4.5367541001,-0.2488211345
H,-0.6108879803,-4.9259798009,-2.8793283916
F,2.2232490191,-1.8987006368,5.2151288554
F,-5.2634897316,2.9923039729,0.8515143049
F,-2.8214280751,-5.9797751956,-2.0613126355

H,1.4206361558,-0.9060346227,-3.1281330696
H,-0.2641862949,-0.420746693,-3.5082389912
H,1.0057940117,0.8125804864,-3.4294525732
H,-3.0689335284,-2.3772421461,0.594391693
H,0.3251207165,-2.7976225658,-2.0292441757
H,-0.4331196293,-3.1412007889,1.8242711778
H,1.1978256461,0.8486106412,1.8292841787
H,-3.3026061726,-0.4151966082,-1.3017601364
H,-1.3082840124,1.2988948523,2.1123386327

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B,-0.1789546158,-0.6652253106,0.1035359324
Si,1.8659408333,-0.5054545657,0.220563087
C,-0.9621570439,0.6769944577,0.3692998527
C,-0.8469813196,1.3568337616,1.5762226336
C,-1.6939773458,1.3152927405,-0.6274999593
C,-1.4145713549,2.6037774413,1.7967689339
C,-2.2607022808,2.5692828876,-0.4569744986
C,-2.1182289022,3.2158970087,0.766283548
C,-0.9836603932,-1.9562405609,-0.2627741227
C,-2.3843981342,-2.0527891956,-0.1879994085
C,-0.3360792408,-3.1304206205,-0.6761309224
C,-3.0843549795,-3.2091966927,-0.4984721422
C,-1.0011598268,-4.3020565958,-1.002401766
C,-2.3869789127,-4.3382995288,-0.9109423314
C,2.3397861356,1.2770502614,0.6754970647
C,2.0478007719,2.3284334543,-0.40507005
H,3.419925957,1.2661657416,0.8764982459
H,1.8692828998,1.5606802352,1.6238876899
H,2.3599789766,3.3280686533,-0.0873572384
H,2.5801001898,2.1008730566,-1.3346655726
H,0.9800682815,2.3823564721,-0.6466227509
C,2.6177004604,-0.8497231568,-1.4929714382
C,1.6604129427,-0.5576024223,-2.6588716684
H,2.9588005761,-1.8893052202,-1.5432103876
H,3.5172880687,-0.226258312,-1.5836547129
H,2.1492013602,-0.6826440793,-3.6299472902
H,0.7977568695,-1.2335110239,-2.6413787819
H,1.2696530314,0.4655528097,-2.6180764926
C,2.5699790834,-1.6662876819,1.5433124476
C,4.1061618913,-1.6762263671,1.5673781885
H,2.1946707323,-2.6810850919,1.3699448129
H,2.1812830289,-1.3522632864,2.520331577
H,4.4900516178,-2.3613395947,2.3293851864
H,4.5168225884,-1.9930826651,0.6030143627
H,4.5105753355,-0.6834471485,1.7878802771
F,-3.0421020233,-5.4469201452,-1.2140565768
F,-4.409893715,-3.2507086526,-0.4063041045
F,-3.1233385255,-1.0170587165,0.2076561535
F,0.9933781437,-3.1598134208,-0.7833384113
F,-0.3339057416,-5.3829451207,-1.3955038825
F,-0.180530377,0.7796632688,2.5895303868
F,-1.2928818362,3.2144683402,2.9729010563
F,-2.6635164041,4.41261942,0.9523613413
F,-2.9405440344,3.1542636738,-1.4400788522
F,-1.8493592779,0.7112696422,-1.815018336

M13_TS

0 1

B,0.5425006316,0.3576808581,0.3184874859
Si,-1.611880249,0.1390418171,0.037912374
C,1.4410354421,-1.1727898526,0.8666791978
H,1.2317092932,-2.1498536917,0.4284001801
H,1.4101609052,-1.2204509676,1.9543503204
H,2.4189852521,-0.8378601834,0.5208936928
H,0.1271098264,-0.7989115845,0.5909661855
C,0.941649722,1.3594861886,1.506880521
C,0.2065223503,1.5220909708,2.6765733704
C,2.1256007073,2.0979155808,1.4622953742
C,0.5694493949,2.3759200917,3.71017887
C,2.5274042472,2.9684818747,2.4662695046
C,1.7394246393,3.1128999145,3.6002645345
C,0.9782874644,0.7081296307,-1.1830002564
C,1.2923571042,-0.236372514,-2.1581584321
C,1.0034375847,2.0304467883,-1.630953007
C,1.6225544297,0.0852293746,-3.4682737347
C,1.3351780065,2.3985796626,-2.9275269515
C,1.6458107772,1.4164159303,-3.8583348378
F,1.9575245931,1.7466396158,-5.1076134449
F,1.346816346,3.6806420526,-3.286570559
F,0.6935216841,3.028792647,-0.7894274699
F,1.9063477903,-0.8723561944,-4.3498082835
F,1.2622557301,-1.5497859333,-1.8605815191
F,2.9516956568,1.9792493261,0.4119817786
F,3.6642645261,3.6530510981,2.3575693925
F,2.1099641311,3.9358179871,4.5757547011
F,-0.1891920898,2.4850964467,4.8001342718
F,-0.9210422799,0.8115772631,2.8558599425
C,-2.5497038555,-0.9885904702,1.2411208958
C,-1.8794902233,-2.3526589874,1.4594631932
H,-3.5419736637,-1.1357787161,0.79368503
H,-2.7146628524,-0.4909012532,2.2002903737
H,-2.5268418107,-3.0391068736,2.0126285952
H,-1.6269077345,-2.8395039512,0.5092631804
H,-0.9554648636,-2.2506223105,2.0397934869
C,-1.9196843951,-0.6080775556,-1.6872845189
C,-2.0426119088,0.3888727257,-2.8491578341
H,-2.8560275282,-1.1763989969,-1.6047311999
H,-1.1493874712,-1.3552081615,-1.9142061096
H,-2.2268992311,-0.1287582865,-3.7954597579
H,-2.8710382973,1.086208221,-2.6893816675
H,-1.1374887269,0.9900932033,-2.9753262809
C,-2.2593475808,1.9113259459,0.0999197787
H,-1.8687658594,2.4564554041,-0.7677827922
H,-1.8686108994,2.4262823943,0.9843348938
C,-3.7963288854,1.9425138657,0.104486665
H,-4.1982402542,1.4838213402,1.0130752607
H,-4.1731389445,2.9684421054,0.0573227689
H,-4.215981741,1.3993805692,-0.7499591626

M14

0 1

B,-1.471203995,0.7260545476,0.0019162475

Si,0.5265882841,0.740516023,-0.3160844269
C,-2.3876109118,-0.514031616,-0.1689972241
C,-1.8496363893,-1.7474540316,-0.5742298771
C,-3.7670703406,-0.5208090115,0.1013581898
C,-2.613072651,-2.8945282264,-0.7283685269
C,-4.5586535082,-1.6491194092,-0.0407424825
C,-3.9755907258,-2.8395965064,-0.4619085
C,-2.0247249782,2.1296343208,0.4457525433
C,-2.9563073073,2.8609503451,-0.2859716254
C,-1.4594612279,2.7722368581,1.5454501321
C,-3.3110802247,4.1611752114,0.0437457419
C,-1.802877303,4.0623851514,1.9207944416
C,-2.7307821425,4.7609507987,1.1563398103
F,-3.5182011718,2.3153150075,-1.3713263481
F,-4.1960134032,4.8360531871,-0.685993927
F,-3.0693298667,5.9998348825,1.4930606048
F,-1.2591914097,4.6351389014,2.9915860282
F,-0.5701511648,2.1108846295,2.2968548808
F,-0.5485341937,-1.8631242991,-0.8174225286
F,-2.0609690991,-4.0398730851,-1.1166727457
F,-4.7198281243,-3.9246204581,-0.5989252241
F,-5.8610117092,-1.6110429885,0.2249802823
F,-4.3825906015,0.5794110521,0.5299664423
O,0.7709753043,0.3702626879,-1.9053606595
O,1.3303130852,-0.2579919267,0.7114521367
O,1.1516840664,2.252513004,-0.0275786358
C,0.9782538567,3.3348665194,-0.9236527754
H,1.612174842,4.1577169135,-0.5869114879
H,1.2611600476,3.0575540493,-1.9457640923
H,-0.0649971378,3.679185817,-0.9338961322
C,2.0753915036,0.1339421564,-2.4135314001
H,2.4815502637,-0.7987455174,-2.0074523376
H,2.0055951235,0.0503918153,-3.499639825
H,2.7566219743,0.9581463477,-2.1644880255
C,2.4298031872,0.1320644215,1.5228461332
H,2.1992469622,1.038895572,2.0892298997
H,2.6367741001,-0.688242397,2.2124496728
H,3.3181322863,0.3169898226,0.9094065102

M14_TS

0 1

B,0.8023644933,0.0683713413,0.1951130294
Si,-1.2637029672,-0.3976885593,-0.2266351863
C,1.7389856558,-1.2666374652,0.9721262994
H,1.7954880953,-2.2331008349,0.4705354041
H,1.4404192535,-1.3923351391,2.011604616
H,2.7135562069,-0.7830458651,0.9117231274
H,0.4180498382,-1.089194598,0.4513093072
C,0.6999351125,1.1721776659,1.353767661
C,-0.0461227725,0.9217041758,2.5064576262
C,1.3230286905,2.417151784,1.3162906295
C,-0.20926622,1.8363293163,3.5344448982
C,1.1829470223,3.366796713,2.3233722077
C,0.4062681756,3.0784549144,3.4356018841
C,1.3776603394,0.4357388597,-1.2582704636
C,2.2997994067,-0.286344047,-2.0104073258
C,0.8754225105,1.5726976563,-1.895497994

C,2.7139431584,0.0938521149,-3.2843919036
C,1.2607237295,1.992726739,-3.1568040437
C,2.1956144418,1.2420201874,-3.861148479
F,2.5815014361,1.6189049323,-5.0757144566
F,0.7428627995,3.0913840431,-3.7017259692
F,-0.0524881815,2.3105442349,-1.2661349245
F,3.6015002145,-0.643033569,-3.9515039249
F,2.8336656748,-1.4284208808,-1.5447533569
F,2.11799023,2.7543481656,0.2907406585
F,1.7988980617,4.5443304385,2.2323672518
F,0.2691499597,3.973267535,4.4093680372
F,-0.9406157985,1.538528966,4.6069116478
F,-0.6374987159,-0.2765939246,2.6488392635
O,-2.2717786823,0.6098225407,0.5674995071
O,-1.557510945,-1.9489442552,0.2364455477
O,-1.5441529761,-0.185573257,-1.8349795014
C,-2.583337418,1.9520162527,0.2183219279
H,-2.6646685828,2.0696793956,-0.8658225909
H,-1.8076739623,2.6269482016,0.5969754006
H,-3.5367095573,2.1998427703,0.6878601945
C,-1.02456443,-1.0404250617,-2.8414280914
H,-1.856508038,-1.4494463407,-3.4204439309
H,-0.4486405842,-1.8745438173,-2.4204053608
H,-0.3761283849,-0.4627098392,-3.5081326551
C,-2.8691776988,-2.5057383094,0.2666082257
H,-3.3438730832,-2.4371588192,-0.7185014126
H,-2.7767633577,-3.5557549009,0.547164243
H,-3.4858650901,-1.9833976006,1.0032642553

M15

0 1

B,-0.142886165,0.3419756389,-0.5674193465
Si,0.7061569269,1.9883168231,-1.4318276626
C,0.7403418542,-0.8284669441,-0.0417397716
C,2.0539018494,-1.0247326393,-0.4873814366
C,0.2909701801,-1.7461102937,0.9199724093
C,2.8730079197,-2.0430455749,-0.0302947112
C,1.0865513708,-2.7692794562,1.4143129013
C,2.382080274,-2.9187902974,0.9324238224
C,-1.7046958905,0.2721788174,-0.4670006063
C,-2.4016605582,-0.7968100127,-1.0327761777
C,-2.4849519169,1.2869839226,0.0855761252
C,-3.7861582408,-0.8390439669,-1.0996441826
C,-3.871719858,1.2718084819,0.0539885577
C,-4.5241676698,0.2060771012,-0.5547435223
C,2.2135193019,2.5031889777,-0.4211709227
C,3.5160511332,2.6544544618,-0.8835177373
C,2.0198045874,2.6841717159,0.9445791906
C,4.5672929306,2.9949319764,-0.0399904634
C,3.0377643768,3.0225535286,1.8206257321
C,4.3238565854,3.1821170608,1.3150378798
F,-0.9391829739,-1.6552680183,1.4231298725
F,0.625197553,-3.6070238815,2.3355151672
F,3.1482210458,-3.894591678,1.388601869
F,4.1078013596,-2.1923557018,-0.4964753885
F,2.564763052,-0.2189399247,-1.42639836
F,-1.7257226065,-1.8269917124,-1.5520837166

F,-4.4114227384,-1.8655393682,-1.6665515802
F,-5.8479974945,0.1780455147,-0.6012500755
F,-4.5750699214,2.2613737929,0.5969304518
F,-1.8947243643,2.3117188825,0.7141518509
C,1.1458311043,1.6259186712,-3.2274057359
C,0.8946955803,0.3909419957,-3.8078757529
C,1.6634715591,2.6120801047,-4.059127036
C,1.1626612711,0.1188926704,-5.1414673007
C,1.9474317675,2.3850853165,-5.3978005688
C,1.6968437451,1.1269551033,-5.9360862052
C,-0.5402644091,3.4068745564,-1.543662623
C,-0.4514845666,4.6363389111,-0.900029416
C,-1.7028714642,3.1841710253,-2.2776123519
C,-1.4614483389,5.5883042429,-0.964777917
C,-2.7377237416,4.1028155026,-2.361988294
C,-2.6124222127,5.3153803586,-1.6936965178
F,-3.5850598731,6.213230485,-1.760476566
F,5.3196790193,3.5034448031,2.1289976661
F,1.9605741241,0.8909110672,-7.2136978462
F,0.6285321861,4.9506417552,-0.1762211725
F,-1.8554316633,2.0190440604,-2.9336545193
F,1.9000402514,3.8321038098,-3.5631027024
F,0.3549336017,-0.5929504192,-3.0663156996
F,3.8112017809,2.4595227794,-2.1715184737
F,0.7823950725,2.5237683167,1.4431365308
F,-3.8362848728,3.8353379552,-3.0623653331
F,-1.3394736302,6.7520575327,-0.3348043288
F,0.9128865241,-1.0780284279,-5.6632039993
F,2.4487929356,3.3463315092,-6.1666033049
F,2.8050373087,3.1899507911,3.1185927299
F,5.8010190382,3.1347776368,-0.5148073897

M15_TS

0 1

B,0.004485199,-0.7791718937,1.2237958549
H,0.97956213,-2.2846699565,2.7954403376
H,-0.7978247058,-2.3166503986,3.018256477
H,-0.0893009938,-2.9402978356,1.5205010009
H,-0.1352400079,-0.678983967,2.4691382584
C,-1.2818432031,-0.8405526031,0.268899231
C,-2.546636029,-1.2262688742,0.7098262009
C,-1.210656323,-0.5204839282,-1.0888942047
C,-3.6621985041,-1.297111761,-0.1117100547
C,-2.2974096505,-0.5931804577,-1.9493848291
C,-3.5358310362,-0.9799566331,-1.4570413582
C,1.4601974474,-0.8538221018,0.5447165007
C,2.5472016237,-0.0218657173,0.764497747
C,1.7054927459,-1.8986133058,-0.3511086885
C,3.7874828665,-0.1846041556,0.1574389681
C,2.9215997459,-2.1023292092,-0.9838901488
C,3.9766489126,-1.2350365026,-0.7261915474
F,5.1510358105,-1.4138950156,-1.318011267
F,3.0854881997,-3.1141237243,-1.8316374594
F,0.7211570564,-2.7620263368,-0.650261472
F,4.7836632448,0.6573349901,0.4206414167
F,2.4299979002,1.0208573103,1.6023254966
F,-0.0617666253,-0.086378211,-1.6311047071

F,-2.1638327719,-0.2724222237,-3.2334133034
F,-4.5887823795,-1.0417580369,-2.2616129253
F,-4.8434873673,-1.6643288356,0.3793758206
F,-2.736453476,-1.5421357559,2.0040848041
C,-0.3555489067,2.4118439018,0.7584998881
C,0.6948817737,3.2999842033,0.5218782866
C,-1.4008893133,2.4540779938,-0.1679047613
C,0.7420070058,4.1253092077,-0.5957104718
C,-1.3856449446,3.259272901,-1.294915054
C,-0.2965290811,4.093974214,-1.5156771551
Si,-0.4057185214,1.2121370309,2.2132787237
C,0.0126918089,-2.1884072808,2.3051739136
C,0.7044286991,1.7791244642,3.631032127
C,0.5771660956,3.0776700456,4.1129970486
C,1.6156094641,0.9640109323,4.2875273793
C,1.3236033338,3.5612447654,5.1768264554
C,2.380543579,1.4034179097,5.3584576122
C,2.231840185,2.7126761491,5.8010842788
C,-2.1134599972,1.3006973257,3.037521666
C,-2.4043115725,0.3718313502,4.0330582539
C,-3.0616018084,2.308813056,2.8637326242
C,-3.5748751037,0.370242452,4.7717083038
C,-4.2525137073,2.3447137804,3.580871753
C,-4.5140794137,1.3663697702,4.530965914
F,-0.2963988477,3.907952702,3.5273856611
F,1.1800066372,4.8112062412,5.6041221789
F,2.9519187912,3.1511848492,6.8235449381
F,3.2440345437,0.5918458529,5.9605686287
F,1.7817063286,-0.3065279171,3.8876844466
F,1.6977997267,3.427792881,1.3928102789
F,1.7657407114,4.9520545715,-0.7797083207
F,-0.2635777914,4.8756972467,-2.5836494831
F,-2.4038145174,3.2499996698,-2.1485116531
F,-2.5078690931,1.7249310687,0.0292062142
F,-2.8505016498,3.321732523,2.0209280156
F,-5.1318556658,3.3200193884,3.3784039889
F,-5.6425136122,1.3966540666,5.2236753417
F,-3.7999982233,-0.5537012574,5.6999437834
F,-1.4926000125,-0.5755827282,4.3205298056

M16

0 1

B,-0.0955136359,0.2222414804,-0.5436553096
Si,0.6448061825,1.90129553,-1.4579953765
C,0.7270536825,-1.0403555115,-0.1364599731
C,2.0794326229,-1.1786471044,-0.4854253779
C,0.2035484668,-2.0988249576,0.6274538956
C,2.8581154612,-2.2667908236,-0.1229345812
C,0.9533195761,-3.1985340068,1.0154682334
C,2.2875717954,-3.2820379605,0.6343153882
C,-1.6531654701,0.2462945306,-0.2914677572
C,-2.5288217563,-0.5935877868,-0.97172915
C,-2.2365888259,1.1797418615,0.5569633716
C,-3.9067699649,-0.5112301406,-0.8371631917
C,-3.6083781556,1.284640616,0.7368340842
C,-4.4477949942,0.4352910357,0.0260880022
C,2.0658235381,2.6450184505,-0.4681251425

C,3.379113434,2.6755008443,-0.9583957979
C,1.8207580426,3.212659301,0.7925318132
C,4.4118504577,3.2519302523,-0.2198617767
H,3.6038248042,2.2414662522,-1.9301384505
C,2.849295588,3.7866145962,1.5382085659
H,0.8118788327,3.2119925372,1.2006869952
C,4.148018132,3.8071977866,1.0313572346
H,5.4211037,3.2670378942,-0.6201193374
H,2.6373000116,4.2194163745,2.5111805362
H,4.9507888029,4.2559843883,1.6083341176
F,-1.06474241,-2.0867681384,1.0367699533
F,0.4138401919,-4.1711947278,1.7438946494
F,3.012991201,-4.3285465361,0.9926465013
F,4.1332980973,-2.3500288117,-0.4896644796
F,2.6825498928,-0.2410512664,-1.2149147612
F,-2.0317133719,-1.5246083949,-1.8001361771
F,-4.711416437,-1.3270091677,-1.5138305797
F,-5.7647756649,0.5230961777,0.1748017468
F,-4.1232360258,2.1831962243,1.5725357248
F,-1.4444034184,2.002287325,1.2652553684
C,1.1784977853,1.5056140704,-3.2252001266
H,0.3235153692,1.1428195726,-3.804974704
H,1.5335074989,2.4252638709,-3.7036146392
H,1.9721926507,0.758220335,-3.2831249797
C,-0.7368791399,3.1824948912,-1.5769071322
H,-1.6172338957,2.7711211761,-2.0832699362
H,-1.0489999033,3.5554468263,-0.5973928503
H,-0.3829072585,4.0385049039,-2.1607334839

