

# Supporting Information for “Mechanism of the Aerobic Oxidation of Alcohols by Palladium Complexes of N-Heterocyclic Carbenes”

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Table 1: Thermodynamic data

Species	$E_{\text{Elec}}$ (Hartree)	$G_{\text{Solv}}$	ZPE	$H_{\text{vib}} + 3kT$ (kcal/mol)	$\Delta E_{\text{Sol}}$	$\Delta H$	Imaginary Frequencies ( $\text{cm}^{-1}$ )
1-phenylethanol	-386.11129	-0.00456	102.00	6.33			
acetophenone	-384.90815	-0.00463	87.50	5.94			
benzyl alcohol	-346.79020	-0.00494	84.40	5.34			
O <sub>2</sub>	-150.32549		2.35	2.32			
benzene	-232.25314	-0.00181	63.85	3.33			
AcOH	-229.10117	-0.00640	38.71	3.37			
AcOH-HOAc	-458.22851	-0.00569	79.19	7.50	-12.0	-9.4	
1	-1743.88200	-0.01147	427.83	31.69	0	0	
TS1	-1900.84903	-0.01030	487.19	34.07	20.6	17.4	-259.66,-30.61
TS2	-1900.84901	-0.00937	487.44	34.85	21.2	19.0	-13.76
TS3	-1900.85075	-0.00742	486.64	34.77	21.4	18.3	-999.33
TS4	-2129.95233	-0.01015	526.05	38.06	29.4	25.7	-446.82,-18.22 <sup>a</sup>
TS5	-2129.95535	-0.01151	526.27	38.40	26.6	23.5	-762.94
TS6	-2129.93497	-0.00846	525.62	39.05	41.3	38.2	-1144.17,-7.60
2a	-2129.99729	-0.01060			0.9		
2b	-2129.99139	-0.00770			6.4		
3	-2130.01110	-0.01058	531.66	38.73	-7.8	-5.2	
4	-2129.97612	-0.00989	530.04	38.74	14.6	15.6	-99.57,-9.87 <sup>b</sup>
5	-1900.88036	-0.00724	491.18	34.71	2.9	4.3	-27.66
6	-1900.85447	-0.01088	488.13	35.32	16.9	15.8	
7	-1748.19295	-0.01104	464.24	32.85	19.1	17.9	
8	-1748.19008	-0.00813	463.27	32.58	22.7	20.3	-98.29
9	-1900.84062	-0.00857	485.49	34.94	27.0	22.9	-666.37,-13.22 <sup>b</sup>
10	-2129.97600	-0.00855			15.5		
11	-2129.96704	-0.00969	528.82	39.47	20.4	20.9	-36.78
12	-1900.85146	-0.01152			18.3		
13	-1900.88983	-0.00868			-4.0		
14	-1515.98123	-0.00889	399.88	28.19	-6.7	-9.7	-34.81 <sup>a</sup>
15	-1515.96366	-0.01221	398.64	28.06	2.2	-2.1	-38.21,-12.06 <sup>b</sup>
16	-1671.78225	-0.00736	445.99	31.97	-9.1	-12.3	
17	-1519.12742	-0.00440			-9.1		
triplet 18	-1437.20916	-0.00813			-18.5		
singlet 18	-1437.19440	-0.01101			-11.0		
19	-1669.45649	-0.01150			-15.8		
20	-1666.34593	-0.00925	405.97	29.60	-31.5	-31.7	
3b	-2090.69380	-0.01030	513.87	36.83	-9.7	-8.3	-9.23 <sup>c</sup>
TS3b	-1861.53224	-0.00782	469.08	33.51	19.7	16.4	-1062.42
9b	-1861.51796	-0.00860	468.11	33.02	28.2	23.4	-735.49,-15.19 <sup>b</sup> , -9.39

Despite the convergence of forces and energies during relaxation, normal mode analysis yielded imaginary frequencies in some cases, corresponding to <sup>a</sup> acetate methyl group rotation, <sup>b</sup> rotation around the Pd-carbene bond and <sup>c</sup> rotation around the substrate O-C bond.

Table 2: Thermodynamic data for L=pyridine analogues

Species	$E_{\text{Elec}}$ (Hartree)	$G_{\text{Solv}}$	ZPE	$H_{\text{vib}} + 3kT$ (kcal/mol)	$\Delta E_{\text{Sol}}$	$\Delta H$	Imaginary Frequencies ( $\text{cm}^{-1}$ )
1-phenylethanol	-386.11	-0.0046	101.32	6.43			
AcOH-HOAc	-458.23	-0.0057	78.87	7.48			
1	-832.07	-0.0136	121.75	12.55	0	0	
3	-1218.21	-0.0131	224.34	19.78	-12.1	-10.1	
TS1	-989.04	-0.0132	180.61	15.67	17.1	14.5	-503.21
5	-989.08	-0.0091	184.19	14.98	-0.8	-0.5	
TS2	-989.05	-0.0098	180.55	15.76	13.2	10.7	-485.05
6	-989.06	-0.0127	181.44	15.06	3.6	1.2	-10.34
9 <sup>‡</sup>	-989.05	-0.0097	179.2	15.8	12.8	8.9	-784.61

Cartesian coordinates of structures (in Angstroms):

#### 1-phenylethanol

O74	-1.2008390604	1.4249965149	3.6980844068
H75	-.2366445812	2.7064462595	5.0179711954
C76	-1.1664888696	2.6603002725	4.4298117435
C77	-2.3521474382	2.6143861603	5.3920874989
C78	-1.2039101515	3.8687608182	3.5080980660
H79	-2.2841032050	1.7261234808	6.0272737896
H80	-2.3648655931	3.5046134951	6.0280381973
H81	-3.2921891354	2.5728584684	4.8332845791
C82	-.3817496622	4.9746644744	3.7548553194
C83	-.4342131822	6.1006018172	2.9309237537
C84	-1.3055253475	6.1286131396	1.8420793546
C85	-2.1235863050	5.0268529230	1.5822765076
C86	-2.0753805209	3.9056430234	2.4099279619
H87	.3057408859	4.9532832046	4.5980956480
H88	.2098829337	6.9511226171	3.1361361218
H89	-1.3445763268	7.0015149103	1.1965468861
H90	-2.8009723583	5.0416685697	.7328071898
H91	-2.7082417980	3.0466026825	2.2057853866
H92	-.5013126881	1.4415001371	3.0314420924

#### Structure 1

Pd1	0.0552188836	0.5773724405	3.9481561175
O2	-0.4360618937	-1.3576579991	3.5334647863
O3	-1.7535826580	-1.2997575659	5.3670419498
C4	1.9401398430	-0.0055255117	4.1555265382
N5	2.6504825500	-0.2098375819	5.2989617394
N6	2.8139451654	-0.2619777410	3.1432597432
C7	3.9579714139	-0.5822032621	5.0000293513
C8	4.0606834504	-0.6147661983	3.6502846192
C9	2.5569027909	-0.1112030858	1.7258675422
C10	2.7503499339	1.1589224162	1.1442760554
C11	2.5550249570	1.2670163032	-0.2374741608
C12	2.1918863485	0.1623588494	-1.0009678608
C13	2.0175874986	-1.0797543614	-0.3992922830
C14	2.1944886887	-1.2495114265	0.9790081570
C15	2.1921834985	0.0058271376	6.6576107007
C16	1.6469398199	-1.0805587561	7.3716589225
C17	1.2684747732	-0.8450128782	8.6979774878
C18	1.4324679327	0.4063594232	9.2834115089
C19	1.9855280926	1.4551514586	8.5570081863

C20	2.3812123215	1.2822489757	7.2255802129
C21	3.2167567734	2.3732380856	1.9442642774
C22	4.7215892187	2.6250183073	1.7136208552
C23	2.3961282532	3.6386543629	1.6412448559
C24	2.0435085808	-2.6311383506	1.6094264172
C25	3.3212316841	-3.4700604378	1.3930172287
C26	0.8053899988	-3.3829985155	1.0922935830
C27	1.5159463861	-2.4761064939	6.7658404566
C28	2.7817613528	-3.3147690726	7.0512747772
C29	0.2644487471	-3.2274527767	7.2521311550
C30	3.0476563906	2.4330683642	6.4742482464
C31	4.5203201036	2.5811602424	6.9126837966
C32	2.2945738860	3.7658054858	6.6298475076
C33	-1.3607860397	-1.8402644078	4.3340790490
C34	-1.9291648024	-3.1695507771	3.8530821631
H35	4.6796903788	-0.7793801871	5.7754241324
H36	4.8901915957	-0.8461286198	3.0024009847
H37	2.6948759441	2.2283303182	-0.7216548173
H38	2.0468721755	0.2694417852	-2.0726351056
H39	1.7379702839	-1.9325460141	-1.0092430912
H40	0.8348386427	-1.6513230219	9.2791950925
H41	1.1281870517	0.5640026369	10.3146418441
H42	2.1143633557	2.4235523567	9.0298839746
H43	3.0757529831	2.1566606646	3.0060209856
H44	5.3238044380	1.7498765029	1.9793220616
H45	5.0672035402	3.4691435327	2.3204369288
H46	4.9238106387	2.8611786284	0.6632113498
H47	2.5248181821	3.9761913843	0.6069880475
H48	2.7208565635	4.4560720690	2.2940174344
H49	1.3328815570	3.4655477284	1.8242899719
H50	1.8996915144	-2.4926682466	2.6840900297
H51	4.2081168527	-2.9816145794	1.8105175735
H52	3.5058769596	-3.6356671073	0.3253219499
H53	3.2224870426	-4.4503087601	1.8725924201
H54	-0.0972645186	-2.7868615178	1.2425997998
H55	0.8900109807	-3.6398709146	0.0304320594
H56	0.6890666737	-4.3236686351	1.6415801625
H57	3.0408806026	2.1921708869	5.4075378261
H58	2.6884028501	-4.3102414465	6.6028879959
H59	3.6877043475	-2.8517733237	6.6480814231
H60	2.9247971228	-3.4442415980	8.1302422186
H61	-0.6380053788	-2.6298856344	7.1057512976
H62	0.1540474941	-4.1583008313	6.6850598037
H63	0.3414664773	-3.5072352029	8.3091925603
H64	1.4222530853	-2.3598787245	5.6812535761
H65	5.0116171165	3.3797801846	6.3457259173
H66	5.0874085320	1.6577368678	6.7537414489
H67	4.5886510129	2.8333092434	7.9769458745
H68	2.7765475444	4.5356034896	6.0170888864
H69	2.3016083590	4.1244270454	7.6650612066
H70	1.2600424934	3.6664910088	6.2940517639
H71	-2.5700754743	-3.5969901692	4.6250167333
H72	-2.5190690478	-3.0046665345	2.9453349418
H73	-1.1271529981	-3.8681086640	3.5990306128
O74	-1.7802900216	1.7844858179	3.7163156998
C75	-1.0886980053	2.8082599332	3.9869230899
O76	0.1759132711	2.6661325991	4.2045059598
C77	-1.6967387309	4.1836595376	4.0356908237
H78	-2.7697282162	4.1128592725	4.2223414509
H79	-1.2113121454	4.7881820763	4.8053995324
H80	-1.5416266359	4.6773205509	3.0695253123

TS1

Pd1	0.0826051191	0.5966915643	3.8226578594
O2	-0.6762856556	-0.8405134751	5.1205121236
O3	-1.1624262937	0.8920902173	6.4882005543
C4	2.0109936114	0.0045422365	4.0154804833
N5	2.7356709816	-0.3030345489	5.1306573659
N6	2.8953646972	-0.1745902381	2.9863082585
C7	4.0396060014	-0.6581510580	4.7998654463
C8	4.1392631017	-0.5852675323	3.4528180138
C9	2.6285788571	0.0271975339	1.5829760034
C10	3.0934417144	1.2155897140	0.9812051642
C11	2.8846252758	1.3652397441	-0.3942044327
C12	2.2368711788	0.3796002848	-1.1335294022
C13	1.7922172346	-0.7832581272	-0.5129031141
C14	1.9832658744	-0.9939790273	0.8583124704
C15	2.2863126105	-0.3323123515	6.5062843564
C16	2.0295611239	-1.5928571957	7.0834429455
C17	1.7026676453	-1.6196825023	8.4431610493
C18	1.6377615220	-0.4462101754	9.1898691684
C19	1.8946941033	0.7815782391	8.5899334482
C20	2.2244251083	0.8703982160	7.2323907192
C21	3.8252363379	2.3046591554	1.7646407577
C22	5.3118606446	2.3738351029	1.3612781820
C23	3.1535563084	3.6822305364	1.6141643947
C24	1.5281774259	-2.3052851053	1.4942013669
C25	2.3048617177	-3.5023175520	0.9085689197
C26	0.0071032677	-2.5066800831	1.3614803061
C27	2.1218352186	-2.9005594717	6.2978973532
C28	3.2990554917	-3.7631022783	6.7958204395
C29	0.8020732642	-3.6937618759	6.3275855111
C30	2.5231519849	2.2318717432	6.6122166182
C31	3.8724997649	2.7837049369	7.1153390798
C32	1.3779153781	3.2324029576	6.8583990164
C33	-1.2847899149	-0.2851475813	6.1395313583
C34	-2.1980372672	-1.2443552475	6.8972585991
H35	4.7580402093	-0.9300771220	5.5558748296
H36	4.9602569807	-0.7842695878	2.7834416122
H37	3.2310566661	2.2660976738	-0.8924459396
H38	2.0788622568	0.5187375862	-2.1994657779
H39	1.2934318227	-1.5465482349	-1.1029928616
H40	1.4967015501	-2.5722945604	8.9230128122
H41	1.3808927584	-0.4896930217	10.2448783347
H42	1.8313661805	1.6894430050	9.1819837056
H43	3.7857362620	2.0457720853	2.8263763637
H44	5.8156117625	1.4132523107	1.5117350517
H45	5.8372163347	3.1272779909	1.9583072039
H46	5.4241363815	2.6446275160	0.3057299778
H47	3.1775825528	4.0384409206	0.5786500932
H48	3.6714237102	4.4252745549	2.2307395060
H49	2.1081567375	3.6457710588	1.9334089847
H50	1.7511245189	-2.2624377120	2.5634027728
H51	3.3862880830	-3.3798937914	1.0331580758
H52	2.1053206779	-3.6273139980	-0.1616352647
H53	2.0091229421	-4.4297532053	1.4111012370
H54	-0.5382397425	-1.6855034613	1.8356723327
H55	-0.3024981107	-2.5663146683	0.3119210202
H56	-0.2937461483	-3.4388392234	1.8514568166
H57	2.6040855838	2.0994672548	5.5296808597
H58	3.3886769924	-4.6739815503	6.1936542379
H59	4.2518470310	-3.2253864562	6.7376951067

H60	3.1556918901	-4.0665404550	7.8386730965
H61	-0.0071686541	-3.0974974556	5.8995143145
H62	0.9057703731	-4.6144640677	5.7413492488
H63	0.5258572554	-3.9855157854	7.3473451340
H64	2.3140393949	-2.6556388413	5.2497488783
H65	4.0910395826	3.7505872639	6.6475289217
H66	4.6992677922	2.1019268436	6.8861255730
H67	3.8575959097	2.9351589325	8.2006465962
H68	1.5582543539	4.1546625668	6.2933456653
H69	1.3045514553	3.5100366705	7.9159709776
H70	0.4195147509	2.8015317331	6.5564532473
H71	-2.7125884369	-0.7105969220	7.6970882732
H72	-2.9299986615	-1.6800275724	6.2104842286
H73	-1.6159875328	-2.0670174268	7.3223779881
O74	-1.7367875956	1.4358022922	3.2738958491
H75	0.2479108706	1.8931553876	2.6839685968
C76	-1.0302315561	2.3189167762	2.5873815475
C77	-0.9400860309	3.7098998304	3.2301139597
C78	-1.2056271589	2.2871487477	1.0720983360
H79	-0.8046181612	3.5896341726	4.3060452028
H80	-0.1285120894	4.3218209008	2.8271016173
H81	-1.8880321449	4.2289924633	3.0496194871
C82	-0.6617374494	3.2726852086	0.2372668700
C83	-0.8706234556	3.2266620340	-1.1417213840
C84	-1.6235356691	2.1949117893	-1.7023023591
C85	-2.1683091327	1.2101373014	-0.8755080728
C86	-1.9613644318	1.2549531184	0.5021495253
H87	-0.0712546556	4.0819999260	0.6549103642
H88	-0.4452647232	3.9993330093	-1.7769300206
H89	-1.7885408660	2.1609546624	-2.7760539604
H90	-2.7630371105	0.4081053799	-1.3045589149
H91	-2.3901319719	0.5061285749	1.1598755756

TS2

C1	0.2050349270	3.1428152113	1.8606499037
C2	-0.6154669946	2.7810740777	0.7722682495
C3	-0.6932378935	3.5459812797	-0.4103722271
C4	0.0846044112	4.7080851283	-0.4754514998
C5	0.9012027979	5.0911085243	0.5851857890
C6	0.9590766954	4.3169684374	1.7390303359
N7	-1.4259114295	1.5906202060	0.8972626729
C8	-1.0455352202	0.3397140187	0.5011383792
N9	-2.0739252188	-0.4563214315	0.9166226146
C10	-3.0663038717	0.2804333318	1.5590844845
C11	-2.6580522374	1.5721916884	1.5455330888
C12	-2.0850408053	-1.9005798632	0.8512058573
C13	-1.5538714389	-2.6137090870	1.9447439228
C14	-1.5962751330	-4.0123867035	1.8877696873
C15	-2.1515187449	-4.6682662662	0.7949539787
C16	-2.6740074807	-3.9382010120	-0.2692707106
C17	-2.6519988201	-2.5386622346	-0.2713303919
Pd18	0.6728661017	-0.1306245567	-0.7375208478
H19	1.8112537894	-0.3989342221	-1.7716534965
O19	2.1966356380	-0.2207578874	0.8212007611
C20	3.0950706985	-0.1317840697	-0.0709998593
C21	-0.9537645980	-1.9312822209	3.1723139950
C22	0.5419535113	-2.2641544779	3.3314908391
C23	-3.2527066690	-1.7505361029	-1.4324550813
C24	-3.0397128677	-2.4331423773	-2.7933950525
C25	-1.6161974121	3.1634768941	-1.5646320482
C26	-1.0116729484	3.4732177929	-2.9447038051

C27	0.2826408897	2.3316391571	3.1530195449
C28	1.7286357295	1.9274661456	3.4989463131
O29	-0.4965477725	-0.0772094697	-2.4423858548
C30	0.0773318195	0.1004953342	-3.6013885365
C31	-0.9072739225	0.0862644999	-4.7698346884
O32	1.2859650973	0.2459461093	-3.8125873772
C33	-1.7425347396	-2.2805849270	4.4498933361
C34	-4.7548236323	-1.4867744200	-1.1933594095
C35	-2.9891040124	3.8525994863	-1.4087850562
C36	-0.3741615527	3.0937132399	4.3222840943
C37	3.5925784373	1.2371120008	-0.4939864359
H38	-3.1134907110	2.4680611600	1.9359517178
H39	-3.9491080279	-0.1837434261	1.9682969601
H40	-1.1901657893	-4.5921351599	2.7119924628
H41	-2.1776601897	-5.7546320008	0.7699965236
H42	-3.1011062426	-4.4659612797	-1.1153378693
H43	0.0537460801	5.3207613099	-1.3701752334
H44	1.4960015287	5.9977440552	0.5101014547
H45	1.6007108538	4.6251645874	2.5594515246
H46	-1.0269171394	-0.8496229465	3.0332370341
H47	-2.8009524965	-2.0165151758	4.3524528046
H48	-1.3356366648	-1.7373860003	5.3101100562
H49	-1.6864912535	-3.3505691850	4.6786222427
H50	0.7016702814	-3.3402790334	3.4649029840
H51	0.9516114243	-1.7575615298	4.2128942751
H52	1.1092070823	-1.9325443305	2.4576758245
H53	-2.7332786075	-0.7901240583	-1.4838448113
H54	-4.9297195137	-0.9280176583	-0.2685620007
H55	-5.3120467153	-2.4284850008	-1.1255650529
H56	-5.1776328017	-0.9044170901	-2.0198863853
H57	-1.9830325863	-2.6592798142	-2.9585564538
H58	-3.6160178494	-3.3607162506	-2.8894429958
H59	-3.3695415534	-1.7640786116	-3.5945109270
H60	-0.2787778316	1.4051750118	3.0063195594
H61	-3.6602435683	3.5582960627	-2.2236073101
H62	-3.4732235868	3.5858972032	-0.4637399692
H63	-2.8852812635	4.9438642826	-1.4355509040
H64	-0.0228185541	3.0203117774	-3.0592854035
H65	-1.6596014483	3.0677356461	-3.7284921160
H66	-0.9227919368	4.5502850210	-3.1277086706
H67	-1.7685041124	2.0814525821	-1.5256813001
H68	-0.3502651396	2.4887320491	5.2356856775
H69	-1.4194361533	3.3408970571	4.1073786280
H70	0.1526946455	4.0318870626	4.5304373279
H71	2.3610026183	2.8014437074	3.6922086142
H72	2.1721651698	1.3460649453	2.6867918865
H73	-0.5059861941	0.6667650765	-5.6023233966
H74	-1.0349752490	-0.9492612814	-5.1053733647
H75	-1.8874873800	0.4669750085	-4.4744825458
H76	4.5810429749	1.4081610459	-0.0460339959
H77	2.8975302999	1.9980238004	-0.1376494621
H78	3.6906762437	1.3221917284	-1.5781998333
C80	3.8830928678	-1.3443137311	-0.4485127687
C81	4.8504495362	-1.3091403552	-1.4655361575
C82	3.6636335985	-2.5446124710	0.2462870501
C83	5.5788757177	-2.4541389916	-1.7831214915
H84	5.0177010035	-0.3986001807	-2.0306478631
C85	4.3981578677	-3.6837110034	-0.0684954976
H86	2.9116259891	-2.5654394257	1.0273769723
C87	5.3562673956	-3.6419014214	-1.0850150313
H88	6.3157250994	-2.4198100294	-2.5804638917
H89	4.2230807757	-4.6070560420	0.4765935658

