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Cocatalyst Binding Effects in Organocatalytic Ring-Opening Polymerization of L-Lactide

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Supporting Information for *Cocatalyst Binding Effects in Organocatalytic Ring-Opening Polymerization of L-Lactide*

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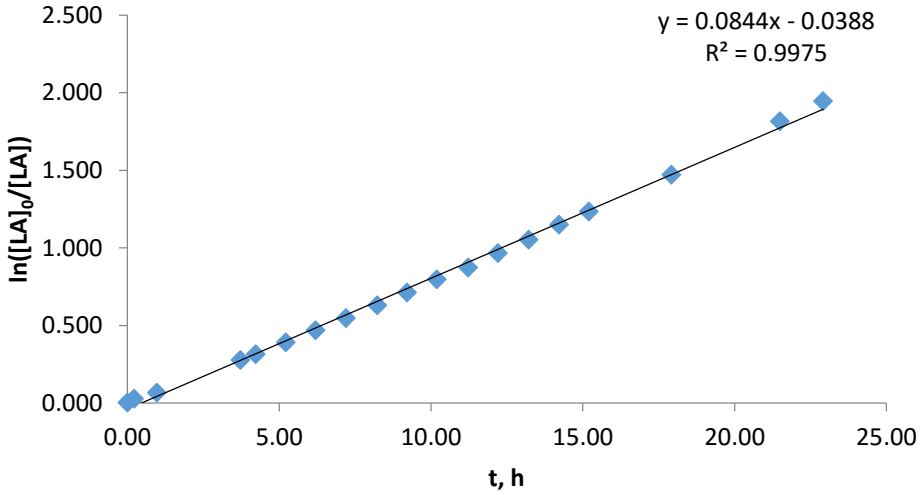


Figure S1. First order evolution of [LA] versus time in the **1**/HMTETA catalyzed ROP of LA from benzyl alcohol in $CDCl_3$. $[LA]_o$ = 0.5 mmol; $[HMTETA]_o = [1]_o$ = 0.025 mmol; $[benzyl\ alcohol]_o$ = 0.010 mmol.

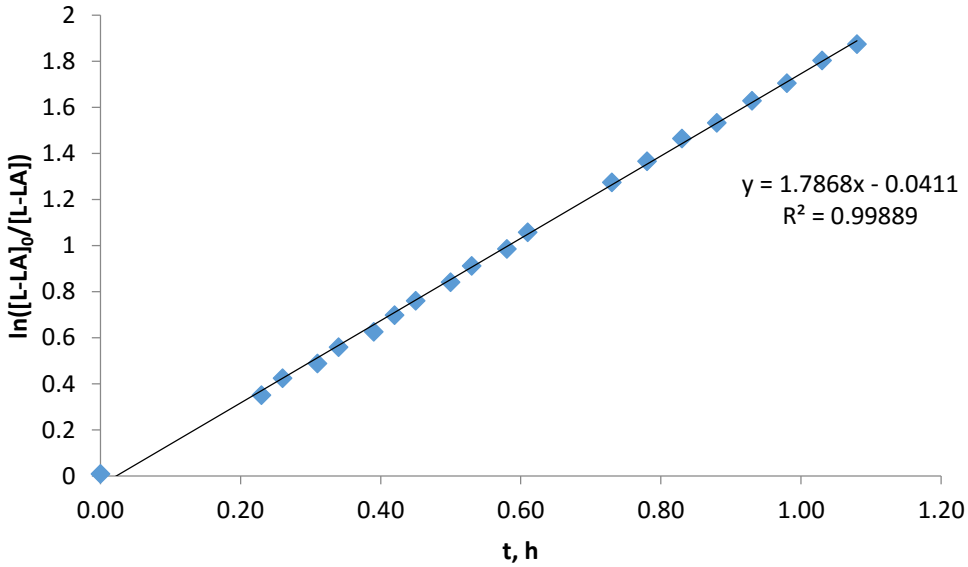


Figure S2. First order evolution of [LA] versus time in the **1**/Me_6TREN catalyzed ROP of LA from benzyl alcohol in $CDCl_3$. $[LA]_o$ = 0.5 mmol; $[Me_6TREN]_o = [1]_o$ = 0.050 mmol; $[benzyl\ alcohol]_o$ = 0.010 mmol.