M16_TS

0 1

B,0.0893890816,-0.9180218932,1.1057243749
H,1.3865869655,-2.7665974606,2.015377456
H,-0.3014478712,-3.0266010828,2.5754814468
H,0.0743042922,-3.1354928215,0.8496556602
H,0.123522758,-1.3471415432,2.285690602
C,-1.3110406072,-0.8290938034,0.3339888295
C,-2.4583713663,-1.5298825812,0.7001548339
C,-1.484931094,0.0497469176,-0.7387047082
C,-3.6840994977,-1.3959863268,0.0619809911
C,-2.6925440679,0.2163352681,-1.4036116561
C,-3.8033605309,-0.5122965616,-1.0012750493
C,1.4503636013,-0.730421121,0.2791765505
C,2.6253404737,-0.196281818,0.7949759125
C,1.5486309857,-1.1664236204,-1.0437069315
C,3.796484894,-0.0418122492,0.0649687633
C,2.694766893,-1.031665426,-1.8150764599
C,3.8293076914,-0.4572855167,-1.2576241431
F,4.9386380674,-0.324486665,-1.9774611253
F,2.7195425892,-1.4580448835,-3.0762273469
F,0.5011499197,-1.7609313405,-1.6340376012
F,4.8810443572,0.4928828048,0.6259678993
F,2.6690759516,0.1936283381,2.081761673
F,-0.4581134447,0.7852317307,-1.1808820873
F,-2.7941667251,1.0727032248,-2.4184388534
F,-4.968466164,-0.3637572029,-1.6247442344
F,-4.7426269991,-2.0952168243,0.4711233234

F,-2.4257805416,-2.3651592085,1.7557122602
C,-0.2505368481,2.1649741265,1.6149733092
C,0.9598882934,2.7990404557,1.295268253
C,-1.4356195319,2.6990997704,1.085850983
C,0.987405497,3.9164925239,0.4634122653
H,1.8958129973,2.4210320495,1.700077147
C,-1.4137053617,3.8159389738,0.2522590813
H,-2.3929061103,2.2380243821,1.3201663156
C,-0.1997011421,4.4224061837,-0.0648440333
H,1.9346413619,4.3908195158,0.2258141079
H,-2.3416767626,4.2090756909,-0.1515947481
H,-0.1787056949,5.2884218913,-0.7190058982
Si,-0.2969017697,0.5977087577,2.6444771228
C,0.3319855442,-2.6298856828,1.7803350452
C,-2.0340838512,0.3142040608,3.3194434718
H,-2.81484347,0.2907130859,2.5558084071
H,-2.0902203497,-0.6218399519,3.8848253259
H,-2.2642450982,1.1327251108,4.0105581887
C,0.8443562447,0.6837141153,4.1445837849
H,1.1945571107,-0.305032206,4.4585139551
H,1.7235630169,1.3033329745,3.959485795
H,0.2854123321,1.1213137386,4.9780170205

M17

0 1

B,0.074007202,0.6569342746,-0.015312562
Si,-0.0345926799,2.6875601374,-0.1964453506
C,1.4188978344,-0.0737406167,0.1628086713
C,2.6406321039,0.6226933013,0.1607491555
C,1.5181114296,-1.4587650547,0.3997149731
C,3.8691339815,0.013501247,0.343747098
C,2.7299529743,-2.10165023,0.5919146002
C,3.9082279177,-1.3612185654,0.5579604831
C,-1.3101468134,-0.0515959162,-0.1149649026
C,-2.3591071617,0.3702197602,0.7021449166
C,-1.6077532809,-1.0471365903,-1.0462296658
C,-3.6349983555,-0.1634508775,0.6290188004
C,-2.8767299386,-1.5913574906,-1.1662542007
C,-3.8901064658,-1.1483789868,-0.3202271636
F,-5.1012147924,-1.6716925503,-0.4171700428
F,-3.1349584199,-2.5281015837,-2.0710798038
F,-0.655574115,-1.4795116826,-1.8765457405
F,-4.6000936541,0.2458770003,1.4406722102
F,-2.1090900099,1.312401258,1.622650064
F,0.4287893323,-2.2148508852,0.4729450681
F,2.7806833543,-3.4080941765,0.8146266219
F,5.0664667008,-1.9638977472,0.739873816
F,4.9938100434,0.7138891585,0.3266232853
F,2.6464511476,1.9453167285,-0.0178946177
C,-1.7887745244,3.2054243197,-0.4960603181
C,0.5704419438,3.6260307592,1.2737516787
C,0.8600867372,3.2938120166,-1.6984704887
N,-2.9028934261,3.4320062189,-0.713874886
N,1.4100841842,3.6072449057,-2.6675095746
N,0.9569443905,4.1501300978,2.2306053951

M17_TS

0 1

B,0.6442442369,0.1409380051,0.1796938706
Si,-1.4836888782,-0.1830525852,-0.2858559705
C,1.5444885169,-1.3072278867,0.6046136389
H,1.4679205872,-2.1984094639,-0.017273212
H,1.3857568738,-1.551053574,1.6547945466
H,2.5413778064,-0.8785671732,0.4681252222
H,0.0921166197,-0.9987475767,0.2482203701
C,0.6952762848,1.0579695658,1.4868507507
C,-0.2294965752,1.0245553615,2.521445615
C,1.7754856956,1.9169249255,1.6798937598
C,-0.1385260525,1.8063950515,3.6636757889
C,1.9110751435,2.7190219668,2.8037460091
C,0.9439912043,2.6653858832,3.8010266712
C,1.0056554977,0.7253391171,-1.2652839669
C,1.3828512413,-0.086355037,-2.3376096735
C,0.9360210734,2.0922707795,-1.5514075414
C,1.7012947811,0.4019146724,-3.594423297
C,1.2509479101,2.6215080155,-2.7966128058
C,1.6364356306,1.7709589651,-3.8239865525
F,1.9357778443,2.260670848,-5.0173354455
F,1.1832432382,3.930444772,-3.0096907227
F,0.5553934108,2.9615744465,-0.6110020499
F,2.047864719,-0.422549994,-4.5755670969
F,1.3971170996,-1.4191849041,-2.1841829523
F,2.7404258533,1.984259841,0.7531223507
F,2.9567241878,3.5275196889,2.937884556
F,1.0621624153,3.4209850092,4.8838397702
F,-1.0611102287,1.7330885104,4.6157132699
F,-1.2824081839,0.1854368358,2.4252952697
C,-2.5322716754,-1.4540941773,0.5455616424
C,-2.1918405054,1.4879481818,0.0041790406
C,-1.6545658717,-0.5449149364,-2.0877309336
N,-3.1169961152,-2.3072758236,1.0655232445
N,-1.7236587383,-0.7687577623,-3.2215060051
N,-2.5880808969,2.5555772119,0.2108391184

M18

0 1

B,0.61713732,-1.2019873439,0.1938535215
C,2.08092192,-1.57437773,0.6158690834
C,2.4072605924,-2.824917053,1.1621943
C,3.156779577,-0.6856429118,0.4968028812
C,3.6877718519,-3.1657969852,1.5708885224
C,4.4540317987,-0.9958533811,0.8742158036
C,4.7183523712,-2.2459167415,1.4195965999
C,-0.3650811657,-2.349599905,-0.2431610939
C,-1.6626293153,-2.4534389002,0.2547755925
C,-0.0041424649,-3.2988393975,-1.2009902743
C,-2.5589470706,-3.4259023335,-0.1641228312
C,-0.8762679885,-4.2729016752,-1.6624147895
C,-2.1617964842,-4.3361984921,-1.1358963476
F,1.4654710869,-3.7548079733,1.3385538239
F,3.9402521997,-4.3594444579,2.0981862058
F,5.9481680811,-2.5593645402,1.7955077854
F,5.4386958628,-0.1164155985,0.7214871402
F,2.973686698,0.5315244518,-0.0319936328

F,-2.074464911,-1.6084359724,1.2104322659
F,-3.7831323017,-3.4945947256,0.3505214022
F,-3.0062675097,-5.2675091927,-1.5581682541
F,-0.4971492383,-5.1475742534,-2.5898167981
F,1.2298631604,-3.2803636819,-1.7203743051
Si,0.0001507357,0.7074133128,-0.015671617
Si,0.8661989711,1.0882503402,-2.1821902603
H,-0.2518976448,1.2924412314,-3.1364175393
H,1.7464498452,2.2798708001,-2.1919441367
H,1.6499891438,-0.0908567771,-2.6314004138
Si,0.9893264816,2.1766324265,1.5236304855
H,1.8142103654,3.1940085355,0.831253899
H,-0.060761878,2.8628648481,2.3154796767
H,1.8537741166,1.4069844818,2.4542986964
Si,-2.3138309396,1.0137598536,-0.1790630901
H,-2.9189607746,-0.0779653802,-0.9840253585
H,-2.9651817435,1.0753566757,1.1492832826
H,-2.5503935189,2.2979108658,-0.8853531858

M18_TS

0 1

B,0.445786163,0.1392851946,0.2278320123
Si,-1.6950467994,-0.2206570894,-0.1644270581
C,1.2919972148,-1.3735328295,0.8164170063
H,1.1667972459,-2.323647331,0.2942341836
H,1.1269433975,-1.4943107504,1.8866178175
H,2.2988104757,-1.0026638715,0.6224138802
H,-0.0133595236,-1.0224982401,0.4393138049
C,0.6459315476,1.1328851376,1.4664042748
C,-0.1037726126,1.043975035,2.6365401019
C,1.6246544153,2.1263526128,1.4792366431
C,0.0537062116,1.88551515,3.7273561637
C,1.8153579957,2.9975404525,2.5451581052
C,1.0218090758,2.8794574577,3.6773546608
C,0.9287463091,0.5549406802,-1.2404085199
C,1.5149265592,-0.2857987173,-2.1841464055
C,0.6763025134,1.8515852087,-1.6946188701
C,1.8434801967,0.1209833096,-3.4731332958
C,0.9914100812,2.3011066744,-2.9665631287
C,1.582634855,1.4240378764,-3.868091729
F,1.8900940916,1.8291808511,-5.0951747115
F,0.728140039,3.5529015978,-3.332029394
F,0.0805275762,2.7306154683,-0.8712200568
F,2.3994584376,-0.734528225,-4.3281306822
F,1.7727464469,-1.5714191509,-1.8880304983
F,2.4530956153,2.2745560509,0.4362020199
F,2.7620895269,3.9315180115,2.4944031658
F,1.1959130727,3.6986633386,4.7083882034
F,-0.7088934787,1.7485601519,4.8101000266
F,-1.0524799005,0.0917073186,2.7418550338
Si,-1.8662102331,-0.8702500099,-2.409365306
H,-1.4328086654,0.2270856869,-3.3110147404
H,-1.0189454017,-2.0628776582,-2.6620310129
H,-3.2778301338,-1.2139719855,-2.7080091987
Si,-2.7044704082,-1.8822910353,1.1591916714
H,-1.6478966979,-2.7578107888,1.7311121935
H,-3.4914951906,-1.2929698361,2.2657160817

H,-3.5935478377,-2.7188602963,0.3161678561
Si,-2.7526390701,1.8477377862,0.1697375684
H,-2.0947022318,2.600285669,1.2634678237
H,-2.7254211021,2.6381641356,-1.0819848924
H,-4.1639279465,1.5790041493,0.5398896416

M19

0 1

B,-0.1380043635,0.3683192208,-0.606132888
Si,0.6999599549,2.0196247751,-1.4652802707
C,0.7563163005,-0.782737723,-0.043964206
C,2.0640929753,-0.9950822951,-0.4971647916
C,0.3250638843,-1.6490419567,0.9702052634
C,2.8936122165,-1.9853335061,0.003724744
C,1.132371559,-2.6403210803,1.509099284
C,2.4216163567,-2.8096817312,1.018670392
C,-1.7013379642,0.2672879602,-0.508252988
C,-2.3790438759,-0.8073158491,-1.0839412063
C,-2.4980357507,1.2581118687,0.0632407053
C,-3.762821927,-0.8771801021,-1.1447603254
C,-3.884797097,1.2135263237,0.0390061178
C,-4.5187465732,0.1440744384,-0.5811451784
C,2.2079564636,2.4832368297,-0.4384372081
C,3.5215552217,2.6448024108,-0.8715833725
C,2.0364318002,2.6019414224,0.9389273046
C,4.5893838739,2.9299885621,-0.0317827908
C,3.0381002026,2.8849576887,1.8499838363
C,4.3110005554,3.0482373714,1.3208168234
H,5.5937869357,3.049895382,-0.4172950139
H,2.8419189396,2.974693025,2.9106391526
F,-0.8998827259,-1.5367398843,1.485943239
F,0.6874961562,-3.4296169276,2.4819799217
F,3.2001092276,-3.7574193164,1.5168867121
F,4.123755592,-2.1556672139,-0.4709192457
F,2.558689616,-0.2399307574,-1.4830006869
F,-1.6863017042,-1.8202530279,-1.6173998392
F,-4.3706599117,-1.9099395714,-1.7230793045
F,-5.8443419705,0.0896536331,-0.6218388477
F,-4.607977165,2.178525759,0.6017313773
F,-1.9275608529,2.2835517018,0.7064516093
C,1.1249622028,1.6435797145,-3.2564164317
C,0.860463399,0.4135965419,-3.8452787065
C,1.6506505575,2.6022956277,-4.1182911465
C,1.1087527003,0.1008729872,-5.1714073177
C,1.9344936098,2.381403835,-5.4562017982
C,1.6534102652,1.1141532724,-5.9471404677
H,0.8857756019,-0.8754433144,-5.5819922952
H,2.3513504596,3.1562259459,-6.0867467155
C,-0.5505162061,3.4299213665,-1.5420443501
C,-0.4792194695,4.6534980255,-0.8794418468
C,-1.7199161758,3.2452599763,-2.2793451128
C,-1.4675381706,5.6257895212,-0.9186378899
C,-2.7586928242,4.1563108412,-2.3720268892
C,-2.5966181163,5.3424607994,-1.670825752
H,-1.3623270133,6.5599104971,-0.381847892
H,-3.646398638,3.9547233668,-2.9580829765
F,-3.5735553373,6.2566598012,-1.7284150393

F,5.3188072764,3.3244912274,2.158974943
F,1.9127263668,0.8588318263,-7.2364896669
F,0.6109353192,4.9268809468,-0.1429318944
F,-1.8595303891,2.0787632833,-2.9493925684
F,1.8929346917,3.8258393515,-3.6180819693
F,0.3069339954,-0.5490619687,-3.0713898423
F,3.7954262013,2.5058712604,-2.1775677452
F,0.7847234933,2.4173802771,1.4138161821

M19_TS

0 1
B,-0.722940815,-0.4623291452,-1.220463274
H,0.1532336787,0.2392105347,-1.7799691765
C,-0.4151882753,-1.986711988,-0.8053202984
C,0.5673961999,-2.7735940872,-1.4052759949
C,-1.1723823809,-2.6534556173,0.1582067801
C,0.7959373047,-4.1059443383,-1.0866827027
C,-0.9884965995,-3.9845908223,0.5000469116
C,0.0077969529,-4.7203247204,-0.1254491488
C,-2.204314373,0.1234223505,-1.002020068
C,-2.5230376102,1.4114148395,-0.592410406
C,-3.3075160067,-0.6702838644,-1.3235091571
C,-3.8231282164,1.8853845602,-0.4617306575
C,-4.6221521609,-0.2442393874,-1.2077493184
C,-4.8837506458,1.0474967319,-0.7681356449
F,-6.1358359129,1.4775778764,-0.655469085
F,-5.630299343,-1.0553225645,-1.5205976719
F,-3.1200147633,-1.9201448605,-1.7752246336
F,-4.0516471604,3.1327263424,-0.0543461951
F,-1.542150491,2.284022383,-0.3054698221
F,-2.1192831968,-1.9958227985,0.843488452
F,-1.7412969529,-4.5509417666,1.4420095876
F,0.2070868038,-5.99416282,0.1957026891
F,1.7565575799,-4.7937048588,-1.7034663224
F,1.3596624332,-2.254638377,-2.3588634213
C,0.0008809099,0.757177037,1.7488133794
C,-0.4213001437,1.9377129803,2.3717798691
C,-0.1711746012,-0.385379065,2.53390131
C,-1.0031016631,1.9973044276,3.629317341
C,-0.7399130536,-0.4148441375,3.7944121815
C,-1.1560575372,0.8017100463,4.3116494821
H,-1.3122468658,2.9423178605,4.0572226347
H,-0.8478490665,-1.3410687077,4.3439442502
Si,0.7626350195,0.6740524582,0.0259466311
C,-0.5355347807,-0.3178336558,-2.9974331498
C,2.3973357681,-0.2710686241,0.0202424369
C,3.0645143219,-0.3979767588,-1.1983078426
C,3.116572771,-0.7575664909,1.1133742163
C,4.2902002725,-1.0091026426,-1.3872418015
C,4.3485319077,-1.3891849228,1.0183699528
C,4.9012137815,-1.5096030033,-0.2468377885
H,4.7449280269,-1.0902657207,-2.3660192897
H,4.8612006996,-1.7546170664,1.8990163197
C,1.3133231855,2.3948927917,-0.51997631
C,2.2236334521,3.0910107752,0.2744249812
C,0.9446241785,3.0584004129,-1.6827360296
C,2.7388744946,4.3412286431,-0.0199287622

C,1.4068462867,4.3088892677,-2.0619192352
C,2.3042357633,4.9232064582,-1.2023583168
H,3.4377184318,4.8400121627,0.6392464384
H,1.0841610564,4.7801602389,-2.9813593075
F,-1.7155703438,0.8242861136,5.5266856791
F,6.0883519196,-2.1148342842,-0.3715720677
F,2.7760297185,6.1331329254,-1.5294965783
H,-1.0733306511,0.5625660764,-3.339399662
H,0.4549141209,-0.3631939772,-3.4486983098
H,-1.0809459171,-1.2279382857,-3.2539674258
F,2.6270332171,-0.5828624428,2.3489365728
F,2.466000065,0.1433763481,-2.2850521357
F,0.0798918079,2.4439067948,-2.5170763472
F,2.618017234,2.5050033648,1.4211575665
F,-0.2450684411,3.1116858758,1.7486317374
F,0.2663516054,-1.5569618756,2.0411559581

M20

0 1

B,0.2370990791,0.7874845653,-0.1813486621
Si,0.1390427508,-1.2489810367,0.0756015248
C,1.5314629963,1.6485762251,-0.2232307265
C,2.8039928622,1.0641373421,-0.1068963901
C,1.5274030595,3.0422102188,-0.4113016974
C,3.9834257549,1.7903008557,-0.1687948623
C,2.6871787635,3.7985558804,-0.478957292
C,3.9195063544,3.1658978344,-0.3571093291
C,-1.1912981481,1.4452630233,-0.2646134433
C,-1.7424822101,2.1420987069,0.802562297
C,-2.0513010596,1.1439469106,-1.3140926173
C,-3.0818478254,2.5022909251,0.8480219591
C,-3.3910065498,1.4972024357,-1.3185890388
C,-3.9086381216,2.1745270052,-0.2200077744
C,1.1091254545,-2.1909847896,-1.2322884464
C,2.0277999654,-3.1925030677,-0.8876860737
C,0.9350406698,-1.8914475748,-2.5933585546
C,2.7397769798,-3.8812698706,-1.869000006
H,2.1988418702,-3.431837377,0.1592982625
C,1.6451865449,-2.5772564515,-3.5777866436
H,0.2351069544,-1.1139931161,-2.8940824997
C,2.5482358011,-3.5757726024,-3.2155255623
H,3.4471878357,-4.6532819432,-1.5818741165
H,1.4951603178,-2.3310462742,-4.6245898881
F,0.3830268197,3.7095896839,-0.5394779448
F,2.6376002823,5.1148445829,-0.6590377454
F,5.0336649147,3.8761691631,-0.4181995256
F,5.1651095477,1.1934832324,-0.0508640675
F,2.9238218783,-0.2476768367,0.0813372609
F,-0.9674523651,2.4471239706,1.856028739
F,-3.5804991782,3.1529876262,1.8977085896
F,-5.192687839,2.5171889866,-0.1950915595
F,-4.1796849785,1.196845622,-2.3471633483
F,-1.5627933405,0.4778850845,-2.3741648429
C,0.6938517697,-1.6783089758,1.826033102
C,1.3441405011,-0.7714561821,2.6739126148
C,0.4015861029,-2.9563410279,2.3308051514
C,1.7027976864,-1.1264147673,3.9743813443