H90	5.9246895777	-4.5338597184	-1.3343045379
H91	1.7384289877	1.3115378344	4.4055197176

TS3

Pd1	.1337114956	.7898605997	4.2242619371
O2	-.6443676820	-1.2144235395	4.0959620861
O3	-2.5820572064	-.1033988323	3.8516985253
C4	2.1309279881	.1667354299	4.3012013258
N5	2.8868894356	-.1567414929	5.3902290118
N6	2.9430571807	-.1147597693	3.2409630425
C7	4.1447051476	-.6232147155	5.0157754598
C8	4.1804710061	-.5951808342	3.6614207335
C9	2.6155739161	.1406491697	1.8565905165
C10	2.9271854614	1.4063542140	1.3212126698
C11	2.6359433291	1.6229103061	-.0315860826
C12	2.0635043507	.6251167096	-.8127077446
C13	1.7629081098	-.6152765500	-.2559297165
C14	2.0253966412	-.8872839109	1.0914554120
C15	2.4850580930	.0389424428	6.7646105157
C16	1.7745654423	-.9868857887	7.4221652923
C17	1.4279374393	-.7695567621	8.7603398373
C18	1.7661027709	.4146698018	9.4105734475
C19	2.4655698324	1.4098914157	8.7368347477
C20	2.8454045984	1.2447615864	7.3980161658
C21	3.5642505510	2.5258907134	2.1407313628
C22	4.9718011028	2.8691385793	1.6130462238
C23	2.6642831218	3.7759483309	2.1927601314
C24	1.7043787869	-2.2587259381	1.6808947961
C25	2.8524244469	-3.2548386501	1.4116661496
C26	.3691577448	-2.8283160808	1.1705777105
C27	1.4283324255	-2.3039885303	6.7313788043
C28	2.5213156578	-3.3607220731	6.9974896492
C29	.0445971605	-2.8452598588	7.1277494690
C30	3.6207605829	2.3541989139	6.6908572746
C31	4.9642766032	2.6352948280	7.3925277109
C32	2.7785354970	3.6375304272	6.5561818178
C33	-1.9085632175	-1.1748469393	3.9327900568
C34	-2.6550666491	-2.4905584199	3.8564844754
H35	4.8849546140	-.9161331216	5.7428558243
H36	4.9588675739	-.8569986574	2.9630153774
H37	2.8601229101	2.5884828005	-.4757406739
H38	1.8467815610	.8144234519	-1.8607893026
H39	1.3112809981	-1.3818465974	-.8773571288
H40	.8814512792	-1.5351574025	9.3012589497
H41	1.4811331974	.5607128393	10.4492233247
H42	2.7214208865	2.3303181517	9.2536354019
H43	3.6784252345	2.1732183410	3.1688579395
H44	5.6264142788	1.9906683367	1.6067444925
H45	5.4382464150	3.6349752295	2.2427368890
H46	4.9319611480	3.2614544572	.5907249444
H47	2.5006833565	4.1947725784	1.1931097647
H48	3.1400947821	4.5542334396	2.8005596073
H49	1.6932508365	3.5442034559	2.6392550654
H50	1.6003472816	-2.1392178547	2.7626455424
H51	3.8004715099	-2.9068288344	1.8342443097
H52	3.0000632658	-3.3997713509	.3350634814
H53	2.6263553072	-4.2314830632	1.8547055387
H54	-.4442961355	-2.1116475444	1.3095414773
H55	.4125260647	-3.1008020681	.1100264541
H56	.1187475337	-3.7373925288	1.7276631570
H57	3.8508543197	2.0166614821	5.6771374119

H58	2.2842707441	-4.2967774039	6.4794530821
H59	3.5037069488	-3.0251176636	6.6495635863
H60	2.6029359572	-3.5792632959	8.0685800861
H61	-.7308882721	-2.0906880333	6.9727241450
H62	-.2015124258	-3.7141123827	6.5086267192
H63	.0083006302	-3.1711695366	8.1735765588
H64	1.3908002524	-2.1164994608	5.6552170433
H65	5.5348843189	3.3860975618	6.8348310867
H66	5.5768278858	1.7301913323	7.4665540939
H67	4.8171489811	3.0207022477	8.4074362713
H68	3.3562324459	4.4161421122	6.0448268620
H69	2.4911838803	4.0317409082	7.5378115025
H70	1.8703776756	3.4527393999	5.9752991902
H71	-3.1889699145	-2.6441080164	4.8004607566
H72	-3.4018952847	-2.4526439205	3.0599228549
H73	-1.9682212897	-3.3221208371	3.6964649425
O74	.0231911347	2.8493690809	4.3006416064
H75	-1.6000774033	.9839164572	4.0638878708
C76	-1.2692683597	2.5604078573	4.2358114590
C77	-1.9607241847	2.9372909058	2.9226911261
C78	-2.0680378868	2.7395687500	5.5105210478
H79	-1.2890366237	2.7196490391	2.0895130231
H80	-2.8996130875	2.4022899611	2.7666852384
H81	-2.1718407837	4.0140944116	2.9346642936
C82	-3.4532652799	2.5150526629	5.5547792996
C83	-4.1634423223	2.6908379200	6.7428750583
C84	-3.5040714407	3.0945314349	7.9043938113
C85	-2.1265674824	3.3208016984	7.8689625920
C86	-1.4142841922	3.1435285218	6.6840508955
H87	-3.9783366313	2.1758324489	4.6683284887
H88	-5.2345865590	2.5072718202	6.7595741146
H89	-4.0584451112	3.2314031490	8.8292277764
H90	-1.6038256682	3.6379091233	8.7678701298
H91	-.3448743347	3.3168324414	6.6498041588

TS4

Pd1	0.0949200533	0.0599645608	-0.0847322354
O2	0.5368686965	-0.4209548811	1.9709551356
O3	-0.4693944835	0.7359151919	-1.9402885320
C4	-1.2781969172	-1.5568900903	-0.1223670907
N5	-1.0479860681	-2.8697680555	-0.4223043477
N6	-2.5984942478	-1.5199172598	0.2261126341
C7	-2.2004834073	-3.6330140489	-0.2527211412
C8	-3.1756688391	-2.7854654746	0.1507375017
C9	-3.3672444067	-0.3436542944	0.5821048397
C10	-3.9805414079	0.3982463297	-0.4503392268
C11	-4.7857054958	1.4798938770	-0.0744064968
C12	-4.9778608411	1.8069007402	1.2637227805
C13	-4.3624906400	1.0594323463	2.2615312252
C14	-3.5414985780	-0.0308397114	1.9461987161
C15	0.1905707604	-3.4465341508	-0.9133788182
C16	1.1476998180	-3.9022551370	0.0166838854
C17	2.3024086845	-4.5091752960	-0.4907987198
C18	2.4940961429	-4.6614045354	-1.8593997061
C19	1.5301956504	-4.2118298232	-2.7538284413
C20	0.3562657036	-3.5950268051	-2.3069338683
C21	-3.8384800594	0.0263891386	-1.9246828583
C22	-5.0035990089	-0.8837470502	-2.3709414005
C23	-3.7361765695	1.2551267785	-2.8436589294
C24	-2.9052689419	-0.8537805084	3.0635627265
C25	-3.8964821953	-1.9040848839	3.6092431019



C26	-2.3799496860	0.0241610512	4.2130426827
C27	0.9363992023	-3.8053666210	1.5255267924
C28	0.2859849961	-5.0964722777	2.0685156958
C29	2.2370872106	-3.5039693757	2.2903681428
C30	-0.6980419962	-3.1527801770	-3.3200222181
C31	-1.6357478613	-4.3238076480	-3.6880916370
C32	-0.0827994334	-2.5583004940	-4.6010546474
C33	1.3495421928	-0.1335454086	2.8758043420
C34	1.1348914617	-0.6909998475	4.2665297984
H35	-2.2110531861	-4.6947643679	-0.4362979575
H36	-4.2138602273	-2.9537768097	0.3857436957
H37	-5.2724089521	2.0731011498	-0.8413719849
H38	-5.6109744435	2.6492466730	1.5300223176
H39	-4.5214550710	1.3270066211	3.3007507936
H40	3.0634848555	-4.8671693465	0.1942113121
H41	3.4016396733	-5.1300708572	-2.2304870523
H42	1.6966282479	-4.3304303037	-3.8189506037
H43	-2.9025828444	-0.5261720890	-2.0393468633
H44	-5.0533294531	-1.8043032437	-1.7810962641
H45	-4.8867495783	-1.1668774082	-3.4231713083
H46	-5.9646636234	-0.3667035017	-2.2667826565
H47	-4.6694240447	1.8286332153	-2.8783342237
H48	-3.5234182391	0.9297094479	-3.8675045674
H49	-2.9261227138	1.9139428621	-2.5220086910
H50	-2.0441776130	-1.3800255408	2.6411535519
H51	-4.2359648930	-2.5904262593	2.8277728780
H52	-4.7822529109	-1.4190540403	4.0351869728
H53	-3.4281492661	-2.5024765472	4.3989365428
H54	-1.6975870726	0.7951605265	3.8438293085
H55	-3.1909939219	0.5194582084	4.7576670189
H56	-1.8414134575	-0.5940325217	4.9383767453
H57	-1.3003122186	-2.3667879177	-2.8530532732
H58	0.1184882789	-5.0197774910	3.1492226900
H59	-0.6797949029	-5.2962655889	1.5937741351
H60	0.9324103210	-5.9632624973	1.8890335055
H61	2.7388217645	-2.6160553519	1.8943456602
H62	2.0156543394	-3.3327201029	3.3486837846
H63	2.9447991929	-4.3386410770	2.2473783710
H64	0.2530349605	-2.9731206516	1.7156650113
H65	-2.3919084478	-3.9951151693	-4.4101833424
H66	-2.1596485368	-4.7294710919	-2.8176837246
H67	-1.0667236562	-5.1407414109	-4.1466165366
H68	-0.8708868948	-2.0971289167	-5.2072932455
H69	0.3838681132	-3.3308649983	-5.2230272135
H70	0.6678186617	-1.8013065636	-4.3638810777
H71	2.0831082427	-1.0483042202	4.6743842524
H72	0.7809674289	0.1158438537	4.9166586505
H73	0.3959546846	-1.4911770561	4.2551187128
O74	3.2055067813	1.7230705285	0.7794753868
H75	1.1372448448	1.2916879547	-0.0999081927
C76	2.3664403356	2.3764955740	0.0835744368
C77	2.6826285534	2.5564423610	-1.3854554990
C78	1.5005342155	3.4147234855	0.7531427371
H79	3.0317799445	1.6162714851	-1.8112051994
H80	1.8298478421	2.9250307728	-1.9564930115
H81	3.4833885852	3.3067027037	-1.4447516050
C82	0.3404929267	3.9202009946	0.1445277298
C83	-0.4063105433	4.9126957113	0.7728497556
C84	-0.0034003201	5.4174997904	2.0131537558
C85	1.1487751785	4.9214522889	2.6228426798
C86	1.8973801116	3.9226514793	1.9980896821
H87	0.0001163215	3.5005701456	-0.7971374352

H88	-1.3090583113	5.2888911708	0.2994436539
H89	-0.5873401979	6.1938304708	2.5004685629
H90	1.4692798734	5.3133031554	3.5843230232
H91	2.7994929839	3.5375100020	2.4625017880
H92	2.6914102087	1.1151215228	1.8613985682
O93	1.4184729534	-0.0834429024	-2.8795226858
C94	0.3679525089	0.5615058260	-2.9270660327
O95	2.3923325414	0.6260198313	2.7898835146
C96	-0.0430643217	1.2781659919	-4.2125731580
H97	0.5498052264	2.1962694034	-4.3006938541
H98	-1.1002054705	1.5465982281	-4.2183766191
H99	0.1955963392	0.6521102656	-5.0754953724

TS5

Pd1	-0.0147866631	-0.0263006265	-0.0405188746
O2	-0.0459259990	0.0607619807	2.1224252861
O3	2.0532513296	-0.1450998249	0.2438520877
C4	0.1959844191	0.1316917797	-2.0177696893
N5	0.2645559988	-0.7947846247	-3.0228587170
N6	0.3797791882	1.3360635628	-2.6408636014
C7	0.4799180759	-0.1666444225	-4.2481965672
C8	0.5542751216	1.1617148608	-4.0088134724
C9	0.4828504270	2.6437400764	-2.0124572155
C10	1.7495843997	3.0647808735	-1.5498943069
C11	1.8347325594	4.3445056680	-0.9896104506
C12	0.7215619589	5.1738454183	-0.9088423069
C13	-0.5043077739	4.7475915903	-1.4057784429
C14	-0.6545718578	3.4781637263	-1.9770869404
C15	0.2131036083	-2.2466372985	-2.9314277598
C16	-1.0018511814	-2.9035092343	-3.2248941691
C17	-1.0035353403	-4.3038551711	-3.2008408882
C18	0.1510906745	-5.0198594522	-2.9118377834
C19	1.3413306350	-4.3493573564	-2.6567829438
C20	1.4105888795	-2.9515925501	-2.6706757073
C21	3.0131447376	2.2224697022	-1.7138614290
C22	3.7417486611	2.6031357442	-3.0216315487
C23	3.9718155144	2.3337821887	-0.5169783426
C24	-1.9942217567	3.0852134225	-2.5949292106
C25	-2.1063053865	3.6314727101	-4.0357124707
C26	-3.2023034893	3.5514505888	-1.7612445195
C27	-2.2778942041	-2.1642252260	-3.6234532683
C28	-2.4027825501	-2.0660329355	-5.1600113918
C29	-3.5494998386	-2.8191792955	-3.0498639266
C30	2.7589337428	-2.2593618802	-2.4772592894
C31	3.4328367212	-1.9795768442	-3.8398704849
C32	3.7282889543	-3.0606947962	-1.5894845891
C33	-0.5338831336	0.7659447381	3.0306762267
C34	0.0891378915	0.7103992263	4.4074340664
H35	0.5696233086	-0.7312971773	-5.1608866081
H36	0.7193611264	1.9964525722	-4.6694279612
H37	2.7893541959	4.6985951902	-0.6157250077
H38	0.8120254679	6.1617451761	-0.4652533929
H39	-1.3602409576	5.4112740602	-1.3508919310
H40	-1.9219537064	-4.8401824419	-3.4138564681
H41	0.1255866398	-6.1060858885	-2.8915536787
H42	2.2357154656	-4.9221808631	-2.4417604419
H43	2.7163143170	1.1734879780	-1.7733286897
H44	3.1044888431	2.4721836635	-3.9020962311
H45	4.6317309697	1.9785333042	-3.1585465605
H46	4.0659547994	3.6499798783	-2.9981228781

H47	4.4152821146	3.3323022757	-0.4306228994
H48	4.7976943763	1.6260296072	-0.6445792901
H49	3.4586680943	2.0853562468	0.4140351455
H50	-2.0277237757	1.9919144440	-2.6516936403
H51	-1.3001610081	3.2678578128	-4.6802138688
H52	-2.0656372286	4.7264191192	-4.0382769850
H53	-3.0580952207	3.3291089589	-4.4865703605
H54	-3.1434254149	3.1972350035	-0.7285397353
H55	-3.2918685592	4.6430145328	-1.7544392124
H56	-4.1281699890	3.1657539677	-2.2028740406
H57	2.5759675868	-1.3047585626	-1.9759326576
H58	-3.3205194433	-1.5351949783	-5.4368805927
H59	-1.5608385357	-1.5335205455	-5.6105643460
H60	-2.4435517164	-3.0656179232	-5.6069624578
H61	-3.4691372777	-3.0021427282	-1.9743205413
H62	-4.4162365983	-2.1732304465	-3.2248311974
H63	-3.7653152482	-3.7768453680	-3.5349877747
H64	-2.2178475084	-1.1459839222	-3.2251796776
H65	4.3987882765	-1.4853772310	-3.6874237167
H66	2.8289440294	-1.3349870748	-4.4836587135
H67	3.6174915831	-2.9164195029	-4.3783891957
H68	4.5958640281	-2.4386200387	-1.3454215652
H69	4.1115747119	-3.9498831801	-2.1038373968
H70	3.2540083817	-3.3687861121	-0.6555374208
H71	0.0167701171	1.6828158704	4.8988278568
H72	-0.4704971606	-0.0135481796	5.0104000303
H73	1.1263317411	0.3799580743	4.3440768820
O74	-2.9871353513	1.3874000914	0.9716880334
H75	-1.6813628371	0.0993793745	-0.2066997756
C76	-2.9470968524	0.2312530778	0.3849057941
C77	-3.7882745951	0.1195081629	-0.8855745885
C78	-3.0229677015	-1.0156077063	1.2567353621
H79	-3.5988875498	0.9577192149	-1.5541140173
H80	-3.6128101772	-0.8220591715	-1.4016161920
H81	-4.8404892454	0.1522928656	-0.5758228601
C82	-2.4516281477	-2.2395597797	0.8861977521
C83	-2.6290575807	-3.3700709266	1.6810024352
C84	-3.3869799757	-3.2927845685	2.8524616524
C85	-3.9589156617	-2.0771166999	3.2274573261
C86	-3.7766156554	-0.9416125147	2.4358399901
H87	-1.8200795253	-2.2990139068	0.0033317252
H88	-2.1581343228	-4.3060807416	1.3945469209
H89	-3.5211992639	-4.1739416358	3.4740597716
H90	-4.5461656021	-2.0078655868	4.1395635753
H91	-4.2152716618	0.0084555745	2.7248591701
H92	-2.1911099341	1.4595490088	2.0017308374
O93	1.7161019806	-2.2535316791	0.9862582688
C94	2.3980133580	-1.2312391899	0.8896650945
O95	-1.5647945377	1.5405721164	2.9303488426
C96	3.7686989046	-1.1249542610	1.5527444104
H97	3.6776508129	-0.4954690031	2.4449049110
H98	4.4945130985	-0.6471851953	0.8891945230
H99	4.1191170258	-2.1144842327	1.8501596019

TS6

Pd1	.3087213431	-.1270847593	.0461397688
O2	.2572183071	-.0978907154	2.4069649981
O3	2.3727140604	.7084961900	-2.6113194014
C4	-.5392592226	-2.0358339174	.1051018990
N5	.0742667625	-3.2489059377	.2552549416
N6	-1.8713785519	-2.3429746496	.0793055240

C7	-.8572345778	-4.2836052791	.3230758377
C8	-2.0802709156	-3.7134382115	.2132032160
C9	-2.9558848625	-1.4076792190	-.1337275101
C10	-3.4406769862	-1.2352328426	-1.4471719207
C11	-4.5354439974	-.3815346557	-1.6265005465
C12	-5.1198058660	.2746238271	-.5490333460
C13	-4.6196166110	.0898839407	.7357510521
C14	-3.5284612056	-.7536332921	.9764862878
C15	1.5026119706	-3.4820542736	.3220431268
C16	2.1241876461	-3.5293943415	1.5877188251
C17	3.4934908385	-3.8200060499	1.6236666503
C18	4.2116268591	-4.0528412098	.4559161402
C19	3.5740197622	-4.0019414375	-.7790556120
C20	2.2070402743	-3.7181093484	-.8785085778
C21	-2.8490619081	-1.9695572264	-2.6477762692
C22	-3.7165153817	-3.1894904104	-3.0231961576
C23	-2.6582603912	-1.0487628983	-3.8656702513
C24	-3.0305691224	-.9735350686	2.4022449796
C25	-3.8526622195	-2.0778926855	3.0996926525
C26	-3.0426631745	.3158410691	3.2419365756
C27	1.3509635720	-3.3222226345	2.8882397579
C28	.9065615762	-4.6757026881	3.4840359302
C29	2.1469801861	-2.5204809278	3.9324783250
C30	1.5236910058	-3.7165882304	-2.2442524582
C31	1.0713300271	-5.1415995831	-2.6317083148
C32	2.4074430457	-3.1216138975	-3.3551589933
C33	.6242569334	.8547242514	3.1181265571
C34	.4956973075	.8182665372	4.6228442484
H35	-.5592748738	-5.3126122461	.4421382665
H36	-3.0684112127	-4.1435975988	.2147849010
H37	-4.9339359455	-.2277602215	-2.6243082886
H38	-5.9685229719	.9338273566	-.7109793898
H39	-5.0856127070	.6096647409	1.5661542986
H40	4.0052040001	-3.8629904000	2.5794376917
H41	5.2744585186	-4.2735799406	.5081567869
H42	4.1481389964	-4.1821967309	-1.6817475846
H43	-1.8558274779	-2.3290918591	-2.3666398334
H44	-3.8121883042	-3.8930746516	-2.1903600741
H45	-3.2768275498	-3.7289338322	-3.8693666099
H46	-4.7264602175	-2.8768457389	-3.3119812440
H47	-3.6128014081	-.7057051250	-4.2797543918
H48	-2.1401371766	-1.5934030299	-4.6628193314
H49	-2.0575804319	-.1751204985	-3.6032090111
H50	-1.9904848749	-1.3035253401	2.3493131616
H51	-3.7978456571	-3.0267966733	2.5568760585
H52	-4.9087211727	-1.7937690993	3.1710270137
H53	-3.4809491920	-2.2508817935	4.1161034403
H54	-2.5071268741	1.1246101266	2.7364562399
H55	-4.0594769293	.6624720027	3.4565770767
H56	-2.5558118442	.1340315181	4.2058144440
H57	.6359787738	-3.0827938187	-2.1711628361
H58	.3368149090	-4.5204684280	4.4074356778
H59	.2728631029	-5.2384472275	2.7917394855
H60	1.7746567167	-5.3000342844	3.7250889592
H61	2.5057525609	-1.5759881488	3.5156765328
H62	1.5065429471	-2.2930605175	4.7911966651
H63	3.0097584720	-3.0771171605	4.3145392726
H64	.4573525670	-2.7366675331	2.6564112719
H65	.5694183908	-5.1330549026	-3.6059044895
H66	.3743739347	-5.5631213539	-1.9007929906
H67	1.9318296388	-5.8170878570	-2.7023600533
H68	1.8150910901	-2.9895872985	-4.2669703581

H69	3.2458604168	-3.7791333868	-3.6114867685
H70	2.8142542082	-2.1488058816	-3.0670274026
H71	1.4784120851	.9745019489	5.0781009211
H72	-.1494504078	1.6391515020	4.9511894682
H73	.0808602907	-.1345353820	4.9501756622
O74	.9668579320	1.8178487175	.1939229169
H75	2.1948726431	1.3352034450	-1.6922204364
C76	1.8534738748	2.3929448552	-.6508910444
C77	3.2451342232	2.6109806848	-.0724428666
C78	1.2807838771	3.3818688742	-1.5866331469
H79	3.5445312859	1.7310499023	.5053116363
H80	3.9984207532	2.7635812933	-.8516439062
H81	3.2778044387	3.4844608557	.5978269822
C82	2.0929908277	4.2572672682	-2.3420479491
C83	1.5344707179	5.1386791376	-3.2648627428
C84	.1529796135	5.1753292328	-3.4691930868
C85	-.6649558240	4.3173769286	-2.7280280965
C86	-.1143769565	3.4339456342	-1.8041606125
H87	3.1704900076	4.2451142944	-2.2111965979
H88	2.1847445044	5.8029180214	-3.8292904450
H89	-.2789782660	5.8621020447	-4.1921658322
H90	-1.7432663385	4.3390024399	-2.8697701221
H91	-.7539868312	2.7718699607	-1.2300554373
H92	1.1337701663	1.9300980254	1.5851387114
O93	.4485404487	-.3989861558	-2.2516527930
C94	1.2425382809	.1885241559	-3.0152452732
O95	1.1430388175	1.9562590268	2.6487633380
C96	.9383905218	.3550519828	-4.4868871506
H97	.1725059546	-.3504332404	-4.8105056037
H98	1.8523038462	.2242956047	-5.0722748391
H99	.5813159352	1.3774961575	-4.6568901653

2a

Pd1	-.0065234133	.6891906189	3.6078242190
O2	-.3642619447	-1.2952997043	3.3100404492
O3	-1.9640693091	-1.0407360874	4.8853325489
C4	1.8662908913	.1558517533	4.1557773777
N5	2.5017966814	-.0716739789	5.3425343389
N6	2.7682004257	-.2319474814	3.2055703797
C7	3.7713246666	-.6034944426	5.1292948514
C8	3.9393915614	-.6979275105	3.7915998404
C9	2.6123709788	-.1605248269	1.7651419555
C10	2.7794707716	1.0900484984	1.1282387209
C11	2.7105137146	1.1093494474	-.2686906205
C12	2.5013708707	-.0578912997	-.9979717709
C13	2.3483928968	-1.2740935567	-.3432037274
C14	2.3945960403	-1.3572308072	1.0541838186
C15	2.0866338910	.3583287375	6.6615846995
C16	1.2291668824	-.4586479349	7.4253326418
C17	.8755271813	.0078400115	8.6969523529
C18	1.3726209025	1.2106478256	9.1918954884
C19	2.2564104775	1.9699114142	8.4336466818
C20	2.6394172255	1.5612389958	7.1505708729
C21	3.0837146561	2.3755271998	1.8982425075
C22	4.6071762360	2.5397220341	2.0941296750
C23	2.4901420119	3.6340504550	1.2390139824
C24	2.2395159635	-2.7148286909	1.7354648993
C25	3.5273295377	-3.5549069885	1.5999903038
C26	1.0293099006	-3.4968810270	1.1943292531
C27	.7731936279	-1.8326661287	6.9382320831
C28	1.8508643422	-2.8928250288	7.2613025986