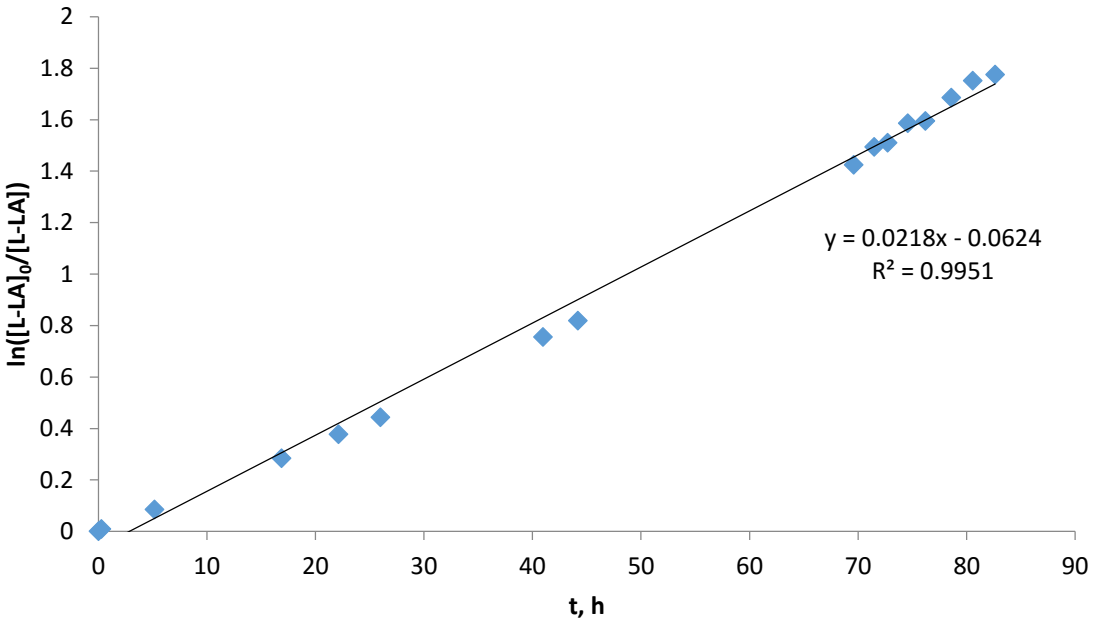
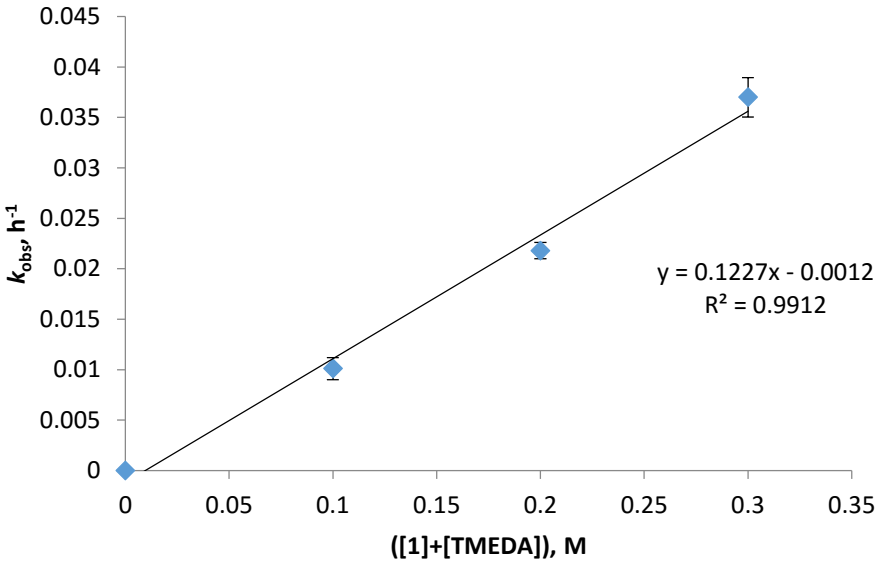
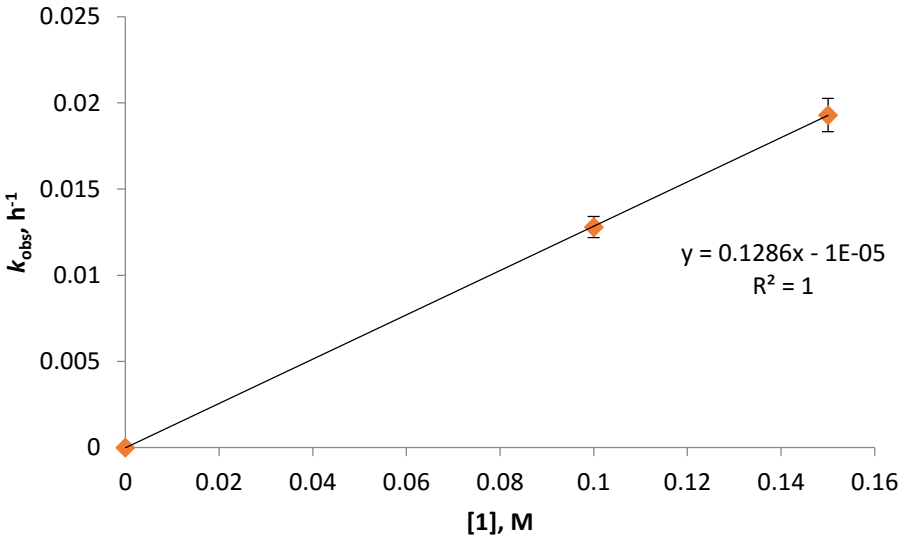


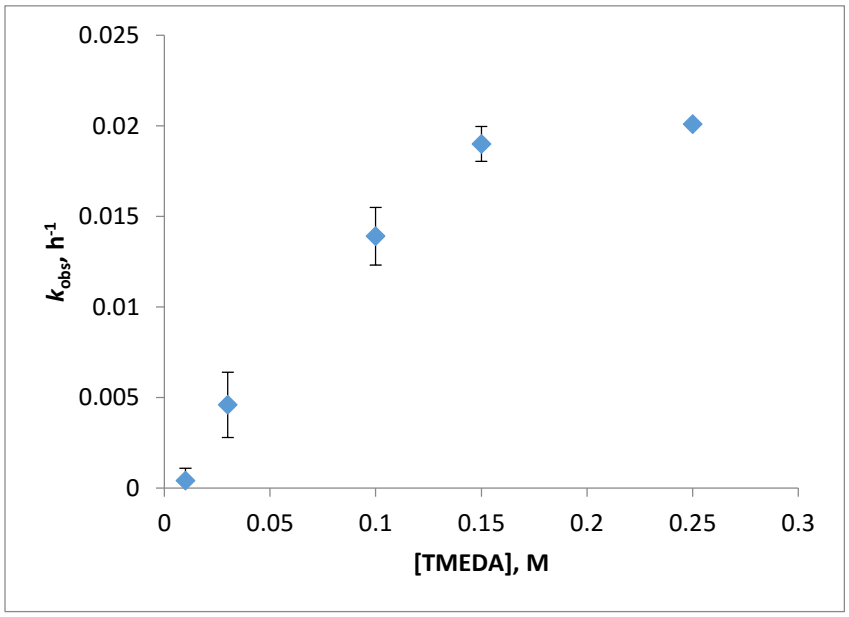
Figure S3. First order evolution of [LA] versus time in the **1**/TMEDA catalyzed ROP of LA from benzyl alcohol in $CDCl_3$. $[LA]_o$ = 0.5 mmol; $[TMEDA]_o = [1]_o$ = 0.050 mmol; $[benzyl\ alcohol]_o$ = 0.010 mmol.



A)



B)



C)

Figure S4. Observed rate constant (k_{obs}) vs concentration plots for the **1**/TMEDA catalyzed ROP of L-LA: A) [**1**] = [TMEDA], B) [**1**] > [TMEDA], [TMEDA] = 0.05 M, C) k_{obs} vs [TMEDA], [1] = 0.05 M (bottom).