H,1.5747544806,0.2336780546,2.3263165165
C,0.766235965,-3.3217736374,3.6246656031
H,-0.1271078096,-3.6742557564,1.7060240296
C,1.4188540009,-2.4048764305,4.449072199
H,2.2009262057,-0.4052519284,4.6149488837
H,0.5352191545,-4.3169583705,3.992035684
C,-1.6987682225,-1.6761862586,-0.0231645624
C,-2.2968671098,-2.2310628386,-1.1613889115
C,-2.5357555677,-1.2843215773,1.0363459218
C,-3.6838006308,-2.3638719656,-1.2544504838
H,-1.6776409634,-2.5521054026,-1.9956596262
C,-3.9199727338,-1.4113206449,0.949837836
H,-2.0990777128,-0.8667381402,1.9432136307
C,-4.4974602215,-1.9449002832,-0.2040839547
H,-4.127488352,-2.78750056,-2.1502259536
H,-4.5476118633,-1.0946104125,1.7777898513
H,1.6989411514,-2.6848041275,5.459887275
H,3.1035299632,-4.1108598468,-3.9797266988
H,-5.5765327856,-2.037504051,-0.2800753569

M20_TS

0 1

B,0.6881206369,0.4225408054,-1.2537712904
H,0.0342098028,-0.5111226972,-1.7885462816
C,0.005317848,1.868657182,-1.1510107017
C,-1.1326966934,2.2043092808,-1.8844753297
C,0.3839290608,2.8310830806,-0.2155837264
C,-1.8433625405,3.3842720092,-1.7239629712
C,-0.2870475887,4.0323831339,-0.0296326017
C,-1.4145470277,4.3121191456,-0.7861640784
C,2.2278723516,0.194092456,-0.8832641851
C,2.7417728621,-1.0337753097,-0.4714027109
C,3.1793331785,1.2033299497,-1.031701241
C,4.0705997886,-1.2406652992,-0.1309769109
C,4.5187075947,1.0441083013,-0.6986186206
C,4.9657121621,-0.1845683872,-0.2326849564
F,6.2460417205,-0.3577895426,0.0808665404
F,5.3796768976,2.0496385522,-0.8469035816
F,2.8292412307,2.3906857271,-1.546384386
F,4.494340918,-2.4378368067,0.2703845952
F,1.9335403017,-2.107642639,-0.4277878395
F,1.4218803193,2.6104299447,0.6104144208
F,0.1264800366,4.901118176,0.8926961867
F,-2.0851143306,5.4460740011,-0.6048158451
F,-2.9370986985,3.621844232,-2.4463303019
F,-1.6348419175,1.3246091632,-2.771271593
C,0.2759072502,-1.1160614193,1.6677550006
C,0.1690296714,-2.3770559427,2.2741650865
C,1.0737668338,-0.1458347023,2.2927784229
C,0.8295643173,-2.6559216824,3.4695458773
C,1.7362573709,-0.4220584159,3.4882328403
C,1.6145310748,-1.6786120803,4.0788961419
H,0.7366070805,-3.6391930304,3.9202320133
H,2.3505423267,0.3431895646,3.9527603142
Si,-0.6575318583,-0.7829063007,0.0698004732
C,0.6656725359,-0.1405297953,-3.0077023241
C,-2.1449611811,0.3281539784,0.3870313111

C,-3.2579325573,0.3114179011,-0.4687993572
C,-2.1215778591,1.2776829331,1.4200904427
C,-4.2991706264,1.225130729,-0.3141014023
C,-3.1606043383,2.1938778857,1.5797695134
C,-4.2481371659,2.1736991843,0.7069206186
H,-5.1436850163,1.2031942249,-0.9958599395
H,-3.1188074645,2.9244914324,2.3821340136
C,-1.3078299563,-2.399407423,-0.6602396802
C,-2.5166694501,-2.9193692969,-0.1643172708
C,-0.6392335307,-3.1359394846,-1.6494734407
C,-3.0336751281,-4.1240333134,-0.6359670855
C,-1.156312291,-4.3378861157,-2.1324232638
C,-2.3549816691,-4.8342873944,-1.6256849827
H,-3.9668389845,-4.5058159405,-0.233449517
H,-0.6193249981,-4.8873296712,-2.8993595537
H,1.4277085566,-0.9097089634,-3.1222379599
H,-0.2591670123,-0.4361105394,-3.5064737522
H,1.0028997613,0.8062894439,-3.4302402801
H,-3.0646308448,-2.3740856527,0.6011769116
H,0.3108232874,-2.7870415184,-2.0446950549
H,-0.4248715729,-3.15709142,1.8043740752
H,1.1972395882,0.8346438265,1.8422950816
H,-3.3081656406,-0.4122000563,-1.279276204
H,-1.2811031309,1.3072152292,2.1107098294
H,-2.7582660057,-5.7706388124,-1.9985507675
H,-5.0533293304,2.892537935,0.8233165351
H,2.133687664,-1.8969493755,5.0069725439

M21

0 1

B,-1.022416633,0.7683701587,0.0396872377
Si,1.0180465106,0.9711074113,0.0166122334
C,-1.7923028556,2.1352220059,0.2101990771
C,-1.6248580179,2.9057228367,1.3552962889
C,-2.5699459102,2.6969385793,-0.7971514506
C,-2.1985674777,4.1589731441,1.5138009037
C,-3.1447648775,3.9545743957,-0.6899750959
C,-2.9588171118,4.6872619001,0.477401006
C,-1.8295001973,-0.555811361,-0.1599956381
C,-3.23332042,-0.6361318148,-0.1200014146
C,-1.1788551344,-1.7817471977,-0.370920746
C,-3.932563162,-1.8221272302,-0.2871932495
C,-1.843053402,-2.9859361042,-0.5447657869
C,-3.2315246336,-3.0023831626,-0.5040195197
F,-2.7737859979,2.006671776,-1.9287930894
F,-3.8746454944,4.461090496,-1.6808907961
F,-3.5105153411,5.8890209265,0.6023524504
F,-2.0258585955,4.8554799847,2.6346529974
F,-0.8929011558,2.4145938487,2.3688575262
F,0.1534345174,-1.8379082985,-0.4084822547
F,-1.1720385266,-4.116417752,-0.7442206871
F,-3.9768997332,0.4472926445,0.0965952907
F,-5.2608251707,-1.8440823001,-0.2399881146
F,-3.8855410803,-4.1406609566,-0.6656033193
C,1.4332906971,2.8031410289,0.2290401581
H,0.908373514,3.4255096181,-0.5040777883
H,1.189437542,3.1725635315,1.2293785672

H,2.5082294391,2.949803707,0.0757785381
C,1.867068177,0.0165119377,1.4045779618
H,1.4947271465,0.3449282128,2.3800186409
H,1.7218352888,-1.0628289737,1.322490767
H,2.9431733935,0.219601854,1.3746418632
C,1.6867958636,0.4760226545,-1.6819718483
H,1.2110960039,1.0624580302,-2.4749389477
H,2.7603952403,0.692805743,-1.7144405711
H,1.5471241446,-0.5832367347,-1.9058714999

M21_TS

0 1

B,-0.1491811252,-1.1674660288,0.0605638332
Si,-0.114551476,-2.3714856468,-1.759956754
C,-0.1910960875,-2.1654341757,1.6225620784
H,0.4600248576,-3.0289219485,1.7673414549
H,-1.2261101613,-2.4166572907,1.8499917733
H,0.160181171,-1.3565560836,2.263015425
H,-0.1706520329,-2.4083440675,0.2517231921
C,-1.5056960554,-0.3281745618,0.2142319733
C,-2.7564844113,-0.8136166705,-0.1559837142
C,-1.5285108214,0.932347889,0.8126210933
C,-3.9399985755,-0.1030119656,-0.0115332512
C,-2.6856557824,1.684044209,0.972433555
C,-3.9021413292,1.1649335876,0.5510812249
C,1.2554151316,-0.4117172226,-0.0711932828
C,2.4672829934,-0.9171504159,0.3936334755
C,1.3644869704,0.7823441756,-0.7856616057
C,3.6904219889,-0.2860451473,0.2097816081
C,2.5639446731,1.4491732101,-0.9930261572
C,3.7403164005,0.9122535921,-0.4873449265
F,4.9001918599,1.5335445012,-0.6766580605
F,2.5958029565,2.5918603011,-1.6757441719
F,0.2703532505,1.3391563781,-1.3304017835
F,4.8111200589,-0.828837534,0.6833201613
F,2.501850609,-2.1068867291,1.0242397557
F,-0.3976462266,1.4734801182,1.2880870565
F,-2.6403052348,2.8874943992,1.5400256013
F,-5.0208979113,1.865917256,0.7029064712
F,-5.1019061906,-0.629259526,-0.3965191259
F,-2.859052997,-2.0556914521,-0.6659522036
C,-0.8313274681,-4.1120009684,-1.6153447827
H,-0.2441594051,-4.7217871072,-0.9193012196
H,-1.8738309384,-4.1223731436,-1.2917603332
H,-0.7752122333,-4.5997146036,-2.5950042038
C,-1.003048764,-1.3305599698,-3.0472814291
H,-2.0817450494,-1.2982867752,-2.8780265038
H,-0.6209178466,-0.3057457459,-3.05469984
H,-0.825807897,-1.7666875415,-4.036781723
C,1.6905501689,-2.5798758767,-2.2618742482
H,2.1630490957,-1.625015352,-2.5115862013
H,2.2831544906,-3.0606323469,-1.476512632
H,1.7351862339,-3.2210187598,-3.1494389691

M22

0 1

B,0.069898813,-1.1453967276,0.2115581106

Si,-0.0549420213,-3.1238943583,0.6884941144
C,-1.3204558585,-0.4310487623,0.117988279
C,-2.277220229,-0.8725627287,-0.7915698185
C,-1.6999991291,0.6052302401,0.9669091692
C,-3.5455194679,-0.3191387971,-0.8751820002
C,-2.9651045657,1.170578216,0.9311439938
C,-3.8889272105,0.7049964691,0.0004194422
C,1.4039838728,-0.3850754095,0.0096833752
C,1.463751328,0.9716568223,-0.3667434265
C,2.6530298167,-1.016427119,0.1465214165
C,2.6556588378,1.6477863252,-0.570686932
C,3.8630838726,-0.3702147916,-0.0459485445
C,3.8603403689,0.9724408427,-0.40546128
F,-0.8231736343,1.0735205091,1.862240513
F,-3.3004279225,2.1513581461,1.7633988295
F,-5.0986234491,1.2443811429,-0.0546643588
F,-4.4263600839,-0.7523067976,-1.770602991
F,-1.950024672,-1.8530688201,-1.6435010608
F,2.7163707993,-2.3043322032,0.4719122816
F,5.0140917093,-1.0144621389,0.1005771784
F,0.3543049898,1.6778763529,-0.5620430729
F,2.6612893089,2.927092923,-0.9259589652
F,5.0022521031,1.6063826685,-0.597390173
Cl,0.7332723493,-4.3614774417,-0.7416470492
Cl,0.8400980119,-3.4678131719,2.5064628333
Cl,-2.0243863876,-3.6620479903,0.9441089661

M22_TS

0 1
B,-0.0538000252,-1.2006487711,0.1852969476
Si,-0.1231780546,-2.3157912783,-1.7843897691
C,-0.2266369211,-2.3437847638,1.523740829
H,0.4886581323,-3.1633754222,1.5986240113
H,-1.2472615148,-2.7167833713,1.6050136509
H,-0.0241712684,-1.6346990156,2.3286475166
H,-0.1786506222,-2.4441882994,0.0397799348
C,-1.3916681137,-0.3259283497,0.2029042137
C,-2.6375972801,-0.9048078186,-0.0296399927
C,-1.4237429242,1.0317918644,0.5146651631
C,-3.835950694,-0.2117445801,0.007246569
C,-2.6025331963,1.7682747557,0.5632026684
C,-3.8150304403,1.1453612091,0.304908447
C,1.3915113379,-0.5225540443,0.107962233
C,2.5028804329,-0.8429422615,0.8843746178
C,1.6019078717,0.4964777471,-0.8235496567
C,3.7271501036,-0.1937074449,0.7618364351
C,2.79912914,1.1732414924,-0.9753556079
C,3.8762652892,0.8218461947,-0.1699735555
F,5.0383066394,1.4492981617,-0.2962082958
F,2.9318225793,2.1356873859,-1.8830725117
F,0.5994117648,0.8334240935,-1.6484349989
F,4.7532165754,-0.5416326718,1.5348710493
F,2.4509459566,-1.8190708451,1.8031641424
F,-0.297961505,1.6946011657,0.8063331584
F,-2.5753713934,3.0630089268,0.8666340488
F,-4.9470076094,1.8367306395,0.3520953354
F,-4.9899889341,-0.826429897,-0.2354792313

F,-2.6915442572,-2.2191875057,-0.3219319181
Cl,-0.7076569041,-4.2862079316,-1.6740895651
Cl,-1.3676407741,-1.3216498188,-3.0536694482
Cl,1.7643120292,-2.3165426958,-2.5746087905

M23

0 1

B,0.2268445098,0.8260545131,-0.1817732522
Si,0.1268918409,-1.210181872,0.0554315479
C,1.5293046879,1.668104559,-0.1925803511
C,2.794936325,1.066691766,-0.0791507362
C,1.5450464593,3.0660161389,-0.3566090712
C,3.9841306077,1.7756040498,-0.1157633216
C,2.7154732654,3.8074938524,-0.3983118164
C,3.9389325361,3.1565465573,-0.2768613543
C,-1.1940574958,1.4906053248,-0.2705073774
C,-1.7170424284,2.2669569031,0.7575320843
C,-2.0708027439,1.1516103831,-1.2951043492
C,-3.044328105,2.6716448652,0.7867251353
C,-3.3982563008,1.5478564381,-1.3166770569
C,-3.8871290063,2.3089756073,-0.2590807817
C,1.0843409831,-2.1687197373,-1.2510894197
C,2.0073595602,-3.1594172172,-0.893409905
C,0.8860089303,-1.8774324625,-2.6096623167
C,2.7027258812,-3.8427198768,-1.8788088969
H,2.2125069268,-3.4085736609,0.1434081937
C,1.5948188149,-2.5737922366,-3.5759889346
H,0.1861971553,-1.1155202679,-2.942428982
C,2.5072438976,-3.5619245224,-3.2256490769
F,0.4114858977,3.7479168127,-0.4886090391
F,2.6840375332,5.125193622,-0.555171806
F,5.0604711737,3.8517250073,-0.3146174415
F,5.1544133018,1.1597950483,-0.0019894779
F,2.8938118555,-0.2538888059,0.0792426342
F,-0.9263809344,2.6115427075,1.784243014
F,-3.5135483399,3.401788613,1.7929285182
F,-5.1540478934,2.6990589743,-0.2539589742
F,-4.2006272445,1.2090078082,-2.3206070646
F,-1.6093738286,0.4076898603,-2.3157263506
C,0.6845986809,-1.670014612,1.7995206081
C,1.3443514689,-0.7676264137,2.6430168699
C,0.3844790112,-2.9534451668,2.2828017835
C,1.7027827386,-1.1499971523,3.9269409933
H,1.5919529185,0.2439209756,2.3346739455
C,0.7591003032,-3.3171264,3.5656297613
H,-0.149788761,-3.6836783352,1.6803568841
C,1.4205886419,-2.423858811,4.402000644
C,-1.7005030316,-1.6902480825,-0.0275905159
C,-2.2602972054,-2.3555956575,-1.1235677131
C,-2.5438085444,-1.2656078173,1.0122848861
C,-3.630165036,-2.5718931277,-1.178033456
H,-1.6559321773,-2.707554288,-1.9541902142
C,-3.9080923465,-1.4843523769,0.9338547513
H,-2.1602837171,-0.7562590487,1.8936743132
C,-4.4689542675,-2.1357922319,-0.1607175831
F,-5.7802733661,-2.3442511888,-0.2245072968
F,3.1828071848,-4.2223562705,-4.1609883549

F,1.7696843002,-2.7812827642,5.6332175125
F,1.4191026566,-2.3090352188,-4.8736388629
F,3.5867268543,-4.7905311714,-1.5560847512
F,0.4877372949,-4.5365305556,4.0368394769
F,2.3293533513,-0.2955746499,4.7405608654
F,-4.177988676,-3.2065365731,-2.2177720222
F,-4.7245604989,-1.0728481837,1.9091483315

M23_TS

0 1

B,0.6961032438,0.4293842221,-1.2804388719
H,0.0208468605,-0.5078354,-1.7747365907
C,0.0106322231,1.8716776555,-1.1402844227
C,-1.1372732034,2.2167054171,-1.853889715
C,0.4136082527,2.8286554436,-0.209318999
C,-1.8354606791,3.4021867329,-1.6790419172
C,-0.2425059655,4.0371894449,-0.0104228477
C,-1.3807386068,4.3277894615,-0.7487967648
C,2.2324858887,0.1884284952,-0.9064111321
C,2.743402703,-1.0336563599,-0.478538594
C,3.187097401,1.1896145343,-1.086163164
C,4.075383348,-1.2453718423,-0.1548716973
C,4.5307914147,1.0262481204,-0.7734450254
C,4.9768015742,-0.1979551926,-0.2926755423
F,6.258114928,-0.3748922488,0.0033424277
F,5.3937929345,2.0219323126,-0.9518706934
F,2.8301030828,2.369987926,-1.6097298518
F,4.4927769739,-2.4365731485,0.2659758702
F,1.9226712902,-2.0995260033,-0.3950175584
F,1.4682310633,2.5991238298,0.5923272531
F,0.2020925628,4.9034313971,0.8950361072
F,-2.0317569006,5.468723253,-0.5636897735
F,-2.9409724992,3.6456636609,-2.3785096405
F,-1.6592131691,1.3416961341,-2.7335142764
C,0.2580928102,-1.0845183023,1.667845837
C,0.0854324738,-2.319032793,2.3096340727
C,1.0820355935,-0.1170899039,2.2595770572
C,0.7203393412,-2.564701972,3.5164347065
C,1.7079584204,-0.389273132,3.4663542895
C,1.5367785183,-1.6091895947,4.1091688513
Si,-0.6489516178,-0.7804520237,0.0479106742
C,0.6566732601,-0.1131765939,-3.0192288914
C,-2.1565125259,0.3047242869,0.3627133534
C,-3.2629870653,0.2648408545,-0.498046178
C,-2.1330981423,1.2518013767,1.3965241659
C,-4.3045244144,1.1638161112,-0.3310257254
C,-3.1836073967,2.1438282058,1.5415278505
C,-4.2768797619,2.1153269292,0.6824290612
C,-1.2884547663,-2.4180166297,-0.646242273
C,-2.5001563665,-2.9300699476,-0.1529874094
C,-0.5916360377,-3.1550313962,-1.6141963084
C,-2.985613304,-4.141004339,-0.6194940266
C,-1.100335011,-4.3608555625,-2.0716068788
C,-2.2975015498,-4.8688880909,-1.5838693171
F,2.1456081344,-1.8588061437,5.2633464593
F,-5.2778737542,2.9749847761,0.8325092159
F,-2.7755220726,-6.024567386,-2.0294836001

H,1.3994298474,-0.8989825583,-3.1501594517
H,-0.2792784571,-0.38107637,-3.5122206855
H,1.0147969989,0.8261649055,-3.4434614047
H,0.3628047731,-2.8326531181,-2.0171365972
H,-3.0865880929,-2.402499099,0.5940789834
H,-0.5248936905,-3.1112161172,1.8872621371
H,1.2720775843,0.8477208829,1.8010026974
H,-1.3079374014,1.3192786149,2.1003682956
H,-3.3311039798,-0.4420005804,-1.3197347104
F,-5.3617103532,1.140230799,-1.145097417
F,-3.1691893674,3.0598101465,2.5129250114
F,-4.1340153095,-4.6379841468,-0.1561593487
F,-0.4450833039,-5.0661292363,-2.9965752829
F,2.5010999956,0.5193847909,4.0391985045
F,0.5663404797,-3.7359632284,4.1390650523

M24

0 1

B,-1.251845275,0.2191361998,-0.1242924343
Si,0.7646620044,0.0358413588,0.1437091866
H,1.1734776529,0.7115405294,1.3992009885
H,1.101730736,-1.4037217875,0.2645728543
C,-1.939970059,1.5943681847,-0.4012601115
C,-1.2896106368,2.806889079,-0.1309291372
C,-3.2092915056,1.7214364614,-0.9889214573
C,-1.8412824727,4.0492979617,-0.4024165621
C,-3.7873632401,2.9450346503,-1.288828654
C,-3.0990779193,4.1150397029,-0.9884821817
C,-2.1142408613,-1.0915685894,-0.048750119
C,-3.2646511519,-1.1873257389,0.7364952177
C,-1.7325738895,-2.2588176456,-0.7099827232
C,-3.9815363305,-2.3642438012,0.8837029831
C,-2.4366998922,-3.4502224633,-0.6099506615
C,-3.564050556,-3.5016302842,0.200449778
C,1.6830474082,0.7887959841,-1.3151774796
C,2.3952185551,1.9913792516,-1.2004440176
C,1.6505500308,0.153802896,-2.5672164363
C,3.0518516877,2.5439580556,-2.2996187729
H,2.4416524385,2.5029704843,-0.2426553276
C,2.3044078625,0.7034772052,-3.6685265232
H,1.1163225442,-0.7863982127,-2.6849964201
C,3.0053229356,1.9015350679,-3.5357111446
H,3.6016412555,3.4737165481,-2.1895830447
H,2.2696995985,0.1959969591,-4.6276826201
H,3.5172060397,2.330432182,-4.3916637508
F,-3.9206637201,0.6412510397,-1.3147302747
F,-4.9875494301,3.0131521946,-1.8567429243
F,-3.6418018809,5.2903051134,-1.2625852172
F,-1.1852605843,5.1687227078,-0.1125124487
F,-0.0825875891,2.8059925455,0.4373461113
F,-3.7052514648,-0.1106008716,1.3983101548
F,-5.0630292992,-2.4161995927,1.6562981215
F,-4.2457167682,-4.6331090075,0.3184227476
F,-2.0489050849,-4.5332289302,-1.2777970006
F,-0.667592388,-2.239929698,-1.5227457089