C29	-.5842123403	-2.2684110351	7.5125764162
C30	3.6807304234	2.3789191266	6.3834551155
C31	5.0494886276	2.3109109659	7.0909056916
C32	3.2518744429	3.8386748992	6.1574648051
C33	-1.4235307226	-1.6850164873	3.9866939142
C34	-1.9483849109	-3.0454070477	3.5491685542
H35	4.4289034185	-.8373848550	5.9502741229
H36	4.7720910421	-1.0391445146	3.1994333322
H37	2.8246948008	2.0511422683	-.7941077938
H38	2.4581259654	-.0167499622	-2.0831999334
H39	2.1856360204	-2.1766327514	-.9239010535
H40	.2042068071	-.5807181981	9.3116108265
H41	1.0793091811	1.5495596201	10.1817973347
H42	2.6594746297	2.8919373422	8.8429016541
H43	2.6257464439	2.2934868911	2.8882321638
H44	5.0463088991	1.6922042119	2.6306847410
H45	4.8232682280	3.4490365243	2.6666794345
H46	5.1160430278	2.6236355258	1.1267986556
H47	3.0059192417	3.8900592360	.3060046254
H48	2.6053553197	4.4888968647	1.9137007570
H49	1.4246201916	3.5136143276	1.0236818957
H50	2.0493376575	-2.5381136237	2.7973069196
H51	4.4005448411	-3.0466959975	2.0221086461
H52	3.7477650226	-3.7677754467	.5477670874
H53	3.4161645211	-4.5135855140	2.1191922435
H54	.1201642455	-2.8983927851	1.2777050331
H55	1.1649514410	-3.7937357521	.1483868564
H56	.8922453041	-4.4160923419	1.7750926120
H57	3.8043973754	1.9394975006	5.3914443662
H58	1.5372668517	-3.8763706197	6.8928411811
H59	2.8165568262	-2.6574999785	6.8020393971
H60	2.0046605972	-2.9721895669	8.3437848914
H61	-1.3599549732	-1.5279687695	7.3072196861
H62	-.8953857251	-3.2060346353	7.0407180079
H63	-.5323969326	-2.4545960986	8.5917661973
H64	.6634585176	-1.7807533156	5.8515887748
H65	5.8077262785	2.8433774049	6.5067410246
H66	5.3866828292	1.2772926284	7.2222042948
H67	5.0084347160	2.7727786327	8.0833282724
H68	4.0423102590	4.3866539679	5.6329548980
H69	3.0579833363	4.3640484668	7.0990454578
H70	2.3508620221	3.8814217694	5.5427824316
H71	-2.6713640680	-3.4121111335	4.2788221987
H72	-2.4428979510	-2.9400066396	2.5778913069
H73	-1.1338618253	-3.7637695973	3.4279542946
O74	.1182029478	2.8237154015	3.8836248396
H75	-1.9090177377	2.9612398155	4.3016215066
C76	-.9756077981	3.3527507865	4.7176641400
C77	-.8212068486	2.8302873098	6.1372577222
C78	-.9935700289	4.8671778475	4.5925709428
H79	.1335889134	3.1221553014	6.5795093704
H80	-1.6273670054	3.2333278625	6.7585902500
H81	-.8934312485	1.7395165996	6.1482480707
C82	-1.9862931045	5.4867223376	3.8220150449
C83	-2.0160458161	6.8745064341	3.6747885179
C84	-1.0434006420	7.6634217790	4.2903940043
C85	-.0481153971	7.0577897753	5.0595617548
C86	-.0272485314	5.6729932833	5.2132059170
H87	-2.7317035643	4.8741577680	3.3215325540
H88	-2.7941991264	7.3371499170	3.0741914484
H89	-1.0600033749	8.7431314273	4.1732902264
H90	.7116589757	7.6665488886	5.5422235515

H91	.7496299977	5.2146180099	5.8148915602
H92	-.1859972508	3.0082020864	2.9203065965
O93	-1.8203633797	1.0670593310	2.5648994247
C94	-1.8294030087	1.9822772755	1.6669664634
O95	-.9995021111	2.9306973076	1.5899434786
C96	-2.9334752513	1.8786271793	.6306135255
H97	-3.8562605899	1.5133921772	1.0883860803
H98	-2.6287038681	1.1491849440	-.1292617755
H99	-3.0958545282	2.8421668980	.1446645403

2b

Pd1	-0.0340003595	0.8744139903	3.8739247982
O2	-0.6130689582	-0.5383926098	2.4054367080
O3	-0.4722618772	-2.3884132332	3.6786683958
C4	1.8144781792	0.1710025762	4.1998532401
N5	2.5043754900	0.0879265519	5.3735990659
N6	2.7021329807	-0.2545905989	3.2452054444
C7	3.7948082595	-0.3837170848	5.1528843918
C8	3.9246737517	-0.5793354585	3.8246836412
C9	2.4818218476	-0.4440887041	1.8252100635
C10	2.3307964213	0.6855738019	0.9936668919
C11	2.1575648041	0.4568708425	-0.3764798495
C12	2.1539316538	-0.8316937873	-0.9003771280
C13	2.3409858684	-1.9250219805	-0.0622770816
C14	2.5129727638	-1.7645800998	1.3184213570
C15	2.1100067602	0.4364973416	6.7254426060
C16	1.2221273743	-0.4011644625	7.4245252401
C17	1.0105959295	-0.1160538579	8.7809161525
C18	1.6610542014	0.9393392795	9.4112324152
C19	2.5321725389	1.7507213441	8.6901071528
C20	2.7753109855	1.5240525435	7.3319483223
C21	2.4295174846	2.1179850840	1.5181370876
C22	3.8888715670	2.6141894162	1.4338732322
C23	1.4785473525	3.0913552552	0.7992764827
C24	2.8002452954	-3.0023037829	2.1756562958
C25	4.2446631979	-3.4981822751	1.9358261269
C26	1.8195727104	-4.1651631266	1.9354372537
C27	0.5351450847	-1.6087938530	6.7948018540
C28	1.1435892918	-2.9226106152	7.3259908860
C29	-0.9899795056	-1.5811633091	7.0048720427
C30	3.7302693521	2.4523668122	6.5791699485
C31	5.1645269912	2.3614325289	7.1389748275
C32	3.2350797592	3.9112575832	6.5825451659
C33	-0.8695822852	-1.8029768396	2.6757795206
C34	-1.6808416756	-2.5087473842	1.5969766887
H35	4.4864980950	-0.5242021967	5.9663996601
H36	4.7570441029	-0.9191149569	3.2338933500
H37	2.0325514363	1.3018298947	-1.0451220968
H38	2.0190933831	-0.9828656115	-1.9681488108
H39	2.3593089624	-2.9245969507	-0.4856657218
H40	0.3344961719	-0.7449029424	9.3526766869
H41	1.4873203762	1.1324140092	10.4667787749
H42	3.0255802939	2.5809229165	9.1876299961
H43	2.1382238675	2.1181130508	2.5710884559
H44	4.5678132819	1.9695118121	2.0030172039
H45	3.9729213965	3.6303940940	1.8360130348
H46	4.2374781345	2.6319614412	0.3945882479
H47	1.7819272389	3.2804138618	-0.2367170377
H48	1.4717585996	4.0554274656	1.3173873931
H49	0.4528685238	2.7098840001	0.7887840327
H50	2.7030580713	-2.7242683817	3.2282873376

H51	4.9928951648	-2.7126777061	2.0803130946
H52	4.3617295593	-3.8699287715	0.9119141152
H53	4.4837164030	-4.3205103851	2.6188472860
H54	0.7969351535	-3.8811679955	2.1842447595
H55	1.8511210274	-4.5253622751	0.9014512251
H56	2.0927057160	-5.0087885222	2.5789463106
H57	3.7617868069	2.1394385733	5.5326906046
H58	0.6765245289	-3.7820371539	6.8332961014
H59	2.2226125518	-2.9697886216	7.1372860649
H60	0.9905206935	-3.0274935159	8.4067699029
H61	-1.4192809868	-0.6479732320	6.6255638876
H62	-1.4489865962	-2.4090811916	6.4563199370
H63	-1.2659426423	-1.6789711446	8.0614274785
H64	0.6883885144	-1.5894683792	5.7154467343
H65	5.8429670218	2.9952385406	6.5571051102
H66	5.5536811172	1.3375915370	7.1103566768
H67	5.2080309860	2.6990558591	8.1802912810
H68	3.9288451541	4.5450761055	6.0174086236
H69	3.1712104220	4.3177191983	7.5982099052
H70	2.2487749691	3.9768369728	6.1194516198
H71	-1.9894255703	-3.4941575153	1.9474769238
H72	-2.5615499363	-1.9223527754	1.3166782714
H73	-1.0652188462	-2.6213248023	0.6980274020
O74	0.3934452007	2.3087924897	5.2124280257
H75	-1.6412403222	2.4001144470	5.6226665696
C76	-0.7271547533	3.0064647618	5.7107398239
C77	-0.5259714070	3.2790289821	7.2159429915
C78	-0.9898114045	4.3139966383	4.9607125311
H79	0.3366983336	3.9292438127	7.3839632472
H80	-1.4102664366	3.7718168983	7.6372512007
H81	-0.3615528736	2.3373931072	7.7454214023
C82	-2.2086100943	4.9904590673	5.1199901948
C83	-2.4516823575	6.1983772634	4.4637499481
C84	-1.4749949761	6.7533748947	3.6320995086
C85	-0.2608640967	6.0871617311	3.4639766942
C86	-0.0220755903	4.8769644300	4.1217734574
H87	-2.9798315578	4.5605367767	5.7578531255
H88	-3.4034200352	6.7069023887	4.6001314741
H89	-1.6616334244	7.6935322291	3.1190499170
H90	0.5046618212	6.5108363265	2.8175828205
H91	0.9129503024	4.3433156219	3.9856023940
H92	-1.5338135928	0.3137775762	1.6402195591
O93	-1.9735815722	1.7989974473	3.3942521736
C94	-2.5438329074	1.8127997244	2.2893002337
O95	-2.2349015770	1.0065190518	1.3023547310
C96	-3.6703115925	2.7694728191	2.0127387245
H97	-3.6244589624	3.6069976839	2.7089596626
H98	-4.6219493802	2.2418269442	2.1443179610
H99	-3.6237256244	3.1187811375	0.9790703528

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Pd1	0.1190402985	0.7546604961	4.0040103960
O2	-0.4262122306	-1.2755423399	3.9781743391
O3	-2.6819317411	-1.0377073558	4.0334399745
C4	2.0007097710	0.1607971850	4.2617748003
N5	2.6939958995	-0.1657393396	5.3888626874
N6	2.8606805635	-0.0777549439	3.2320486167
C7	3.9702575646	-0.6140031686	5.0577249205
C8	4.0753755687	-0.5569280648	3.7100782485
C9	2.6187761360	0.1447469810	1.8178387118
C10	2.9822881416	1.3894246687	1.2623109761



C11	2.8131301640	1.5501342778	-0.1174421969
C12	2.3096704012	0.5229256349	-0.9068789562
C13	1.9646934606	-0.6953144072	-0.3324292143
C14	2.1115703822	-0.9180198803	1.0417029333
C15	2.2761452741	-0.0379499459	6.7756704635
C16	1.6145712188	-1.1215058611	7.3895685079
C17	1.3050571385	-0.9973700158	8.7493091617
C18	1.6463736951	0.1449390580	9.4644921540
C19	2.3112118340	1.1920042523	8.8368292020
C20	2.6461740243	1.1281646027	7.4794252635
C21	3.5876016705	2.5214927364	2.0885306143
C22	5.1281605266	2.5072293030	1.9855708802
C23	3.0365823617	3.9019026923	1.6927816077
C24	1.7739154172	-2.2844248012	1.6333181911
C25	2.9594310280	-3.2582395153	1.4634682293
C26	0.4955284681	-2.8905365135	1.0285140272
C27	1.2935781688	-2.4171078023	6.6483347191
C28	2.4261580903	-3.4483160381	6.8434918222
C29	-0.0558742366	-3.0231290805	7.0694288636
C30	3.4224192575	2.2780932933	6.8392365080
C31	4.9387617191	2.1360908725	7.0965014837
C32	2.9425887245	3.6599832882	7.3209099386
C33	-1.6362516182	-1.7248632084	3.9842891422
C34	-1.7789552489	-3.2360879725	3.8938794582
H35	4.6696761634	-0.9271160388	5.8149825514
H36	4.8860271191	-0.8067216494	3.0455262123
H37	3.0795011569	2.4947922367	-0.5795327888
H38	2.1861296338	0.6719049262	-1.9762238876
H39	1.5759296902	-1.4884967665	-0.9622763013
H40	0.7922749763	-1.8079890760	9.2554896637
H41	1.3928898576	0.2194289046	10.5183922980
H42	2.5697142692	2.0775570752	9.4069799109
H43	3.3077947899	2.3611351449	3.1326489033
H44	5.5534128356	1.5594672268	2.3304790114
H45	5.5609614331	3.3097143275	2.5937835496
H46	5.4520910711	2.6593855716	0.9496822192
H47	3.3535354099	4.2024718958	0.6882030970
H48	3.4145686679	4.6609640010	2.3865141982
H49	1.9452796593	3.9108835579	1.7357892727
H50	1.5829407655	-2.1528651286	2.7014088943
H51	3.8668302560	-2.8860085263	1.9494311975
H52	3.1892323987	-3.4131070637	0.4031635070
H53	2.7212756687	-4.2338103478	1.9026756795
H54	-0.3437314327	-2.1927148417	1.0978310082
H55	0.6258512784	-3.1682012576	-0.0233222711
H56	0.2261140164	-3.8029589734	1.5710246414
H57	3.2566242796	2.2344951545	5.7586915436
H58	2.2020089495	-4.3725127454	6.2979565550
H59	3.3882567043	-3.0720916331	6.4813721693
H60	2.5455655235	-3.7033950161	7.9025910081
H61	-0.8664205418	-2.2963351593	6.9680198816
H62	-0.2900721744	-3.8847264050	6.4370528285
H63	-0.0451469039	-3.3808171108	8.1044477706
H64	1.2161036798	-2.1869571392	5.5828440583
H65	5.4834801787	2.9672466728	6.6329576494
H66	5.3448233560	1.2042266416	6.6908342620
H67	5.1509185575	2.1534146972	8.1715444586
H68	3.4042167712	4.4436568574	6.7090876349
H69	3.2377947466	3.8523999865	8.3583333624
H70	1.8560271264	3.7503151049	7.2457572731
H71	-2.5046521659	-3.5784125573	4.6354295387
H72	-2.1799228910	-3.4868878423	2.9063477862

H73	-0.8250322438	-3.7455068592	4.0312666027
O74	-1.8906364298	1.2884672079	3.4800891326
H75	-1.8548230451	3.2921147110	3.7668603339
C76	-2.6139184855	2.5149654765	3.6550479649
C77	-3.4606556864	2.4607688269	4.9300095435
C78	-3.4322253018	2.8339225922	2.4110785675
H79	-2.8121460079	2.2914907092	5.7941770965
H80	-3.9941407306	3.4060382189	5.0723662746
H81	-4.2041923150	1.6584410348	4.8648617330
C82	-3.8144728055	4.1606142114	2.1680537397
C83	-4.5898657473	4.4891692790	1.0564838557
C84	-4.9921351213	3.4920289688	0.1661761419
C85	-4.6135245329	2.1701119459	0.3984153671
C86	-3.8382021488	1.8416229343	1.5124997899
H87	-3.4974602323	4.9447174226	2.8538647907
H88	-4.8738297685	5.5240386217	0.8819530366
H89	-5.5930195475	3.7454108962	-0.7031918451
H90	-4.9184257653	1.3880503494	-0.2922534895
H91	-3.5343270072	0.8126763223	1.6774924856
H92	-2.3954031906	0.4529762855	3.7529461355
O93	0.7495904572	2.7004000465	3.9114081889
C94	0.3945932878	3.4824075514	4.8983078464
O95	-0.1571889192	3.1194136957	5.9393175452
C96	0.6849772833	4.9585951984	4.6387106766
H97	1.4381236813	5.1014618781	3.8623453194
H98	0.9961082406	5.4415665561	5.5672552513
H99	-0.2453367079	5.4384778621	4.3095723060

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Pd1	.5224888041	.8069427897	3.6391511388
O2	-.4744401616	-1.1001415296	3.3287216563
O3	-1.5660336194	.7879732560	3.0549747230
C4	2.3257501243	.1644855798	4.1115092778
N5	2.7717188487	-.2021411285	5.3472144832
N6	3.2765682759	-.2830320517	3.2419571545
C7	3.9781343128	-.8881592290	5.2450439061
C8	4.2924578384	-.9377614734	3.9308275510
C9	3.3631180639	-.0833773793	1.8053510648
C10	4.0939333639	1.0284563045	1.3379396229
C11	4.2699688724	1.1402322169	-.0446933115
C12	3.7371297436	.1965886036	-.9169793473
C13	3.0145598792	-.8846338361	-.4247977134
C14	2.8105920356	-1.0544922616	.9503894180
C15	2.2220841289	.1430636049	6.6436745208
C16	1.2010119820	-.6545949020	7.1966022267
C17	.7928222819	-.3538449426	8.5025753681
C18	1.3784761203	.6845907245	9.2213085589
C19	2.3862271206	1.4534446072	8.6473794684
C20	2.8363779104	1.2016251573	7.3461139196
C21	4.7154296718	2.0640955191	2.2735719782
C22	6.2022268117	1.7442210471	2.5433015880
C23	4.5751193576	3.5053685524	1.7520142153
C24	2.0569877711	-2.2770972001	1.4675349568
C25	2.9853688131	-3.5086054157	1.5214615351
C26	.7969255398	-2.5858187496	.6392340218
C27	.5950369147	-1.8472765592	6.4624404728
C28	1.2301251848	-3.1642239751	6.9564573815
C29	-.9382795856	-1.8987055168	6.5854513090
C30	3.9804261359	2.0364120386	6.7717205350
C31	5.2912560892	1.7714273907	7.5412711406
C32	3.6507578826	3.5400869563	6.7389869474

C33	-1.5560492685	-.4831829821	3.0196717356
C34	-2.7876922799	-1.2602047147	2.6476345604
H35	4.4905686519	-1.2565283247	6.1185825520
H36	5.1351994244	-1.3646166633	3.4128232921
H37	4.8253460229	1.9822448927	-.4446611330
H38	3.8854370358	.3055035004	-1.9882167657
H39	2.6047287541	-1.6120611754	-1.1180268437
H40	.0147609865	-.9509624627	8.9675489647
H41	1.0512134355	.8911294963	10.2370179658
H42	2.8328959722	2.2632791906	9.2160197760
H43	4.1785490842	2.0203060846	3.2260180455
H44	6.3390200903	.7549541889	2.9907965204
H45	6.6346999739	2.4833525499	3.2271732797
H46	6.7794326197	1.7715433372	1.6119371684
H47	5.1911418721	3.6821684839	.8629133374
H48	4.9095296835	4.2102284425	2.5208882816
H49	3.5374713073	3.7354670989	1.5059226368
H50	1.7158839900	-2.0642360131	2.4834961076
H51	3.8543631156	-3.3354086653	2.1651341007
H52	3.3569192216	-3.7615244188	.5219988780
H53	2.4471916863	-4.3797046129	1.9121413464
H54	.1607142933	-1.7015827887	.5476372897
H55	1.0414520096	-2.9394049184	-.3686773504
H56	.2157937018	-3.3730466367	1.1305027348
H57	4.1425678001	1.7285714554	5.7357454456
H58	.8190487219	-4.0180428705	6.4063360859
H59	2.3164909828	-3.1653483529	6.8163457170
H60	1.0318068968	-3.3224609415	8.0228697739
H61	-1.3913415427	-.9565949614	6.2627927093
H62	-1.3323940763	-2.6984576684	5.9503788269
H63	-1.2661602649	-2.1013126223	7.6110940554
H64	.8162040071	-1.7468770301	5.3977533665
H65	6.1165749642	2.3338437231	7.0913422417
H66	5.5628849823	.7099225652	7.5341452738
H67	5.2082273078	2.0841140369	8.5879978440
H68	4.4858630660	4.0921661775	6.2924248565
H69	3.4873468719	3.9470377370	7.7426770023
H70	2.7535536756	3.7283366501	6.1462660819
H71	-3.2680799383	-1.6277562777	3.5611845266
H72	-2.5189478801	-2.1254821185	2.0372006166
H73	-3.4907233556	-.6181735720	2.1142630140
O74	.6252181915	2.7847645074	4.9136841568
H75	-.4164919309	2.2554872295	6.5703809289
C76	-.3970352099	3.1060526980	5.8798580781
C77	-1.7781282113	3.2637089962	5.2313512794
C78	-.0203437270	4.3498909464	6.6737662926
H79	-2.0558003599	2.3619801036	4.6814095255
H80	-2.5314576254	3.4593414380	6.0031173303
H81	-1.7792469819	4.1056990015	4.5319168960
C82	-.0462744947	4.3266782458	8.0731153527
C83	.2578836855	5.4710106441	8.8146142174
C84	.5988528769	6.6549085262	8.1609391660
C85	.6280649045	6.6874336795	6.7644920553
C86	.3172116332	5.5471619633	6.0239242891
H87	-.2975000418	3.4006805107	8.5858790380
H88	.2317895999	5.4354204393	9.9011246337
H89	.8407722089	7.5463102272	8.7340291208
H90	.8936672496	7.6065526612	6.2482157136
H91	.3481919013	5.5827038130	4.9379746867
H92	.6084918409	3.4448385843	4.1216081474
O93	1.2000966141	2.3352526854	1.9141270949
C94	.8559038475	3.5546800819	1.8666616952

O95	.5780919227	4.2825152877	2.8690148152
C96	.7522478041	4.2018731483	.4888023455
H97	1.2700624948	3.6078748804	-.2662652610
H98	1.1479238360	5.2206381474	.5171290101
H99	-.3074422737	4.2679021705	.2174658465