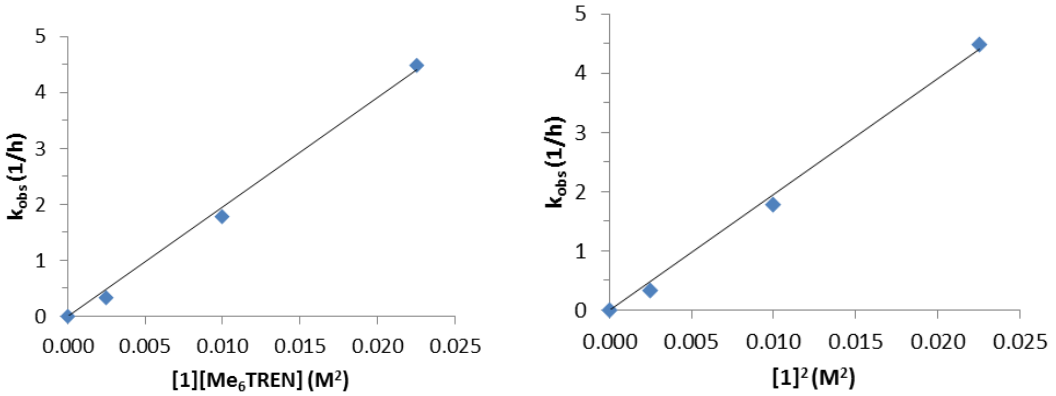


Figure S5. (left) Observed rate constant (k_{obs}) vs [**1**][Me$_6$TREN], and (right) observed rate constant (k_{obs}) vs [**1**]^2 for the **1**/Me$_6$TREN catalyzed ROP of L-LA.

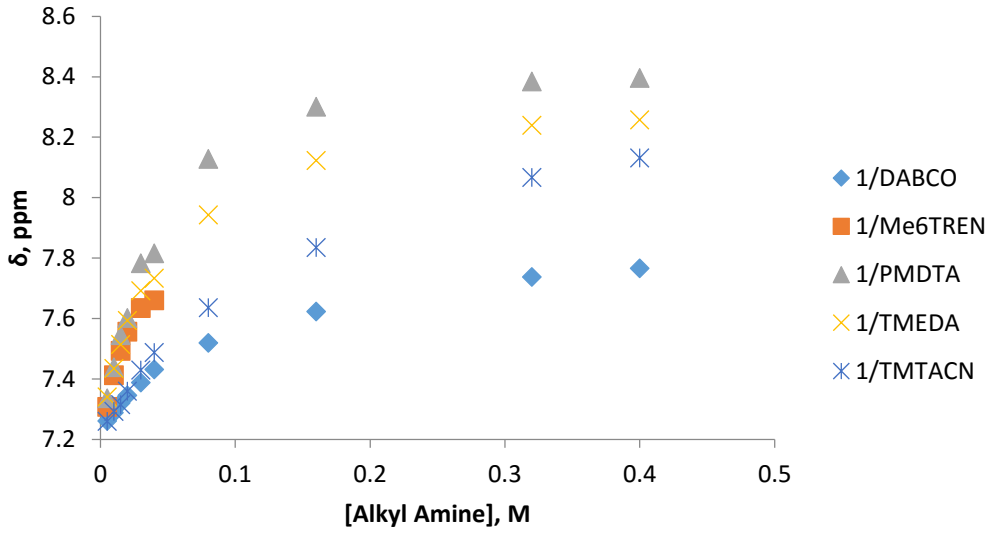


Figure S6. Binding curves for the association of **1** with alkylamine cocatalysts. The curve fitting method was used to extract binding constants, see Experimental Section. The chemical shift is of the *ortho*-protons of **1**.

Equation used for binding studies.[1-3]

$$\delta_{obs} = \delta_H - (\Delta\delta/2[H]_o)\{[H]_o + [G]_o + 1/K - (([H]_o + [G]_o + 1/K)^2 - 4[H]_o[G]_o)^{1/2}\}$$

Where: δ_{obs} is the observed chemical shift of the TU in the presence of base
δ_H is the chemical shift of free TU in the absence of base
$\Delta\delta$ is the difference in the chemical shift of host and complex, ($\Delta\delta = \delta_C - \delta_H$)
K is the binding constant, K_{eq}

The binding constants were determined by fitting the binding curve with the quadratic form of the binding equation shown above (K_{eq} and $\Delta\delta$ variables).[1-2] The value of the binding constants determined from curve fitting are within experimental error of those

determined from the slope of the linear (Lineweaver-Burke) forms of the binding equation.[4-5]

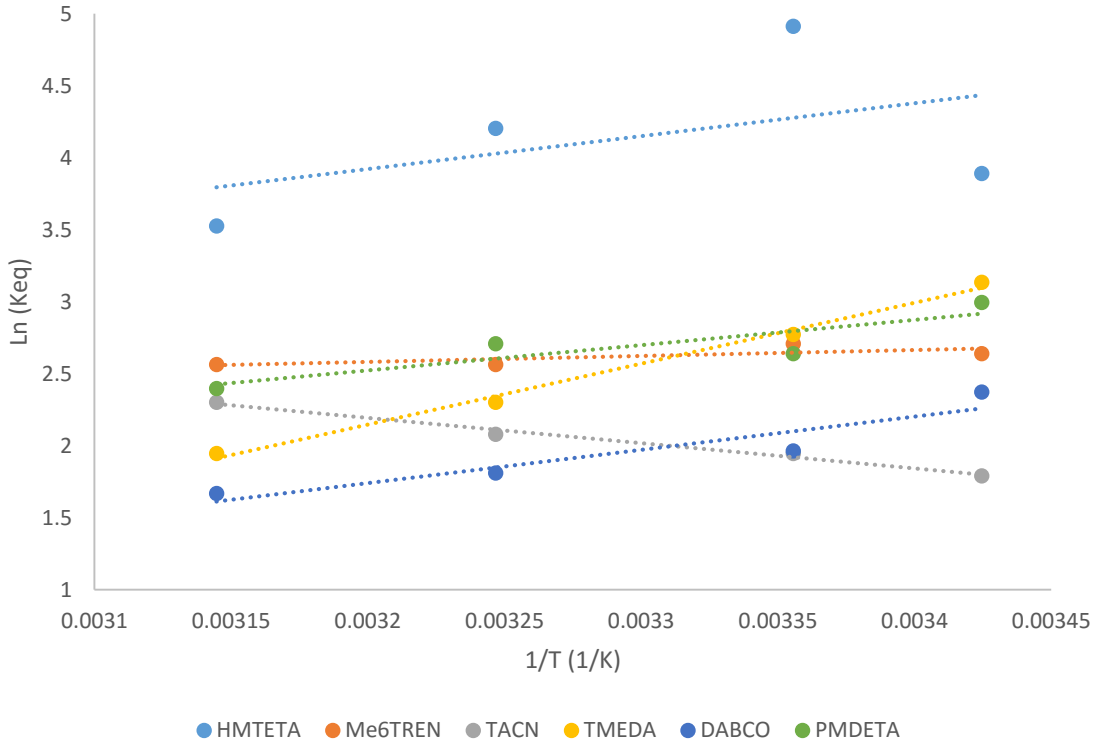


Figure S7. Temperature dependent binding.