M24_TS

0 1

B,0.1316254137,-0.9591690877,1.0726693255
H,1.3244885276,-2.8889082864,1.9292408319
H,-0.3944672888,-3.086944746,2.4147521499
H,0.0454329146,-3.1400157746,0.7005103457
H,0.7382706973,0.5858744655,3.7289157031
H,-1.5742599846,0.2528382393,3.1139601133
H,0.1368392041,-1.4071421797,2.24532501
C,-1.269317611,-0.7802845762,0.3174087593
C,-2.4630402019,-1.3256659154,0.7888778533
C,-1.4026274506,0.0276630902,-0.8139470607
C,-3.6967942239,-1.1212800547,0.1865658528
C,-2.6161453413,0.2550335724,-1.4493642571
C,-3.7732294994,-0.324120985,-0.9471846721
C,1.5099467299,-0.757986633,0.2839823834
C,2.642626262,-0.1274520057,0.7840791388
C,1.6496647965,-1.2757825293,-1.0039381096
C,3.8205839653,0.0262582429,0.0633194212
C,2.8034050205,-1.1469615584,-1.7627304498
C,3.8991656509,-0.4839736882,-1.2239030225
F,5.0166935519,-0.3525462518,-1.9305136425
F,2.8731458185,-1.6536817696,-2.9916695831
F,0.6254029523,-1.9373293695,-1.5638431871
F,4.8677719241,0.6520689428,0.5989991232
F,2.6370866829,0.3676517003,2.0356078129
F,-0.3377771471,0.6535086808,-1.3283456975
F,-2.6813879375,1.0407862523,-2.522364356
F,-4.9437936591,-0.1114294689,-1.5403310693
F,-4.7994028262,-1.6752393962,0.6888166239
F,-2.455216224,-2.0777753702,1.904281568
C,-0.2631283931,2.1186596714,1.6017585561
C,0.8883657367,2.8581378751,1.2943285071
C,-1.4937968816,2.553045271,1.0840083092
C,0.8130852357,3.9878094587,0.4814284806
H,1.8522651369,2.5573219747,1.6952611111
C,-1.5710536958,3.6794213708,0.2677029401
H,-2.4046658227,2.0048115608,1.3191582566
C,-0.4145180518,4.3949662381,-0.0386149682
H,1.7138583887,4.5487339726,0.2526907191
H,-2.530750905,3.9970020673,-0.1282852965
H,-0.4709078689,5.2707718868,-0.6773877333
Si,-0.2135850035,0.5361430351,2.5981983899
C,0.2876154073,-2.6880669224,1.6630788196

M25

0 1

B,-0.1128603407,-0.7812496313,-0.5728298123
Si,-0.1110004373,-2.4842395667,-1.6851166122
C,-1.4054014516,-0.0820678359,-0.0195838301
C,-2.6840671187,-0.4784058829,-0.4304430206
C,-1.3894189087,0.962528922,0.9182371115
C,-3.8565567106,0.1086024463,0.0183406512
C,-2.5399227045,1.5655409477,1.4053675343
C,-3.7803539241,1.1392926694,0.9464441134
C,1.2706585494,-0.0434506492,-0.4288308076
C,2.3981033185,-0.7013509234,0.0553715009
C,1.472087684,1.2664760575,-0.8603986474

C,3.6511964846,-0.1108086157,0.1196063371
C,2.7119210643,1.8867607019,-0.8375240302
C,3.8077045093,1.1910169353,-0.3397089002
F,5.0009335304,1.7718114059,-0.2986800411
F,2.8624845832,3.1352069142,-1.2745597362
F,0.4367754269,1.9739323922,-1.334526333
F,4.6974140418,-0.7734916771,0.6084465599
F,2.2802673041,-1.9525335527,0.5261199016
F,-0.2380099092,1.4209271903,1.4102835263
F,-2.469931411,2.5459132216,2.3006786565
F,-4.8868307153,1.710060364,1.3965928807
F,-5.0425219472,-0.3051343598,-0.4203153216
F,-2.8261176143,-1.4747480339,-1.3153428098
N,-0.6986099129,-2.1050548446,-3.277254689
N,-1.0106671266,-3.7083135737,-0.8656906023
N,1.5065674482,-2.9878311054,-2.0229613141
H,2.1264533339,-3.297938478,-1.2877744289
H,1.668695945,-3.4941876126,-2.8839224026
H,-0.8791018107,-4.6772690777,-1.1257154973
H,-1.942695295,-3.5454916645,-0.5108373374
H,-0.1182430443,-1.5994707123,-3.9335237054
H,-1.6818542008,-1.9511151108,-3.4507389141

M25_TS

0 1

B,-0.0556077475,-1.1837259612,0.1425999739
Si,-0.17361514,-2.2315840479,-1.7705025993
C,-0.2030739775,-2.3212842777,1.5799246191
H,0.4914319045,-3.1564166319,1.6797287054
H,-1.2313135383,-2.6621161168,1.6969724924
H,0.0376907792,-1.5716360451,2.3313119211
H,-0.1379365154,-2.4318392804,0.200461609
C,-1.3919890722,-0.3099103045,0.2692493971
C,-2.6436834959,-0.8699015608,0.0231464174
C,-1.4244748919,1.034180815,0.6360988332
C,-3.8411103508,-0.1785457294,0.1045825783
C,-2.6004692641,1.7731325426,0.7240156437
C,-3.8176748689,1.1655318508,0.454464774
C,1.3773712825,-0.4674240481,0.1125559943
C,2.5011110332,-0.7581157302,0.8797031183
C,1.5694254786,0.5442801429,-0.8310382768
C,3.7163535197,-0.0908025806,0.7417161526
C,2.7528720345,1.2399086411,-0.999250964
C,3.8436026705,0.917612808,-0.1992658635
F,4.996180625,1.5654939773,-0.341778357
F,2.8624730959,2.1963200076,-1.9200015461
F,0.5502977379,0.8704599368,-1.6456616164
F,4.7545328077,-0.4169870786,1.5117594452
F,2.4763823387,-1.731512542,1.8080637133
F,-0.2942729711,1.6878376798,0.9389362087
F,-2.5662264577,3.0569821665,1.0757927584
F,-4.9503729138,1.8566839293,0.5405553451
F,-5.0007102805,-0.7848414536,-0.1502547387
F,-2.7186427791,-2.1773632258,-0.3129446973
N,-1.2014584916,-1.4087806989,-2.8735660433
N,-0.7037548394,-3.860000589,-1.4994605375
N,1.4065866084,-2.1953270525,-2.4279182558

H,2.2590266322,-2.3004615673,-1.8986876866
H,1.5511340884,-2.1886923897,-3.4275448196
H,-0.3098253326,-4.5959625517,-2.0710315008
H,-1.644246241,-4.0802696001,-1.1996970536
H,-1.0827310341,-0.4204804907,-3.0549991311
H,-2.1565827932,-1.7114426834,-3.0058040331

M26

0 1

B,0.0135107999,0.1207634345,0.0317872048
Si,0.0530707017,2.1539212593,0.1357065612
C,-1.3791446884,-0.5842212572,-0.0133697069
C,-2.5225536817,0.019755503,0.5451190013
C,-1.5522041786,-1.8282657568,-0.6522314941
C,-3.7682035981,-0.5992608825,0.5035795144
H,-2.4330224498,0.9877927539,1.0336187986
C,-2.8016337125,-2.4387319437,-0.7276771321
H,-0.6952360134,-2.3130650826,-1.1124627623
C,-3.9095706303,-1.8294284207,-0.1392568224
H,-4.6298089771,-0.120096042,0.9578925204
H,-2.9119524919,-3.3896874331,-1.2397218455
H,-4.8829925907,-2.3081944738,-0.1878889213
C,1.3338254781,-0.7098174128,0.0368079847
C,1.3867905458,-1.9900985061,0.6254308204
C,2.5253367427,-0.2041105169,-0.5184386703
C,2.5675472756,-2.7266954323,0.6574465971
H,0.4902401699,-2.4031917504,1.0801071001
C,3.7003054224,-0.9509021244,-0.5244173261
H,2.5284949781,0.7880366271,-0.9614569878
C,3.723944805,-2.2119750309,0.0707379004
H,2.5868928958,-3.7026698418,1.1326198172
H,4.6000233768,-0.5455682538,-0.9768137908
H,4.6434888128,-2.7894135932,0.0842047449
H,1.3850641909,2.7494866454,-0.1423368123
H,-0.9290414268,2.7793577965,-0.7879730991
H,-0.3297939061,2.5693443248,1.5137354856

M26_TS

0 1

B,0.0541094851,0.1017761947,0.7144464289
Si,-0.1406159866,1.9218168301,-0.3728675571
C,0.1307738297,0.3058399079,2.5272293358
H,-0.6431278728,0.8686021592,3.0551816078
H,1.1214957818,0.6120014124,2.8630026924
H,-0.010852237,-0.758707928,2.7215189092
H,0.0345980981,1.1569393902,1.4159553797
C,1.4786586453,-0.5130285419,0.335997215
C,2.6688713331,0.2311002959,0.4031673851
C,1.5904379682,-1.86606395,-0.0188499863
C,3.9086601366,-0.3411161389,0.1280233053
C,2.8276520021,-2.4472594117,-0.299531578
C,3.9922463923,-1.6864432468,-0.2297646509
C,-1.3224073672,-0.6125729624,0.3300274969
C,-2.4146675529,-0.7388336184,1.2024885101
C,-1.479370276,-1.1438338694,-0.96383239
C,-3.5999961621,-1.3623620002,0.8105532928
C,-2.6544048437,-1.7759650537,-1.3612837379

C,-3.724097758,-1.8868849389,-0.4729114728
H,-2.3532905963,-0.3475529743,2.2141745133
H,-4.4246679452,-1.4404775047,1.5128462229
H,-2.7363111564,-2.1801135072,-2.3658787906
H,-0.6588349351,-1.0642443789,-1.6739529959
H,-4.643260423,-2.3765033525,-0.7792090272
H,0.6951709903,-2.4801738648,-0.0712138652
H,2.6319101685,1.2840177074,0.6787844721
H,4.8086379406,0.2636947091,0.1884578877
H,4.9556322006,-2.1356439949,-0.450241825
H,2.879616962,-3.4976542599,-0.5706975186
H,-0.0627119958,1.4392328878,-1.7689514513
H,-1.453042976,2.5703492691,-0.1330052922
H,0.9260719597,2.9351085836,-0.1580967262

M27

0 1

B,-0.3655156967,0.5835023941,-0.6268474141
Si,0.4797336242,2.2474052124,-1.4612811604
H,0.7870498944,1.9379916487,-2.8781984862
H,-0.4386656795,3.4102953851,-1.4506253883
C,0.6216532279,-0.498284756,-0.0551426659
C,1.8686229666,-0.7427466553,-0.6358959614
C,0.3702893031,-1.1896231401,1.1347614979
C,2.8089877847,-1.6033461043,-0.0907974661
C,1.2914351339,-2.0416128369,1.7245452203
C,2.517412606,-2.2506796077,1.1032836545
C,-1.9092862607,0.336920973,-0.5094052465
C,-2.4675089243,-0.9359927055,-0.6820064823
C,-2.8253513399,1.3631907054,-0.2588344104
C,-3.8312228043,-1.1787313426,-0.6381779718
C,-4.1954083303,1.1550220158,-0.1817410198
C,-4.6994610974,-0.1236576985,-0.3809088632
C,2.0436329276,2.6008169548,-0.4637657298
C,3.329088349,2.6778582775,-1.0426702517
C,1.9202740391,2.7093936933,0.9372337834
C,4.4467472242,2.8183480925,-0.2181924286
C,3.0608898293,2.8525906889,1.731930143
C,4.3355151032,2.898427728,1.1712859292
H,5.4342500408,2.8722945027,-0.672786742
H,2.9496240774,2.9357787058,2.811266749
F,-0.7897409318,-1.0171665027,1.7801820188
F,1.0156170533,-2.6608886802,2.8694167306
F,3.4045091316,-3.0712725094,1.6479491475
F,3.9755926712,-1.8150200054,-0.6931991606
F,2.1831736192,-0.1585235057,-1.7965439512
F,-1.6779288631,-1.987500758,-0.9233797215
F,-4.3157008577,-2.4025367861,-0.8293637726
F,-6.0055771051,-0.3391193728,-0.3230308193
F,-5.0251699946,2.1613129155,0.0793625632
F,-2.3952903214,2.6076715032,-0.0367666589
C,5.5619126621,3.0703501456,2.0303512744
H,5.9530430416,4.0897587146,1.947199711
H,5.3378957176,2.8823970831,3.0830226612
H,6.3577795054,2.3868127856,1.7215742568
C,3.5357352767,2.6300043499,-2.5390898769
H,4.5831059367,2.8159593648,-2.7870532924

H,3.2585820352,1.6566139473,-2.9533257214
H,2.9305796375,3.3866859375,-3.0477610508
C,0.5657451372,2.6893676495,1.6101938503
H,-0.1472889212,3.3536329541,1.1116931632
H,0.1254599299,1.6820258163,1.6237525293
H,0.6436779015,3.0065016123,2.6527278505

M27_TS

0 1

B,-0.2624196084,0.0311543014,-0.4423796323
Si,1.1506994301,-0.1328628901,1.2326114654
H,0.6339916238,-1.2852443987,2.0048515931
H,0.9910013462,1.1160154341,2.0034395551
C,0.5760256869,-0.0082711901,-2.0683354077
H,1.2043270433,-0.8619075339,-2.3282525728
H,1.0986325072,0.9260760345,-2.2677749336
H,-0.3435170778,-0.0616931069,-2.6489184644
H,0.954932402,-0.1097690857,-0.7252060325
C,-0.8473238647,1.5201406335,-0.3854004554
C,0.0073039566,2.6209685039,-0.350727044
C,-2.2038830688,1.8390717126,-0.3986653081
C,-0.4182062316,3.9384761519,-0.3056060951
C,-2.6782228915,3.146206311,-0.3489264923
C,-1.7819047079,4.2034198178,-0.3000569043
C,-1.2235502263,-1.2350526741,-0.2377978985
C,-1.3683152611,-2.3470595457,-1.0625914326
C,-2.0162215533,-1.2609144296,0.912855245
C,-2.2346015655,-3.4001756638,-0.7824481436
C,-2.8963918792,-2.2814700678,1.2285091067
C,-3.0071223228,-3.3669878006,0.3670162759
F,-3.8397811276,-4.3640129532,0.6476413024
F,-3.6274833827,-2.2371810351,2.3400196524
F,-1.9307817247,-0.2371229666,1.7776510402
F,-2.3220174528,-4.4384496471,-1.6130685856
F,-0.6499757068,-2.4716791521,-2.1933609581
F,-3.1335743668,0.8771259043,-0.4749240497
F,-3.9870005078,3.3893909166,-0.359897772
F,-2.2210525316,5.4572181461,-0.2584900545
F,0.4588583626,4.9405559956,-0.2712899993
F,1.3394893691,2.4073902,-0.3679445339
C,2.9372946772,-0.4478539192,0.724645692
C,3.9756221703,0.4864359456,0.9418257056
C,3.2410595663,-1.6693304455,0.0810350235
C,5.2636747536,0.1966347491,0.4879350197
C,4.5413187997,-1.9208395123,-0.3609021952
C,5.5651681014,-0.9932393577,-0.1758794732
H,6.0578882945,0.9196786263,0.6622788254
H,4.7605465168,-2.8659509939,-0.853298774
C,2.1956883254,-2.747824696,-0.0985821039
H,1.8921880187,-3.1644281311,0.8683470768
H,1.2853325444,-2.3830926462,-0.5856524399
H,2.5805879165,-3.5656771049,-0.7113555838
C,3.752580459,1.780500866,1.6910573997
H,3.0119623352,2.415073655,1.1992196193
H,3.3986435131,1.5907149273,2.7093004106
H,4.6850515869,2.3443823025,1.76233211
C,6.9569531076,-1.2585458321,-0.6880740307

H,7.1053996441,-0.7825888038,-1.6632460533
H,7.7114912972,-0.8566917808,-0.0069151157
H,7.1373827042,-2.3293207711,-0.8092595787

M28

0 1

B,-0.0394196851,0.7533687239,-0.0602933609
Si,-0.1039092193,2.7813964961,-0.3151648782
C,-1.3851984578,-0.0566891183,-0.103514842
C,-2.4886917629,0.2987130694,0.6700196749
C,-1.5634324955,-1.1547029523,-0.9475307613
C,-3.6990226116,-0.3783529843,0.621111743
C,-2.7624781161,-1.8427180924,-1.045591265
C,-3.8352023524,-1.4521372093,-0.2503765817
C,1.3072590074,-0.0192588581,0.0958985743
C,1.3977498798,-1.3048328497,0.6555944244
C,2.5309379143,0.5475125566,-0.2866897694
C,2.6005922143,-1.9697458377,0.8328098047
C,3.7517126585,-0.0928337032,-0.1426997417
C,3.7827210478,-1.3605279228,0.42558715
F,-0.548893003,-1.5703173813,-1.7156900093
F,-2.8952599497,-2.8714659865,-1.8768106368
F,-4.9852811543,-2.1064268225,-0.3224759541
F,-4.7183237805,-0.014542976,1.3925122195
F,-2.3819507397,1.31491688,1.5356565228
F,2.5548063148,1.7594114303,-0.8465954126
F,4.8801888555,0.485536866,-0.5376015452
F,0.3047864763,-1.9442318026,1.0735021415
F,2.6376183242,-3.1796170437,1.3803554929
F,4.935823816,-1.988783461,0.5790714798
C,-1.870418489,3.4939131283,-0.1456309682
H,-2.6480046804,2.8886308742,-0.6264415996
H,-2.1532909614,3.6470834852,0.8996019403
C,0.9693240036,3.6889564598,0.9658989952
H,2.0389502885,3.4978083522,0.850738544
H,0.8040110514,4.7707387365,0.9238749093
C,0.5090848156,3.3228106146,-2.0528832343
H,-0.2355718343,3.9659672354,-2.5321603294
H,0.746688024,2.4921136391,-2.7247336842
F,1.6766471464,4.0797924884,-1.8923756196
F,-1.8699474984,4.7510371094,-0.7718403042
F,0.575879033,3.2406766863,2.2393723811

M28_TS

0 1

B,0.0364798011,0.7610090736,0.6965550324
Si,-0.2240095104,2.4979298018,-0.5555825039
C,0.0596497308,1.0574766668,2.497130834
H,-0.671547915,1.7142474693,2.9700895882
H,1.0723034111,1.3145769465,2.8057514681
H,-0.1737071767,0.0281827425,2.7738834474
H,-0.0362523567,1.848385339,1.3155198396
C,1.45706049,0.0606634167,0.4632029941
C,2.6000142756,0.6897708667,-0.0143689412
C,1.6188759164,-1.2863648177,0.7884571084
C,3.8196755745,0.0457431458,-0.1851143457
C,2.8133097072,-1.9733171324,0.6310533134