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Pd1	0.0066991723	0.3498634625	4.1423607782
O2	-0.7353703263	-1.5793118619	4.7417941801
O3	-2.1938020985	-0.0188179231	4.2059326977
C4	1.9780310362	0.1163663286	4.2696451080
N5	2.6804705606	-0.1611410605	5.4041548003
N6	2.9052658540	0.1009921711	3.2723616618
C7	4.0291873636	-0.3475692792	5.1167405936
C8	4.1688126678	-0.1907928279	3.7800937943
C9	2.6884624780	0.3552476476	1.8656047244
C10	3.1589804236	1.5739997576	1.3375804050
C11	3.0395601738	1.7647266813	-0.0434422047
C12	2.4700843551	0.7904594230	-0.8579361111
C13	2.0072333222	-0.3995235470	-0.3056594999
C14	2.1082371889	-0.6508373277	1.0688812463
C15	2.1404675914	-0.2964112464	6.7398614237
C16	1.9640219156	-1.5959981270	7.2542942747
C17	1.5111604905	-1.7060940892	8.5751098705
C18	1.2396236286	-0.5749942814	9.3363105567
C19	1.4163519804	0.6966360243	8.7959214828
C20	1.8746570495	0.8714124714	7.4852705295
C21	3.7879075329	2.6654528415	2.2008090811
C22	5.2952396309	2.8126442525	1.9084082750
C23	3.0571947532	4.0100009627	2.0347097360
C24	1.6429427885	-1.9931866651	1.6287651166
C25	2.6229604253	-3.1155202560	1.2346519085
C26	0.2044079766	-2.3339572724	1.2030269058
C27	2.2721544670	-2.8575151500	6.4492078585
C28	3.5642260041	-3.5316466333	6.9559916622
C29	1.0980441149	-3.8543359595	6.4497012743
C30	2.1250405786	2.2699411340	6.9220198574
C31	3.5874468064	2.6976972038	7.1758630566
C32	1.1551627112	3.3298316706	7.4707897336
C33	-1.9521116513	-1.2034523365	4.5976402210
C34	-3.0766949654	-2.1659521245	4.8730077743
H35	4.7467851944	-0.5725217191	5.8885718857
H36	5.0337005297	-0.2535224065	3.1405446029
H37	3.3913493424	2.6923425488	-0.4847328629
H38	2.3861573603	0.9596867833	-1.9281862732
H39	1.5680598846	-1.1525707937	-0.9528997948
H40	1.3662710189	-2.6909576401	9.0085520983
H41	0.8872705690	-0.6828224733	10.3588208348
H42	1.1971211797	1.5675993693	9.4036794178
H43	3.6753144046	2.3786232763	3.2504144322
H44	5.8375188892	1.8743858285	2.0666426246
H45	5.7403799849	3.5705696486	2.5624681106
H46	5.4693115223	3.1223346565	0.8722528556
H47	3.1341433888	4.3956861074	1.0126793875
H48	3.4918884140	4.7602499928	2.7044720876
H49	2.0040313165	3.8890174987	2.2882046737
H50	1.6363127431	-1.9306797117	2.7186752995
H51	3.6376061735	-2.9025760123	1.5861120804
H52	2.6678118363	-3.2391271958	0.1472228861
H53	2.3078501509	-4.0706409717	1.6688895220
H54	-0.4856951415	-1.5371638630	1.4916488531

H55	0.1207234590	-2.4850723225	0.1219721817
H56	-0.1213091118	-3.2576640942	1.6926423707
H57	1.9612081417	2.2330936896	5.8410016789
H58	3.8027241401	-4.4114439200	6.3477729905
H59	4.4228695050	-2.8530451523	6.9167515860
H60	3.4530918949	-3.8629531285	7.9942138301
H61	0.1944543079	-3.3797524436	6.0589786886
H62	1.3419606872	-4.7141957400	5.8138571010
H63	0.8908391810	-4.2418678521	7.4542147773
H64	2.4359502157	-2.5647233757	5.4082432916
H65	3.7727005605	3.6900139495	6.7517341137
H66	4.3041566716	2.0016307006	6.7263463358
H67	3.7983852722	2.7468066006	8.2502584569
H68	1.2870241801	4.2674589574	6.9229351306
H69	1.3312212506	3.5436876569	8.5322933838
H70	0.1130665207	3.0220788729	7.3464854688
H71	-3.8586051949	-1.6670383118	5.4505889694
H72	-3.5177048999	-2.4801069750	3.9213795368
H73	-2.7132595903	-3.0456948325	5.4060681797
074	0.3217096842	2.2296918897	3.5279357715
H75	-1.7468635221	2.1460864851	3.3918409190
C76	-0.9196929960	2.8507581125	3.2218318299
C77	-0.9653136483	3.2435802009	1.7359970996
C78	-1.1638967294	4.0380155269	4.1471636131
H79	-0.8135464140	2.3535354722	1.1168680849
H80	-1.9320558308	3.6921549951	1.4792899850
H81	-0.1807491325	3.9669357010	1.4925196985
C82	-2.2492580121	4.0361422267	5.0304707637
C83	-2.4768528827	5.1122015275	5.8918573269
C84	-1.6177533032	6.2100542837	5.8817097068
C85	-0.5295209304	6.2232325705	5.0062719098
C86	-0.3056194543	5.1471003718	4.1491290766
H87	-2.9167384379	3.1776195865	5.0459556163
H88	-3.3249850717	5.0906028861	6.5707288375
H89	-1.7921521850	7.0491589396	6.5495846147
H90	0.1451561245	7.0755524963	4.9918672387
H91	0.5495948429	5.1617304005	3.4812203582

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Pd1	-0.0907588312	0.7066621437	3.8947825984
02	-0.7085759122	-1.2509734392	3.6634068025
03	-2.0761259028	-1.0170119864	5.4543720696
C4	2.0064419811	0.1301399594	4.2213453705
N5	2.7692798027	-0.0937304770	5.3431386901
N6	2.8579280779	-0.1480483199	3.1789381018
C7	4.0587851860	-0.4991578381	4.9976696864
C8	4.1142832773	-0.5307623862	3.6440964981
C9	2.5174860224	-0.1012212332	1.7751385047
C10	2.6057177512	1.1310990155	1.0924090883
C11	2.3344311618	1.1278968641	-0.2799509268
C12	1.9904315528	-0.0473081246	-0.9434773539
C13	1.9052218761	-1.2463686880	-0.2451649768
C14	2.1612398284	-1.3029956709	1.1303291854
C15	2.3514738524	0.0782549085	6.7152415627
C16	1.7312428688	-0.9994139299	7.3813304942
C17	1.3995861514	-0.8150633550	8.7289875839
C18	1.6761386061	0.3803157254	9.3850051808
C19	2.2919598396	1.4258199422	8.7057492065
C20	2.6424175048	1.3009331309	7.3560396472
C21	3.0275414024	2.4200849082	1.7953222789
C22	4.5562213832	2.6075597057	1.7161332537

C23	2.3067214143	3.6627922575	1.2503841716
C24	2.0846464532	-2.6399285834	1.8608087976
C25	3.3270645191	-3.5005049269	1.5512373678
C26	0.7906537775	-3.4071846977	1.5394881240
C27	1.4666994672	-2.3377690744	6.6944921085
C28	2.6776219695	-3.2831378760	6.8617810806
C29	0.1834263228	-3.0265019428	7.1898967483
C30	3.3491127575	2.4507229941	6.6407271398
C31	4.8546449613	2.4725573559	6.9801805214
C32	2.7164460032	3.8195860789	6.9504640764
C33	-1.6361057023	-1.6498170906	4.4856362730
C34	-2.1809664780	-3.0374384808	4.1480613783
H35	4.8050369732	-0.7258995429	5.7419829322
H36	4.9180705789	-0.7932640450	2.9751763106
H37	2.3929246079	2.0560138395	-0.8394533995
H38	1.7861940100	-0.0259360039	-2.0106512585
H39	1.6307572214	-2.1549280557	-0.7732047564
H40	0.9142857211	-1.6184630724	9.2719551737
H41	1.4074714985	0.4981217883	10.4316071262
H42	2.5013760046	2.3530190821	9.2303809328
H43	2.7511756456	2.3307015202	2.8492197474
H44	5.0930487940	1.7707611487	2.1733121539
H45	4.8602395577	3.5250504606	2.2354538165
H46	4.8822823921	2.6840793106	0.6726201125
H47	2.6048719841	3.8947612953	0.2226368447
H48	2.5635998168	4.5364744939	1.8615590369
H49	1.2221191465	3.5356895232	1.2731465708
H50	2.0704757141	-2.4354218053	2.9347138281
H51	4.2566709533	-2.9902243402	1.8266511691
H52	3.3833229132	-3.7384809984	0.4821619509
H53	3.2859252961	-4.4456535533	2.1037834090
H54	-0.0817184940	-2.7972131089	1.7833315576
H55	0.7390254969	-3.7085897383	0.4868446717
H56	0.7477691660	-4.3233238852	2.1389525697
H57	3.2487717649	2.2869382358	5.5638156369
H58	2.4914870036	-4.2349207368	6.3515768166
H59	3.5955640648	-2.8559303516	6.4466297028
H60	2.8576507742	-3.4999176141	7.9218438542
H61	-0.6795651064	-2.3579428595	7.1266897770
H62	-0.0223668471	-3.9041485271	6.5671267472
H63	0.2816518893	-3.3855399451	8.2221607010
H64	1.3320877286	-2.1393581709	5.6265455232
H65	5.3571286028	3.2938157165	6.4561458249
H66	5.3488113287	1.5393414468	6.6934119820
H67	5.0084125214	2.6152169206	8.0560281248
H68	3.1535260421	4.5907717238	6.3063878040
H69	2.8913179963	4.1287107455	7.9865083581
H70	1.6365578506	3.8017884228	6.7852329205
H71	-2.8103821451	-3.4026694981	4.9610667973
H72	-2.7783227758	-2.9767903685	3.2311527685
H73	-1.3655856233	-3.7420546192	3.9582394112
O74	0.2423804665	2.8177633659	4.0715573801
H75	-1.5639649073	1.0513406405	3.5446878266
C76	-0.3055606659	3.7572920912	4.6750479350
C77	0.1658687096	5.1512965706	4.3073291400
C78	-1.3658466780	3.5981249583	5.6967710263
H79	0.9990291232	5.0676017306	3.6106014078
H80	-0.6430897542	5.7101269845	3.8235678199
H81	0.4786592349	5.7177757434	5.1897584466
C82	-2.0267456548	4.7377120377	6.2035831582
C83	-3.0353012580	4.6102249100	7.1515218849
C84	-3.4013321099	3.3436119066	7.6156789705

C85	-2.7534488214	2.2081693506	7.1290811597
C86	-1.7404927079	2.3299225642	6.1809005329
H87	-1.7633316130	5.7281405774	5.8494436695
H88	-3.5391095779	5.4964282871	7.5265742172
H89	-4.1929224434	3.2457487335	8.3545159429
H90	-3.0328223931	1.2165293299	7.4704047377
H91	-1.2669340923	1.4256598543	5.8104893061

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Pd1	-.1790161660	.4627530826	4.0808811547
O2	-.4842470176	-1.6040687038	3.9133303657
O3	-2.7498538399	-1.4466361906	3.9840757211
C4	2.0541175700	.1558949590	4.1543442667
N5	2.8336629228	-.0357531381	5.2642968009
N6	2.8955330427	-.1727840432	3.1247204360
C7	4.1128435661	-.4775503341	4.9348629362
C8	4.1525150739	-.5606414732	3.5841546677
C9	2.5996385756	-.0435096696	1.7138511304
C10	2.8632623675	1.1947114343	1.0883085318
C11	2.6435588738	1.2856198150	-.2908520293
C12	2.1819773331	.1922198918	-1.0165024009
C13	1.9273017368	-1.0150444038	-.3752430167
C14	2.1276910302	-1.1654814352	1.0028745254
C15	2.4436893256	.2794946186	6.6197056767
C16	1.7071754779	-.6661690884	7.3638831538
C17	1.3807188098	-.3302778055	8.6836281970
C18	1.7711801242	.8843351451	9.2402901137
C19	2.5028266172	1.7959878601	8.4869672735
C20	2.8556419675	1.5174312232	7.1602722179
C21	3.4150439741	2.3981623986	1.8511483574
C22	4.9484591583	2.4912986128	1.7017449711
C23	2.7596373403	3.7273437892	1.4321726681
C24	1.8738599185	-2.5111429229	1.6769584948
C25	3.1273883000	-3.4095900299	1.5976937048
C26	.6571534859	-3.2470598556	1.0915292794
C27	1.3189102019	-2.0257486523	6.7884824107
C28	2.4216452272	-3.0652380418	7.0841097539
C29	-.0453769356	-2.5260343496	7.2905012345
C30	3.6921826652	2.5306242836	6.3778140999
C31	5.1421652286	2.5641764115	6.9040648539
C32	3.0826256506	3.9462794148	6.3913844013
C33	-1.6958233284	-2.0879324861	3.9367988164
C34	-1.7528762996	-3.6164793362	3.8844126497
H35	4.8609701660	-.6827294965	5.6836957272
H36	4.9435993687	-.8522094768	2.9125468195
H37	2.8380225624	2.2223988050	-.8037026531
H38	2.0181028778	.2823888203	-2.0871447472
H39	1.5621231484	-1.8563693996	-.9542908025
H40	.8112090188	-1.0306332461	9.2850446580
H41	1.5044987172	1.1200888995	10.2672004049
H42	2.8060762696	2.7383788974	8.9338384801
H43	3.1952606284	2.2493156128	2.9128524654
H44	5.4464144708	1.5907041626	2.0733635227
H45	5.3402015029	3.3485109386	2.2615067701
H46	5.2275475960	2.6190391898	.6499814958
H47	3.0459509877	4.0237066781	.4174769322
H48	3.0785688615	4.5319224435	2.1038554994
H49	1.6677390605	3.6693331581	1.4656553082
H50	1.6440403716	-2.3178649310	2.7279616497
H51	3.9954149505	-2.9497011278	2.0798955185
H52	3.3954514464	-3.6170201384	.5549498523

H53	2.9410015903	-4.3687353305	2.0937530596
H54	-.2290277922	-2.6073688221	1.0929712377
H55	.8351514076	-3.5960480819	.0677139197
H56	.4357142791	-4.1296707191	1.6990419801
H57	3.7306792383	2.2063857791	5.3342593973
H58	2.1594724753	-4.0342873860	6.6452697139
H59	3.3886879528	-2.7615592090	6.6697011578
H60	2.5496026586	-3.2072266318	8.1638288743
H61	-.8291901412	-1.7834124720	7.1165062752
H62	-.3229849663	-3.4349478807	6.7482284540
H63	-.0329907876	-2.7770585398	8.3575933479
H64	1.2275199422	-1.9211458009	5.7047462508
H65	5.7496052276	3.2619890019	6.3169457432
H66	5.6132432840	1.5774724988	6.8497414765
H67	5.1739629712	2.8897661157	7.9497702403
H68	3.6869049947	4.6206468701	5.7741866769
H69	3.0529765466	4.3700432999	7.4008316593
H70	2.0623984158	3.9529277679	5.9972432854
H71	-2.4899066176	-3.9761880086	4.6066364301
H72	-2.0942434510	-3.9216525399	2.8898163412
H73	-.7801895486	-4.0720232304	4.0787794361
H75	-1.7038072138	.4801190622	4.0104862367
C76	-.4301731951	2.5419063333	5.2649467737
C77	-.0874107694	2.8061947708	3.9167259183
C78	-1.0926479083	3.2399420891	3.0178150564
C79	-2.3851948114	3.4575974741	3.4694583374
C80	-2.7151251314	3.2279114542	4.8171200028
C81	-1.7593217335	2.7545583076	5.7016762247
H82	.3403788072	2.3204437572	5.9953144484
H83	.9518535505	2.8397870980	3.6133802228
H84	-.8338401763	3.4373117458	1.9815299721
H85	-3.1485169894	3.8058222164	2.7795977343
H86	-3.7306887305	3.4042577146	5.1596402048
H87	-2.0156787321	2.5661441036	6.7397689582

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Pd1	.0155528748	-.1848872470	-.0771177414
O2	-.0390428198	-2.0527766072	1.1427993484
O3	2.1608446461	-1.6274967757	1.2767696858
C4	-2.2106134343	.0473746725	-.5967508885
N5	-3.2636476999	.2110335443	.2666344889
N6	-2.8374169532	-.0632040540	-1.8127310017
C7	-4.4927915080	.2029856784	-.3906027556
C8	-4.2242278211	.0247936012	-1.7053000827
C9	-2.1668980397	-.2472619467	-3.0757417246
C10	-1.7337237348	-1.5377848427	-3.4410154917
C11	-1.1132315166	-1.6812318419	-4.6891131686
C12	-.9374248705	-.5935563428	-5.5385909861
C13	-1.3771228513	.6706519972	-5.1553653739
C14	-1.9957343106	.8747434724	-3.9161567067
C15	-3.1601876048	.3289732299	1.7025028003
C16	-2.8731875645	1.5872949417	2.2688880352
C17	-2.8457755828	1.6786990276	3.6653302048
C18	-3.0929116975	.5661914207	4.4637351773
C19	-3.3704031683	-.6653230175	3.8794585126
C20	-3.4082953395	-.8154234857	2.4881618406
C21	-1.9392367208	-2.7649131264	-2.5571615379
C22	-2.9536170328	-3.7344408180	-3.1972940753
C23	-.6094221936	-3.4744371853	-2.2405784824
C24	-2.4751697148	2.2731990019	-3.5277085208
C25	-3.7374322723	2.6623645826	-4.3239317323



C26	-1.3812173988	3.3455347543	-3.6963589443
C27	-2.6438624615	2.8340188754	1.4196430813
C28	-3.9071864015	3.7193266961	1.3949943817
C29	-1.4164927363	3.6413097406	1.8795863816
C30	-3.7492421495	-2.1744789680	1.8809671297
C31	-5.2516937834	-2.4837065608	2.0443403826
C32	-2.8875383250	-3.3106725498	2.4601964882
C33	1.1386633563	-2.3302381016	1.5387849146
C34	1.3191378583	-3.5746506767	2.3909396779
H35	-5.4267650337	.3201131521	.1354191021
H36	-4.8747240117	-.0524099313	-2.5617482360
H37	-.7654868525	-2.6623490592	-4.9991650360
H38	-.4546232711	-.7301923590	-6.5027362921
H39	-1.2320067153	1.5129067862	-5.8256150052
H40	-2.6319105677	2.6343734548	4.1342936249
H41	-3.0688977264	.6599042196	5.5463419647
H42	-3.5587126628	-1.5268924766	4.5130547197
H43	-2.3542175622	-2.4310926026	-1.6034455629
H44	-3.9153649209	-3.2439786540	-3.3834382360
H45	-3.1317714402	-4.5901264938	-2.5366500310
H46	-2.5874646292	-4.1235577639	-4.1544010936
H47	-.1226584557	-3.8536374992	-3.1467003408
H48	-.7889316703	-4.3282948284	-1.5786081511
H49	.0806519205	-2.7960529756	-1.7308263083
H50	-2.7459653284	2.2528314255	-2.4681055737
H51	-4.5490379289	1.9439677373	-4.1705455491
H52	-3.5268275588	2.7009757046	-5.3985968400
H53	-4.0979305662	3.6501863429	-4.0161810475
H54	-.4750485247	3.0903311639	-3.1401244048
H55	-1.1009423735	3.4840128499	-4.7461385107
H56	-1.7443507825	4.3115642240	-3.3278911642
H57	-3.5316033253	-2.1277830659	.8104352201
H58	-3.7509658991	4.6001449716	.7614843936
H59	-4.7719247437	3.1716948034	1.0056454699
H60	-4.1610919357	4.0700686863	2.4019397367
H61	-.5279592287	3.0060019455	1.9372837410
H62	-1.2144890051	4.4557911309	1.1745720090
H63	-1.5688967731	4.0979202259	2.8636045531
H64	-2.4474734892	2.5065262061	.3952155592
H65	-5.4996721448	-3.4412466746	1.5731256549
H66	-5.8799187732	-1.7114334716	1.5877952979
H67	-5.5266181400	-2.5505012104	3.1031303833
H68	-3.1335415662	-4.2537596248	1.9583905098
H69	-3.0686062592	-3.4581145745	3.5311242341
H70	-1.8275454931	-3.1004430126	2.3006603857
H71	2.3729189359	-3.8395317569	2.4803182983
H72	.9150085551	-3.3806466450	3.3902489846
H73	.7540983835	-4.4066232527	1.9630960419
H75	1.4706348207	-.5794679629	.4519631080
C76	1.1697389568	.9666036796	-1.8209162842
C77	.8834053179	1.8828795421	-.7772101765
C78	1.9230167326	2.2732707687	.1011045051
C79	3.2138239641	1.7961087223	-.0793130050
C80	3.4983490113	.9011071127	-1.1235982658
C81	2.4872374025	.4764097546	-1.9744650018
H82	.4327611363	.7614992611	-2.5889960109
H83	-.0644175612	2.4097045614	-.7509780176
H84	1.7092881398	2.9797818103	.8981924763
H85	4.0061946163	2.1116841913	.5935395982
H86	4.5106393018	.5296075196	-1.2545429865
H87	2.7057787480	-.2155411727	-2.7826769815

Pd1	-.0908255988	-.3473284798	.3765643775
O2	-.3234001396	-1.4652307553	2.3009424007
O3	1.8962325137	-1.1787137057	2.3010024996
C4	-2.2362276808	-.0935795186	-.3195687740
N5	-3.2534110493	-1.0045030600	-.4505973681
N6	-2.8870620854	1.1044906818	-.4860445942
C7	-4.4833750212	-.3938362446	-.6920359815
C8	-4.2536006755	.9405500213	-.7104484246
C9	-2.2264794326	2.3835665598	-.5699111498
C10	-1.9861943472	2.9242729422	-1.8508917353
C11	-1.3636691674	4.1757448813	-1.9222832265
C12	-.9876824461	4.8573058790	-.7681060415
C13	-1.2306076522	4.2984399105	.4827463606
C14	-1.8530804829	3.0505470753	.6130834316
C15	-3.0907287503	-2.4374364705	-.4052517154
C16	-3.3773234752	-3.1163582821	.7975361625
C17	-3.2664746131	-4.5114615824	.7940777435
C18	-2.8811165692	-5.2012233560	-.3519085984
C19	-2.5962675797	-4.5066631065	-1.5227841412
C20	-2.6938428318	-3.1108831858	-1.5779176815
C21	-2.3656905264	2.1976592126	-3.1411786108
C22	-3.3799617819	3.0067816854	-3.9726635400
C23	-1.1213505052	1.8426519499	-3.9789216745
C24	-2.1397634695	2.4886816564	2.0021560753
C25	-3.2703588293	3.2813730595	2.6880502387
C26	-.8741464675	2.4404302328	2.8780381699
C27	-3.8416252811	-2.3835983941	2.0544305916
C28	-5.3789567051	-2.4275212538	2.1808756659
C29	-3.1817526056	-2.9196954553	3.3363132178
C30	-2.4010473675	-2.3852687216	-2.8887347177
C31	-3.4940731118	-2.6781386651	-3.9365290439
C32	-1.0033734262	-2.7248354287	-3.4389499916
C33	.8156552533	-1.6086637194	2.8317278182
C34	.9329330358	-2.2996268208	4.1750119511
H35	-5.3898315539	-.9605222328	-.8315869858
H36	-4.9178162814	1.7765437033	-.8624762633
H37	-1.1670768758	4.6198486515	-2.8944994482
H38	-.5057269037	5.8286909021	-.8439978072
H39	-.9326350223	4.8393480510	1.3761207372
H40	-3.4815317692	-5.0655062374	1.7023210205
H41	-2.8019534659	-6.2851062346	-.3310463685
H42	-2.2959496099	-5.0557056706	-2.4108461584
H43	-2.8476537830	1.2544488435	-2.8731145541
H44	-4.2819977847	3.2317488406	-3.3940570019
H45	-3.6810258548	2.4441867898	-4.8635332779
H46	-2.9567436629	3.9591721047	-4.3107117520
H47	-.5844833753	2.7413299813	-4.3033564944
H48	-1.4119436818	1.2873159438	-4.8782943704
H49	-.4303844364	1.2223724343	-3.4014103249
H50	-2.4767478101	1.4564333074	1.8835913627
H51	-4.1887536840	3.2682951942	2.0909506043
H52	-2.9870005666	4.3294215284	2.8391999088
H53	-3.4985527686	2.8522692384	3.6700498597
H54	-.0886751423	1.8578712636	2.3868638999
H55	-.4816304474	3.4411268154	3.0919645758
H56	-1.1008348303	1.9633085175	3.8376443101
H57	-2.4120905870	-1.3110292628	-2.6888863921
H58	-5.7059671625	-1.8763433149	3.0699013151
H59	-5.8759748119	-1.9861956204	1.3116314459
H60	-5.7322622458	-3.4607706761	2.2780658528