Computational Images of Cocatalyst Complexes.

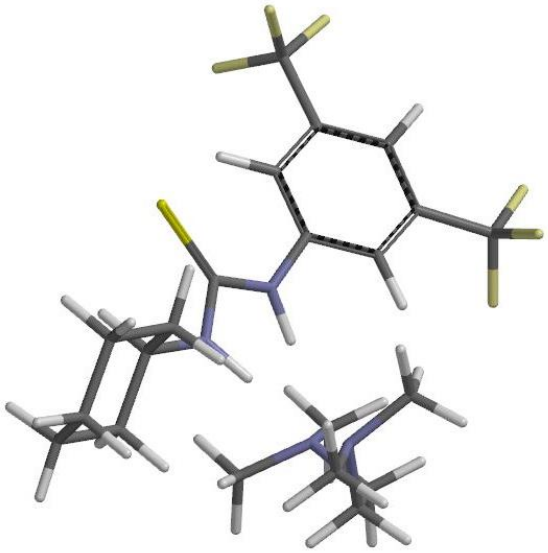


Figure S7. **1** + TMEDA. See Experimental Section for computational details and below for optimized coordinates.

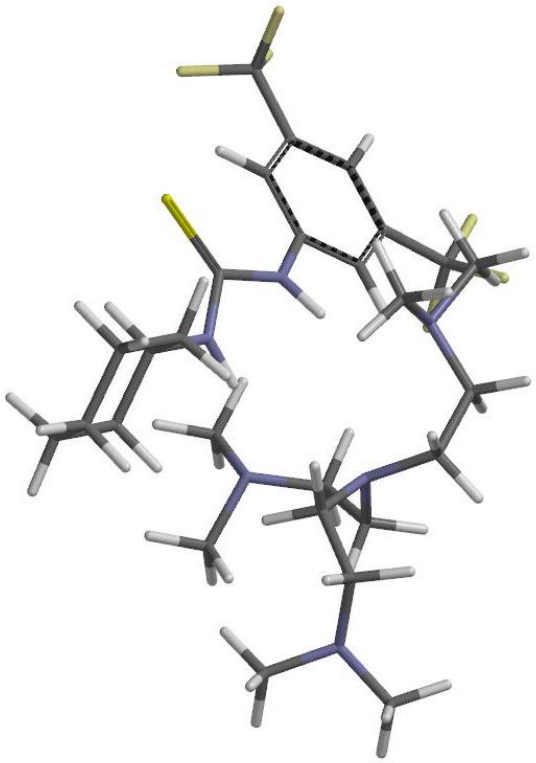


Figure S8. **1** + Me_6TREN. See Experimental Section for computational details and below for optimized coordinates.

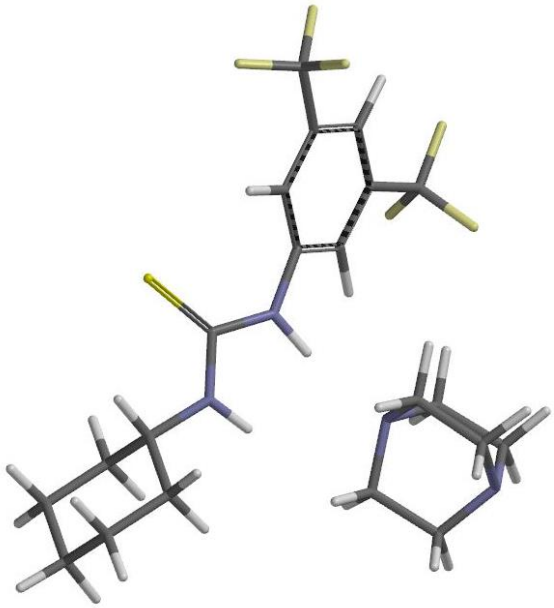


Figure S8. **1** + DABCO. See Experimental Section for computational details and below for optimized coordinates.

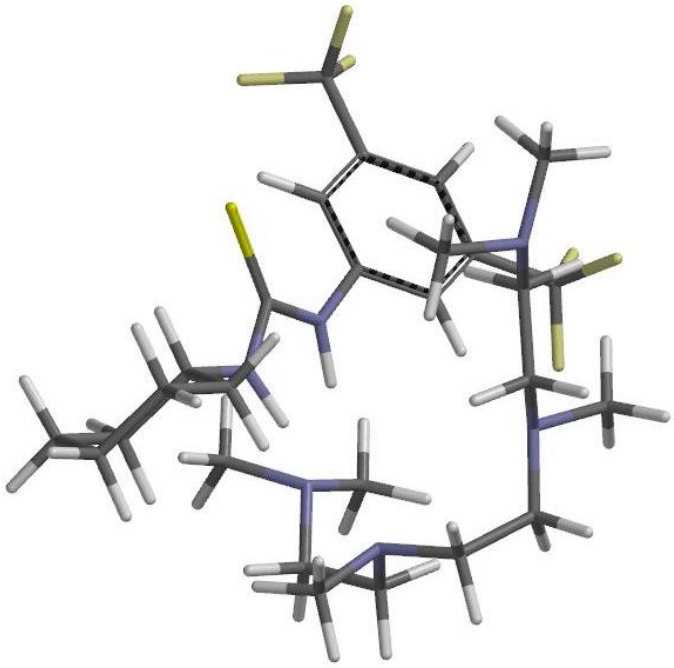


Figure S9. **1** + HMTETA. See Experimental Section for computational details and below for optimized coordinates.