C,3.9244097492,-1.2994750032,0.137738502
C,-1.3068790272,-0.00661156,0.2768413694
C,-2.5460051331,0.1882595549,0.8848564356
C,-1.3160695388,-0.897118571,-0.7986507234
C,-3.7104163077,-0.4511761287,0.4840560501
C,-2.4562360716,-1.5601251467,-1.2313030771
C,-3.6646265466,-1.3352268117,-0.5855182205
F,-4.7659124994,-1.9593139838,-0.9854866129
F,-2.4008986394,-2.4033963256,-2.257088684
F,-0.1852552558,-1.1485832215,-1.4691390656
F,-4.8626708277,-0.2168732624,1.1084776794
F,-2.6626933171,1.0648580824,1.9025505916
F,0.5786078447,-1.9763807933,1.2802504176
F,2.9073757931,-3.2607368825,0.9520844726
F,5.0791156542,-1.9366358007,-0.0140131382
F,4.8779559546,0.7053056014,-0.6484745724
F,2.5555139733,1.9951767514,-0.3388543027
C,0.72470248,4.1225110585,-0.1961611682
H,0.0253707638,4.9648330743,-0.1700329099
H,1.2947261562,4.104777171,0.7389344904
C,0.2090900684,1.8975979889,-2.3131137481
H,0.3845374247,2.7582832117,-2.9665990511
H,1.0821803927,1.2402465272,-2.3516269118
C,-2.0806010478,2.9427709627,-0.5874958968
H,-2.6529327959,2.2162262667,-1.1739219177
H,-2.5417749009,3.0388109378,0.4013290627
F,1.629859094,4.3588558462,-1.2346599932
F,-2.1864399712,4.1851204677,-1.2296057189
F,-0.8888116568,1.1871177295,-2.8130594437

M29

0 1

B,0.0230946177,0.2924352728,0.0589978611
Si,0.1507588731,2.32166093,0.2661943022
C,-1.3549884361,-0.448650007,0.0636009067
C,-2.3919152487,-0.0934480657,0.9466097067
C,-1.6102173717,-1.4976922136,-0.8425961647
C,-3.6106462158,-0.7676142592,0.9487693915
H,-2.2354196925,0.7141650296,1.6555895658
C,-2.8417558932,-2.147073069,-0.8763974528
H,-0.8311031331,-1.7989495036,-1.5384763905
C,-3.841497365,-1.7894673704,0.0281278431
H,-4.3849621185,-0.4877276346,1.6565230401
H,-3.0186610664,-2.939167903,-1.5976681815
H,-4.7978178538,-2.3036493068,0.0140331295
C,1.3233467991,-0.5436818354,-0.1917869764
C,1.3988072905,-1.8967537169,0.196037583
C,2.4735722353,0.0205954938,-0.7770923562
C,2.5608798412,-2.6434167234,0.0171149512
H,0.5330742594,-2.3642584784,0.6578463092
C,3.6275991635,-0.7272223787,-0.9923323756
H,2.4605306064,1.0630083548,-1.084464882
C,3.6746708104,-2.0614046602,-0.5872107079
H,2.5966798479,-3.6793182476,0.3403380877
H,4.4926785679,-0.2703554152,-1.4630237538
H,4.5784625867,-2.6439878164,-0.7387454381
C,-1.3632112761,3.1462510121,1.0496533001

H,-2.2867575634,2.8934587229,0.519503956
H,-1.4871107695,2.8760543405,2.1034710504
H,-1.2360589361,4.2338877095,1.0031216315
C,0.3031296821,3.0681731533,-1.4736193546
H,0.3504482686,4.1605314711,-1.3986409856
H,1.1952348359,2.730623705,-2.0091808675
H,-0.5693250716,2.8128524141,-2.0838989195
C,1.653674027,2.8454783159,1.2908696778
H,2.591814238,2.4641774123,0.8774223429
H,1.7188276262,3.9384635404,1.3315398341
H,1.5726951445,2.4771147172,2.318860556

M29_TS

0 1

B,-0.0147864658,0.7401378126,0.6212977229
Si,-0.227384045,2.3921107422,-0.7422824346
C,-0.021087285,1.2743105615,2.400157986
H,-0.8055215106,1.9289425648,2.7895981528
H,0.9610651225,1.6277452456,2.7138699474
H,-0.1892421907,0.2611681634,2.7663366311
H,-0.078451058,1.8817848657,1.1596251268
C,1.4303932371,0.0836055332,0.4521690821
C,2.6102081218,0.8475380397,0.4494343374
C,1.5781107063,-1.308728891,0.3567937649
C,3.8692724931,0.2614910465,0.3446486949
C,2.8346387095,-1.9069323007,0.247058833
C,3.9864180215,-1.1242976412,0.2359584579
C,-1.3617014138,-0.0657994264,0.3403003555
C,-2.5187466883,0.0345207373,1.1299030981
C,-1.4486285182,-0.8814748549,-0.8035162782
C,-3.6995609484,-0.6290599754,0.7957604719
C,-2.6206407725,-1.5535079884,-1.1430899515
C,-3.7570775272,-1.4265768611,-0.3446024134
C,0.8232449118,3.9291741102,-0.3769007214
H,0.7096126323,4.2829546908,0.6539630031
H,1.8869607274,3.7529816896,-0.5609316925
H,0.5063392466,4.7433070994,-1.0386826593
C,0.2894281013,1.7079174673,-2.418033085
H,1.2725916738,1.2303665736,-2.3630278257
H,-0.4341408761,0.9764063471,-2.787408246
H,0.3436976812,2.5283765825,-3.1423388439
C,-2.0349446419,2.9275898794,-0.7750756992
H,-2.6815493526,2.1021629252,-1.0881617622
H,-2.3754995816,3.2588700213,0.212638555
H,-2.1707094823,3.7614917258,-1.4723463916
H,-2.5143985469,0.649938443,2.0257586808
H,-4.5747722125,-0.5227036091,1.4300954828
H,-2.6468429764,-2.1762303237,-2.0325877701
H,-0.5754626215,-0.9932033803,-1.4425936527
H,-4.6736133558,-1.9460323485,-0.606331808
H,0.6950021462,-1.9418497217,0.3763806374
H,2.5464741022,1.9305293039,0.5390688915
H,4.7584715346,0.8852158973,0.3453512293
H,4.9646727675,-1.5867867117,0.1484354761
H,2.9112767546,-2.9879805548,0.1744424964

M30

0 1

B,-0.1186857436,0.0590909322,-0.1028561534
Si,-2.0864395721,-0.4332116473,-0.2123370215
H,-2.6971537233,-0.1149699717,1.0909773188
H,-2.2142395348,-1.8614865831,-0.5582743829
H,-2.6104539102,0.429120049,-1.2937692568
S,1.3136007947,-0.5794994117,-1.1362267772
O,2.270907813,-1.3484985656,-0.3609845829
O,1.6801631153,0.5645421741,-1.9670567419
C,0.5179289683,-1.7987431655,-2.2994693821
F,0.1213405017,-2.8695884089,-1.6248384585
F,1.3936253233,-2.144222295,-3.2235059477
F,-0.5423838537,-1.2286154589,-2.8732939534
S,0.2429237852,1.3456275479,1.2103891611
O,0.3739413253,0.4541149529,2.3647927354
O,-0.7254161941,2.4304589611,1.1586888057
C,1.9061849352,2.1615342307,0.9713805328
F,2.8345469151,1.2345096015,0.7937170328
F,2.1667008891,2.8588735685,2.0645656673
F,1.8595588958,2.96360773,-0.0777184157

M30_TS

0 1

B,0.007585092,0.2055073202,0.3225385767
Si,-0.0283850374,2.3439396703,0.1090651579
H,-1.4430890833,2.7553419102,0.1477470733
H,0.7103635389,2.9331845019,1.2452615536
H,0.6333886967,2.6145184777,-1.1746695024
C,-0.0130884517,-0.469887475,1.9787171163
H,-0.9659124518,-0.3342153042,2.4917108667
H,0.8334789642,-0.1765552057,2.6032976581
H,0.1201173577,-1.5154592783,1.6791974823
H,-0.0526837086,0.8278890605,1.3966102746
S,-1.5895867857,-0.6196402932,-0.3021669853
S,1.7749532781,-0.3400299968,-0.1762681833
O,-2.6794877708,-0.0626589551,0.5001189952
O,-1.390396717,-2.0589159634,-0.4275866586
O,2.0868510545,-1.68128747,0.3049279338
O,2.6420498909,0.7978682404,0.1477643323
C,-1.9527533562,-0.0210472251,-2.0390277301
C,1.8121215505,-0.4774778988,-2.0368823924
F,1.2531762775,-1.6100089245,-2.42415508
F,1.1390918247,0.5493438595,-2.5645183512
F,3.070080609,-0.4307693007,-2.4372028626
F,-1.2500715979,-0.7034915092,-2.9269233294
F,-3.2428971498,-0.1819977895,-2.2704874167
F,-1.6434515045,1.2758264388,-2.1409865786

M31

0 1

B,-0.0100952442,1.3875153067,0.0038981885
H,-0.2296763267,4.267233441,0.0733359975
H,-2.0356696228,3.1191082521,1.1674718654
H,-1.9224653356,3.1860198607,-1.2370249525
O,0.7701504965,0.9947097,-1.0529100387
O,0.0570886387,0.515021312,1.0588626653
C,1.1276561178,-0.4217539296,0.7808347701

C,1.2315855194,-0.351204091,-0.7766395991
C,2.6370088173,-0.5144317018,-1.331742624
H,3.0444648879,-1.4934427404,-1.0577289895
H,2.6073443433,-0.4480520292,-2.4223532022
H,3.3058998898,0.2634585408,-0.9601131431
C,0.2661394309,-1.3005406028,-1.4839739934
H,0.2460220118,-1.0506693582,-2.5476180471
H,0.5805294929,-2.3425929019,-1.3748405437
H,-0.7485860625,-1.1965734298,-1.0884104298
C,0.7464481306,-1.7845084369,1.335389878
H,1.4981324789,-2.5322747099,1.0608627753
H,0.6963712332,-1.732408356,2.4260257155
H,-0.226881011,-2.1087535939,0.9637119084
C,2.3723231181,0.1119030997,1.4877593859
H,2.1495450001,0.2239080912,2.5517277385
H,3.217766323,-0.5733708199,1.3772727325
H,2.6597174313,1.0908564739,1.0927327051
Si,-1.1171287586,3.0786146234,0.0044082371

M31_TS

0 1

B,-0.9668599884,-0.5478747738,0.1278682384
Si,-2.7155430079,0.8123819388,-0.3209959749
H,-4.0875156594,0.2567257171,-0.492248695
H,-2.7616758042,1.8030182569,0.7812542673
H,-2.3214958359,1.4670028717,-1.5904003831
C,-1.5974395583,-2.1803976479,0.6380782009
H,-0.7816726164,-2.7400876369,0.1792512706
H,-2.5415034145,-2.6286847403,0.3113643536
H,-1.537463171,-2.1757948433,1.7261509652
H,-2.1739252085,-0.9578985195,0.1917640397
O,-0.2195206912,-0.037538102,1.2149845246
O,-0.1907541446,-0.5954597086,-1.0554199063
C,1.1580446631,-0.295441,-0.6559281236
C,0.9436293228,0.5699582392,0.6304925985
C,2.0809798286,0.5020194716,1.6382047774
H,3.0174143585,0.8454789132,1.1856052207
H,1.8535151185,1.1494057834,2.4895814044
H,2.2180172123,-0.5148065189,2.0100592085
C,0.6205929822,2.028979944,0.3017540882
H,0.2384335158,2.5151629303,1.2033766291
H,1.5107442612,2.5676071238,-0.0371650349
H,-0.139864152,2.1036952777,-0.4820701324
C,1.8514884071,0.4290693529,-1.7995043019
H,2.8421054773,0.7800056431,-1.4903680967
H,1.9779208817,-0.2555947993,-2.6427599889
H,1.261453867,1.2820958013,-2.139572515
C,1.8787421012,-1.61126819,-0.3520379187
H,1.7770179995,-2.2728706462,-1.2167860634
H,2.9441640984,-1.4486815147,-0.1613996165
H,1.4448961573,-2.1072646237,0.5213379641

M32

0 1

B,0.1086403238,-0.1366034244,0.248810516
Si,-1.8930414091,-0.4604943135,0.0558632978
H,-2.3479290019,-1.3338532783,1.1708310161

H,-2.2321379321,-1.1486074412,-1.2164888345
H,-2.676359674,0.7998783145,0.1285562559
C,0.5179496503,1.1216297162,1.0848307387
H,-0.0580223461,1.1178959611,2.0333650511
H,0.1053974691,1.9939343238,0.5314391584
C,1.0392481305,-1.1575086352,-0.4868915961
H,0.6978461383,-2.1850549326,-0.2439006838
H,0.8016220138,-1.051498714,-1.5683861171
O,1.8870245568,1.2981585486,1.3381248984
O,2.4197304636,-1.030242473,-0.2682719749
C,2.1453123716,2.469179107,2.0705357198
H,1.641052262,2.4484511837,3.0486720148
H,3.2238143524,2.5272503967,2.2249631595
H,1.8096987025,3.3639343231,1.5244215572
C,3.1623488095,-1.9758301945,-0.9954596612
H,3.0046854505,-1.8600766589,-2.0786085081
H,4.2162442887,-1.8099128561,-0.7670674086
H,2.8887081497,-3.0033937528,-0.7113950995

M32_TS

0 1

B,-0.0070359832,-0.5756885418,0.2381136118
Si,0.0490691537,-2.6085897836,-0.3622920573
H,1.1287939243,-3.4340055586,0.2334447256
H,-1.2452855383,-3.3101295847,-0.1858940735
H,0.3252788098,-2.442746871,-1.8102825025
C,0.0137863092,-0.2189470935,1.961368929
H,0.9311593616,-0.4802741472,2.4921361657
H,-0.8661555956,-0.5347013988,2.5258214993
H,-0.0175470346,0.8632806216,1.8174977644
H,0.0280367285,-1.4442401199,1.1443800403
C,-1.4372042562,-0.0813375584,-0.3099236491
H,-2.2721346034,-0.6781066142,0.1015905388
H,-1.4916159029,-0.1824359885,-1.4093794202
C,1.3776779155,-0.0155702942,-0.3691815921
H,2.2340531473,-0.6943156431,-0.1916648132
H,1.2793991054,0.0780966032,-1.4653719906
O,-1.6185289079,1.2802494581,0.0403374567
O,1.676692666,1.2530246842,0.1863455379
C,2.8137907495,1.8391498665,-0.3917740758
H,2.9766372361,2.8001085334,0.0999158325
H,3.7033139549,1.2058957057,-0.2515395535
H,2.6710254932,2.0053258451,-1.469830339
C,-2.8242463432,1.8074110122,-0.4494276177
H,-3.690138392,1.2560482545,-0.0521116301
H,-2.8842258006,2.8491444904,-0.1286091143
H,-2.8596991971,1.7660291226,-1.5483366731

M33

0 1

B,0.55438,-0.000097,0.041523
Si,2.57678,-0.000085,-0.040689
H,3.100923,0.013207,1.350263
H,3.104769,1.19908,-0.738668
H,3.106676,-1.211123,-0.716324
C,-0.272191,-1.333141,0.046783
H,0.07932,-2.027958,0.819464

C,-0.272002,1.333136,0.04665
H,-0.087687,1.854095,-0.914059
O,-1.674528,-1.1673,0.242809
O,-1.674315,1.16725,0.243103
C,-2.158239,0.000105,-0.35552
H,-3.240032,0.000174,-0.226552
H,-1.897552,0.000221,-1.432287
H,-0.087508,-1.854191,-0.913841
H,0.079606,2.027964,0.819268

M33_TS

0 1
B,-0.2059117509,0.3167389929,0.003972344
Si,-1.9319305352,-0.86381224,0.0272379103
H,-2.7149449478,-0.7509038399,1.2836071888
H,-2.8516499464,-0.6606148088,-1.1211044848
H,-1.3329048277,-2.2152234988,-0.0607821892
C,-0.3501545562,2.0896140836,-0.0973838852
H,-0.912073359,2.6219224833,0.6740687194
H,-0.6214388766,2.4628867538,-1.0864333161
H,0.718257381,2.248275609,0.0764027412
H,-1.2642582511,0.9852452714,-0.0534379453
C,0.6093912946,0.0068472661,1.3622587987
C,0.67616238,-0.1575299279,-1.2728436789
O,1.5441142697,-1.1880348253,-0.78741967
O,1.9807745215,0.2590297971,1.0152294431
C,2.490293609,-0.7094258761,0.1297433043
H,3.3280836099,-0.2184515901,-0.3857118623
H,2.8381072285,-1.5958273104,0.677093856
H,0.3796168873,0.6777087318,2.195414307
H,0.510410651,-1.0262118049,1.7279233824
H,0.1332286924,-0.5999151721,-2.113176239
H,1.2828320061,0.6710436954,-1.6786090946

M34

0 1
B,-1.2302508343,-0.6025907667,0.0753433023
Si,0.6654362697,0.1401855406,0.1227588367
H,1.6680509253,-0.9416981783,0.2564640267
H,0.9657531701,0.9138791422,-1.111964803
H,0.8364156245,1.0826260979,1.2611720457
C,-2.2751033357,1.54321809,-0.3972549445
H,-1.9877854399,1.7290728618,-1.4366395097
H,-1.5558456491,2.0338278241,0.2677958698
H,-3.26481946,1.9662522992,-0.2199494977
C,-2.6925709955,-2.5070066149,0.263369812
H,-3.1715298262,-2.3476730152,-0.7066019794
H,-3.3199787766,-2.061832552,1.0404617167
H,-2.5792828464,-3.5755275857,0.4479092274
O,-2.3481529676,0.1511026589,-0.1437804739
O,-1.3883759883,-1.9355999635,0.2809162288

M34_TS

0 1
B,0.0074321449,0.0852408677,0.5812684755
Si,-2.1771895801,-0.2984457366,0.536465776
H,-2.5940496435,-1.6412894328,1.0081915323

H,-3.0224115599,0.7271044188,1.2001479235
H,-2.3708291558,-0.2141760916,-0.9299030986
C,0.6724490724,-0.1374941401,2.241769586
H,0.7579694122,-1.1762381874,2.5636785474
H,0.3168880797,0.5041831799,3.0502580097
H,1.6469624271,0.2434871524,1.9218573837
H,-0.6242962396,-0.20950198,1.6565429599
O,0.2897417237,1.4385126498,0.3063373113
O,0.427595898,-0.9662465463,-0.2620749858
C,1.8119898187,-1.0419378086,-0.5452107469
H,1.9401961463,-1.6937371472,-1.4116040941
H,2.2284348529,-0.0532321768,-0.7766941525
H,2.3691531,-1.4702627494,0.298365039
C,-0.1138424536,1.944488673,-0.9496738055
H,0.0682316381,1.2188443805,-1.7524675325
H,-1.1812805092,2.2025949865,-0.9469772558
H,0.4618703177,2.8510134482,-1.1480594024

M35

0 1

B,-0.2034483041,-0.1810540044,0.1427174762
Si,-2.1840750016,-0.5821882642,0.1789640251
H,-2.6429257506,-0.3997322526,1.5752443745
H,-2.4764803442,-1.9497939167,-0.2941102472
H,-2.8381073755,0.4226490259,-0.6909997997
C,0.3597280235,1.1873332928,0.7654566503
C,0.9061745082,-1.1438502884,-0.5026594907
F,0.8062762058,0.8885205704,2.0089086169
F,-0.5773822085,2.1450001219,0.9031171062
F,1.3788374475,1.7350520902,0.0854225622
F,2.1262336328,-1.0575144272,0.0492378487
F,0.5688970685,-2.4457626373,-0.5000494867
F,1.0158760981,-0.7612252003,-1.7994813259

M35_TS

0 1

B,0.3352759136,0.346696072,-0.3815063945
Si,1.1682947404,-0.5632692545,1.3593800973
H,1.7210564512,-1.8789858491,0.9819483512
H,2.2211368902,0.263957607,1.9905592861
H,-0.0031857306,-0.6809070069,2.2467238731
C,1.403556599,1.2744643271,-1.4607537524
H,2.2357553181,0.7369538298,-1.9166917482
H,1.7331005204,2.2249308907,-1.0405658642
H,0.6419273852,1.4590718568,-2.220887524
H,1.5561657066,0.5337007233,-0.2517880449
C,-0.2094430839,-0.8697081231,-1.2796908543
C,-0.7100120573,1.439236486,0.1715103093
F,0.8028647094,-1.5878115303,-1.8299151144
F,-0.9717811913,-0.4438903956,-2.3124842985
F,-0.9667765089,-1.7494375713,-0.5888610861
F,-1.2227622747,2.2256294531,-0.8021825144
F,-1.7656559355,0.887475918,0.8010300113
F,-0.125808892,2.2860270171,1.0626082475

M36

0 1

B,-0.0549956129,-0.1283479435,0.2270279879
Si,-2.033775599,-0.4577245051,0.0257285024
H,-2.6714959372,-0.7874785417,1.3274497262
H,-2.2959526795,-1.5950083427,-0.8953484543
H,-2.7406612268,0.7320214303,-0.5160227376
N,0.5769937042,1.005125335,0.8115636091
N,0.9801464901,-1.009822554,-0.1915283481
C,2.0128019307,0.7595676144,0.9648345874
C,2.2856498308,-0.3598514619,-0.0575223418
H,0.145134421,1.7244262457,1.3683001456
H,0.8896162131,-1.8034069021,-0.8048474898
H,2.6121148024,1.6509253253,0.757922462
H,2.2456269002,0.4137961924,1.9816376812
H,2.6102914978,0.0677335945,-1.0163331725
H,3.0601296952,-1.0479611564,0.2933504623