H61	-2.0945548080	-2.8918088768	3.2416799540
H62	-3.4678794282	-2.2915756836	4.1874400215
H63	-3.4995884185	-3.9425956513	3.5692650953
H64	-3.5346964842	-1.3383143783	1.9570775828
H65	-3.3000917537	-2.1236897131	-4.8619163641
H66	-4.4853373530	-2.3899912643	-3.5707125591
H67	-3.5291394315	-3.7442306088	-4.1882716590
H68	-.8019938663	-2.1425731976	-4.3454691635
H69	-.9137953018	-3.7843490630	-3.7041142672
H70	-.2252389028	-2.4919543232	-2.7068384169
H71	1.7684807286	-3.0038260090	4.1645793225
H72	1.1498669328	-1.5464456909	4.9401177024
H73	.0069019626	-2.8135134801	4.4350136259
074	1.0958676455	.9418076086	-.9687511222
H75	1.3374175025	-.6066471064	1.1695709839
C76	2.0425799047	.9553444396	-1.7642723935
C77	2.4625374817	2.2947662494	-2.3383716518
C78	2.7763527177	-.2766847533	-2.1533537373
H79	1.7863507813	3.0618261919	-1.9596068101
H80	3.4892058978	2.5398315122	-2.0418957486
H81	2.4287673258	2.2887364702	-3.4335998762
C82	3.8729022889	-.2256640950	-3.0350020104
C83	4.5585895277	-1.3876109862	-3.3790127248
C84	4.1622307398	-2.6170279860	-2.8468638560
C85	3.0747911621	-2.6804637852	-1.9731069351
C86	2.3834751880	-1.5219675108	-1.6301284338
H87	4.1978842982	.7226325755	-3.4508768019
H88	5.4038457243	-1.3348548650	-4.0594453639
H89	4.6993428375	-3.5230715806	-3.1146080228
H90	2.7645967640	-3.6341281882	-1.5553416997
H91	1.5386180457	-1.5658396803	-.9430299551

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Pd1	.4202112690	1.2669315969	3.6653647744
02	-.7298563690	-.1314286105	4.6993301507
03	-1.0109063243	1.6326458435	6.0934871064
C4	2.2150890454	.3664776121	4.0777201018
N5	2.7757120844	-.1639963353	5.2048491028
N6	3.1788020165	.2115287323	3.1198216642
C7	4.0609505629	-.6375647837	4.9464918794
C8	4.3108285232	-.4081378758	3.6370802097
C9	3.0166489985	.4880487341	1.7089259044
C10	3.6021175269	1.6529749622	1.1704031601
C11	3.4911442457	1.8482238650	-.2109862410
C12	2.8221367574	.9308222339	-1.0166540926
C13	2.2532944422	-.2084227827	-.4579114276
C14	2.3431756533	-.4649300778	.9155611043
C15	2.1476161242	-.3964759340	6.4900766315
C16	1.6632807122	-1.6951621516	6.7536487160
C17	1.1586461643	-1.9465243692	8.0356194333
C18	1.1390906810	-.9513786274	9.0068107896
C19	1.6208966512	.3215281846	8.7161947758
C20	2.1376855128	.6315020338	7.4535886717
C21	4.3644597804	2.6582216906	2.0303833387
C22	5.8869684860	2.4244714059	1.9380227933
C23	4.0270709197	4.1159351624	1.6708048890
C24	1.7638699514	-1.7628001751	1.4746588485
C25	2.5502468980	-2.9820384163	.9490417116
C26	.2577948168	-1.9046705292	1.1843334472
C27	1.6824398614	-2.8234408924	5.7228531784
C28	2.6405817507	-3.9526097447	6.1538082077

C29	.2683065949	-3.3686884787	5.4408769428
C30	2.7095300690	2.0170682200	7.1669160755
C31	4.2170371244	2.0631977109	7.4966207054
C32	1.9651003152	3.1401016097	7.9088930039
C33	-1.2726104985	.4709704110	5.7074249097
C34	-2.3179905740	-.3438603793	6.4485976906
H35	4.6572574359	-1.0980197673	5.7173671861
H36	5.1679476246	-.6335979487	3.0238215138
H37	3.9323878137	2.7310538285	-.6626237108
H38	2.7470798449	1.1044828787	-2.0868355455
H39	1.7349385792	-.9170590073	-1.0967162159
H40	.7766975345	-2.9354231569	8.2726045921
H41	.7441340541	-1.1667419854	9.9957418245
H42	1.5906094554	1.0875414850	9.4825923627
H43	4.0590461521	2.5045502038	3.0693344353
H44	6.1680624577	1.4147906581	2.2516829963
H45	6.4241244887	3.1346911384	2.5766226235
H46	6.2397815256	2.5625242254	.9099856892
H47	4.4076170671	4.3941624045	.6818749835
H48	4.4905121163	4.7942383013	2.3959807211
H49	2.9470028446	4.2766349497	1.6863940539
H50	1.8769842312	-1.7483059158	2.5612160350
H51	3.6174331056	-2.9076236212	1.1859784282
H52	2.4559941837	-3.0805383729	-.1380712607
H53	2.1663687920	-3.9041440882	1.3996098250
H54	-.3116136970	-1.0706220101	1.6019749987
H55	.0478926614	-1.9489196786	.1102063382
H56	-.1211521167	-2.8296293751	1.6337629424
H57	2.5960884676	2.2044722629	6.0946994131
H58	2.6742204967	-4.7381835432	5.3901183446
H59	3.6616466236	-3.5831494899	6.3028991457
H60	2.3164984401	-4.4153596789	7.0926762699
H61	-.3869988816	-2.5694991190	5.0834187861
H62	.3143590234	-4.1508787012	4.6735112430
H63	-.1780821446	-3.8152597066	6.3368846983
H64	2.0582619180	-2.4194456076	4.7792638575
H65	4.6295688005	3.0529719782	7.2700226987
H66	4.7845208661	1.3239515762	6.9225006311
H67	4.3865997527	1.8643199435	8.5607882539
H68	2.3141645009	4.1149622724	7.5521554025
H69	2.1529579327	3.1102094576	8.9880960968
H70	.8872686143	3.0830155349	7.7421479586
H71	-2.5212431298	.1013599190	7.4234087933
H72	-3.2405011393	-.3424509010	5.8582971319
H73	-1.9962893898	-1.3811269373	6.5633185826
O74	-1.3170566565	2.1640100643	3.1647241780
H75	-.3929623208	2.7489668065	1.4044450591
C76	-1.3967628845	2.5234566969	1.8150952734
C77	-2.2306324833	3.8179477175	1.7068827995
C78	-2.0109515792	1.4314699791	.9361439914
H79	-1.7552399682	4.6191914931	2.2834881704
H80	-2.3328668870	4.1428717759	.6651136835
H81	-3.2300902650	3.6452177648	2.1190050627
C82	-1.7714202469	1.4004896230	-.4438033835
C83	-2.3657037106	.4301217373	-1.2523866059
C84	-3.2116482696	-.5271098502	-.6883932118
C85	-3.4533267959	-.5061544014	.6870570605
C86	-2.8562210397	.4645810139	1.4937780080
H87	-1.1052449280	2.1395418306	-.8881261716
H88	-2.1669819478	.4189934419	-2.3217002723
H89	-3.6755323901	-1.2851955584	-1.3151773145
H90	-4.1067298763	-1.2516810319	1.1342096877

H91	-3.0156767617	.4805249252	2.5678466350
O93	1.2560374551	3.2683462485	3.3923806665
C94	.7867305233	4.1103685355	4.1874567329
O95	.0184713808	3.8684318961	5.2114409975
C96	1.1172843271	5.5729926853	4.0257442000
H97	1.7856325275	5.7242701988	3.1801088566
H98	1.5777423962	5.9507725251	4.9431596578
H99	.1900897699	6.1330748196	3.8737824476
H100	-.3281799698	2.9141925409	5.3490552838

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Pd1	.2413281693	1.0423192045	3.8312126095
O2	-.6605362856	-.0600747126	5.3479305073
O3	-1.0410634098	1.8077988799	6.5732433806
C4	2.1018523639	.2317386796	4.0799948183
N5	2.7538267099	-.2685945646	5.1718665856
N6	3.0262041489	.1391496854	3.0738471786
C7	4.0478662946	-.6654357948	4.8453303807
C8	4.2187100353	-.4127680659	3.5282386546
C9	2.8176741178	.4323330605	1.6741979308
C10	3.2588867692	1.6724485703	1.1655187011
C11	3.1650799860	1.8669880921	-.2181437708
C12	2.6503148042	.8774252649	-1.0524024238
C13	2.2067971537	-.3287171941	-.5200458245
C14	2.2835870031	-.5841044012	.8545253939
C15	2.2387522547	-.5192066749	6.5031761639
C16	1.7768918988	-1.8194701840	6.7887021896
C17	1.4016324513	-2.0935116153	8.1090535878
C18	1.4814597515	-1.1145530413	9.0941061347
C19	1.9323648659	.1640628016	8.7784173763
C20	2.3235088063	.4960074563	7.4756949126
C21	3.8595053420	2.7555611822	2.0595430603
C22	5.4012681728	2.7233112034	1.9960935858
C23	3.3373618795	4.1622845246	1.7189399431
C24	1.8202014976	-1.9338656592	1.3973782743
C25	2.6921474379	-3.0829666453	.8522730045
C26	.3270572965	-2.1828890812	1.1088005084
C27	1.6667883504	-2.9148142493	5.7300436036
C28	2.6061716792	-4.0969941673	6.0400172106
C29	.2098424202	-3.3876343014	5.5563351377
C30	2.8497598554	1.8919242722	7.1506412415
C31	4.3777516447	1.9654247778	7.3613092026
C32	2.1469267524	2.9975004283	7.9576355610
C33	-1.1892182651	.5955570324	6.3265342057
C34	-2.0823377241	-.2461112476	7.2270534155
H35	4.7071921904	-1.0935058291	5.5827282128
H36	5.0566273479	-.5761809456	2.8706289660
H37	3.5027869924	2.8044647172	-.6487354264
H38	2.5921071452	1.0498753678	-2.1241286791
H39	1.7974658553	-1.0877640094	-1.1801972036
H40	1.0389546804	-3.0850188674	8.3652750416
H41	1.1854420343	-1.3463978013	10.1138859973
H42	1.9765302962	.9187144010	9.5560788887
H43	3.5549538153	2.5501406308	3.0893249150
H44	5.8027053823	1.7516092143	2.3010760794
H45	5.8271383407	3.4842517612	2.6593662660
H46	5.7560218192	2.9261907126	.9789839547
H47	3.6581630420	4.4946177685	.7251470643
H48	3.7271139848	4.8832918994	2.4449345204
H49	2.2465056576	4.2004665768	1.7673450616
H50	1.9371805916	-1.9235298986	2.4838710742

H51	3.7507487303	-2.9323124121	1.0897666636
H52	2.6033944028	-3.1730612666	-.2360494645
H53	2.3802979675	-4.0377259474	1.2895889341
H54	-.2982645946	-1.3928329483	1.5340678085
H55	.1227670110	-2.2292973265	.0336660899
H56	.0147574891	-3.1372927099	1.5471076811
H57	2.6407373532	2.0906677081	6.0952479127
H58	2.5458404401	-4.8519522019	5.2480995497
H59	3.6499740288	-3.7741482687	6.1195084547
H60	2.3377389059	-4.5859515549	6.9830384166
H61	-.4402201560	-2.5435668993	5.3113402509
H62	.1468201749	-4.1280361420	4.7501612974
H63	-.1683920913	-3.8638688908	6.4683186797
H64	1.9794558676	-2.4942528189	4.7706729593
H65	4.7495566039	2.9648995076	7.1089973862
H66	4.9140798200	1.2430631197	6.7378378061
H67	4.6371332132	1.7634930545	8.4073656096
H68	2.4520382875	3.9783766029	7.5772475056
H69	2.4185421603	2.9686414169	9.0194378208
H70	1.0596784123	2.9213279913	7.8753611133
H71	-2.1729413439	.2235824517	8.2073885231
H72	-3.0769532573	-.2977231786	6.7703212006
H73	-1.6995538478	-1.2635809322	7.3226587867
074	-1.4942230996	1.9369129567	3.3045281031
H75	.1222809321	2.0123781659	2.0619547173
C76	-1.0317629392	2.2726271104	2.0650337938
C77	-1.0835145530	3.7876531482	1.7870967238
C78	-1.6436364943	1.4543114950	.9248941305
H79	-.5492464858	4.3305687350	2.5668045672
H80	-.6499361030	4.0375417771	.8140585859
H81	-2.1326280824	4.1008779443	1.7911620723
C82	-1.1376312504	1.5267408145	-.3797883119
C83	-1.7271850739	.7948986973	-1.4109782767
C84	-2.8346598401	-.0150477093	-1.1506696154
C85	-3.3430764663	-.0910608114	.1467661331
C86	-2.7499218902	.6367177141	1.1800400923
H87	-.2667521968	2.1429724413	-.5907844754
H88	-1.3215050716	.8564891269	-2.4178950213
H89	-3.2968340612	-.5826008187	-1.9542154659
H90	-4.2046199711	-.7199053420	.3566896713
H91	-3.1260688081	.5819622584	2.1964775805
093	1.2822398539	3.5938173740	4.4063010097
C94	.6006107566	4.4462604439	4.9751818629
095	-.4215858636	4.1863168338	5.7668667950
C96	.8546959964	5.9312376309	4.8281943533
H97	1.7099698490	6.1038029723	4.1750367588
H98	1.0372703753	6.3770026012	5.8107740043
H99	-.0344302080	6.4177504189	4.4143713791
H100	-.5934807427	3.1979259023	5.8970732401

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Pd1	-.0662229490	-.0214536957	-.0211186311
02	-.0039817461	-.1426302548	2.0518887307
03	2.2436465829	-.0744241942	1.8476894315
C4	-.7303562303	1.9045607660	-.1580024675
N5	-1.0027361499	2.8451002874	.7962434233
N6	-1.0933433299	2.5208444567	-1.3274257219
C7	-1.5281682330	4.0026610521	.2324676648
C8	-1.5843864141	3.8008796812	-1.1030141464
C9	-1.0323160470	1.9530572992	-2.6491398635
C10	.1343355468	2.1549441400	-3.4139165124

C11	.1440009856	1.6401770072	-4.7145152752
C12	-.9583510040	.9625854989	-5.2268458626
C13	-2.1035385556	.7939418557	-4.4520756170
C14	-2.1733069563	1.2955122012	-3.1473912067
C15	-.7937329266	2.7766371751	2.2270558781
C16	-1.8108709852	2.2365612243	3.0321462457
C17	-1.6332958559	2.2989110040	4.4171011955
C18	-.4944652558	2.8742038094	4.9712045797
C19	.4951683841	3.4011364944	4.1479117806
C20	.3668867209	3.3730459414	2.7538935485
C21	1.3224506710	2.9596498612	-2.8891171717
C22	1.3251956726	4.3697849619	-3.5167278242
C23	2.6749613595	2.2576619846	-3.1081533889
C24	-3.4555890925	1.1407146483	-2.3317675555
C25	-4.6532711482	1.7986711769	-3.0441748089
C26	-3.7500232747	-.3323386318	-1.9946853390
C27	-3.0737901731	1.6062067537	2.4546741520
C28	-4.3287899593	2.4182600502	2.8293722749
C29	-3.2151377949	.1318503540	2.8766736312
C30	1.4562152827	3.9967356424	1.8832090377
C31	1.5271504269	5.5237583656	2.1038035400
C32	2.8267894824	3.3312843315	2.1111975430
C33	1.2122464219	-.2650217856	2.5049105829
C34	1.2699967814	-.6798098968	3.9697021540
H35	-1.8010744469	4.8490589503	.8407471338
H36	-1.9235290791	4.4293144235	-1.9101365083
H37	1.0246910244	1.7767204871	-5.3343318276
H38	-.9287647304	.5713366726	-6.2399650310
H39	-2.9603921581	.2725843044	-4.8689752090
H40	-2.3974382950	1.8892823002	5.0705863629
H41	-.3773059695	2.9126845451	6.0510262999
H42	1.3799114699	3.8472393618	4.5925617208
H43	1.1966355243	3.0820445292	-1.8093990208
H44	.3923743363	4.9065676096	-3.3116663975
H45	2.1526131099	4.9642697644	-3.1152624585
H46	1.4462344897	4.3162025578	-4.6046827654
H47	2.9082763307	2.1356044379	-4.1721151583
H48	3.4778349513	2.8583402746	-2.6669001862
H49	2.6982044714	1.2699712766	-2.6408918176
H50	-3.3201510023	1.6659465955	-1.3819154366
H51	-4.4603569756	2.8547983724	-3.2599138487
H52	-4.8828695627	1.3009082126	-3.9923127515
H53	-5.5474727537	1.7396646295	-2.4145572739
H54	-2.9414873713	-.7664498533	-1.4002207409
H55	-3.8717960934	-.9366485551	-2.9006221866
H56	-4.6755141591	-.4107400273	-1.4138224291
H57	1.1928934356	3.8293170429	.8354843212
H58	-5.2202020959	1.9754596329	2.3707095958
H59	-4.2560724296	3.4575347326	2.4922481051
H60	-4.4850702005	2.4307084223	3.9132601532
H61	-2.3193545303	-.4323603393	2.6091310203
H62	-4.0844760587	-.3176789624	2.3827276863
H63	-3.3660278408	.0391009960	3.9578250239
H64	-2.9902042878	1.6178222093	1.3640669566
H65	2.2782841967	5.9720761098	1.4423229620
H66	.5651702656	6.0103267036	1.9015718161
H67	1.8076757584	5.7631267140	3.1357980280
H68	3.5719999886	3.7764080642	1.4438254464
H69	3.1769408468	3.4775924565	3.1389642981
H70	2.7806233188	2.2565701366	1.9152492500
H71	2.2990957360	-.6374794540	4.3293874837
H72	.8918916829	-1.7027405613	4.0685981987

H73	.6291929600	-.0296148419	4.5734256769
074	.5029602276	-1.9764284005	-.3224227604
H75	.0904009277	-.4644733121	-1.7083062620
C76	.5460398155	-1.6926828620	-1.6236526250
C77	-.4876854906	-2.4383829180	-2.4772638648
C78	1.9436703557	-1.5606059953	-2.2159699347
H79	-.1186430135	-3.4539488583	-2.6535251311
H80	-.6723729687	-1.9578765563	-3.4401078201
H81	-1.4242890555	-2.5023169194	-1.9221200427
C82	2.1818091893	-1.6643548300	-3.5923188602
C83	3.4826071598	-1.5762281439	-4.0945815782
C84	4.5554916210	-1.3798205347	-3.2258342229
C85	4.3211894920	-1.2667316874	-1.8518689831
C86	3.0247575539	-1.3548639266	-1.3452793957
H87	1.3589918951	-1.8149836958	-4.2831108129
H88	3.6553558420	-1.6640627526	-5.1644082664
H89	5.5677975667	-1.3120378718	-3.6163168343
H90	5.1511762727	-1.1067909702	-1.1694430904
H91	2.8375228997	-1.2597305961	-.2799060763

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Pd1	0.7400148658	1.1053154546	3.7816157697
02	-0.5980415309	-0.5310420451	3.1992100151
03	-2.0216638884	-0.1217455775	4.9061092072
C4	2.3410304339	-0.0090046801	4.0713196930
N5	2.8943967045	-0.4042926061	5.2547987715
N6	3.1605949069	-0.5375613740	3.1155306662
C7	4.0387404868	-1.1684054907	5.0376369547
C8	4.2059093889	-1.2510391476	3.6966184091
C9	3.0092671491	-0.3848347026	1.6845296393
C10	3.5603001400	0.7533657554	1.0614776933
C11	3.4484399928	0.8447814088	-0.3321401288
C12	2.8229919041	-0.1548342927	-1.0690419406
C13	2.2911016285	-1.2691172065	-0.4268960008
C14	2.3671722155	-1.4121382367	0.9638503419
C15	2.4160827429	-0.0575998742	6.5754351495
C16	1.5118838518	-0.9253032633	7.2214235209
C17	1.1153353417	-0.5859662591	8.5204022219
C18	1.5980880683	0.5583601409	9.1469437173
C19	2.4920607463	1.3943433640	8.4863197820
C20	2.9218914848	1.1083288214	7.1851534325
C21	4.2893264859	1.8512596072	1.8311245135
C22	5.7962131304	1.8465306652	1.5040128697
C23	3.6661569516	3.2368392664	1.5804893500
C24	1.8057421601	-2.6623811818	1.6376794935
C25	2.7634061528	-3.8588956765	1.4514327828
C26	0.3891997269	-3.0098606639	1.1482848784
C27	1.0116276614	-2.2158576448	6.5754947404
C28	1.8748925421	-3.4136731924	7.0289795836
C29	-0.4777782761	-2.4885771446	6.8485783688
C30	3.9297620612	2.0279882518	6.5012633941
C31	5.3294234190	1.8686278484	7.1295144231
C32	3.4817617243	3.5006942411	6.5159739347
C33	-1.7075866287	-0.6823208190	3.8355037824
C34	-2.6925226070	-1.6570513192	3.1851920165
H35	4.6141328522	-1.5725253571	5.8544233683
H36	4.9580934249	-1.7418081347	3.1002104683
H37	3.8624388072	1.7084026464	-0.8444786225
H38	2.7503803272	-0.0664575446	-2.1500869144
H39	1.8054931844	-2.0414236955	-1.0142865042
H40	0.4165624239	-1.2265849542	9.0475099170



H41	1.2761734142	0.7987741742	10.1568380830
H42	2.8656203481	2.2818706418	8.9881392989
H43	4.1833363399	1.6453646366	2.8990984998
H44	6.2536617721	0.8773123875	1.7308114743
H45	6.3182365880	2.6115652717	2.0894585275
H46	5.9758270327	2.0575248682	0.4433315920
H47	3.7539883723	3.5396493031	0.5308814603
H48	4.1766229182	3.9944139826	2.1855577715
H49	2.6071394615	3.2392633053	1.8521326459
H50	1.7217876862	-2.4567469808	2.7081052821
H51	3.7635799784	-3.6489034099	1.8466559449
H52	2.8737002259	-4.1122972868	0.3908546404
H53	2.3763196018	-4.7443809417	1.9691500358
H54	-0.2838917570	-2.1664502343	1.3153249275
H55	0.3735712136	-3.2858116376	0.0880570757
H56	0.0064558251	-3.8693808915	1.7107108017
H57	4.0014198801	1.7301241160	5.4521777443
H58	1.5329766024	-4.3358653312	6.5446939266
H59	2.9332384386	-3.2758853905	6.7810858718
H60	1.8036043438	-3.5574933851	8.1131728439
H61	-1.0999940190	-1.6445270833	6.5414899666
H62	-0.7963337602	-3.3699467192	6.2792728543
H63	-0.6681347498	-2.7071244239	7.9048922339
H64	1.1225585484	-2.1113322072	5.4927970848
H65	6.0582107098	2.5010131601	6.6110640985
H66	5.6794002055	0.8322956996	7.0721394650
H67	5.3249479187	2.1582759114	8.1865677726
H68	4.1984203765	4.1176069338	5.9633608314
H69	3.4219180199	3.9028827344	7.5335791513
H70	2.5018565522	3.6136127691	6.0432676332
H71	-3.6370207384	-1.6707920974	3.7321670127
H72	-2.8711321978	-1.3725205040	2.1435677867
H73	-2.2659713434	-2.6658524271	3.1742857474
O74	-0.8602079800	2.4877044741	3.3670987915
H75	1.7083303694	2.2593673831	4.1248321339
C76	-1.6325143567	3.0281804219	4.1756954627
C77	-1.4290191837	2.8371886839	5.6480213754
C78	-2.7743099042	3.8067995201	3.6210352193
H79	-1.6720919864	1.7804623442	5.8332119264
H80	-0.3675636910	2.9674395384	5.8840824729
H81	-2.0408624489	3.4808028993	6.2775747395
C82	-3.5804568870	4.6441912161	4.4112680151
C83	-4.6267073378	5.3612141722	3.8354451514
C84	-4.8888235057	5.2422323412	2.4702888413
C85	-4.0985999765	4.4053120297	1.6765733842
C86	-3.0468103282	3.6969625802	2.2449400027
H87	-3.3900590430	4.7494984208	5.4731860837
H88	-5.2402149102	6.0102195223	4.4539522856
H89	-5.7065155833	5.7993350666	2.0238794403
H90	-4.3060103293	4.3073157654	0.6150916658
H91	-2.4211294139	3.0437888224	1.6452873686