Optimized Energies and Atomic Coordinates:

1 + HMTETA

		Cartesian Coordinates (Angstroms)		
	Atom	X	Y	Z
1	C C16	0.9894109	-1.4727979	-0.8215657
2	S S1	0.6430497	-3.1250735	-0.7542201
3	N N2	2.2567399	-0.9719702	-0.8520693
4	H H10	2.3673275	0.0235565	-0.6697293
5	N N3	0.0487468	-0.4735353	-0.8389453
6	H H27	0.3951613	0.4802393	-0.9934503
7	C C17	-1.3536643	-0.5391003	-0.7540792
8	C C18	-4.1633420	-0.3832505	-0.6479231
9	C C19	-1.9865385	0.5674783	-0.1699250
10	C C20	-2.1363603	-1.5750872	-1.2837411
11	C C21	-3.5270611	-1.4876128	-1.2149658
12	C C22	-3.3773418	0.6461909	-0.1317388
13	H H28	-1.3716619	1.3511466	0.2606122
14	H H30	-1.6591248	-2.4294477	-1.7419244
15	H H33	-5.2436517	-0.3196712	-0.6245901
16	C C23	3.4701700	-1.7767561	-0.9681170
17	C C24	5.5695445	-2.1977026	-2.3280808
18	C C25	5.5868573	-2.5902270	0.1753813
19	C C26	6.4142148	-2.1636308	-1.0458813
20	C C27	4.3109634	-1.7460253	0.3199323
21	C C28	4.2993162	-1.3453127	-2.1899404
22	H H36	5.2810725	-3.2358982	-2.5429145
23	H H37	5.3070792	-3.6475100	0.0713954
24	H H38	6.7954007	-1.1439239	-0.8892658

25	H	H39	4.5881530	-0.7059347	0.5478426
26	H	H40	4.5825388	-0.2874051	-2.0865219
27	H	H41	3.1194264	-2.8008227	-1.1250681
28	H	H42	6.1596642	-1.8546386	-3.1858855
29	H	H43	6.1865864	-2.5166078	1.0900585
30	H	H44	7.2930945	-2.8102422	-1.1530313
31	H	H45	3.7014172	-2.1056411	1.1552688
32	H	H46	3.6812193	-1.4246690	-3.0915252
33	C	C29	-4.0219879	1.8357875	0.5235128
34	C	C30	-4.3547243	-2.6287743	-1.7476187
35	F	F1	-5.5818693	-2.2155149	-2.1391270
36	F	F2	-3.7685601	-3.2213670	-2.8097864
37	F	F3	-4.5413966	-3.5874171	-0.8127692
38	F	F4	-5.2949743	2.0148487	0.1170267
39	F	F5	-4.0544452	1.7135871	1.8754090
40	F	F6	-3.3459894	2.9820225	0.2594708
41	N	N1	2.6702447	2.5108853	-0.0118602
42	C	C1	2.6570347	2.9767424	1.3897007
43	H	H4	3.2432810	3.9126873	1.4845602
44	H	H5	3.1977183	2.2290948	1.9783196
45	C	C13	2.0303958	3.4807450	-0.9151633
46	C	C3	4.0732986	2.3157114	-0.3913989
47	H	H3	4.5422410	1.5921227	0.2811281
48	H	H11	4.1548068	1.9264769	-1.4083824
49	C	C4	1.7418670	2.9416491	-2.3207297
50	H	H12	2.5907757	2.3487832	-2.6729730
51	H	H13	1.6614474	3.8004166	-3.0132225
52	C	C5	1.3082839	3.2790767	2.0514547
53	H	H14	0.8102258	4.0953529	1.5175889
54	H	H15	1.5640309	3.6946784	3.0481068
55	N	N4	0.5390989	2.1003618	-2.4028408
56	N	N5	0.3383679	2.1868039	2.1794641
57	C	C7	0.5648099	1.2835707	-3.6206611
58	H	H17	-0.3264400	0.6517953	-3.6579922
59	H	H21	1.4424875	0.6313873	-3.6100076
60	H	H22	0.5926992	1.8941239	-4.5403678
61	C	C8	-0.6814797	2.9130532	-2.3783385
62	H	H18	-0.7233249	3.6257529	-3.2220017
63	H	H23	-0.7539024	3.4803785	-1.4475546
64	H	H24	-1.5575433	2.2633073	-2.4307914
65	C	C11	0.8643401	1.1098113	3.0334914
66	H	H32	1.0817197	1.4774447	4.0546627
67	H	H34	1.8121501	0.7804380	2.6016355
68	C	C12	-0.9051967	2.7439296	2.7220489
69	H	H1	-1.2482672	3.5624784	2.0830226
70	H	H19	-0.7831571	3.1389513	3.7484449
71	H	H47	-1.6979603	1.9967027	2.7363261
72	H	H48	1.0878049	3.7985586	-0.4684969
73	H	H49	2.6541594	4.3908863	-1.0099409
74	H	H7	4.6567605	3.2541004	-0.3405876
75	C	C2	-0.0642334	-0.1064021	3.1496429
76	H	H6	-0.2826709	-0.5014797	2.1411538
77	H	H8	-1.0186322	0.2058965	3.5825641
78	N	N6	0.4913164	-1.1243020	4.0439486
79	C	C6	1.5968539	-1.8693305	3.4473450
80	H	H9	2.4082860	-1.1931472	3.1644554
81	H	H16	1.2996867	-2.4454297	2.5515433
82	H	H20	1.9997711	-2.5700019	4.1857611
83	C	C9	-0.5421762	-2.0403384	4.5146340

84	H	H2	-0.1055393	-2.7459537	5.2285419
85	H	H25	-1.0128186	-2.6285078	3.7041436
86	H	H26	-1.3292775	-1.4814082	5.0312808

1 + TACN

Cartesian Coordinates (Angstroms)