M36_TS

0 1

B,0.2921168379,0.4904608843,-0.488282777
Si,1.085786759,-0.4715158284,1.3135930586
H,1.7050277516,-1.7889527451,1.0207095274
H,1.9930627889,0.2662807459,2.240280316
H,-0.2101859419,-0.6709188945,2.0051995343
C,1.6156238373,1.2161360531,-1.5421441951
H,2.3342954481,0.5298037515,-1.9972928413
H,2.1180128705,2.1071985425,-1.1582305545
H,0.8639027889,1.5189908053,-2.27279721
H,1.5473827149,0.5446915253,-0.2918786974
N,-0.7059693016,1.5358109338,-0.1590220277
H,-0.6083803719,2.1046320552,0.6715708312
C,-2.0138713797,0.8853759455,-0.2868005401
C,-1.7874121387,-0.1147369214,-1.4230763728
H,-2.800974997,1.6067646476,-0.528046899
H,-2.3056719035,0.3393178422,0.6242047304
H,-1.8526629089,0.4100620289,-2.3892863519
H,-2.5310470177,-0.9178772834,-1.4135784789
N,-0.4390937517,-0.6183012705,-1.1447214211
H,-0.0162576444,-1.1587186876,-1.8869215911

M37

0 1

B,1.3160763959,0.0223451991,0.0002018693
H,3.8651219178,-0.2625775099,1.3709483133
H,3.9459266974,1.2293980526,-0.501713547
H,3.8426289769,-1.1369866678,-0.8492645696
C,-0.9180837092,0.7361163246,-0.2287154323
C,-0.9058897507,-0.7326726967,0.2241357996
Si,3.334207274,-0.0280970575,0.0018242053
H,-1.2051071223,-1.4035221123,-0.5974042415
H,-1.5827097729,-0.9137111076,1.0677271159
H,-1.2375119859,1.4016854252,0.5892039909
H,-1.5900697937,0.9040834008,-1.0788207295
N,0.4871842865,-0.9753671553,0.5878416117
N,0.4734731607,1.0099554898,-0.5810636486
C,0.831258048,-2.2912073086,1.062379507
H,0.5938421523,-3.0685426851,0.3202491129
H,1.9019011543,-2.3408116621,1.2776576268

H,0.2893087695,-2.5305317805,1.9858272017
C,0.7795412244,2.3266127245,-1.079691902
H,0.484485083,3.1088248141,-0.3641100947
H,1.8527871046,2.415155951,-1.2596154731
H,0.2555458594,2.5210220216,-2.024012856

M37_TS

0 1
B,-1.0572764271,0.6004411889,-0.1711378763
Si,-2.6845923766,-0.8728706094,-0.0603686527
H,-3.235434785,-0.8875680302,1.317856169
H,-3.8331609296,-0.9135629067,-1.0113763356
H,-1.8641850193,-2.0879227985,-0.2822795824
C,-1.6717018851,2.3224179633,-0.4246684129
H,-0.7001728881,2.7329158593,-0.143620482
H,-2.4508255199,2.7613048661,0.205439355
H,-1.8646097734,2.5285818474,-1.4788498968
H,-2.25003606,1.0273945291,-0.3190782623
C,1.0248740992,0.1863825711,0.8222903412
C,1.0076967209,-0.4095147409,-0.5856895928
H,1.9553481132,-0.2612035603,-1.1172885419
H,0.8083290612,-1.4958010357,-0.5326269928
H,1.5623415525,1.1530683353,0.8155350285
H,1.5133485649,-0.4700166971,1.5522806668
N,-0.082995948,0.3044214407,-1.240210445
N,-0.3906927078,0.361272354,1.1275106705
C,-0.7034724308,1.0941543522,2.3286373331
H,-0.2488971647,0.6113553017,3.2011439587
H,-0.3501657143,2.1409794171,2.3025623731
H,-1.787586354,1.1063752286,2.4863822309
C,-0.4601761604,-0.1937083964,-2.5412723481
H,0.3830668064,-0.1244768348,-3.2378974307
H,-0.7909622224,-1.2481400593,-2.5171096678
H,-1.2771457317,0.4083034743,-2.9525300278

M38

0 1
B,-0.0354432911,0.2839401867,-0.0074228904
Si,-0.2516814947,2.3012458319,0.0002134165
H,-1.4775937934,2.7240573127,-0.7294051582
H,0.9086356245,2.9856570118,-0.6313543169
H,-0.3659674952,2.8382298753,1.3826760367
N,-1.1832385905,-0.5365914672,-0.1498604447
N,1.2552252137,-0.2833434362,0.1464532696
H,-1.1576435452,-1.5463956106,-0.1427308401
H,-2.1087684845,-0.1625568394,-0.2802715796
H,2.090540074,0.2722341943,0.2303035474
H,1.4331091525,-1.2773408693,0.1721708696

M38_TS

0 1
B,0.2665443502,0.3749161034,-0.4829317722
Si,1.2629417238,-0.4565326285,1.3046083433
H,2.4471472275,-1.3294426819,1.0761445856
H,1.6064590725,0.5189610208,2.3744366764
H,0.1383317551,-1.3022624361,1.7693912648
C,1.5009285853,1.1924919391,-1.5767534724

H,2.3105192314,0.6017298995,-2.0155565172
H,1.8740198124,2.1553559562,-1.2225994153
H,0.7269638039,1.354273329,-2.3316550466
H,1.5358764719,0.5398666159,-0.3153129444
N,-0.2679427163,-0.72909484,-1.3010533158
H,0.3611255411,-1.2498802721,-1.8967626777
H,-0.901794276,-1.3575265977,-0.8231128254
N,-0.699578232,1.3161927468,0.1010193393
H,-0.3862738089,2.0472571207,0.7241483736
H,-1.3872300919,1.6690767551,-0.5553006561

M39

0 1

B,-0.5801016531,-0.0267284251,0.0261217348
Si,1.4634138448,0.0267487376,0.1038693218
H,2.0256285054,0.496653554,-1.1937433456
H,2.1178082761,-1.2773637824,0.3880929335
H,1.9515054686,0.9883509603,1.1304931402
N,-1.2620597917,1.2294112597,0.0013443027
N,-1.2943539689,-1.2630410964,-0.0360148061
C,-0.606006549,2.4930560557,-0.2810419237
H,0.3995856026,2.3369181776,-0.6747490264
H,-1.1687884429,3.0569545368,-1.0366836508
H,-0.535199405,3.1172642485,0.6211851611
C,-2.6314767891,1.4255471115,0.4471025347
H,-3.3052086566,1.706269838,-0.3754881142
H,-3.0142480371,0.5231089628,0.9241246837
H,-2.6610664538,2.2350781418,1.188599952
C,-2.6026017651,-1.4106319856,-0.6519508053
H,-3.3873112896,-1.6528786875,0.0797031875
H,-2.8837181298,-0.5007964321,-1.1827980877
H,-2.5699932418,-2.2301066846,-1.3823878079
C,-0.7523665941,-2.5445769071,0.3764317496
H,-0.6330651562,-3.2208358545,-0.4822744138
H,0.2166273287,-2.4207175193,0.8578951372
H,-1.4259295123,-3.0324033199,1.0938967628

M39_TS

0 1

B,0.4009627934,0.3568523317,-0.6395236616
Si,0.6347014998,-0.0833081428,1.5402228211
H,1.7905770681,-0.8299459105,2.1073956538
H,0.4943198775,1.1754386591,2.315660239
H,-0.5841877068,-0.9085490535,1.7242026433
C,2.0269740857,0.8687465293,-1.3399470575
H,2.5986095876,-0.0098367387,-1.6432445212
H,2.6934092499,1.6070775667,-0.8860126738
H,1.5429856151,1.3229663113,-2.2104117661
H,1.5625549238,0.4543446086,-0.0570844249
N,-0.0156944951,-0.9072482849,-1.2838262
N,-0.5148521259,1.5140237035,-0.7194131367
C,-0.0701064082,2.8487735979,-0.3774450092
H,-0.7999438285,3.584024701,-0.7358584298
H,0.0411618936,2.9993328245,0.7117176076
H,0.8867644608,3.0791579411,-0.8506522108
C,-1.8808831048,1.2757790672,-0.2781775309
H,-2.005443284,1.4159478073,0.8106256759

H,-2.5621258925,1.9740247333,-0.7796717373
H,-2.1756912042,0.2542897823,-0.5279997665
C,-0.3445480945,-0.7898192439,-2.6964580044
H,-0.982125118,-1.6281123776,-3.002035327
H,-0.8850646449,0.1428669703,-2.8743726308
H,0.5501709424,-0.8005810627,-3.3460138638
C,0.6914781401,-2.1375042999,-1.0076025305
H,1.7034956792,-2.1718582801,-1.4539363895
H,0.7962910637,-2.2998611419,0.0698982792
H,0.1316417266,-2.9885985986,-1.4126828478

M40

0 1

B,-0.0361075837,0.3942231426,-0.236871242
Si,-0.2397206338,2.3938261181,-0.058398979
H,-1.4566516618,2.9012926264,-0.7404367757
H,0.9424507305,3.1303914629,-0.5717770531
H,-0.370277792,2.6931243504,1.3919317515
H,-1.3652961972,-1.8199917949,0.1264148497
H,-2.5343954554,-0.0311005623,0.20215839
H,2.4106736879,0.4411058572,0.5539402662
H,1.6221981166,-1.5346827775,0.3386341049
P,-1.566223996,-0.6405488561,-0.623536287
P,1.7005241551,-0.3285033768,-0.3912871156

M40_TS

0 1

B,0.3314798286,0.2593193032,-0.3129447189
Si,1.1736736994,-0.4484825226,1.4726385106
H,2.2152069065,-1.482647891,1.2501922223
H,1.7538208152,0.6336342667,2.3070560281
H,0.0125063577,-1.0465125663,2.1633577949
C,1.4071521125,1.0833120398,-1.4902006476
H,2.1766593409,0.4598533234,-1.9532984643
H,1.8307725132,2.0373333253,-1.1651049854
H,0.6309959393,1.2827685381,-2.230023786
H,1.5579839387,0.4769912904,-0.2107058405
H,-0.7234669459,-0.8065927547,-2.3572683199
H,0.8683212501,-1.8907744801,-1.6002464307
H,-0.1147031999,2.5953460053,0.64213901
H,-1.3499403934,2.0548056015,-0.9276814566
P,-0.3704004209,-1.3955160148,-1.1111339822
P,-1.0120232919,1.5325445659,0.3519350061

M41

0 1

B,-0.112828,-0.161485,0.203819
Si,-2.110017,-0.468304,-0.01841
H,-2.672561,-0.904173,1.29023
H,-2.453025,-1.517334,-1.015038
H,-2.824856,0.779692,-0.400583
C,0.379756,1.234041,0.73586
H,-0.347089,1.74109,1.379568
H,1.327444,1.169744,1.283481
C,0.900532,-1.264772,-0.280734
H,0.535904,-2.25714,0.021875
H,0.785286,-1.285823,-1.379322

C,0.595655,2.09598,-0.535094
H,0.942258,3.098509,-0.270833
H,1.343469,1.651057,-1.199991
H,-0.33257,2.207701,-1.105221
C,2.376837,-1.094882,0.09045
H,2.770766,-0.138285,-0.268107
H,2.515144,-1.115554,1.176045
H,2.997528,-1.88801,-0.336354

M41_TS

0 1
B,-0.4976343423,0.7931720854,-0.0271923372
Si,1.3588904721,-0.2492818563,0.0822475313
H,1.6475322698,-0.8677570096,1.4019312171
H,1.5372188036,-1.2876014092,-0.9666777917
H,2.3486286911,0.8269813708,-0.1567395672
C,-1.93388108,-0.3067700099,0.0066212133
H,-2.0935412316,-0.9493445904,0.8767253144
H,-2.0897362038,-0.8703239048,-0.9154300569
H,-2.6528967998,0.5145616598,0.0525440014
H,-0.5255212069,-0.4707741356,0.0926224835
C,-0.6356404405,1.6908200327,1.3060215005
H,-1.4453230743,2.4098648543,1.0980856453
H,-1.0045105837,1.0751292292,2.1379989215
C,-0.5459054962,1.4294769899,-1.5119315354
H,-0.2993625654,0.6827930869,-2.2799464299
H,-1.5935683504,1.7083995941,-1.7078028445
C,0.6014130803,2.4636751724,1.7849985768
H,0.3536919626,3.1489407134,2.6017524125
H,1.3757227071,1.7845149528,2.1592638528
H,1.0514187841,3.0541139097,0.9814505879
C,0.3169799193,2.6802450703,-1.7207897236
H,0.2202780323,3.0659597393,-2.7404111501
H,0.0134801985,3.4807117325,-1.0382094403
H,1.3789607042,2.4826927023,-1.5430937215

M42

0 1
B,-1.3348280168,-0.3174000741,0.0034655352
Si,0.6837031573,-0.3082332254,0.0092053174
H,1.2317421002,-1.6019559366,0.4747734471
H,1.1547666354,-0.0287726418,-1.3683424309
H,1.1445785827,0.7833079786,0.9001410403
Br,-2.2619506073,1.2518579965,-0.5627783778
Br,-2.3470975016,-1.8376275314,0.5435354956

M42_TS

0 1
B,0.4354884013,0.1955194559,0.0000486826
Si,-1.6516350296,-0.1735676114,0.0001975957
H,-2.0856134395,-0.9075897747,-1.2117398859
H,-2.0854762671,-0.9073812914,1.2123104533
H,-2.1818434472,1.2029561078,0.0001094315
C,1.5329907859,-1.2246050354,0.0001101407
H,1.5139798468,-1.8345645774,-0.9049680173
H,1.5140810606,-1.8344076827,0.9052961284
H,2.4381782348,-0.6153764004,0.0000067544

H,0.1453316634,-1.0195966113,0.0001700958
Br,0.7626954229,1.1329538565,1.7059698203
Br,0.7625056079,1.1326600343,-1.7060700694

M43

0 1

B,0.0582192499,0.3708818954,0.0020177837
Si,0.1470680741,2.3920775767,-0.0000797196
Br,1.6849221268,-0.6422067166,0.0052895361
Br,-1.5985116777,-0.5842694314,0.000901617
C,1.0995719822,2.926589364,-1.5377343833
H,1.2079052346,4.0162473692,-1.5534531593
H,2.1012171958,2.4859684924,-1.5468479743
H,0.5869108046,2.6260165509,-2.4563529101
C,1.0943905787,2.9298835867,1.5396368393
H,2.0960739181,2.4894598082,1.5529902329
H,1.2024840222,4.0195929725,1.5534502234
H,0.5787275426,2.6311341515,2.4571690501
C,-1.5878548115,3.1201048921,-0.0037316046
H,-2.1477065481,2.8008821935,-0.88826162
H,-2.1505982841,2.8028042388,0.8796534326
H,-1.5469987881,4.2142826863,-0.0048561239

M43_TS

0 1

B,-0.0535632746,0.1598303057,0.3502036817
Si,0.0166076093,2.2077094277,-0.2352007112
C,-0.0551533454,-0.1744658695,2.1418649093
H,-0.9464874025,0.1536109024,2.6804585708
H,0.8636194043,0.0885756236,2.6699364902
H,-0.0947767945,-1.2552688015,2.0058042009
H,-0.0199537151,0.9380097536,1.3214061628
Br,1.6172851819,-0.6621490808,-0.3171984319
Br,-1.786730551,-0.5398511763,-0.2973958201
C,1.5951796603,3.0169177929,0.3977441538
H,2.4773840216,2.4597185732,0.0696559371
H,1.6751956403,4.0388663698,0.012212477
H,1.6155484909,3.0754418323,1.4914212069
C,0.0027911888,2.1261642527,-2.1087278085
H,-0.9045320737,1.6350979008,-2.4702923709
H,0.0368678163,3.1411715559,-2.5192167002
H,0.8682844638,1.571413602,-2.480592828
C,-1.49237674,3.1278403276,0.4156852837
H,-1.4957924343,3.1872298474,1.5094999498
H,-1.5033304918,4.153052968,0.0306720957
H,-2.4160374343,2.6355112126,0.0981002011

M44

0 1

B,-0.1979417709,-0.5606595041,-0.0577982355
H,-1.9911904382,-2.8141322709,0.4111211273
H,-0.8893575059,-2.895388707,-1.7169632811
H,-2.7093979409,-1.3701912762,-1.3506772882
C,-0.7302407284,0.6195533269,0.8432000724
H,0.080191088,1.0199430005,1.4691000393
C,1.3343550851,-0.7206099116,-0.396199701
H,1.4787575866,-1.2571835575,-1.3426578102

C,-1.127796365,1.7315910721,-0.1574265988
H,-1.4953370721,2.6097676167,0.3847766226
H,-0.2878079885,2.0524859041,-0.7812589405
H,-1.9342110643,1.3949726634,-0.8196048438
C,2.1935561791,0.5472464819,-0.4103423282
H,1.9244548851,1.2098166843,-1.2385888557
H,2.0875765523,1.1157997517,0.5200673568
H,3.2548699806,0.2969652126,-0.5213829679
C,1.8097920168,-1.6717485285,0.7347266344
H,1.6851036226,-1.2069636946,1.7202152453
H,1.2694263787,-2.6248265088,0.7392697692
H,2.8744445844,-1.8960940002,0.6096279109
C,-1.9223286257,0.2751166266,1.7423761296
H,-1.6788694563,-0.5205308099,2.453853802
H,-2.2512181766,1.1493195205,2.3160019242
H,-2.7773922315,-0.0657001456,1.1456110981
Si,-1.5050977849,-1.9779306163,-0.7213702011

M44_TS

0 1

B,-0.536987335,0.7479707964,-0.009236453
Si,1.3630153844,-0.2693428826,0.0677961085
H,1.6850327458,-0.7078472584,1.4487015695
H,1.5488147381,-1.4395493969,-0.8301341332
H,2.3205439558,0.7824124673,-0.3471377252
C,-1.9147751648,-0.4398340367,0.0376299298
H,-2.0912898513,-0.8509631687,1.0335199432
H,-1.9792151359,-1.2375255387,-0.7069054772
H,-2.6867751911,0.295269468,-0.1965949716
H,-0.4945797735,-0.5255081731,0.0118369651
C,-0.6535797029,1.5536674377,1.3995098903
H,-0.8156874382,0.8124168237,2.1972244151
C,-0.6482380301,1.4648193725,-1.4622797128
H,-1.7022314745,1.7824404759,-1.5434951481
C,0.5853045979,2.369358967,1.8065147661
H,0.3934499689,2.9214200412,2.7340541177
H,1.4608070349,1.7367753012,1.9857222341
H,0.8606859791,3.1018904333,1.0417012408
C,0.1968469878,2.7374786753,-1.6124511806
H,0.066389887,3.168349822,-2.612362142
H,-0.0834108762,3.5054017343,-0.8862604513
H,1.2655699073,2.5318530939,-1.4827763219
C,-1.8789477552,2.483588749,1.3867599329
H,-2.8140545555,1.9472346588,1.1958735787
H,-1.9897151189,2.9957771986,2.3493726263
H,-1.7785209326,3.2570279882,0.6164256869
C,-0.3663474066,0.534900758,-2.6518034753
H,-0.9270118455,-0.4044453043,-2.598055395
H,-0.6254676415,1.0187683858,-3.6002622236
H,0.6999115618,0.2800026614,-2.7056421441

M45

0 1

B,-0.1072935475,0.1992846873,-0.0065731964
Si,1.7397104742,1.0543985942,-0.0003643716
C,-1.394821078,1.0232988243,0.0979905457
C,-0.2198152572,-1.3263590758,-0.1200081913

N,-2.321185325,1.7170765017,0.1809579177
N,-0.2102930495,-2.483229406,-0.2090701755
C,2.5751191489,0.5562714683,-1.6143147022
H,3.5985784099,0.9455984298,-1.6325094771
H,2.6256821061,-0.532411792,-1.711417432
H,2.0501438573,0.9552196576,-2.4869835986
C,2.6746121734,0.3192960448,1.4612903547
H,3.6990315142,0.7063379649,1.473089925
H,2.2087464467,0.5773647347,2.4166342898
H,2.7259414608,-0.771157884,1.3871825057
C,1.5860955682,2.9201799354,0.1483922947
H,1.0183641967,3.33929157,-0.6878879
H,1.0753487911,3.2034896727,1.0737099411
H,2.5760048397,3.3876527822,0.1524136503