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C1	.0058499949	.0365523689	-.1637446245
C2	-.0646513017	.0369785107	1.2432078977
C3	1.0782315523	-.0151359924	2.0663533566
C4	2.3246558436	-.0620175491	1.4307436725
C5	2.4258881655	-.0621305383	.0430782774
C6	1.2788356306	-.0160488229	-.7433145811
N7	-1.3640544055	.0564894863	1.8737838063
C8	-2.0379051815	1.1799135111	2.2555875202

N9	-3.1796637936	.7100344577	2.8362611008
C10	-3.2113903349	-.6813585831	2.8225818334
C11	-2.0708400552	-1.0922151389	2.2180239823
C12	-4.2066202936	1.5235402909	3.4463979605
C13	-5.2742997481	1.9807518447	2.6494576025
C14	-6.2695948558	2.7358924207	3.2805450119
C15	-6.2038849987	3.0195389239	4.6409829554
C16	-5.1391064307	2.5504463592	5.4038988173
C17	-4.1147722208	1.7897880576	4.8275488462
Pd18	-1.4727163780	3.0666087572	2.0290971133
H19	-2.1317378001	2.8549080293	.6694190224
C21	-5.3832563997	1.6781415518	1.1574922692
C22	-5.4310265829	2.9690609942	.3174674767
C23	-2.9703531779	1.2805400490	5.7006619290
C24	-2.1990551320	2.4374345742	6.3647444739
C25	1.0048255441	-.0486994289	3.5910260281
C26	1.7576017494	1.1337863212	4.2306216903
C27	-1.2328870125	.0733319175	-1.0534529767
C28	-1.2051507211	1.2674708943	-2.0259908304
O29	-.3599309862	3.9821587628	3.8252716804
C30	-.2751670821	5.0529444989	3.1423061230
C31	.4044224651	6.2685076744	3.7285051082
O32	-.7715354500	5.1127477407	1.9668716013
C33	-6.5957549659	.7715283840	.8632022228
C34	-3.4822394379	.2721739024	6.7498240117
C35	1.5140428346	-1.3988864006	4.1360530951
C36	-1.4092919770	-1.2592937533	-1.8084762523
H38	-1.6897953635	-2.0779801602	2.0053320111
H39	-4.0349303128	-1.2336409807	3.2453266963
H40	-7.1057493374	3.1086491169	2.6963662306
H41	-6.9859540550	3.6109669639	5.1092871491
H42	-5.0985360556	2.7793664621	6.4647936603
H43	3.2272999117	-.0991041624	2.0333156294
H44	3.4041482254	-.0988510248	-.4284641841
H45	1.3714587590	-.0173551866	-1.8255534419
H46	-4.4848185780	1.1324432818	.8557360858
H47	-6.5400949241	-.1670878197	1.4254390204
H48	-6.6406751543	.5254670618	-.2038734971
H49	-7.5377884170	1.2634965089	1.1303601464
H50	-6.3222502201	3.5654481321	.5420207259
H51	-5.4577230336	2.7251566141	-.7506382084
H52	-4.5493154566	3.5881092661	.5058608433
H53	-2.2614837743	.7493138625	5.0589703896
H54	-3.9984858737	-.5729138845	6.2811436052
H55	-4.1833152648	.7426791908	7.4483156045
H56	-2.6463962457	-.1245953530	7.3366178476
H57	-1.7645655191	3.1069302500	5.6171750683
H58	-2.8466425246	3.0237400686	7.0266549463
H59	-1.3816296855	2.0381125184	6.9759697393
H60	-2.1072160393	.2028317996	-.4100606518
H61	1.4078736704	-1.4345416204	5.2261939615
H62	.9557179074	-2.2413977196	3.7136836313
H63	2.5731960273	-1.5520990812	3.9005849223
H64	1.3331200954	2.0906517458	3.9146215733
H65	1.6819912375	1.0773941505	5.3221324658
H66	2.8229681578	1.1197685082	3.9741307642
H67	-.0446838328	.0455764013	3.8844739653
H68	-2.3307392819	-1.2461654048	-2.4004237293
H69	-1.4644561284	-2.1074026719	-1.1174305309
H70	-.5741376693	-1.4424650290	-2.4932321049
H71	-.3734339935	1.1941001023	-2.7353956034
H72	-1.1067726180	2.2115485629	-1.4826253936

H73	.5318040845	7.0449891278	2.9734405197
H74	-.2063760839	6.6592129923	4.5489195143
H75	1.3739769287	5.9854483953	4.1477428789
H91	-2.1328910506	1.3014745905	-2.6086868319

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C1	.0879448383	.1054997669	.1340298539
C2	.0492024567	-.0604785709	1.5323036496
C3	1.2086074699	-.2311996437	2.3138090371
C4	2.4396254411	-.2362971207	1.6476248183
C5	2.5089739293	-.0811579694	.2663003916
C6	1.3463380040	.0876719660	-.4794681992
N7	-1.2361060195	-.0901467125	2.1886132437
C8	-1.8653225425	.9908800734	2.7418846662
N9	-3.0316902955	.4713170964	3.2323832350
C10	-3.1200490269	-.8958966688	2.9944538489
C11	-1.9889750034	-1.2493218248	2.3366412392
C12	-4.0547498068	1.2207137864	3.9220668878
C13	-5.1406537384	1.7226855178	3.1784672672
C14	-6.1375424592	2.4092834464	3.8814933738
C15	-6.0543545676	2.5882041297	5.2589292446
C16	-4.9672526232	2.0841168929	5.9669229423
C17	-3.9422911385	1.3877826750	5.3164315155
Pd18	-1.2283651852	2.9021242987	2.7790285550
H19	-1.8486201315	3.2143631561	1.4295172049
C21	-5.2611646146	1.5482211402	1.6669594781
C22	-5.2945573104	2.9078919031	.9409971843
C23	-2.7570005914	.8571036489	6.1184270078
C24	-1.9499819797	2.0100320640	6.7470741897
C25	1.1649992692	-.3928191374	3.8309924519
C26	1.8555413231	.7909788590	4.5368589172
C27	-1.1684895092	.2910376770	-.7125159964
C28	-1.1317448642	1.6096916788	-1.5096007861
O29	-.6407804303	4.9000276303	2.6368665548
C30	-1.0213234090	5.4947534210	1.5563926744
C31	-.6201297845	6.9597198317	1.4506722779
O32	-1.6879749652	4.9665097661	.6386399152
C33	-6.4874806110	.6874239666	1.3012392359
C34	-3.2019850939	-.1610357750	7.1859978939
C35	1.7677089507	-1.7386284947	4.2780820542
C36	-1.3937808160	-.9195391932	-1.6414763203
H38	-1.6484524571	-2.2016414030	1.9629024467
H39	-3.9709364831	-1.4757641581	3.3140490047
H40	-6.9875295420	2.8137331191	3.3399109994
H41	-6.8392842227	3.1265609866	5.7834571218
H42	-4.9109967019	2.2361897333	7.0408074936
H43	3.3548783799	-.3610175376	2.2188690392
H44	3.4748361766	-.0895604394	-.2316049492
H45	1.4148221894	.2136539904	-1.5558105593
H46	-4.3727726256	1.0169589732	1.3142360831
H47	-6.4540027535	-.2919831471	1.7910498557
H48	-6.5301005327	.5232915284	.2189092257
H49	-7.4222847065	1.1752549489	1.5986808443
H50	-6.1687729166	3.4995404817	1.2354857753
H51	-5.3505785968	2.7543544836	-.1423445485
H52	-4.3974211912	3.4963653830	1.1526706057
H53	-2.0885490124	.3324714261	5.4301859980
H54	-3.7442774733	-.9990684227	6.7356246224
H55	-3.8592643802	.2979079076	7.9324874065
H56	-2.3322409005	-.5654530895	7.7154089100
H57	-1.6165798361	2.7208352814	5.9834799923

H58	-2.5472771998	2.5654850980	7.4781374663
H59	-1.0662189943	1.6211915570	7.2652760871
H60	-2.0267172041	.3489474815	-.0371782157
H61	1.6833471843	-1.8535706943	5.3642706604
H62	1.2528505492	-2.5825590457	3.8071919809
H63	2.8296595105	-1.8107768454	4.0202441278
H64	1.4064082811	1.7443659015	4.2381965142
H65	1.7653946724	.6932087145	5.6246912575
H66	2.9228488830	.8364829836	4.2935028796
H67	.1168984010	-.3883989711	4.1436401862
H68	-2.3219598049	-.7972618056	-2.2103597413
H69	-1.4639283684	-1.8551892401	-1.0758360253
H70	-.5750046405	-1.0281078129	-2.3614980755
H71	-.3095797071	1.6211803333	-2.2337653517
H72	-1.0168793943	2.4737156542	-.8490312331
H73	-.7598393691	7.3236122075	.4320357850
H74	-1.2474084165	7.5487411452	2.1285747532
H75	.4180974052	7.0940016263	1.7652950348
H91	-2.0647836553	1.7350109331	-2.0701127954

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Pd1	.5725504545	1.4531898732	5.4040787870
C4	2.2012626922	.4645618387	4.7016871634
N5	3.2236888275	.0414061619	5.5172281182
N6	2.6056442034	.0404850271	3.4597541813
C7	4.2183886529	-.6243193230	4.8080408194
C8	3.8299746064	-.6248071805	3.5113535588
C9	1.8700451544	.2053711488	2.2324200673
C10	2.1844890032	1.2942477273	1.3949093738
C11	1.4923250692	1.3992426580	.1821633975
C12	.5330907895	.4585193061	-.1816722070
C13	.2476536826	-.6114424831	.6613001125
C14	.9109187907	-.7664614110	1.8843422596
C15	3.2411486528	.2156934762	6.9473673927
C16	2.6926715284	-.8017930467	7.7541888385
C17	2.7314777920	-.6186749669	9.1411471491
C18	3.2893794922	.5282337384	9.6987434326
C19	3.8223745906	1.5182324953	8.8784186390
C20	3.8124036160	1.3859022405	7.4850076395
C21	3.2509398830	2.3270967614	1.7518536909
C22	4.4239493788	2.2876058125	.7518499076
C23	2.6588760108	3.7451209099	1.8555577442
C24	.6019832015	-1.9724794424	2.7674410032
C25	.9852718963	-3.2889915407	2.0621786775
C26	-.8692769428	-1.9860181612	3.2216368006
C27	2.0537344382	-2.0590292216	7.1701290238
C28	2.7741170886	-3.3361238624	7.6429094000
C29	.5455444282	-2.1136897914	7.4833816190
C30	4.3820022411	2.4971721341	6.6083122689
C31	5.8642639757	2.7739675247	6.9223708514
C32	3.5326868957	3.7784874346	6.7204795490
H35	5.0949685689	-1.0267176864	5.2902785307
H36	4.2976537081	-1.0277732764	2.6272158297
H37	1.7113572113	2.2263819172	-.4874889827
H38	.0093377819	.5568407364	-1.1290564535
H39	-.4997459465	-1.3419461353	.3651892044
H40	2.3129889552	-1.3814209299	9.7917673538
H41	3.3068445896	.6521648996	10.7783023371
H42	4.2473339782	2.4121521985	9.3259311685
H43	3.6502355772	2.0734143963	2.7374799427
H44	4.8729505958	1.2900000272	.6994729211

H45	5.2056590779	2.9952468652	1.0499460964
H46	4.0998122138	2.5586365205	-.2592330789
H47	2.2215393352	4.0725192668	.9055047712
H48	3.4390803932	4.4655372214	2.1261944989
H49	1.8804010988	3.7843179974	2.6221801140
H50	1.2137877327	-1.8948233070	3.6696499476
H51	2.0409274697	-3.2948872825	1.7697970994
H52	.3886652585	-3.4500556449	1.1573282189
H53	.8139186474	-4.1427826798	2.7273387955
H54	-1.1154801621	-1.0764637955	3.7756151330
H55	-1.5566483002	-2.0616410692	2.3719013698
H56	-1.0539288499	-2.8470031689	3.8748078749
H57	4.3261973611	2.1649055977	5.5683480897
H58	2.3338320905	-4.2205861806	7.1692987624
H59	3.8392638708	-3.3117445701	7.3887564131
H60	2.6941956725	-3.4689665261	8.7274408921
H61	.0365504162	-1.2262012811	7.0936782328
H62	.0930276893	-2.9996578767	7.0229968863
H63	.3610341520	-2.1672385900	8.5621611373
H64	2.1533026914	-2.0150626065	6.0824039994
H65	6.2615613950	3.5330432355	6.2393377660
H66	6.4728619992	1.8697597558	6.8143558130
H67	6.0004759176	3.1472522161	7.9432122180
H68	3.9218644148	4.5539771427	6.0503569120
H69	3.5456749825	4.1791541066	7.7402743392
H70	2.4923853467	3.5736499445	6.4466927036
O74	-1.1008521262	2.5690981200	6.0940143813
C76	-1.2162785475	2.7597694930	4.8363584032
C77	-.7325932318	4.0731075368	4.2453921445
C78	-2.2054546967	1.9491105935	4.0583527115
H79	.0376237691	4.4962420222	4.8911221836
H80	-.3347853781	3.9623307093	3.2347375473
H81	-1.5778210619	4.7752859564	4.1936956213
C82	-2.3512219074	2.0676323601	2.6657341311
C83	-3.3165487493	1.3240274637	1.9872030414
C84	-4.1597466329	.4600050618	2.6866946948
C85	-4.0287086982	.3403720086	4.0737583006
C86	-3.0603424452	1.0735632751	4.7525440246
H87	-1.6976109168	2.7246698314	2.1017540962
H88	-3.4097932303	1.4215345998	.9087354662
H89	-4.9156484243	-.1139805500	2.1571123709
H90	-4.6850204489	-.3271207062	4.6261037311
H91	-2.9468776143	.9911410427	5.8285112422

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Pd1	-.2991111291	-.0648293993	.1125743832
C4	.0044754908	.0557638048	2.1283618305
N5	1.1957709992	.0659273968	2.8135165080
N6	-.9265504089	.0584022352	3.1389888032
C7	1.0067029062	.0782305997	4.1937772810
C8	-.3318932940	.0740065373	4.3996590064
C9	-2.3513756850	.1018269021	2.9338696927
C10	-3.0597614238	-1.1094086085	2.8135480130
C11	-4.4472455893	-1.0342728894	2.6434844342
C12	-5.1003899828	.1938358922	2.5948201672
C13	-4.3756433963	1.3763377727	2.7094044294
C14	-2.9860283021	1.3590415362	2.8776639996
C15	2.4918291919	.1005752761	2.1873261939
C16	3.0673077359	1.3534935309	1.8969473105
C17	4.3340883862	1.3620992323	1.3011356688
C18	4.9959178590	.1747293041	1.0021464669

C19	4.4017492931	-1.0495927123	1.2947789405
C20	3.1386176432	-1.1155569740	1.8945857653
C21	-2.3698578296	-2.4698106568	2.8487964628
C22	-2.9114839576	-3.3545439554	3.9877214634
C23	-2.4737075699	-3.1787198304	1.4844557271
C24	-2.2148423491	2.6732548114	2.9616590177
C25	-2.6757125016	3.5327317041	4.1541837294
C26	-2.3084250594	3.4527327132	1.6349859040
C27	2.3561619351	2.6725227799	2.1856868822
C28	3.1554777490	3.5441404929	3.1732015549
C29	2.0483789173	3.4352222958	.8824164397
C30	2.5001287580	-2.4721150381	2.1771881774
C31	3.3804947952	-3.3454119206	3.0904496380
C32	2.1526729379	-3.2003958825	.8642907846
H35	1.8338855518	.0863539291	4.8856687466
H36	-.9133722580	.0778319954	5.3079447696
H37	-5.0229704884	-1.9504178504	2.5447992436
H38	-6.1790205643	.2295661537	2.4653031565
H39	-4.8956815112	2.3290549749	2.6602632601
H40	4.8039565934	2.3120944589	1.0614612361
H41	5.9774932113	.2038063909	.5360982818
H42	4.9246218523	-1.9696679765	1.0487497737
H43	-1.3071557732	-2.3013329087	3.0403160225
H44	-2.8108852980	-2.8609748059	4.9602383042
H45	-2.3615882776	-4.3012876136	4.0303942249
H46	-3.9708764223	-3.5953091208	3.8453624553
H47	-3.5168073703	-3.3753399759	1.2111787774
H48	-1.9485724761	-4.1405085824	1.5116543041
H49	-2.0211944502	-2.5607497481	.7023497783
H50	-1.1596557894	2.4362066753	3.1201582376
H51	-2.5805755234	2.9887479299	5.1000536868
H52	-3.7219517866	3.8412741905	4.0517357164
H53	-2.0697084445	4.4428983041	4.2253553853
H54	-1.9316549621	2.8480557207	.8042971099
H55	-3.3428045200	3.7381262508	1.4109685389
H56	-1.7139017990	4.3722527453	1.6899812323
H57	1.5588532565	-2.2960336837	2.7036678884
H58	2.6044707620	4.4622152294	3.4061650431
H59	3.3426359372	3.0146101641	4.1135477026
H60	4.1261674813	3.8385043091	2.7586868160
H61	1.4353731935	2.8241770295	.2129730512
H62	1.5015420435	4.3594965625	1.1028229741
H63	2.9670686522	3.7110571556	.3518099328
H64	1.3964855865	2.4422987304	2.6553159183
H65	2.8665390931	-4.2831406695	3.3291969918
H66	3.6100065379	-2.8362521358	4.0325161849
H67	4.3313852079	-3.6053315908	2.6124209196
H68	1.6719074849	-4.1627473008	1.0755484862
H69	3.0498634571	-3.3979726359	.2662844646
H70	1.4637816341	-2.5938226181	.2672336823
C78	.1407842419	-.3945449389	-2.1333683173
C82	-1.2601090439	-.4490937477	-1.9249936740
C83	-2.0473056326	.6986262333	-2.1911246654
C84	-1.4543787894	1.8545354738	-2.6810616279
C85	-.0647037867	1.9066138767	-2.8931693520
C86	.7296261105	.8030412860	-2.6079789757
H87	-1.7475529101	-1.3984616408	-1.7205727798
H88	-3.1223317313	.6545530356	-2.0399150723
H89	-2.0666976943	2.7238332977	-2.9064012121
H90	.3880662976	2.8163253966	-3.2793450520
H91	1.8018975643	.8388669470	-2.7782108383
H92	.7402034532	-1.2988184366	-2.0791825538

triplet 18

Pd1	0.5817262198	1.4707963978	5.2653636882
C4	2.2814588659	0.4496532121	4.8114845011
N5	3.2877063482	0.0268679328	5.6382501863
N6	2.6773413834	0.0086165705	3.5767271955
C7	4.2761103749	-0.6582075408	4.9368511382
C8	3.8909957297	-0.6686069964	3.6371726386
C9	1.9263603884	0.2146044554	2.3617802385
C10	2.1782290168	1.3717689139	1.5988060470
C11	1.4281054659	1.5503331038	0.4308233948
C12	0.4718554686	0.6176369406	0.0407569303
C13	0.2473667391	-0.5190336772	0.8111013304
C14	0.9680846873	-0.7483789588	1.9888481636
C15	3.3166159735	0.2386242325	7.0649248249
C16	2.7175021367	-0.7244097370	7.9008236677
C17	2.7761408049	-0.5056247429	9.2821051848
C18	3.4015590818	0.6219236206	9.8063232882
C19	3.9821744487	1.5597795398	8.9577136215
C20	3.9539207029	1.3905531086	7.5677625114
C21	3.2041190310	2.4240328828	2.0114841092
C22	4.2769278105	2.6333056161	0.9259858505
C23	2.5158885487	3.7521735147	2.3814927818
C24	0.6855545667	-1.9968678741	2.8201209005
C25	0.9349641617	-3.2857626554	2.0129416759
C26	-0.7417873679	-1.9672634728	3.4002955238
C27	2.0082590726	-1.9605743225	7.3542481877
C28	2.6532527951	-3.2623275701	7.8657022993
C29	0.5004246980	-1.9189735417	7.6677353941
C30	4.5788161298	2.4448289224	6.6585072194
C31	6.0767177883	2.6451076285	6.9576111079
C32	3.8061995157	3.7759006571	6.7424366717
H35	5.1459467734	-1.0665215210	5.4260946075
H36	4.3567469283	-1.0870844475	2.7592612384
H37	1.5893515719	2.4363644372	-0.1761797697
H38	-0.1036202188	0.7791017803	-0.8667313401
H39	-0.5057136511	-1.2366471240	0.4984973754
H40	2.3214098217	-1.2263234128	9.9554396222
H41	3.4341748489	0.7718931245	10.8820911163
H42	4.4606507647	2.4392654241	9.3785769412
H43	3.7168867577	2.0655899834	2.9086464589
H44	4.7830460360	1.6948004422	0.6761075232
H45	5.0342921216	3.3453744638	1.2720737782
H46	3.8457103796	3.0347253594	0.0025539478
H47	1.9865014704	4.1799585712	1.5230551479
H48	3.2574055296	4.4862059256	2.7172535766
H49	1.7892561819	3.6033712699	3.1861861413
H50	1.3779025800	-2.0049716509	3.6667565564
H51	1.9576439581	-3.3224065575	1.6221306913
H52	0.2502715322	-3.3684356887	1.1616911644
H53	0.7817171040	-4.1671375441	2.6453156443
H54	-0.8975914775	-1.0704293179	4.0078005971
H55	-1.4965682223	-1.9728462506	2.6063888085
H56	-0.9152441419	-2.8462865414	4.0312352098
H57	4.4987711271	2.0903975674	5.6275703722
H58	2.1623116355	-4.1324790452	7.4164470753
H59	3.7175348135	-3.3071154077	7.6134806483
H60	2.5644873741	-3.3586558245	8.9529062961
H61	0.0404455498	-1.0192579104	7.2473694664
H62	-0.0025837071	-2.7927630395	7.2383981427
H63	0.3145582193	-1.9236928396	8.7471298473