Atom			X	Y	Z
1	N	N1	-3.9631626	-2.3050019	-1.2539444
2	C	C1	-4.8886767	-2.7814741	-2.2730449
3	H	H3	-5.5106800	-3.5872821	-1.8699328
4	H	H4	-4.3243359	-3.1905683	-3.1182340
5	H	H5	-5.5550754	-1.9903955	-2.6683066
6	C	C2	-4.6096232	-1.8619147	-0.0203063
7	H	H6	-5.6039747	-2.3225152	0.0330960
8	H	H7	-4.7757403	-0.7694037	-0.0149363
9	C	C3	-3.8746646	-2.2736638	1.2660706
10	H	H8	-3.8345144	-3.3724584	1.3112164
11	H	H9	-4.5039855	-1.9550676	2.1068505
12	C	C4	-2.9845535	-1.3540467	-1.7997892
13	H	H10	-2.7762733	-0.5859165	-1.0547378
14	H	H11	-3.4073089	-0.8360211	-2.6780426
15	C	C5	-1.6507800	-1.9842827	-2.2135349
16	H	H12	-1.1336123	-1.2736685	-2.8697925
17	H	H13	-1.8429327	-2.8933942	-2.8147716
18	N	N2	-2.5174451	-1.7051403	1.4518723
19	N	N3	-0.7363163	-2.2714848	-1.0950480
20	C	C6	-1.4589247	-2.7161697	1.2812582
21	H	H16	-1.6359694	-3.5752216	1.9584852
22	H	H17	-0.5164651	-2.2576495	1.6011561
23	C	C7	-1.2717620	-3.2679231	-0.1336680
24	H	H18	-0.5711350	-4.1095125	-0.0553601
25	H	H19	-2.2159496	-3.6737321	-0.5068160
26	C	C9	-2.3824622	-1.1029927	2.7873490
27	H	H1	-2.4718091	-1.8446681	3.6018546
28	H	H20	-3.1523584	-0.3409928	2.9316040
29	H	H21	-1.4072375	-0.6139913	2.8755968
30	C	C10	-0.3709184	1.6522465	0.3890683
31	N	N4	-1.7127224	1.4628076	0.5120385
32	H	H24	-2.0527609	0.5029743	0.5790606
33	N	N5	0.3114036	0.4779938	0.1573701
34	H	H23	-0.2268353	-0.3721215	-0.0515139
35	S	S1	0.3784710	3.1575981	0.5371844
36	C	C11	1.7128331	0.2948509	0.1134650
37	C	C12	4.4596054	-0.3015849	-0.0435930
38	C	C13	2.5710317	1.1149817	-0.6330972
39	C	C14	2.2432870	-0.8095529	0.7840138
40	C	C15	3.6013244	-1.1177585	0.6858338
41	C	C16	3.9322063	0.8202717	-0.6889279
42	H	H22	2.1729769	1.9686009	-1.1632310
43	H	H26	1.5910922	-1.4331372	1.3862344
44	H	H29	5.5147685	-0.5351550	-0.1154477
45	C	C17	-2.7057116	2.5371246	0.5439967
46	C	C18	-4.4297349	3.8392205	-0.7904108
47	C	C19	-4.7568961	3.4715049	1.6987798
48	C	C20	-5.4518274	3.6477860	0.3404729
49	C	C21	-3.7303318	2.3278134	1.6697620

50	C	C22	-3.4024262	2.6982701	-0.8204078
51	H	H25	-3.9029409	4.7934909	-0.6477641
52	H	H30	-4.2443530	4.4054508	1.9697636
53	H	H31	-6.0635677	2.7572660	0.1300492
54	H	H32	-4.2580361	1.3728265	1.5166967
55	H	H33	-3.9058246	1.7560227	-1.0849440
56	H	H34	-2.1403753	3.4499352	0.7527893
57	H	H35	-4.9412813	3.9077456	-1.7585613
58	H	H36	-5.4983013	3.2842202	2.4854917
59	H	H37	-6.1436403	4.4987462	0.3773559
60	H	H38	-3.2086290	2.2558407	2.6319109
61	H	H39	-2.6431580	2.8818684	-1.5896707
62	C	C23	4.8568765	1.7480689	-1.4331844
63	C	C24	4.0915529	-2.3847066	1.3275451
64	F	F1	5.3363983	2.7196332	-0.6264127
65	F	F2	5.9269385	1.0900910	-1.9361994
66	F	F3	4.2354730	2.3572002	-2.4653152
67	F	F4	3.6783539	-3.4756434	0.6285434
68	F	F5	3.6082901	-2.5308782	2.5819912
69	F	F6	5.4354727	-2.4444453	1.3964676
70	C	C8	0.5642315	-2.6952970	-1.6307742
71	H	H2	0.9890776	-1.8953792	-2.2459015
72	H	H14	0.4902535	-3.6060394	-2.2524422
73	H	H15	1.2628477	-2.8976087	-0.8149270

1 + Me_6TREN

Cartesian Coordinates (Angstroms)

Atom			X	Y	Z
1	C	C16	-0.3565532	-1.9654632	0.2387363
2	S	S1	-1.1207598	-3.4475029	0.4941631
3	N	N2	0.9719516	-1.8466738	-0.0174063
4	H	H10	1.3074932	-0.9566372	-0.3934779
5	N	N3	-0.9757238	-0.7252759	0.3006581
6	H	H27	-0.3722192	0.0499826	0.5924125
7	C	C17	-2.3084752	-0.3440481	0.0937992
8	C	C18	-4.9143951	0.6752252	-0.3453424
9	C	C19	-2.5400110	1.0365476	-0.0393070
10	C	C20	-3.4058028	-1.2145768	-0.0150334
11	C	C21	-4.6815944	-0.6950182	-0.2357005
12	C	C22	-3.8227716	1.5347176	-0.2418054
13	H	H28	-1.7038945	1.7235529	0.0202816
14	H	H30	-3.2512939	-2.2800549	0.0797111
15	H	H33	-5.9121122	1.0599851	-0.5086353
16	C	C23	1.9047760	-2.9753131	-0.0214730
17	C	C24	3.9118105	-4.0150346	-1.1615347
18	C	C25	3.5684324	-4.3331403	1.3300990
19	C	C26	4.5990173	-4.1959931	0.1998898
20	C	C27	2.5911907	-3.1492103	1.3452993
21	C	C28	2.9328753	-2.8305365	-1.1526160
22	H	H36	3.3649591	-4.9328453	-1.4169447
23	H	H37	3.0021816	-5.2645983	1.1939824
24	H	H38	5.2411063	-3.3255996	0.3987345
25	H	H39	3.1309476	-2.2249158	1.5961858
26	H	H40	3.4964247	-1.8965405	-1.0226784
27	H	H41	1.2995863	-3.8676532	-0.2122285