M45_TS

0 1

B,-0.5048098868,0.7839932584,-0.001483696
Si,1.4188452968,-0.1489962807,0.0013692447
C,-1.994361268,-0.3043667,-0.0047232496
H,-2.1358909011,-0.8982479555,0.8988725869
H,-2.132730815,-0.8969698282,-0.9096440554
H,-2.6926450641,0.5297451041,-0.0053432534
H,-0.632464043,-0.4562595238,-0.0023824082
C,-0.5522518337,1.5345552432,-1.3586186371
C,-0.5569795049,1.5330481208,1.3563117197
N,-0.5430597099,2.0546114867,-2.3941814476
N,-0.5513839204,2.0519491117,2.3924796616
C,1.6084512249,-1.1837549392,-1.555496853
H,1.3910087775,-0.5854856401,-2.4456461148
H,2.635454724,-1.5539673564,-1.6397402067
H,0.9437710198,-2.0540378275,-1.5545346301
C,1.6029395194,-1.1855675758,1.5576917369
H,1.382332355,-0.5883312094,2.4477562369
H,0.9382732107,-2.0558509326,1.5533607466
H,2.6296399593,-1.555873976,1.6451512713
C,2.5673914286,1.33039398,0.0042530191
H,3.6087921095,0.9913853527,0.0059452386
H,2.4083542974,1.9489480315,-0.8836637851
H,2.405157264,1.947988406,0.8922590747

M46

0 1

B,-1.3221146134,-0.2955782732,-0.0002393462
H,-1.9116772114,0.7260625756,-0.1424485771
H,-1.93045642,-1.3102447372,0.1062611166
Si,0.6852093077,-0.2968449253,0.0183455853
F,1.303104298,0.9912419629,0.7400659205
F,1.3214436836,-1.5639312956,0.7603522447
F,1.2454051855,-0.3095287252,-1.4823368998

M46_TS

0 1

B,0.1559881415,0.0000217144,0.2405815953
Si,-1.837182248,-0.0000601446,0.0261790242
C,0.9818897146,0.0000050086,1.8068738631
H,0.8427074087,-0.89533581,2.4128151944

H,0.8425130989,0.8951612885,2.4130471782
H,1.9944169785,0.0001817129,1.4083933472
H,-0.3970338086,0.0000186728,1.3522142453
H,0.3885808528,-1.0514962775,-0.2717204258
H,0.3885115157,1.0515593176,-0.271712205
F,-2.1200055586,-0.0001620246,-1.5465312767
F,-2.5977350624,1.2804375099,0.6202536514
F,-2.5976462231,-1.2805417082,0.6204043283

M47

0 1

C,-0.8049964423,0.3868262922,-0.8118590554
H,-1.6379282712,0.05544146,-0.1848234815
H,-0.9107529732,-0.0307305875,-1.8195302061
Si,0.7637875948,-0.4366277733,-0.099602648
H,1.8428037634,-0.3200770714,-1.1158380221
C,0.4034602184,-2.2476019224,0.2475985847
H,1.2975664933,-2.7621660967,0.6124141648
H,-0.3763271966,-2.3424113028,1.0099927733
H,0.0587788846,-2.762129049,-0.653968
C,1.3059053411,0.4384182011,1.4770359071
H,0.4757263123,0.5043680008,2.1891387998
H,2.1220816178,-0.1062536703,1.9614720773
H,1.6591026039,1.4556449998,1.2773921955
C,0.3574271892,2.577603236,-1.9156435514
H,1.4063917727,2.5147203172,-1.5887226923
H,0.2954729018,2.0492495468,-2.8712908086
H,0.1535337332,3.6403320042,-2.0722377734
C,-1.0292808227,2.7839639336,0.4283260843
C,-0.2171649486,3.758355254,1.0103668423
C,-2.2868225017,2.6315353087,1.0138829061
C,-0.6014461608,4.5203091198,2.1049888024
C,-2.7184865371,3.3857521071,2.097593662
C,-1.8656552796,4.3326789009,2.6488290472
B,-0.5357071997,1.9088116849,-0.8066877216
F,-3.9357333887,3.2129466512,2.6096100626
F,-2.2579005857,5.0580683386,3.6895931976
F,0.2206035942,5.4240731408,2.6347032237
F,1.0166988133,3.9749169578,0.5329569419
F,-3.1632857461,1.747794958,0.517786458

M47_TS

0 1

C,2.2539893055,0.8001974911,0.2619747189
H,3.0164854891,1.0567271358,0.9983905362
H,1.9364073388,1.6741713444,-0.3020793457
C,1.4189690699,-0.6061146897,2.6316826008
H,0.8948165003,0.3211347055,2.8418201006
H,2.4773174568,-0.5102748418,2.8679829774
H,0.9494029939,-1.4273115208,3.175388638
H,1.4301499888,-1.1871222496,1.5538258202
B,1.0758426897,-0.1882148853,0.7236311073
Si,2.4106923722,-0.8459155751,-0.6036743532
C,3.8761001258,-1.9219822718,-0.1207371788
H,3.6777923945,-2.9786916853,-0.3199693636
H,4.7697220279,-1.6300809329,-0.6810771286
H,4.1009305,-1.8130722348,0.9446473116

C,1.9070049703,-0.9341037102,-2.4088083813
H,2.7296839545,-0.6272879869,-3.0618339836
H,1.6031950029,-1.9462970199,-2.6891553375
H,1.0620574013,-0.2625978344,-2.5877986469
C,-0.4862779363,-0.0573587409,0.5518196884
C,-1.3526134206,-1.0700987209,0.970267756
C,-1.1125947023,1.0254758632,-0.0664031931
C,-2.7282235301,-1.0287780766,0.8073591914
C,-2.4870574105,1.1004594623,-0.2646508868
C,-3.3022483118,0.0694802219,0.178725165
F,-3.499765243,-2.0278018798,1.2368369334
F,-4.6204386935,0.131400458,0.0065777767
F,-3.0281856482,2.1595993795,-0.8668295163
F,-0.3916661138,2.0628652462,-0.5174155972
F,-0.8429606319,-2.1636552512,1.5665744508

M48

0 1

C,-1.721942139,0.1574608961,-0.1812175908
C,-1.0234242361,-1.0171067162,-0.9006993047
H,-1.7584211339,-0.0157649448,0.9005583264
H,-2.7825242412,0.2038467514,-0.4907769834
H,-1.6522796757,-1.915566329,-0.8690268276
H,-0.8734273771,-0.7901597408,-1.9627420931
Si,0.6355159111,-1.4467532271,-0.1001094826
H,1.3801179704,-2.3891745969,-0.9774440913
C,0.3337380844,-2.2582614462,1.5722497234
H,1.2784709822,-2.5279977907,2.0538597247
H,-0.2003103112,-1.5791673634,2.2451115406
H,-0.2643236901,-3.1687284355,1.4697966535
C,1.6657021558,0.1127901845,0.1584206093
H,1.1331747332,0.8351509595,0.7896872131
H,2.600655375,-0.1312142024,0.6728486537
H,1.926398338,0.6091614769,-0.7807718174
C,-0.763416465,1.9263482029,-2.0262259064
H,0.2737254537,1.5977578674,-2.1846310376
H,-1.3713305109,1.369052373,-2.7469684759
H,-0.7943655258,2.9901253042,-2.2716446748
C,-1.0882532648,2.7150561213,0.5631282992
C,-0.0744675705,3.675172351,0.5603108806
C,-2.0068640883,2.8175358668,1.6086898213
C,0.0386970836,4.6642545142,1.5277873392
C,-1.9419287135,3.8029907389,2.5843593107
C,-0.9069239188,4.7285251992,2.543555581
B,-1.1764380561,1.5877317558,-0.5485630597
F,-2.8542340741,3.8710030911,3.5516752304
F,-0.8220730921,5.6727121383,3.4726000049
F,1.0349211635,5.5466953528,1.4940458688
F,0.8684211541,3.6506802754,-0.3897026384
F,-3.0319886508,1.9595756227,1.6876514629

M48_TS

0 1

C,2.6430804597,1.1637240764,-0.7687099156
C,2.2860336954,1.3113135112,0.7450766472
H,3.6148198127,1.563820291,-1.071018983
H,1.8679235304,1.6363990552,-1.3829959665

H,1.9316402007,2.3058062336,1.0343581369
H,3.1814817051,1.1021394574,1.345707794
C,1.3129414574,-0.601850553,2.6446203304
H,0.9612078963,0.3522419212,3.0328834869
H,2.3013906076,-0.807621482,3.0604591042
H,0.6049314238,-1.3917683697,2.8937681438
H,1.6257897677,-1.0063392278,1.4348378077
B,1.2388421449,0.0935512465,0.905451235
Si,2.3507747238,-0.7053298329,-0.664930328
C,3.9116542512,-1.6453845253,-0.1752155699
H,3.6820879221,-2.6711508616,0.1306168416
H,4.6077449115,-1.6958912521,-1.0191102362
H,4.4293117814,-1.1486194333,0.6517003107
C,1.4446911895,-1.5817964358,-2.0606528871
H,2.0732305144,-1.6469216754,-2.9549758881
H,1.1649912837,-2.5982494022,-1.7660988729
H,0.5308932487,-1.0414828767,-2.3271070476
C,-0.3053410378,0.1580860715,0.5285346078
C,-1.0725271934,-1.0062777927,0.4511764003
C,-0.9834726711,1.3265671535,0.1869522864
C,-2.4064964484,-1.0323551467,0.0774192921
C,-2.3189247806,1.3463745003,-0.2046236222
C,-3.0366154223,0.1608222709,-0.256406068
F,-3.0841818592,-2.1794313221,0.0270796455
F,-4.3165258214,0.1638179173,-0.6205229676
F,-2.9161728997,2.4952739958,-0.5209644574
F,-0.3562197718,2.5117852452,0.2184293166
F,-0.4959876224,-2.1881157577,0.7438634228

M49

0 1

C,-1.6944420249,0.4242985628,-0.4101914293
C,-1.0866790944,-0.9370929568,-0.7920740194
C,-0.0184807317,-1.39957361,0.2122373266
H,-2.1066753368,0.3604043632,0.6025153213
H,-2.5571561101,0.6120877819,-1.0742945733
H,-1.8876639963,-1.6837675919,-0.8381439087
H,-0.6607592707,-0.8895828689,-1.8029565419
H,-0.4351369872,-1.3653018851,1.227497785
H,0.2428163243,-2.4498966875,0.0233866742
Si,1.592908747,-0.4193534616,0.1807588236
H,1.2788554656,1.0418090349,0.1640006069
C,2.5565380311,-0.8111339813,-1.3885925149
H,3.4703061125,-0.2127751497,-1.4510269695
H,2.8427906458,-1.8679311606,-1.4082000692
H,1.9625107346,-0.6080980025,-2.2851131821
C,2.6188418921,-0.7886140838,1.7113205428
H,2.8450194365,-1.858136669,1.7733663037
H,3.5672959009,-0.2439017318,1.6967469462
H,2.0765193452,-0.5041580485,2.6178842942
C,-0.1942852655,2.0280106985,-2.0449313277
H,0.672180108,2.6936097944,-2.0126679926
H,0.0693661083,1.1245578588,-2.6027299255
H,-0.9645259424,2.5482777632,-2.6327511169
C,-0.7749579448,2.8252319629,0.5044752603
C,-0.887719183,4.1882709125,0.2341609838
C,-0.624479519,2.4947900847,1.8520368054

C,-0.8699325503,5.1648315122,1.2219005575
C,-0.5823041692,3.4389378743,2.8680593108
C,-0.7123726237,4.78458698,2.5478156408
B,-0.8151594381,1.7159301557,-0.6338034686
F,-0.4172444467,3.0729905807,4.1383390319
F,-0.6832506474,5.7033071172,3.5066109009
F,-0.9995523072,6.4539016478,0.9128307688
F,-1.0451246336,4.6125088856,-1.0269076443
F,-0.4715973389,1.2128344878,2.2174628395

M49_TS

0 1

C,3.2962056921,0.7395149028,-0.8576334602
C,2.0091567788,1.4507306627,1.1594644294
C,2.501618859,1.8989958441,-0.228335522
H,4.2716126443,0.6477395057,-0.3617092441
H,3.4899472943,0.8937707321,-1.9246730445
H,1.4470869477,2.2442566392,1.6648624727
H,2.8931206075,1.2500614891,1.7838924438
H,1.6357807591,2.1397317214,-0.8593731431
H,3.1049671932,2.8118327734,-0.1661041628
C,1.2102834568,-0.7024449348,2.7008220511
H,0.7058164468,0.1452670609,3.1621874159
H,2.2066720487,-0.8028446881,3.1356928468
H,0.6225593097,-1.6076225158,2.8560388558
H,1.5969448211,-1.0140468256,1.4442540688
B,1.151098145,0.0970131818,1.02253127
Si,2.2828789909,-0.8301257354,-0.520740178
C,3.3569043876,-2.3139307402,-0.0576925941
H,2.7414951206,-3.1843946531,0.192670615
H,4.0056474113,-2.5935426879,-0.8944638532
H,4.0009742438,-2.0910064658,0.7997007169
C,1.171966583,-1.2761906379,-1.9754590566
H,1.7828300086,-1.5573848408,-2.8400119403
H,0.5162167984,-2.1191061809,-1.7366883964
H,0.5455217624,-0.4262498139,-2.2653673366
C,-0.3915216299,0.0520049454,0.6044500913
C,-1.0589660198,-1.1645646594,0.4548137336
C,-1.1606641407,1.1743651868,0.3059464698
C,-2.3782640194,-1.2849710097,0.0496221728
C,-2.4871093171,1.1026516449,-0.1104901844
C,-3.1017802236,-0.1336954862,-0.2378885766
F,-2.9528104493,-2.4815957237,-0.0745934551
F,-4.3707830785,-0.2188774066,-0.6291739423
F,-3.1727704978,2.2129742733,-0.3819431004
F,-0.638320482,2.4066552114,0.4035454462
F,-0.3881420429,-2.3104979392,0.6966156805

M50

0 1

C,-1.6519468757,-0.0333565206,-0.4680437868
C,-0.9956603867,-1.0791705725,-1.390869442
C,0.3447517311,-1.5812091969,-0.8402632094
H,-1.6752696245,-0.4167797121,0.5585650889
H,-2.7067341473,0.0877815325,-0.7676385049
H,-1.6675613908,-1.9357691086,-1.5158305307
H,-0.8393393471,-0.6559834199,-2.3919181796

H,0.1615115505,-2.0910879165,0.1153455027
H,0.7446020373,-2.3422570072,-1.5230442405
Si,3.0837291595,-1.1034736854,-0.0633754652
H,3.6743870778,-1.9269766197,-1.1541974738
C,2.8858252807,-2.1696325056,1.4757981914
H,3.8595764905,-2.4858864034,1.8618726899
H,2.376685876,-1.6104102202,2.2682622651
H,2.2996448311,-3.0698942702,1.2687923291
C,4.1964086587,0.3695783566,0.2983548649
H,3.781066202,0.9713621919,1.113914497
H,5.1996251992,0.0496017033,0.5951109206
H,4.293722023,1.0184990402,-0.5771923478
C,-0.814676708,2.0869278232,-1.9827584158
H,0.2216883856,1.9099459156,-2.2996890479
H,-1.4596650638,1.6590681667,-2.7565095252
H,-0.9433839653,3.1731481289,-1.96522488
C,-0.7017513832,2.2418079461,0.7324627116
C,0.4320566356,3.0496965992,0.8217440363
C,-1.5052417724,2.2073941189,1.8713727061
C,0.7686045916,3.7641784621,1.9631996615
C,-1.217718518,2.9239845023,3.0257314998
C,-0.0685806203,3.7027864412,3.0705224068
B,-1.0425663419,1.4129528476,-0.5795864234
F,-2.0257354966,2.8736352602,4.0828549521
F,0.2288702254,4.3881169631,4.1683729471
F,1.8755843203,4.5030017981,2.0096218962
F,1.2760653627,3.1329187656,-0.2159080903
F,-2.6315541754,1.4823121789,1.8747673878
C,1.3921607126,-0.480970288,-0.6328392529
H,1.532404512,0.0907623985,-1.5604295413
H,1.0508117736,0.2363834462,0.1295632629

M50_TS

0 1

C,3.2869797429,1.0523325361,-1.5209999855
C,2.0617271786,1.8695026399,1.0702755197
C,2.2917637521,2.8877299848,-0.0701272325
H,4.2291202928,1.2711772639,-1.0013408631
H,3.5485415857,0.7956646307,-2.5554244575
H,1.5899590457,2.3931174645,1.9139539057
H,3.0434902172,1.5511880358,1.4519794532
H,1.5031571721,3.6434870536,-0.0549383609
H,3.2324599108,3.4198198589,0.1216151812
C,1.3393946794,-0.3472526749,2.4055078606
H,0.7326545607,0.4090025285,2.9025460843
H,2.342129401,-0.3458914438,2.836903515
H,0.8675378638,-1.3235992019,2.5227841065
H,1.7325439984,-0.601997823,1.1071345366
B,1.2451060323,0.5114273252,0.76486506
Si,2.4188467692,-0.443270932,-0.7602668135
C,3.6668503146,-1.7023284276,-0.1032133877
H,3.1695419272,-2.5877690204,0.3073949323
H,4.3289619021,-2.0363419401,-0.909078101
H,4.295602965,-1.2680027429,0.6819106851
C,1.3366268246,-1.2365529085,-2.0828526514
H,1.9662017818,-1.5432027248,-2.9255348998
H,0.81017236,-2.1203025779,-1.7136634435

H,0.5928972002,-0.5274461171,-2.4616976123
C,-0.3004938596,0.4084830645,0.3569908572
C,-0.9367805372,-0.8274800299,0.2263797397
C,-1.1148400403,1.505173824,0.0878342459
C,-2.2604344286,-0.9864285097,-0.1516757257
C,-2.4473407132,1.3959304165,-0.2987987559
C,-3.0255797163,0.1417225861,-0.4211277153
F,-2.8017072023,-2.2000252255,-0.2591512636
F,-4.299270212,0.0183721489,-0.7859806245
F,-3.1729915121,2.4865760629,-0.5447505491
F,-0.6310858973,2.7517263167,0.195558523
F,-0.2393202977,-1.9556369777,0.4748327524
C,2.3614725929,2.2782999574,-1.4736217288
H,2.6951098684,3.0465484697,-2.1801876016
H,1.3482605372,1.9920948891,-1.7958924052

M51

0 1

B,1.0133462254,-0.0398762653,-0.0493183619
Si,-1.0208024686,0.0434538839,-0.0157919064
C,1.8934118249,1.2149530526,-0.0650568795
C,1.6965411917,-1.4126625739,-0.0993887047
N,2.4862337578,2.2124807477,-0.0783093226
N,2.1255598071,-2.4900694531,-0.1411397408
C,-1.6129171841,-0.8615481727,1.5360975318
H,-1.2573669604,-1.8982211158,1.4925464743
H,-1.1486345932,-0.4141006881,2.4231703207
C,-1.5837283018,-0.8572927574,-1.5801957878
H,-2.6804770756,-0.8305767121,-1.6115627628
H,-1.3030320453,-1.9143533218,-1.4925436577
C,-1.5882319437,1.8423637443,-0.0022076055
H,-1.1041111377,2.3743579638,-0.830669424
H,-2.6653672243,1.8680307214,-0.2137891607
C,-1.0067219941,-0.2572282794,-2.8708363589
H,-1.3794629684,-0.77632125,-3.7582324139
H,-1.2688137291,0.8005762618,-2.9737653964
H,0.0871617284,-0.3283898277,-2.8924466311
C,-3.1432734921,-0.8256754051,1.6698547028
H,-3.6301251778,-1.3034680567,0.8137334807
H,-3.4771041273,-1.3482210135,2.5709276438
H,-3.5146472104,0.2030159229,1.7293734424
C,-1.2901011841,2.5561812323,1.324463886
H,-1.6115369637,3.6011189064,1.2986350176
H,-1.8052367372,2.0733043214,2.1615350361
H,-0.2179066664,2.553082074,1.5482752086

M51_TS

0 1

B,-1.0051027928,0.0730812666,0.1674275831
Si,1.1382454473,0.0605107885,0.0031239097
C,-1.7266185785,-0.1931511619,1.8478404368
H,-1.5021640111,0.5892719191,2.5735203623
H,-1.5798810601,-1.1903858309,2.2650098754
H,-2.7533980724,-0.0898788342,1.5036808247
H,-0.4809769186,-0.1585001462,1.2764789492
C,-1.5262730874,-1.1187324568,-0.6802577091
C,-1.3881889637,1.5314962756,-0.2017040551