H64	2.1089660667	-1.9553761489	6.2657988608
H65	6.5124856611	3.3614415610	6.2527973461
H66	6.6313108476	1.7047711256	6.8708969337
H67	6.2405506470	3.0364056624	7.9673840508
H68	4.2383715232	4.5126587926	6.0560067208
H69	3.8445756575	4.1977182174	7.7528787457
H70	2.7544630267	3.6337380534	6.4736829947
O71	-1.1804568312	2.4842917939	5.5487539516
O72	-1.6399406752	2.4146141627	4.3487641310

singlet 18

Pd1	.6342835393	1.4675316422	5.4203240066
C4	2.2705655946	.4197452855	4.7815541305
N5	3.2803236157	-.0202639257	5.5892007546
N6	2.6347724266	-.0032255913	3.5373235523
C7	4.2526344109	-.7037881029	4.8654998182
C8	3.8446270745	-.6914287021	3.5720444413
C9	1.8725788110	.2225362754	2.3304522799
C10	2.1114740600	1.3953208323	1.5885318743
C11	1.3740496825	1.5726865333	.4121610119
C12	.4398223307	.6282303012	-.0013287730
C13	.2178378942	-.5163789741	.7578673776
C14	.9265350572	-.7461714497	1.9426438588
C15	3.3026576727	.2106907470	7.0129071783
C16	2.6882595680	-.7349211761	7.8601284185
C17	2.7196688342	-.4822266945	9.2367861841
C18	3.3313989537	.6603607613	9.7450911685
C19	3.9240147395	1.5814912729	8.8858158551
C20	3.9235289695	1.3803483133	7.4997549596
C21	3.1037907443	2.4672409628	2.0290999999
C22	4.2198759098	2.6748498087	.9868793997
C23	2.3790121398	3.7901774743	2.3473381588
C24	.6324794540	-1.9917052963	2.7727804877
C25	.8876663817	-3.2857842201	1.9764636421
C26	-.8036683312	-1.9497359264	3.3318004630
C27	1.9865843445	-1.9824005307	7.3294582796
C28	2.6108717899	-3.2731914179	7.8933213275
C29	.4711965190	-1.9255566525	7.6075235556
C30	4.5537360942	2.4204403880	6.5771181714
C31	6.0424130540	2.6474500840	6.9017789563
C32	3.7626879586	3.7435572593	6.6129482854
H35	5.1277831587	-1.1244712150	5.3342107530
H36	4.2918140775	-1.1002170855	2.6801931807
H37	1.5268508716	2.4689420040	-.1817030303
H38	-.1251320532	.7893342559	-.9153586231
H39	-.5254731714	-1.2386441612	.4329005840
H40	2.2526330504	-1.1872445344	9.9183156813
H41	3.3415811527	.8364463591	10.8172166865
H42	4.3877540932	2.4742087550	9.2948068958
H43	3.5804091980	2.1296071513	2.9538521964
H44	4.7573700301	1.7427261425	.7818907275
H45	4.9455296062	3.4129315529	1.3463849281
H46	3.8194025196	3.0434659810	.0362809900
H47	1.9132663870	4.2139410148	1.4509121547
H48	3.0902505036	4.5299393196	2.7327503831
H49	1.5932996176	3.6387579970	3.0932791231
H50	1.3131272560	-1.9977608718	3.6292890031
H51	1.9164967437	-3.3324691926	1.6033474965
H52	.2169890761	-3.3679618940	1.1142674661
H53	.7166067764	-4.1627769770	2.6106369970
H54	-.9740648900	-1.0358238095	3.9089781779



H55	-1.5440964841	-1.9799486192	2.5250118428
H56	-.9849854678	-2.8131769930	3.9824377341
H57	4.5011758314	2.0411469073	5.5529953133
H58	2.1263796409	-4.1516733063	7.4537483050
H59	3.6815119419	-3.3301598196	7.6712561073
H60	2.4914940200	-3.3407695921	8.9797439970
H61	.0197247621	-1.0380952329	7.1513361994
H62	-.0261081634	-2.8091769493	7.1927183056
H63	.2616036745	-1.8978874161	8.6822764757
H64	2.1152982559	-2.0077361730	6.2438503459
H65	6.4823899495	3.3519919654	6.1877715537
H66	6.6105501675	1.7127372458	6.8493068702
H67	6.1804816800	3.0662161333	7.9043281147
H68	4.2028861196	4.4696208115	5.9204752111
H69	3.7719216150	4.1882813438	7.6142579012
H70	2.7185917483	3.5870424206	6.3211805840
071	-1.1065270003	2.5253793614	5.5343324508
072	-.8476399417	2.2141889436	4.2408932598

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Pd1	.2191072166	-.2610563840	-.0479437432
C4	.0620902873	.0721480034	1.9938472607
N5	1.0728632051	.0957918424	2.9202835485
N6	-1.0725602004	.1042880755	2.7616763528
C7	.5784683567	.1363523834	4.2215500277
C8	-.7714291311	.1455622494	4.1204669476
C9	-2.4329090812	.0445177493	2.2737477757
C10	-3.0448779486	-1.2186776908	2.1313521159
C11	-4.3819642067	-1.2417102195	1.7192520770
C12	-5.0801883608	-.0654901542	1.4654405282
C13	-4.4545578332	1.1667993245	1.6213290507
C14	-3.1177927216	1.2506223074	2.0288389925
C15	2.4811806400	.0277557121	2.6099516033
C16	3.2271721135	1.2264917985	2.6014565406
C17	4.5948595670	1.1348745980	2.3179955687
C18	5.1911793746	-.0946439737	2.0496931107
C19	4.4339887661	-1.2612922840	2.0725325867
C20	3.0623644063	-1.2324156512	2.3595263928
C21	-2.3273930382	-2.5234406294	2.4667709589
C22	-2.7344697869	-3.0115243876	3.8737146212
C23	-2.5596836764	-3.6231107091	1.4157531776
C24	-2.4715511136	2.6184688452	2.2265309342
C25	-3.0470370116	3.3267582258	3.4693032584
C26	-2.6046251120	3.5049694759	.9747880700
C27	2.5990761407	2.5815616175	2.9277067296
C28	2.9354692315	3.0054537802	4.3726953879
C29	3.0026313866	3.6920932515	1.9394054698
C30	2.2817515078	-2.5414937649	2.4532349823
C31	2.7140117523	-3.3271466315	3.7095224332
C32	2.4054352394	-3.4014792651	1.1820327489
H35	1.2287158405	.1460183013	5.0812836691
H36	-1.5418534951	.1746392834	4.8739872876
H37	-4.8831851072	-2.1962857965	1.5960557111
H38	-6.1183611118	-.1101151123	1.1473261568
H39	-5.0125562646	2.0782213902	1.4269839246
H40	5.1998773396	2.0363221898	2.3045361533
H41	6.2536437411	-.1428308823	1.8268126657
H42	4.9131779418	-2.2144397863	1.8717248515
H43	-1.2530920371	-2.3211243092	2.4788655110
H44	-2.5160519409	-2.2652849469	4.6451360859
H45	-2.1947809941	-3.9294740314	4.1313309139

H46	-3.8076977649	-3.2299438867	3.9168970309
H47	-3.6058907273	-3.9486162191	1.3856118032
H48	-1.9566923955	-4.5024880079	1.6669603453
H49	-2.2611138283	-3.2786539088	.4227916475
H50	-1.4029960890	2.4637984727	2.4015171569
H51	-2.9043543842	2.7267368996	4.3742218423
H52	-4.1217146752	3.5082660149	3.3577062261
H53	-2.5574985662	4.2945955860	3.6246787879
H54	-2.2109606276	2.9932220556	.0920702270
H55	-3.6476879299	3.7689435395	.7705833788
H56	-2.0509431009	4.4409629607	1.1088189967
H57	1.2228369280	-2.2985346297	2.5676682287
H58	2.4488934130	3.9559298922	4.6181733063
H59	2.6041577291	2.2592272856	5.1015638901
H60	4.0156958064	3.1365339928	4.4993777771
H61	2.7756882833	3.4199880117	.9051127703
H62	2.4583543035	4.6139455211	2.1726688537
H63	4.0711960656	3.9250163590	1.9979055232
H64	1.5126081020	2.4694145964	2.8629749081
H65	2.1147321849	-4.2383812612	3.8130402227
H66	2.5866194096	-2.7327724055	4.6212869448
H67	3.7669416266	-3.6247429850	3.6514379620
H68	1.8391068173	-4.3305701468	1.3097346431
H69	3.4453548554	-3.6776753521	.9740988520
H70	1.9902336516	-2.8835105523	.3137010255
C78	.7007980787	2.0794639136	-.8645789235
C82	1.9106804833	1.3629693618	-.9724822030
C83	2.3170237572	.8682258812	-2.2270078596
C84	1.5288443312	1.0796116003	-3.3496439963
C85	.3200716717	1.7840143445	-3.2415844461
C86	-.0916632545	2.2816052079	-2.0122489963
H87	2.5734714922	1.2716410276	-.1188532177
H88	3.2489027876	.3173077200	-2.3078436522
H89	1.8420314804	.6893376297	-4.3135365639
H90	-.2960418191	1.9388357229	-4.1226691325
H91	-1.0189584847	2.8414483241	-1.9336070573
H92	.4312957881	2.5600449849	.0700082661
O93	-.3993564281	-2.1412350790	-.5550927839
O94	.0486490304	-1.4886585562	-1.6730940153

20

C1	.2064083638	.3582372810	.1737199616
C2	.0796868644	.3405811282	1.5775444114
C3	1.1795694855	.4509373194	2.4501137300
C4	2.4457031715	.5960277869	1.8701954368
C5	2.6036770754	.6228597202	.4885259550
C6	1.4971630477	.5015638743	-.3478808324
N7	-1.2346215691	.1535367064	2.1514556984
C8	-2.0874756525	1.1447613231	2.5288097658
N9	-3.1739741492	.4989733749	3.0321612398
C10	-2.9968477075	-.8799256367	2.9798939092
C11	-1.7783926619	-1.0971377283	2.4280324229
C12	-4.3529543016	1.1319081150	3.5831969824
C13	-5.4260303193	1.4323644243	2.7183285486
C14	-6.5660800837	2.0024573197	3.2959094709
C15	-6.6315115618	2.2584320046	4.6632136015
C16	-5.5564756830	1.9476602857	5.4892646113
C17	-4.3887260149	1.3761199666	4.9694819445
Pd18	-1.8466834805	3.1179391349	2.3330696423
O19	-2.4725317549	2.9092565113	.4596125188
O20	-3.2335953886	4.1056734637	.2111847650

H21	-2.5417933345	4.7825800687	.1128951161
C22	-5.3856723373	1.1104498175	1.2257167566
C23	-6.0451215577	2.1939479548	.3553765315
C24	-3.2399673706	1.0099612304	5.9059603777
C25	-2.7713879839	2.2068483661	6.7518983711
C26	1.0462044663	.3766287151	3.9686827676
C27	1.6415860067	1.6132162887	4.6660357483
C28	-.9880977231	.1742945245	-.7597976481
C29	-.98868395706	1.1665792923	-1.9352984519
O30	-1.0767778496	3.8863163741	4.2065598092
C31	-1.0372293822	5.0744810830	3.7260879368
C32	-.5320750315	6.2126587595	4.5729485556
O33	-1.4108149608	5.2769752155	2.5265878362
C34	-6.0252274743	-.2686267354	.9562848632
C35	-3.6265653091	-.1870127328	6.7971913781
C36	1.6737573294	-.9254956680	4.5060890057
C37	-1.0537508841	-1.2818162633	-1.2684896843
H38	-1.2456187172	-2.0079528590	2.2083478168
H39	-3.7484084616	-1.5619536996	3.3426653392
H40	-7.4134456883	2.2525428299	2.6661955595
H41	-7.5282910517	2.7029626338	5.0868191745
H42	-5.6222423164	2.1506862043	6.5539642994
H43	3.3179811404	.6852132473	2.5110454533
H44	3.5958259423	.7356204937	.0595303279
H45	1.6368630675	.5200168615	-1.4239193353
H46	-4.3369010617	1.0726566524	.9201289773
H47	-5.5260481181	-1.0691965013	1.5127911544
H48	-5.9662765754	-.5145235618	-.1099925803
H49	-7.0825878011	-.2731082424	1.2442117674
H50	-7.1252960831	2.2631167626	.5254842494
H51	-5.9000980075	1.9502714716	-.7019418885
H52	-5.5911150555	3.1712500276	.5327831563
H53	-2.3866024514	.7014092274	5.2959348611
H54	-3.9160546877	-1.0580896013	6.2002485701
H55	-4.4703765801	.0615873144	7.4495924357
H56	-2.7844916531	-.4781824883	7.4346513448
H57	-2.4314401044	3.0250227180	6.1133510794
H58	-3.5664235473	2.5765318340	7.4076945747
H59	-1.9337466418	1.9058442551	7.3909366702
H60	-1.8973984982	.3753883530	-.1873153684
H61	1.5335171220	-.9986936385	5.5897295694
H62	1.2213662676	-1.8103285286	4.0458606569
H63	2.7503528854	-.9614006868	4.3052669458
H64	1.1322810646	2.5247596524	4.3440024814
H65	1.5188949917	1.5249600241	5.7508633554
H66	2.7134204303	1.7179490968	4.4636633418
H67	-.0182256012	.3538020243	4.2187656985
H68	-1.9338634324	-1.4261946988	-1.9050138986
H69	-1.1147368680	-2.0002836700	-.4437433442
H70	-.1658767525	-1.5315193600	-1.8608173770
H71	-.1397290629	1.0073119078	-2.6121045215
H72	-.9657830712	2.1954640425	-1.5692307219
H73	.4803063389	6.4754432973	4.2480092768
H74	-.5044593163	5.9287208543	5.6260348326
H75	-1.1646642239	7.0923688860	4.4300933810
H76	-1.9015886958	1.0397679971	-2.5238070149

3b

Pd1	0.0489636853	0.4834954252	3.7620086449
O2	-0.3158119680	-1.5829286074	3.9303404851
O3	-2.4119762632	-1.6398663184	3.0713106927

C4	1.9557002917	0.0968136867	4.1840682416
N5	2.5814012580	-0.0702990171	5.3829106115
N6	2.9108135778	-0.1506781944	3.2449420629
C7	3.9119441139	-0.4329139734	5.1874433594
C8	4.1189890516	-0.4805592307	3.8508489572
C9	2.7694333227	-0.0375652456	1.8049707714
C10	3.0981653389	1.1922921225	1.1970464920
C11	3.0298364863	1.2560520281	-0.1996428050
C12	2.6549947317	0.1500229077	-0.9540104970
C13	2.3405764486	-1.0509943734	-0.3269683657
C14	2.3913434583	-1.1773974169	1.0663476515
C15	2.0404512192	0.1490431055	6.7141242116
C16	1.4449066268	-0.9342208921	7.3911570677
C17	1.0080440007	-0.7093337549	8.7024255398
C18	1.1639046800	0.5305756037	9.3115255265
C19	1.7671618263	1.5773911552	8.6233897139
C20	2.2251574290	1.4153837788	7.3111705448
C21	3.5644562300	2.4109719441	1.9893850148
C22	5.1038190666	2.5199264240	1.9614181878
C23	2.9203752523	3.7185799555	1.4976426298
C24	2.0889277090	-2.5202997214	1.7251225814
C25	3.3448604955	-3.4175209405	1.7327904111
C26	0.9115232233	-3.2548486451	1.0599473106
C27	1.3240741257	-2.3255010389	6.7741826467
C28	2.5137783998	-3.2129557382	7.2006108845
C29	-0.0077876316	-3.0130336195	7.1205069986
C30	2.9374291992	2.5713587807	6.6099708237
C31	4.4437055001	2.5829733306	6.9558003737
C32	2.3208875795	3.9438103798	6.9401946755
C33	-1.4004722565	-2.1822668568	3.5767888425
C34	-1.4428623529	-3.6809195651	3.8233984431
H35	4.5722951778	-0.6170324637	6.0185045304
H36	4.9981282719	-0.7109786077	3.2719066567
H37	3.2739469032	2.1861828702	-0.7022315793
H38	2.6086012189	0.2234958797	-2.0373260995
H39	2.0520178116	-1.9053990257	-0.9298867893
H40	0.5422686817	-1.5181186973	9.2554249713
H41	0.8137629165	0.6825589541	10.3291358017
H42	1.8798320783	2.5395125019	9.1112311943
H43	3.2486326227	2.2786590197	3.0274054813
H44	5.5852722132	1.6249959693	2.3688931831
H45	5.4380382836	3.3792621800	2.5533545655
H46	5.4679406051	2.6557886967	0.9366689839
H47	3.2447570611	3.9857849958	0.4857497766
H48	3.2159025635	4.5433194103	2.1557554075
H49	1.8311352497	3.6421008462	1.5133210189
H50	1.7966785876	-2.3290841568	2.7610013990
H51	4.1777391939	-2.9480114966	2.2657764767
H52	3.6802503948	-3.6299754928	0.7112011640
H53	3.1306187770	-4.3736831215	2.2227215917
H54	0.0242009452	-2.6180672914	1.0011635757
H55	1.1543505839	-3.5941768512	0.0469646154
H56	0.6541602151	-4.1454205500	1.6418425924
H57	2.8346902987	2.4220608573	5.5303146416
H58	2.4387724686	-4.2049817176	6.7399322772
H59	3.4741983666	-2.7789932651	6.9036351510
H60	2.5317182487	-3.3476200063	8.2882647965
H61	-0.8583970150	-2.3825409032	6.8477865758
H62	-0.0929080917	-3.9556078009	6.5706468220
H63	-0.0869204970	-3.2545210232	8.1860582266
H64	1.3453025387	-2.2169357744	5.6871265992
H65	4.9457123924	3.4125101846	6.4449205460

H66	4.9480280066	1.6577221411	6.6624256654
H67	4.5897859597	2.7158320307	8.0340015705
H68	2.7532067098	4.7078968221	6.2847038718
H69	2.5395702812	4.2496556644	7.9696916054
H70	1.2378453890	3.9367619854	6.8009805381
H71	-2.0919717832	-3.8736662179	4.6837351953
H72	-1.8872027441	-4.1793221513	2.9588808240
H73	-0.4515932184	-4.0854663279	4.0294624667
074	-1.9729565482	0.8334238993	3.0972229633
H75	-2.5664112610	1.8432817871	4.8107083664
C76	-2.9531175087	1.6002485894	3.8167662322
H77	-3.8477348546	0.9722353540	3.9310618183
C78	-3.3059377991	2.8770338898	3.0823846749
C82	-3.9409679276	3.9114128846	3.7838369037
C83	-4.3080839946	5.0896595062	3.1337271373
C84	-4.0349523752	5.2531181658	1.7735090337
C85	-3.3922987105	4.2320089712	1.0721127483
C86	-3.0308660229	3.0481945747	1.7214606249
H87	-4.1315516332	3.7982223331	4.8493647482
H88	-4.7975179815	5.8848035803	3.6911260072
H89	-4.3146820372	6.1737566293	1.2671827317
H90	-3.1694897457	4.3550505974	0.0150794336
H91	-2.5177858835	2.2565506154	1.1846063784
H92	-2.2701458821	-0.1385653637	3.0202408790
093	0.5081542168	2.4611932872	3.5248723922
C94	-0.0165694646	3.2847468453	4.3970445276
095	-0.5876514266	2.9496913610	5.4390652816
C96	0.1133183421	4.7486119938	3.9956593937
H97	1.1066745413	4.9645581960	3.5959211819
H98	-0.0969890920	5.3882120769	4.8536485292
H99	-0.6172888934	4.9611527797	3.2083743791

TS3b

Pd1	0.1647765020	0.7511912386	4.2787302658
02	-0.6257456581	-1.2485282947	4.2551854298
03	-2.5561706111	-0.1316507236	3.9641913443
C4	2.1516425869	0.1353239959	4.3220856999
N5	2.9298318259	-0.2145481925	5.3863744405
N6	2.9445228023	-0.1054082966	3.2383340142
C7	4.1836790958	-0.6586450958	4.9734867554
C8	4.1926546816	-0.5893962293	3.6202012549
C9	2.5866660423	0.1798618383	1.8673179534
C10	2.8875551677	1.4556505630	1.3506431234
C11	2.5764907759	1.6942829720	0.0060026424
C12	1.9924199101	0.7091507023	-0.7827364209
C13	1.6972630343	-0.5396137722	-0.2417148245
C14	1.9813257131	-0.8340968245	1.0963834319
C15	2.5617610942	-0.0430946859	6.7729276508
C16	1.8954168145	-1.0914829810	7.4404578538
C17	1.5767487439	-0.8923099826	8.7883685017
C18	1.9011585343	0.2959607544	9.4378475332
C19	2.5605764208	1.3114965538	8.7540616570
C20	2.9120533020	1.1657494624	7.4060230009
C21	3.5361884712	2.5598063566	2.1820076476
C22	4.9554057556	2.8785722950	1.6699789679
C23	2.6593071020	3.8261848803	2.2308090595
C24	1.6645173834	-2.2122128045	1.6723873397
C25	2.7954376602	-3.2131696027	1.3553808880
C26	0.3081241283	-2.7590742697	1.1945556716
C27	1.5689000654	-2.4131013597	6.7494780288
C28	2.6975921510	-3.4394194532	6.9828447316

C29	0.2123150284	-2.9967119157	7.1770180747
C30	3.6448426379	2.2987455185	6.6907763668
C31	4.9788607816	2.6338688576	7.3868297197
C32	2.7549405139	3.5497647191	6.5550078489
C33	-1.8910520875	-1.2035809503	4.0925700479
C34	-2.6477221497	-2.5157680019	4.0600999073
H35	4.9406585446	-0.9645559686	5.6775366486
H36	4.9585792347	-0.8243028922	2.8989160799
H37	2.7930367267	2.6673501462	-0.4249908671
H38	1.7604219492	0.9157795601	-1.8242177329
H39	1.2338637611	-1.2950330907	-0.8681619508
H40	1.0634002702	-1.6749186145	9.3372742966
H41	1.6379590888	0.4294243998	10.4838892413
H42	2.8067506777	2.2340045722	9.2720434427
H43	3.6320909462	2.2000845845	3.2099923188
H44	5.5960195659	1.9897762235	1.6731880998
H45	5.4274110209	3.6385662623	2.3026840817
H46	4.9324477075	3.2681371887	0.6460380496
H47	2.5254978737	4.2620994697	1.2341442786
H48	3.1372805294	4.5869106423	2.8588142953
H49	1.6750031182	3.6060192798	2.6533003583
H50	1.5946596560	-2.1107545386	2.7587036571
H51	3.7581081543	-2.8768045922	1.7538568460
H52	2.9097944183	-3.3449931675	0.2733079592
H53	2.5755632655	-4.1934351118	1.7931956486
H54	-0.4933935096	-2.0385595635	1.3776408670
H55	0.3128748172	-3.0060204277	0.1269700136
H56	0.0678485628	-3.6784146683	1.7389381068
H57	3.8867278605	1.9651110935	5.6779326454
H58	2.4755316236	-4.3789054240	6.4645582078
H59	3.6617900153	-3.0740052717	6.6151335562
H60	2.8100649791	-3.6613158308	8.0503289472
H61	-0.5888814085	-2.2657796813	7.0431504520
H62	-0.0223549169	-3.8712078458	6.5613153278
H63	0.2119674703	-3.3270145069	8.2219560099
H64	1.4995820502	-2.2193419636	5.6759700767
H65	5.5212735310	3.3977119625	6.8189416094
H66	5.6228555402	1.7516731241	7.4695647554
H67	4.8209615731	3.0262302076	8.3973507022
H68	3.3020514495	4.3486598893	6.0413581768
H69	2.4566942816	3.9336025289	7.5375865014
H70	1.8520294795	3.3333448062	5.9767633562
H71	-3.3416096184	-2.5479376808	4.9057579217
H72	-3.2470512892	-2.5706710299	3.1469825756
H73	-1.9662338185	-3.3650693719	4.1124140765
O74	0.0439577545	2.8007356057	4.2299483480
H75	-1.6007313288	0.9813408417	4.1167593033
C76	-1.2475609831	2.4824597397	4.2208155840
H77	-1.7673838512	2.6397238491	3.2616289910
C78	-2.0887468442	2.8074823101	5.4229653884
C82	-3.4858399146	2.7400807979	5.3344280511
C83	-4.2794902750	3.0412942666	6.4412505324
C84	-3.6848167354	3.4163924604	7.6474820749
C85	-2.2925506743	3.4908190587	7.7388207725
C86	-1.4972507063	3.1873533151	6.6349389662
H87	-3.9492380619	2.4354701810	4.3989996655
H88	-5.3617902137	2.9827067461	6.3613031298
H89	-4.3021769130	3.6524388879	8.5102770235
H90	-1.8251735078	3.7886958593	8.6741271913
H91	-0.4157093006	3.2473867997	6.6945316559