28	H	H42	4.6595808	-3.8707964	-1.9502402
29	H	H43	4.0723748	-4.4156428	2.3001553
30	H	H44	5.2591200	-5.0710342	0.1762892
31	H	H45	1.8230726	-3.2920537	2.1125161
32	H	H46	2.4117507	-2.7557165	-2.1139955
33	C	C29	-3.9911292	3.0223452	-0.3838011
34	C	C30	-5.8441155	-1.6536240	-0.2865727
35	F	F1	-6.9221760	-1.1022743	-0.8889782
36	F	F2	-5.5367901	-2.7824334	-0.9584769
37	F	F3	-6.2325557	-2.0272279	0.9540142
38	F	F4	-5.2849372	3.3972487	-0.3886396
39	F	F5	-3.3818722	3.6903011	0.6312191
40	F	F6	-3.4330444	3.4828813	-1.5279053
41	N	N1	2.6712172	1.5729156	0.5387792
42	C	C1	2.4560060	2.2769173	1.8008238
43	H	H4	2.9756586	3.2532645	1.8337622
44	H	H5	2.9036435	1.6771309	2.5998396
45	C	C13	2.4717650	2.4043496	-0.6619079
46	C	C3	3.9041124	0.7766860	0.5408367
47	H	H3	3.8188353	0.0434604	1.3526992
48	H	H11	3.9299761	0.1963593	-0.3851796
49	C	C4	1.3290279	1.9414201	-1.5757468
50	H	H12	1.1942213	2.7081642	-2.3651848
51	H	H13	0.4026557	1.9235519	-0.9922123
52	C	C5	0.9979294	2.5652812	2.1696056
53	H	H14	0.5474077	3.2436689	1.4341452
54	H	H15	1.0343664	3.1274073	3.1237948
55	C	C6	5.2465570	1.5178999	0.7283457
56	H	H6	5.9922056	0.8054275	1.1358054
57	H	H16	5.1170011	2.2891301	1.4946283
58	N	N4	1.4987514	0.6069992	-2.1665485
59	N	N5	0.1108668	1.3975211	2.2981623
60	N	N6	5.7523458	2.1697795	-0.4862453
61	C	C7	2.6255564	0.5539074	-3.0974384
62	H	H17	2.7280786	-0.4630850	-3.4868588
63	H	H21	3.5582265	0.8182945	-2.5967624
64	H	H22	2.4975802	1.2371232	-3.9578844
65	C	C8	0.2784606	0.2019085	-2.8696812
66	H	H18	0.0455305	0.8600357	-3.7268575
67	H	H23	-0.5735378	0.2176121	-2.1878272
68	H	H24	0.3922826	-0.8189360	-3.2462111
69	C	C9	6.3856359	1.2148333	-1.3900349
70	H	H9	6.6921431	1.7228455	-2.3095486
71	H	H25	5.6870614	0.4206208	-1.6679526
72	H	H26	7.2800528	0.7354826	-0.9471517
73	C	C10	6.6751609	3.2558425	-0.1697362
74	H	H20	7.5785419	2.9141576	0.3701598
75	H	H29	6.1713257	4.0042144	0.4494834
76	H	H31	7.0001824	3.7443355	-1.0935897
77	C	C11	0.6890679	0.3261788	3.1143348
78	H	H2	-0.0559571	-0.4643574	3.2360790
79	H	H32	0.9924531	0.6695158	4.1201041
80	H	H34	1.5535040	-0.1122512	2.6122861
81	C	C12	-1.1598265	1.8303244	2.8902341
82	H	H1	-1.6168627	2.6163775	2.2837463
83	H	H19	-1.0278637	2.2212039	3.9152612
84	H	H47	-1.8559628	0.9887315	2.9319240
85	H	H48	2.2310503	3.4327438	-0.3603208
86	H	H49	3.4117858	2.4835209	-1.2165070

1 + DABCO

Cartesian Coordinates (Angstroms)

	Atom	X	Y	Z
1	C C16	1.2089310	-1.5514649	-0.1404124
2	S S1	0.8434249	-3.1945276	-0.1898216
3	N N2	2.4839571	-1.0697456	-0.1091368
4	H H10	2.5995125	-0.0695143	-0.2185575
5	N N3	0.2805404	-0.5364245	-0.1334519
6	H H27	0.6405493	0.4273059	-0.1680656
7	C C17	-1.1231022	-0.6064949	-0.1231761
8	C C18	-3.9363673	-0.4603232	-0.0478571
9	C C19	-1.8078393	0.4069801	-0.8032659
10	C C20	-1.8601259	-1.5672325	0.5860731
11	C C21	-3.2515290	-1.4878668	0.6055873
12	C C22	-3.1983255	0.4888863	-0.7479374
13	H H28	-1.2475707	1.1302262	-1.3853439
14	H H30	-1.3468037	-2.3653039	1.1036452
15	H H33	-5.0167641	-0.4085715	-0.0159565
16	C C23	3.6965505	-1.8707133	-0.2670929
17	C C24	5.4163840	-2.7844409	-1.8990332
18	C C25	6.1208369	-2.1025689	0.4379769
19	C C26	6.5465478	-2.2095660	-1.0337670
20	C C27	4.8250903	-1.2914282	0.5990594
21	C C28	4.1212951	-1.9734941	-1.7429378
22	H H36	5.2260834	-3.8256228	-1.6051630
23	H H37	5.9612217	-3.1111195	0.8431719
24	H H38	6.8160151	-1.2103320	-1.4057236
25	H H39	5.0145221	-0.2480021	0.3004993
26	H H40	4.2744714	-0.9583744	-2.1393945
27	H H41	3.4393165	-2.8710308	0.0937622
28	H H42	5.7153918	-2.8097876	-2.9532068
29	H H43	6.9195667	-1.6499140	1.0368580
30	H H44	7.4472147	-2.8280928	-1.1219844
31	H H45	4.5093513	-1.2703692	1.6483144
32	H H46	3.3067623	-2.4256999	-2.3177468
33	C C29	-3.8628339	1.6414512	-1.4475148
34	C C30	-4.0248454	-2.4831993	1.4323407
35	F F1	-5.3007159	-2.6062559	1.0033055
36	F F2	-3.4637370	-3.7081607	1.4066213
37	F F3	-4.0813457	-2.1009652	2.7308812
38	F F4	-5.2067203	1.5672760	-1.4105526
39	F F5	-3.5085914	2.8255572	-0.8790857
40	F F6	-3.4904649	1.7191521	-2.7451072
41	N N1	1.7151695	4.6739524	1.2927295
42	C C1	1.3708245	3.7165088	2.3580458
43	H H1	0.5246207	4.1222409	2.9221435
44	H H4	2.2209661	3.6473364	3.0450267
45	C C2	0.5816590	4.7728135	0.3582372
46	H H3	-0.2885464	5.1329969	0.9165792
47	H H7	0.8213070	5.5280997	-0.3977503
48	C C3	2.8906327	4.1757897	0.5619933
49	H H2	3.1281182	4.8907931	-0.2329674
50	H H9	3.7438368	4.1539792	1.2483343