N,-1.8864907804,-2.0184691736,-1.3154171225
N,-1.6253887898,2.6348862723,-0.4649539872
C,1.8823769369,-1.4813090893,0.8017938414
H,2.9605938009,-1.4568089676,0.5916980937
H,1.7974155768,-1.3990311207,1.8940498597
C,1.7826152925,1.615289773,0.8560679377
H,1.1655926849,2.4668138788,0.5464624769
H,1.6334731322,1.5031719953,1.9389652911
C,1.4085547249,0.0660342902,-1.8640093848
H,0.646102739,-0.5644701546,-2.335491123
H,1.2299664865,1.0863501761,-2.2256985802
C,1.28384766,-2.8102993478,0.3171455918
H,0.2363639803,-2.9145903706,0.6154317326
H,1.3053486893,-2.8885009118,-0.7747721125
H,1.8313623771,-3.6651826737,0.7241687991
C,2.8087972215,-0.4188663919,-2.2743995652
H,2.9385341332,-0.3622042006,-3.3589560418
H,3.6030525608,0.1785480187,-1.816345164
H,2.9696415788,-1.4606840919,-1.9797317634
C,3.2627929534,1.9086775919,0.5635117082
H,3.4156886073,2.130600343,-0.4969741183
H,3.6143877453,2.7746786501,1.1315679607
H,3.9067666356,1.0616356853,0.8234199929

M52

0 1

B,-1.3267679403,0.004276761,-0.0115047835
Si,0.691798719,0.0050783748,-0.0045822255
F,1.2787262297,0.0244233955,1.4910645962
F,1.3412464046,1.2692416063,-0.7517789909
F,1.3197447938,-1.2932889258,-0.7110098589
C,-2.0638896584,-1.3728172215,0.0298757747
H,-3.1041543806,-1.3084384873,0.3617932109
H,-2.0863060289,-1.7097407569,-1.0211502277
H,-1.5453815592,-2.1657933519,0.5760889856
C,-2.0888842713,1.3676414961,-0.0458206638
H,-1.591726047,2.1596304881,-0.6125953565
H,-3.1335267829,1.2815011016,-0.3590770158
H,-2.1027694785,1.71607052,1.0013845551

M52_TS

0 1

B,1.3160539705,0.8166355302,0.0000309425
Si,-0.5374739522,-0.0616386763,0.0000965194
C,2.7452930234,-0.2172390106,-0.0009398904
H,2.910565007,-0.8173753674,-0.8979557195
H,2.9110966577,-0.8182731538,0.8953756281
H,3.4587367336,0.6109835378,-0.0007391965
H,1.2956781541,-0.4441146936,-0.0006463389
F,-1.5548065607,1.1735907977,0.0010704875
F,-0.9137259011,-0.9425542046,1.2863269177
F,-0.9144789402,-0.9411422417,-1.2868793971
C,1.296282191,1.600943164,-1.406029916
H,2.1999170836,2.2231844111,-1.450423715
H,1.3112347933,0.9447362231,-2.2824093699
H,0.4411025819,2.2761545541,-1.5067885983
C,1.2971174347,1.5994252404,1.406948695

H,1.3125120129,0.9422750781,2.2826134476
H,2.200817043,2.2215601603,1.4515132161
H,0.4420363474,2.2745816113,1.5089031778

M53

0 1

B,0.7719808371,1.1748553188,-0.0131287694
Si,-0.9295156459,0.0796217555,-0.001280494
C,1.4572378036,1.4902273683,-1.3780306101
H,2.468747298,1.8949537417,-1.28326488
H,1.452593247,0.6551648435,-2.0851978468
H,0.8383494171,2.27270238,-1.8490313444
C,1.2821852966,1.6940645132,1.3676080527
H,1.8936251636,0.8717369869,1.7764886618
H,1.9365086899,2.5672301988,1.2913390023
H,0.5009599101,1.8769453686,2.1115585338
Cl,-2.5249315132,1.3853950518,0.1275899949
Cl,-1.0304801133,-1.1824551269,1.6257284021
Cl,-1.2017395506,-1.0679409903,-1.690367483

M53_TS

0 1

B,1.3259242147,0.8552821539,-0.0000612079
Si,-0.5682776033,-0.0950426494,0.0006458677
C,2.7018974537,-0.229417374,-0.000692718
H,2.8324854367,-0.8391885931,-0.8972992216
H,2.833276209,-0.8391175757,0.8958446578
H,3.461885532,0.5573409516,-0.0010715521
H,1.2048807026,-0.4038237795,-0.0001212752
C,1.3080375345,1.6282922822,-1.4068743525
H,2.2370972665,2.2104578339,-1.4679507858
H,1.28407376,0.9681064793,-2.2799633394
H,0.481051913,2.3388774458,-1.4968421989
C,1.3091990559,1.6280816487,1.4068824305
H,1.2856856948,0.9677833707,2.2798990354
H,2.2384288255,2.2100328405,1.4674072816
H,0.4824285229,2.3388330426,1.4975050077
Cl,-0.9468426172,-1.2425234111,1.6682025017
Cl,-0.9482723115,-1.2421044749,-1.6668719112
Cl,-1.9212347498,1.4462272187,0.0014190003

M54

0 1

B,-0.9597335376,-0.9854400994,0.1077074334
Si,-2.9178045307,-1.4254938007,0.1555659054
O,-0.2076579619,-0.8110759982,-1.0206164958
O,-0.2299819153,-0.8211603329,1.2599050287
C,1.0598767813,-0.2781787404,0.879632685
C,1.1797331587,-0.7308888449,-0.6110212023
C,1.9047438897,0.2487447929,-1.5191962145
H,2.9340284624,0.3981923012,-1.1758057388
H,1.9361916,-0.1529733685,-2.5351771672
H,1.3975788222,1.2143594773,-1.5494015041
C,1.7642343021,-2.1338502606,-0.7652214254
H,1.6249725712,-2.4582340386,-1.7993308005
H,2.8333335077,-2.1476689747,-0.5337347169
H,1.2529769487,-2.8470160994,-0.1118727671

C,2.1246660756,-0.8412355343,1.8064014983
H,3.1204141303,-0.5190290911,1.4835629434
H,1.9570940213,-0.4714422517,2.8213520089
H,2.0967171392,-1.9317811732,1.8302842537
C,0.9605611163,1.2379407681,1.0380888499
H,0.6800811648,1.4648276141,2.0697446111
H,1.9161081329,1.7239789633,0.8205736365
H,0.1948218785,1.6528462767,0.3760530398
O,-3.7268601055,0.0099399856,-0.0248493338
O,-3.3485322734,-2.5184413064,-0.9975252447
O,-3.386828123,-2.1261065418,1.5863804829
C,-5.138620121,0.0344078667,-0.1449975917
H,-5.4716533522,1.0709269421,-0.0582144647
H,-5.4500155537,-0.3557743372,-1.1209833845
H,-5.6182612172,-0.5581331153,0.6454450351
C,-3.2535843338,-1.4300429807,2.8151548401
H,-3.8863793882,-0.5342318424,2.8286759423
H,-3.5706718621,-2.099481447,3.617681584
H,-2.2130320215,-1.1319536385,2.988769852
C,-4.3752787811,-3.4855279851,-0.8591352204
H,-5.3609616412,-3.0294382494,-1.0104723277
H,-4.2225162573,-4.2486425816,-1.6253829883
H,-4.3490339763,-3.9507447442,0.1308994278

M54_TS

0 1

B,-1.282945993,0.3846822613,-0.1389270402
Si,-3.0938188428,-0.8233149088,0.2199401786
C,-1.7237809416,2.0584689728,-0.689957808
H,-1.2361160373,2.6643496103,0.0740844899
H,-2.7454901392,2.4311133291,-0.827538748
H,-1.2087018832,2.0848233307,-1.6509427725
H,-2.4393149995,0.8658364526,-0.2753791474
O,-0.5360328589,-0.2671254615,-1.1650075111
O,-0.5511161891,0.3957137906,1.082756213
C,0.8078538186,0.1018762991,0.7250705242
C,0.6421468936,-0.805002483,-0.5416172047
C,1.7933954491,-0.7112939427,-1.534172183
H,2.7344042212,-1.0178765733,-1.0643277076
H,1.5997243135,-1.3782664417,-2.3788718158
H,1.9035005506,0.3033401474,-1.9206784097
C,0.3857957508,-2.269159027,-0.1829003944
H,0.1196607287,-2.8105947788,-1.0952098023
H,1.2793815536,-2.7364755515,0.2424974155
H,-0.439650961,-2.3670345316,0.5287283948
C,1.4779930217,-0.5793949377,1.9089585608
H,2.4878339518,-0.9114264798,1.6448716729
H,1.5556207869,0.1274573757,2.740089931
H,0.8996998023,-1.4426889564,2.2448027092
C,1.5205164467,1.41989825,0.4080180684
H,1.3996313326,2.0951702188,1.2597002488
H,2.5898565141,1.265404679,0.2340116583
H,1.0925613474,1.8998261595,-0.477003663
O,-4.3830664993,0.052188762,0.7657195194
O,-3.5738776052,-1.6193004655,-1.1336681842
O,-2.6501514185,-1.9810218639,1.3100817959
C,-5.6542276158,-0.5470403254,0.9874729649

H,-6.310080374,0.2101281753,1.4209703773
H,-6.0810863934,-0.9020500996,0.0445490854
H,-5.574452423,-1.3910928587,1.6825981214
C,-2.3856037592,-1.6925421167,2.6781258268
H,-1.5929565335,-0.9438189579,2.7697577694
H,-3.2903356378,-1.3265371814,3.1769897179
H,-2.0708948769,-2.6228154535,3.1563310629
C,-2.844684906,-2.6699307359,-1.7505973732
H,-3.5066295255,-3.1546736938,-2.4712376619
H,-1.9697289265,-2.2675649832,-2.270319478
H,-2.5202903931,-3.4076193946,-1.0081109313

M55

0 1

B,0.8475961319,1.2868502687,0.3615470166
Si,-0.7350183275,0.0550313003,0.145140736
H,1.3511632495,1.8198787621,-0.5811345264
H,1.2624102983,1.5778137693,1.442906667
C,-0.7560246,-0.8645158996,-1.4994362667
C,0.4091308838,-1.4849500534,-1.9762370108
C,-1.928085122,-0.9948547551,-2.2584096984
C,0.4076336291,-2.211640699,-3.1653201113
H,1.3363370508,-1.4043919881,-1.4107849107
C,-1.9371850867,-1.7203725371,-3.4501339209
H,-2.84600596,-0.5214128759,-1.9165803062
C,-0.7690983325,-2.3297959096,-3.9047973841
H,1.3210050189,-2.682683925,-3.5157874474
H,-2.8552998674,-1.8086884958,-4.0231876635
H,-0.7741424246,-2.8933136286,-4.8328624627
C,-0.8777342923,-1.1939390473,1.548864194
C,-1.2666903422,-2.5208622475,1.3150404139
C,-0.6243536424,-0.8033979595,2.8736308104
C,-1.4039693536,-3.425886003,2.3680424249
H,-1.462433902,-2.8528542605,0.2977585256
C,-0.7631176837,-1.701918432,3.9298279601
H,-0.3143678303,0.2181732451,3.0861196857
C,-1.1534154626,-3.0171102144,3.6766203232
H,-1.7051415497,-4.4494540106,2.1663161429
H,-0.5635527105,-1.3791650687,4.947225478
H,-1.2588277648,-3.7208056295,4.4967699503
C,-2.2110161786,1.2368682237,0.2049099821
C,-2.3454892791,2.2248670212,-0.7856180818
C,-3.1765128221,1.1829900632,1.2201370614
C,-3.4103970792,3.1231948837,-0.7674070111
H,-1.6157236218,2.2851694369,-1.5916499593
C,-4.2449445008,2.0800779984,1.2422312466
H,-3.098474524,0.4269683761,1.9980728415
C,-4.3626064216,3.0512953802,0.2496107643
H,-3.4982705179,3.87689061,-1.5440629524
H,-4.9863629142,2.0186521927,2.0331998792
H,-5.1937614278,3.7496639686,0.2668070901

M55_TS

0 1

B,1.2348677082,0.8352316435,-0.0682095517
Si,-0.634184392,-0.0687802955,0.0342925838
C,2.7082820726,-0.2341410008,-0.1325791007

H,2.823656675,-0.8531644104,-1.0242745855
H,2.9036391136,-0.820520112,0.7664560022
H,3.4154644026,0.5903550776,-0.1813436428
H,1.3304026178,-0.4098484426,-0.0915683311
H,1.2336511882,1.4149910994,-1.1110721727
H,1.3241189399,1.3849048915,0.987250841
C,-1.0105562219,-1.1462793793,-1.4691607082
C,-0.5594067571,-0.7620229089,-2.742513873
C,-1.7689390273,-2.3226625922,-1.3678331375
C,-0.8566741292,-1.5205752922,-3.8738504853
H,0.0280672272,0.1471726545,-2.8535861341
C,-2.0694824081,-3.0860028794,-2.4961121334
H,-2.1295269632,-2.6480383342,-0.3944183761
C,-1.6131448847,-2.6857182466,-3.7510425975
H,-0.4991605233,-1.2037514337,-4.849028451
H,-2.6591659392,-3.9922691924,-2.3953173528
H,-1.8455170212,-3.2793142521,-4.6300453923
C,-0.8268968826,-1.131347884,1.5818569996
C,-0.0764463421,-2.3118457088,1.7133905224
C,-1.6801146822,-0.7770930303,2.6357923959
C,-0.1700791572,-3.10818503,2.852429101
H,0.5824067367,-2.6292500961,0.9046468227
C,-1.7786461759,-1.5693204688,3.7808024815
H,-2.2805678047,0.1265733548,2.5608719197
C,-1.0232874575,-2.7345717348,3.8915238643
H,0.4170101745,-4.0184200354,2.9296446719
H,-2.4478086063,-1.2770253534,4.584520609
H,-1.0997642802,-3.351850873,4.7814296501
C,-1.8581178991,1.3616296994,0.094311933
C,-1.663819425,2.4478694426,0.9619133466
C,-3.0096875702,1.3518470918,-0.7059468852
C,-2.5915301927,3.4849846412,1.0346714063
H,-0.7750635278,2.4872096987,1.5877469298
C,-3.939926605,2.3897933486,-0.6389601762
H,-3.1824588493,0.5259037246,-1.3922569024
C,-3.7325271291,3.4570207808,0.2323653077
H,-2.423098268,4.3162350813,1.7127578228
H,-4.8245078833,2.3646132438,-1.2682333991
H,-4.4547905211,4.2660854225,0.2848372971

M56

0 1

B,-0.5668630137,-0.0094534335,0.0056250623
Si,1.4708174046,0.0130307383,0.0086635954
F,-1.3084143491,1.0207959869,-0.3980282698
F,-1.2549773216,-1.0754244391,0.4148154638
C,2.0731115574,-0.2805274067,1.7721702474
H,1.6922050624,-1.2278617877,2.1656368116
H,3.1672379926,-0.3230509754,1.7918768501
H,1.7570383457,0.5195174469,2.4482246326
C,2.0884916957,1.6729547704,-0.6289560233
H,3.1830239713,1.7006854845,-0.6334004285
H,1.7420728097,1.8585865841,-1.6501506907
H,1.7326364619,2.4955452989,-0.001250809
C,2.0895410954,-1.3873062735,-1.0936997006
H,1.7830845293,-1.2506574079,-2.1350633453
H,3.1836503366,-1.4276125608,-1.0690114247

H,1.7091870517,-2.3547158055,-0.7519439714

M56_TS

0 1

B,0.4578363352,0.1738670742,0.0078221679
Si,-1.6965475984,-0.1338032002,0.0540522207
C,1.4680132567,-1.3188427323,-0.0702804139
H,1.4309296253,-1.8989811329,-0.993272703
H,1.4786103172,-1.9610935129,0.8113380125
H,2.3656222896,-0.6940186787,-0.0724970605
H,0.0720788537,-1.0180657281,-0.0230836465
F,0.7870013394,0.7797551055,1.1981157569
F,0.7249333182,0.8608145402,-1.1536484831
C,-2.2672266347,-1.0553626549,1.5948292263
H,-2.010629654,-2.118857379,1.5532725589
H,-1.8032975425,-0.6279082504,2.4891591671
H,-3.3536087374,-0.9799390753,1.7101498489
C,-2.3492215764,-0.9480742493,-1.5143599552
H,-1.9322030492,-0.4592174889,-2.4002990042
H,-2.0927652882,-2.0114481691,-1.5597031834
H,-3.4400250551,-0.8668176845,-1.5668831381
C,-2.1937209875,1.6779272307,0.129679422
H,-1.7792792503,2.1551660862,1.0218489167
H,-1.8259155866,2.2162497189,-0.7480527181
H,-3.284752765,1.769973601,0.1616042881

M57

0 1

C,-1.5253090585,-2.469327912,0.8081244881
C,-1.2463729728,-1.4890862126,-0.1466832584
C,-2.271369944,-1.2100890305,-1.0471049496
C,-3.5050439055,-1.8449932608,-1.0132549057
C,-3.7466268551,-2.7950256557,-0.0291976252
C,-2.7522136383,-3.1092413257,0.8913386148
C,1.4573409884,-1.5423554808,-0.1439989345
C,2.6660536186,-0.9788183269,0.2789874794
C,3.8689801189,-1.6645176485,0.3033413931
C,3.898527014,-2.9844248396,-0.1308795324
C,2.7303985846,-3.5948024858,-0.5714623497
C,1.5426887125,-2.878188294,-0.5631887711
F,2.7628209841,-4.8551685839,-0.9913029232
F,0.4626733728,-3.5253916985,-1.0031640547
F,2.6942751088,0.2890201126,0.7108393334
F,4.9838054287,-1.0784579285,0.728850324
F,5.0371057541,-3.658369013,-0.1251056379
F,-4.4470726434,-1.5568130737,-1.906901826
F,-4.9210978355,-3.4079461686,0.0284707931
F,-2.9837596325,-4.0253667781,1.82678425
F,-0.5868580589,-2.8194843697,1.6930871842
F,-2.0638929051,-0.3175637422,-2.0253444954
B,0.125667792,-0.7219413271,-0.1647203765
Si,0.1035963078,1.3223768458,-0.110898581
C,-1.5765587835,2.0822397519,-0.5690631857
H,-1.7837367122,2.0048470375,-1.6363198268
H,-2.4113442384,1.6402862951,-0.0196036556
C,0.4274557475,1.7821289416,1.7109683093
H,-0.2404692235,2.5652083587,2.072263334

H,1.4582039059,2.0748716703,1.911757008
C,1.35018544,2.1139260052,-1.2987890413
H,1.1465035465,3.174362304,-1.4609021266
H,2.3892793743,1.9927224863,-0.9936544585
Cl,0.1028206204,0.3005752545,2.7051938662
Cl,1.1547874305,1.2816209397,-2.8920283861
Cl,-1.5485686232,3.8434065028,-0.1676640559

M57_TS

0 1
C,-2.0451252558,1.3091477633,-0.964462581
C,-0.8159229288,1.0377990629,-0.3641502316
C,-0.565859867,1.761670174,0.8020856415
C,-1.4446343762,2.700824156,1.3248744451
C,-2.6493001159,2.9420192044,0.6804474796
C,-2.9546440449,2.2357833414,-0.475901346
C,1.7939180288,0.1725059219,-0.5837004454
C,2.6835186806,-0.7812655383,-0.1078346956
C,4.0246889027,-0.529021531,0.1564719923
C,4.5303430138,0.7431898006,-0.0618793038
C,3.6857145997,1.7369265073,-0.5423152006
C,2.3559483338,1.4341858064,-0.7927679777
F,4.1580904323,2.9612182774,-0.7577613866
F,1.5850576616,2.432345275,-1.2513751994
F,2.2599951821,-2.0394574556,0.1302419242
F,4.8181775459,-1.4954918802,0.6127079059
F,5.807968943,1.0089886561,0.1807756984
F,-1.1464020685,3.3563354528,2.4426025395
F,-3.5055373779,3.8325522496,1.1664929469
F,-4.1130137481,2.4433429718,-1.0981512025
F,-2.4174858114,0.6215898648,-2.060191965
F,0.564557256,1.556816257,1.4940147006
B,0.2379485327,-0.0350091971,-0.9297074419
Si,-0.6070762665,-1.7936209087,0.0192006774
C,0.2365178753,-0.005981542,-2.7315168929
H,-0.1371582216,-0.95645935,-1.6904077867
H,1.1162977698,-0.5291990704,-3.1048664109
H,-0.6513768535,-0.3226795313,-3.2784700852
H,0.3534360753,1.0735932977,-2.8405667364
C,-0.11513285,-3.4854885891,-0.6920080039
H,-0.7238788995,-4.2778409065,-0.2519198531
H,0.9381932982,-3.7368063073,-0.5882824382
C,-2.4967486403,-1.7499120459,-0.1237004039
H,-2.9318598303,-0.8761347425,0.3628815303
H,-2.8387595075,-1.7934484578,-1.1592983467
C,-0.1144511842,-1.6418581189,1.8525579991
H,-0.0106605753,-2.6375535558,2.291486811
H,0.8295588508,-1.10973896,1.9789514644
Cl,-1.3459184132,-0.7633835771,2.8215972986
Cl,-3.1579022428,-3.1983092201,0.7219137248
Cl,-0.4862879545,-3.4616182414,-2.4617123635