Pd1	.0076525288	-.1086621286	.2659187790
O2	-.4113601102	-.5994738603	2.3976735226
O3	1.8230866754	-.5224238168	2.4636210132
C4	-2.1501169149	-.0003460546	-.3944929383
N5	-3.0978876045	-.9820784010	-.5432151527
N6	-2.8941210346	1.1510800200	-.4508637912
C7	-4.3806162366	-.4542489495	-.6933650414
C8	-4.2521503114	.8925697213	-.6316171776
C9	-2.3574149344	2.4923696011	-.3995954947
C10	-2.1064676798	3.1602797947	-1.6150044858
C11	-1.6543916706	4.4843267040	-1.5497081644
C12	-1.4587818302	5.1167123724	-.3263824040
C13	-1.6990974137	4.4296115529	.8602770011
C14	-2.1455956780	3.1018477408	.8543517810
C15	-2.8289178791	-2.4000030653	-.6220072103
C16	-2.8677683448	-3.1742324851	.5580164820
C17	-2.6575773742	-4.5528597990	.4317232341
C18	-2.4174535815	-5.1386032628	-.8088114818
C19	-2.3802181670	-4.3526891317	-1.9550920645
C20	-2.5850521846	-2.9680325672	-1.8886929909
C21	-2.2982656690	2.4950047318	-2.9754945059
C22	-3.4194763198	3.1712421494	-3.7877670491
C23	-.9804476132	2.4560387331	-3.7728824911
C24	-2.4050972043	2.3727181337	2.1699609955
C25	-3.7645929326	2.7847432903	2.7701822774
C26	-1.2701232750	2.5809672889	3.1876589793
C27	-3.1577379361	-2.5565077864	1.9244388913
C28	-4.6691820176	-2.5885820161	2.2376045698
C29	-2.3731141344	-3.2243995806	3.0658954045
C30	-2.5490203348	-2.1401524058	-3.1706218643
C31	-3.7320635170	-2.4889411380	-4.0963214629
C32	-1.2070023717	-2.2888778765	-3.9114196929
C33	.6855186111	-.6868774766	3.0216120403
C34	.6751823844	-.9819952757	4.5068839516
H35	-5.2476559090	-1.0794892203	-.8330094093
H36	-4.9849138719	1.6804094466	-.7017348705
H37	-1.4502185281	5.0240870136	-2.4697581247
H38	-1.1122496002	6.1458752064	-.2960879478
H39	-1.5335960485	4.9307848360	1.8086329151
H40	-2.6796863693	-5.1775337951	1.3181425549
H41	-2.2583717388	-6.2110054361	-.8796455782
H42	-2.1895096817	-4.8184742208	-2.9174339766
H43	-2.5986985321	1.4582539178	-2.8056928413
H44	-4.3721979543	3.1503965949	-3.2487722160
H45	-3.5614300815	2.6580283095	-4.7452584088
H46	-3.1832440474	4.2187526408	-4.0041466614
H47	-.6287655111	3.4639050275	-4.0197092418
H48	-1.1251873269	1.9170643014	-4.7161327954
H49	-.1962392612	1.9539089804	-3.1995086411
H50	-2.4387372021	1.3016752886	1.9606528110
H51	-4.5900848056	2.5733106968	2.0824263782
H52	-3.7881928033	3.8562725842	3.0003254489
H53	-3.9523721890	2.2372578328	3.7002501315
H54	-.3046233165	2.3015486884	2.7586029023
H55	-1.2087096386	3.6188392190	3.5333157372
H56	-1.4441816274	1.9519387890	4.0662463519
H57	-2.6465781015	-1.0871114916	-2.8969319190
H58	-4.8628270953	-2.1385329292	3.2172698191
H59	-5.2544611315	-2.0366617684	1.4966597662
H60	-5.0422431449	-3.6191384899	2.2615445452
H61	-1.3044469611	-3.2637215935	2.8437063989

H62	-2.5029047730	-2.6435435765	3.9841689760
H63	-2.7268157152	-4.2412017076	3.2727894496
H64	-2.8320149409	-1.5142488632	1.8908562066
H65	-3.7126504901	-1.8614366258	-4.9939897045
H66	-4.6922611298	-2.3317684385	-3.5945250894
H67	-3.6933182716	-3.5347952340	-4.4200505161
H68	-1.1900409880	-1.6426797255	-4.7959667810
H69	-1.0427294183	-3.3169182147	-4.2520687525
H70	-.3677914751	-2.0112166334	-3.2669228507
H71	1.3953704109	-1.7707900713	4.7377879899
H72	.9908822478	-.0841639936	5.0482806272
H73	-.3218469969	-1.2715460628	4.8398328570
O74	1.2643063128	.5639712929	-1.3846499315
H75	1.3909858347	-.2500893877	1.1763970510
C76	2.1072450945	.1018257049	-2.1579830114
C78	2.6374384256	-1.2626915973	-2.1740661401
H79	2.5272466816	.7824041039	-2.9214932578
C82	3.6439119592	-1.5725528514	-3.1071810287
C83	4.1906812088	-2.8507860696	-3.1513042194
C84	3.7364847763	-3.8284823454	-2.2608220712
C85	2.7363894476	-3.5282455209	-1.3312713477
C86	2.1800165306	-2.2537286469	-1.2863155306
H87	3.9941427770	-.8016480182	-3.7906170730
H88	4.9672960362	-3.0873783795	-3.8722119011
H89	4.1625237063	-4.8274668471	-2.2928696575
H90	2.3890209926	-4.2923376715	-.6423699865
H91	1.3979862179	-2.0041276652	-.5694652948

L=pyridine analogues:

1-pyr

Pd1	-0.024461836000	-0.043412083300	-0.015202984200
N2	-0.026678193600	-0.018098900000	2.038904681300
O4	1.989991365800	0.050962261600	-0.110645867500
C5	0.715907923500	-0.872712294200	2.769597466100
C6	0.670711486200	-0.856879230500	4.161318306500
C7	-0.153359990300	0.060798079100	4.808612394200
C8	-0.922932812300	0.934735841900	4.040230817800
C9	-0.838087766000	0.863610095500	2.655229878500
C15	2.703311501200	-1.039672007300	0.016529923400
C16	4.161042947600	-0.841772775000	-0.370088352000
O17	2.272127177400	-2.131848837400	0.400407968900
H18	1.332118719200	-1.564788079400	2.203273909200
H19	1.278544586800	-1.562044679800	4.717727245600
H20	-0.200235784800	0.093460554200	5.893042763400
H21	-1.583364437700	1.662400998300	4.498997961100
H22	-1.427030987800	1.505892362300	2.010139934700
H28	4.517325987000	0.147138508500	-0.073369127400
H29	4.772653742900	-1.624796229400	0.080554253800
H30	4.245939662000	-0.913072834500	-1.459743013300
O31	-2.081341076300	0.056197513700	-0.446274155800
C99	-1.827541827300	0.028286903600	-1.706520488000
O100	-0.605382290900	-0.036665470200	-2.062858176300
C101	-2.934112410800	0.098581324500	-2.714637747400
H102	-3.855214329000	-0.309533263400	-2.294549719500
H103	-2.649906282000	-0.438174280700	-3.621663857000
H104	-3.107387339500	1.148154750100	-2.977155743200

3-pyr

Pd1	0.008263801900	0.498103481200	0.377250662300
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N2	-0.3805294827000	-0.0745881731000	2.3053492265000
C3	0.6013171434000	-0.0602341170000	3.2278654791000
C4	0.3540192826000	-0.4198170101000	4.5493482873000
O6	-1.7023604398000	1.6616567614000	0.5584587127000
O7	1.5101959336000	-0.8625093357000	0.2626306601000
C13	-0.9318239963000	-0.8075631593000	4.9209152925000
C14	-1.9393683891000	-0.8128329855000	3.9568756915000
C15	-1.6292410458000	-0.4325588903000	2.6563209746000
C16	-2.1221558316000	2.5118859758000	-0.3168194346000
C17	-3.3715821446000	3.2769691723000	0.0751919087000
C18	2.7075971241000	-0.5451241540000	0.6777499386000
C19	3.7314875682000	-1.6464593003000	0.4519469802000
O20	-1.5699793456000	2.7516831340000	-1.4154117650000
O21	3.0117518699000	0.5341484087000	1.2029465270000
H27	1.5795021486000	0.2538242255000	2.8772764088000
H28	1.1663829697000	-0.3901460890000	5.2673454883000
H29	-1.1474009307000	-1.0966269826000	5.9452610405000
H30	-2.9555773712000	-1.1029355278000	4.2007918073000
H31	-2.3753601286000	-0.3882969336000	1.8726349614000
H32	-3.0751245790000	4.1442537875000	0.6755731250000
H33	-3.8869687445000	3.6343574887000	-0.8173031888000
H34	-4.0349658961000	2.6585887179000	0.6830681880000
H35	4.5886069394000	-1.4945123168000	1.1100444041000
H36	3.2893503138000	-2.6320007492000	0.6158869942000
H37	4.0715358356000	-1.6001677146000	-0.5875577593000
O38	0.3833501064000	1.1632522385000	-1.5837101727000
C39	1.6807603984000	1.7160675184000	-1.9401069651000
C40	2.5355297381000	0.6462619714000	-2.5915919343000
C41	1.9711703845000	-0.4160460481000	-3.3062013155000
C42	2.7898782248000	-1.3497091793000	-3.9434632287000
C43	4.1794026462000	-1.2301950697000	-3.8796201280000
C44	4.7489005991000	-0.1741234418000	-3.1654964906000
C45	3.9303693987000	0.7544120879000	-2.5205748574000
C46	1.4641761973802	2.9150365106017	-2.8712299548698
H47	2.1730574611000	2.0497007555000	-1.0195571533000
H48	0.8915361360000	-0.5190039331000	-3.3370875309000
H49	2.3403225646000	-2.1759832416000	-4.4875972057000
H50	4.8143908533000	-1.9588661349000	-4.3762299370000
H51	5.8294532664000	-0.0782733160000	-3.1000931868000
H52	4.3779029087000	1.5602901541000	-1.9428470746000
H53	-0.3568634820690	1.8702119733661	-1.6444861889062
H54	0.8697561312861	3.6925273388306	-2.3813846109990
H55	0.9501545809105	2.6013865562947	-3.7857931556261
H56	2.4324446247164	3.3401433472098	-3.1519447959073

TS1-pyr

Pd1	0.1438026735000	-0.4518317695000	-2.9520166368000
N3	-1.9194059688000	-0.5537739848000	-2.7148065311000
O4	0.1203472655000	-1.7408684571000	-4.5945014236000
C10	-2.6889132863000	0.5462621675000	-2.8350780015000
C11	-4.0666994271000	0.5058406288000	-2.6582079785000
C12	-4.6696549295000	-0.7117135318000	-2.3407076988000
C13	-3.8693139058000	-1.8450524246000	-2.2193864729000
C14	-2.4946020767000	-1.7360880886000	-2.4164521672000
C15	0.0873322483000	-3.0125150331000	-4.3312632181000
C16	0.3323080697000	-3.9012456671000	-5.5439473452000
O17	-0.1080511009000	-3.5070825122000	-3.2078757841000
H23	-2.1737265865000	1.4688349900000	-3.0771913288000
H24	-4.6479486224000	1.4151038158000	-2.7678902298000
H25	-5.7438204453000	-0.7733065032000	-2.1930789077000
H26	-4.2935890969000	-2.8136243192000	-1.9779073993000

H27	-1.8169230646000	-2.5846998508000	-2.3650462927000
H28	1.4121378984000	-3.9612019627000	-5.7193921975000
H29	-0.0465607646000	-4.9072363276000	-5.3568361814000
H30	-0.1252300236000	-3.4761449393000	-6.4403582966000
H31	0.3815012475768	0.6245588394135	-1.7420027313186
O32	2.1801224592000	-0.0598496460000	-2.8494854041000
C33	1.8985846530595	0.7647140250188	-1.8786240604505
C34	1.9484212541000	2.2490290135000	-2.1812973193000
C35	2.3058390418000	2.6597650590000	-3.4730252203000
C36	2.3775164623000	4.0163789455000	-3.7839383646000
C37	2.0866273468000	4.9773387084000	-2.8132132602000
C38	1.7270449843000	4.5752778940000	-1.5257166676000
C39	1.6599780640000	3.2183212972000	-1.2092300457000
C40	2.2769247499794	0.3118952150533	-0.4698851134851
H41	2.5257844741000	1.9013082214000	-4.2168487949000
H42	2.6612122686000	4.3241125761000	-4.7863737228000
H43	2.1405850830000	6.0344618883000	-3.0581993614000
H44	1.4986391946000	5.3176236039000	-0.7661620276000
H45	1.3706273712000	2.9220343538000	-0.2054392347000
H46	3.3452067793653	0.5178732317995	-0.3331766340201
H47	2.1107990115705	-0.7624772729955	-0.3811326767626
H48	1.7248751549505	0.8337626687451	0.3142645881426

5-pyr

Pd1	0.1268377741000	-0.0621169991000	-0.1169548221000
N3	-0.3025498711000	0.1016886433000	1.8941378038000
O4	2.2155220513000	0.4409248199000	-0.2240136052000
C10	-1.5074866342000	-0.2105381552000	2.3997320116000
C11	-1.7708398262000	-0.1011764121000	3.7618652639000
C12	-0.7627561332000	0.3418681007000	4.6163738585000
C13	0.4845340157000	0.6608908115000	4.0791174349000
C14	0.6805584836000	0.5275987616000	2.7092874787000
C15	2.1884529886000	0.2487819782000	-1.4903735860000
C16	3.4295553496000	0.4268322358000	-2.3169390179000
O17	1.0850027175000	-0.1046356719000	-2.0258061183000
H23	-2.2365955875000	-0.5418044529000	1.6657097875000
H24	-2.7549721152000	-0.3612481782000	4.1369659184000
H25	-0.9444173826000	0.4371126242000	5.6828625626000
H26	1.2990597973000	1.0088189829000	4.7051785217000
H27	1.6280286597000	0.7573691627000	2.2320876738000
H28	4.1681857484000	-0.3268442495000	-2.0259312272000
H29	3.2001925713000	0.3233312476000	-3.3780565662000
H30	3.8655259447000	1.4100671513000	-2.1191884628000
H31	-1.5115537085000	-0.8881606630000	-2.4058564769000
O32	-1.7634849596000	-0.6107490808000	-0.3726583502000
C33	-2.2303277835000	-0.4498823631000	-1.6932034284000
C34	-2.4318791540000	1.0140403953000	-2.0759255770000
C35	-2.9638383110000	1.9276042919000	-1.1559067173000
C36	-3.1686853651000	3.2606669051000	-1.5124728457000
C37	-2.8434407145000	3.7019521049000	-2.7974409234000
C38	-2.3105690324000	2.8012172693000	-3.7201661498000
C39	-2.1052012188000	1.4679363370000	-3.3589154725000
C40	-3.5449609532000	-1.2443924398000	-1.8058797084000
H41	-3.1998402442000	1.5854007578000	-0.1521979033000
H42	-3.5795920646000	3.9581685177000	-0.7866183624000
H43	-2.9987087592000	4.7414568900000	-3.0741657696000
H44	-2.0450875944000	3.1379543740000	-4.7189960992000
H45	-1.6692404397000	0.7736347332000	-4.0740743743000
H46	-4.2913332356000	-0.8384861575000	-1.1146756870000
H47	-3.3678980901000	-2.2949781194000	-1.5556203395000
H48	-3.9468306146000	-1.1822811260000	-2.8229471299000

TS2-pyr

Pd1	-0.1087492225000	-0.1859092492000	0.2126900271000
N3	-0.0812961033000	-0.0657223239000	2.3612113409000
O4	1.9508263197000	-0.2083377358000	0.1568073428000
C10	-1.2420369853000	-0.0228185708000	3.0389829640000
C11	-1.2841287788000	0.0563638571000	4.4272997905000
C12	-0.0827397550000	0.0915221633000	5.1350239904000
C13	1.1174820973000	0.0459310115000	4.4274327838000
C14	1.0795013725000	-0.0326390068000	3.0378685342000
C15	2.4965826004000	-0.3302595810000	-1.0241758151000
C16	4.0192063012000	-0.3337144197000	-0.9920598439000
O17	1.8813690364000	-0.4399460287000	-2.0925502595000
H23	-2.1445005402000	-0.0538529060000	2.4361713010000
H24	-2.2417255140000	0.0893786002000	4.9360635678000
H25	-0.0828932577000	0.1532467930000	6.2193460732000
H26	2.0746746810000	0.0704792730000	4.9374805474000
H27	1.9750918020000	-0.0713811460000	2.4255328997000
H28	4.3734569286000	-1.1986567374000	-0.4221342285000
H29	4.4173320078000	-0.3770809633000	-2.0060492191000
H30	4.3858615776000	0.5641203761000	-0.4856440812000
H31	-0.1432455099911	-0.2826526908546	-1.3802473952569
O32	-2.1501462268000	-0.1980528210000	-0.2066741939000
C33	-1.7493891577375	-0.2323234783848	-1.4500748651378
C34	-1.8627199673000	1.0333052707000	-2.2654220683000
C35	-2.6344923024000	2.0936040047000	-1.7711211040000
C36	-2.7865226614000	3.2597035346000	-2.5200137082000
C37	-2.1608481580000	3.3829683497000	-3.7619908432000
C38	-1.3808213170000	2.3342176657000	-4.2536311012000
C39	-1.2328609840000	1.1630334531000	-3.5125544469000
C40	-1.9009750800855	-1.5563069598450	-2.1925161109405
H41	-3.1094771717000	1.9868632682000	-0.8015281080000
H42	-3.3934763958000	4.0735577101000	-2.1329677226000
H43	-2.2766698840000	4.2940105563000	-4.3427499835000
H44	-0.8793027386000	2.4304557623000	-5.2123116973000
H45	-0.5946876171000	0.3684485020000	-3.8866146411000
H46	-2.9347165034223	-1.6169509250654	-2.5550003426537
H47	-1.7133904861624	-2.3846646816083	-1.5077749059964
H48	-1.2309288123124	-1.6354923768696	-3.0501618736717

6-pyr

Pd1	-0.0683329518000	0.0159216401000	-0.0726633442000
N3	0.0198574666000	-0.2914579410000	2.1720721214000
O4	1.9774794679000	0.0126457333000	-0.1825875349000
C10	-1.0740405086000	-0.3849222491000	2.9451546288000
C11	-1.0081675735000	-0.5495850302000	4.3260804990000
C12	0.2455585987000	-0.6232350428000	4.9324246993000
C13	1.3822309155000	-0.5342376204000	4.1311637500000
C14	1.2272198320000	-0.3695091810000	2.7564578589000
C15	2.5275665082000	1.1624249131000	-0.4793427113000
C16	4.0447483410000	1.0814785560000	-0.6170616650000
O17	1.9275987793000	2.2280726817000	-0.6525699977000
H23	-2.0264023597000	-0.3284508225000	2.4268367776000
H24	-1.9218478982000	-0.6180122343000	4.9075535247000
H25	0.3336860927000	-0.7491994342000	6.0077603446000
H26	2.3785748261000	-0.5896422724000	4.5574619602000
H27	2.0724493999000	-0.2995311249000	2.0785699668000
H28	4.2874329320000	0.6835157471000	-1.6083782110000
H29	4.4834572865000	2.0758698865000	-0.5225487253000
H30	4.4756719434000	0.4017411685000	0.1224791423000

H31	-0.0606273131000	0.1954617677000	-1.5889707956000
O32	-2.1984085325000	0.0948200285000	-0.0775424075000
C33	-3.0774724506000	0.9391609707000	-0.3299175055000
C34	-2.8135975012000	2.3547300974000	-0.6758496454000
C35	-1.5061911930000	2.8803675949000	-0.7012037364000
C36	-1.2902531618000	4.2183657320000	-1.0181219623000
C37	-2.3679987188000	5.0548006577000	-1.3121213662000
C38	-3.6713770224000	4.5492714797000	-1.2920280850000
C39	-3.8935894306000	3.2137703455000	-0.9771654253000
C40	-4.5076233562099	0.4405934422057	-0.2555341479232
H41	-0.6427995192000	2.2550445576000	-0.4890546178000
H42	-0.2718745435000	4.5935739453000	-1.0349521395000
H43	-2.1960083905000	6.0993006430000	-1.5579891510000
H44	-4.5123816934000	5.1965987304000	-1.5224677627000
H45	-4.9118669734000	2.8409418169000	-0.9696677233000
H46	-5.0939713187267	1.0208807823723	0.4640315190926
H47	-4.4978545031787	-0.6081884652091	0.0418775590263
H48	-4.9998960887981	0.5302572343814	-1.2298365612705

9-pyr

Pd1	0.0000000000000	0.0000000000000	0.0000000000000
N3	0.0000000000000	0.0000000000000	2.4400544310600
O4	2.1743460932070	0.0000000000000	-0.1308582902570
H5	0.5106334850621	0.0121932147402	-1.5883858979783
C10	-1.0877684099180	-0.0994623209161	3.2185745936839
C11	-1.0273753477821	-0.1356938370602	4.6109275512436
C12	0.2223692338955	-0.0668212306190	5.2259495046683
C13	1.3580912151930	0.0342830989633	4.4235902636922
C14	1.2011824224325	0.0642360015431	3.0380818127593
C15	2.5007638999910	0.0145646065755	-1.3516463626365
C16	3.9611847754225	-0.0111467613244	-1.7368427895151
O17	1.6375200944343	0.0339466887860	-2.2994269586653
H23	-2.0398655967596	-0.1550655902169	2.6965543443051
H24	-1.9393366908250	-0.2171581373477	5.1945159430850
H25	0.3089791890206	-0.0928662754997	6.3087410088691
H26	2.3515221539082	0.0883320435911	4.8580530362103
H27	2.0548016737880	0.1376559597106	2.3697850416637
H28	4.1972567752734	-0.9923673085743	-2.1613180284856
H29	4.1589826884296	0.7352492643413	-2.5099004343618
H30	4.5942709570650	0.1654218904848	-0.8669311257865
O32	-2.1365921856861	-0.1710039997644	-0.2486492095307
C33	-3.1246311100252	0.4137566717428	-0.7160374923990
C34	-3.0274176758122	1.6706297875187	-1.4983973279699
C35	-1.8027995197196	2.3564526714835	-1.5892031324632
C36	-1.7076974467204	3.5312281589123	-2.3296151436538
C37	-2.8289513352659	4.0401052408652	-2.9882012305167
C38	-4.0520282918879	3.3701326429560	-2.9039013018123
C39	-4.1531141017042	2.1968823657520	-2.1621822734399
C40	-4.4839190951435	-0.2106708456978	-0.4691873808974
H41	-0.9295173905914	1.9528418211068	-1.0767376287658
H42	-0.7555660389950	4.0499259880095	-2.3921931210677
H43	-2.7517326453701	4.9577040665320	-3.5651181132525
H44	-4.9253725407054	3.7620643995915	-3.4170253016652
H45	-5.1086224520414	1.6853505293681	-2.1118085222323
H46	-5.1714216749084	0.5005144729265	0.0011264934750
H47	-4.3579375828135	-1.0806109232434	0.1763016566747
H48	-4.9399928750618	-0.5337533277993	-1.4119127192733