51	C	C4	1.0234908	2.3222680	1.7437244
52	H	H5	-0.0134969	2.0350674	1.9452258
53	H	H11	1.6649400	1.5290914	2.1428162
54	C	C5	2.5997029	2.7557482	-0.0261382
55	H	H12	3.2678858	2.0048223	0.4133317
56	H	H13	2.7378696	2.7304746	-1.1127498
57	C	C6	0.2926558	3.3842379	-0.2965406
58	H	H6	0.4519217	3.4090504	-1.3802941
59	H	H14	-0.7396619	3.0674558	-0.1226144
60	N	N5	1.2031124	2.3573292	0.2707544

1 + PMDETA

Cartesian Coordinates (Angstroms)

Atom			X	Y	Z
1	C	C16	0.9400661	-1.6040524	-0.1443843
2	S	S1	0.6157847	-3.2162549	0.2401523
3	N	N2	2.2057303	-1.1049881	-0.2575092
4	H	H10	2.3141278	-0.0911790	-0.2229078
5	N	N3	-0.0108788	-0.6399799	-0.3807524
6	H	H27	0.3343899	0.2770472	-0.6868464
7	C	C17	-1.4092661	-0.6787211	-0.2598552
8	C	C18	-4.2218703	-0.4910748	-0.1243812
9	C	C19	-2.0383473	0.5523458	-0.0232264
10	C	C20	-2.2035871	-1.8246631	-0.4249482
11	C	C21	-3.5913786	-1.7169660	-0.3403202
12	C	C22	-3.4281184	0.6437516	0.0248336
13	H	H28	-1.4219558	1.4304084	0.1326002
14	H	H30	-1.7344506	-2.7785990	-0.6159406
15	H	H33	-5.3010874	-0.4212929	-0.0872832
16	C	C23	3.4183721	-1.9007813	-0.0703383
17	C	C24	5.7270086	-2.4321396	-0.9765603
18	C	C25	5.2956182	-2.5397073	1.5180724
19	C	C26	6.3278211	-2.2347944	0.4230170
20	C	C27	4.0166113	-1.7098841	1.3349931
21	C	C28	4.4496489	-1.6002796	-1.1700992
22	H	H36	5.4894708	-3.4951540	-1.1209284
23	H	H37	5.0368427	-3.6067652	1.4842987
24	H	H38	6.6714782	-1.1951208	0.5269876
25	H	H39	4.2444625	-0.6444970	1.4896057
26	H	H40	4.7079942	-0.5325104	-1.1504086
27	H	H41	3.1001953	-2.9429187	-0.1617691
28	H	H42	6.4607054	-2.1711481	-1.7482931
29	H	H43	5.7220720	-2.3553794	2.5108448
30	H	H44	7.2138715	-2.8683412	0.5475669
31	H	H45	3.2636358	-1.9894235	2.0795107
32	H	H46	4.0035875	-1.8023337	-2.1506696
33	C	C29	-4.0458593	1.9966866	0.2443854
34	C	C30	-4.4263740	-2.9663093	-0.4550219
35	F	F1	-5.6740186	-2.6933512	-0.9032544
36	F	F2	-3.8798602	-3.8647042	-1.3008540
37	F	F3	-4.5643934	-3.5810240	0.7412260
38	F	F4	-5.3903503	1.9704658	0.1667490
39	F	F5	-3.7241858	2.5068657	1.4596089
40	F	F6	-3.6055217	2.8959611	-0.6722761
41	N	N1	2.8609581	2.3232232	0.1154391

42	C	C1	2.8324698	2.8795208	1.4825166
43	H	H4	3.3972421	3.8318341	1.5240012
44	H	H5	3.3833560	2.1789626	2.1187197
45	C	C13	2.1499982	3.1758319	-0.8518909
46	C	C3	4.2707428	2.1880077	-0.2664492
47	H	H3	4.7820072	1.5175267	0.4301727
48	H	H11	4.3692558	1.7649898	-1.2679621
49	C	C4	1.8813542	2.4867485	-2.1994069
50	H	H12	2.6878678	1.7830710	-2.4216918
51	H	H13	1.9043376	3.2447585	-3.0040595
52	C	C5	1.4701625	3.1761508	2.1151257
53	H	H14	0.9893280	4.0149546	1.5984064
54	H	H15	1.6979940	3.5487139	3.1362736
55	N	N4	0.6135739	1.7393036	-2.2390926
56	N	N5	0.5113127	2.0753433	2.1537552
57	C	C7	0.6267775	0.7602926	-3.3320572
58	H	H17	-0.3204841	0.2153006	-3.3448300
59	H	H21	1.4317413	0.0383152	-3.1681518
60	H	H22	0.7680299	1.2284546	-4.3219965
61	C	C8	-0.5242007	2.6520569	-2.4038536
62	H	H18	-0.4622074	3.2210297	-3.3488124
63	H	H23	-0.5689471	3.3689083	-1.5800036
64	H	H24	-1.4605974	2.0905281	-2.3978799
65	C	C11	1.0194452	0.9197221	2.8888881
66	H	H2	0.2541795	0.1394243	2.9140273
67	H	H32	1.2893103	1.1646713	3.9346331
68	H	H34	1.8998185	0.5035958	2.3953640
69	C	C12	-0.7404767	2.5366942	2.7525669
70	H	H1	-1.1437064	3.3791766	2.1825798
71	H	H19	-0.6162055	2.8633433	3.8027732
72	H	H47	-1.4825717	1.7356678	2.7315969
73	H	H48	1.1920571	3.4624643	-0.4169104
74	H	H49	2.7141533	4.1115312	-1.0283118
75	H	H7	4.8012259	3.1582719	-0.2578458

1 + TMEDA

Cartesian Coordinates (Angstroms)

Atom			X	Y	Z
1	C	C16	1.1570678	1.2675919	0.0222826
2	S	S1	0.9494085	2.9278905	-0.1958706
3	N	N2	2.3798598	0.6712669	0.0681768
4	H	H10	2.4168497	-0.3418869	-0.0773393
5	N	N3	0.1397676	0.3487417	0.1844900
6	H	H27	0.4285296	-0.5907202	0.4873435
7	C	C17	-1.2463911	0.4684560	0.0007023
8	C	C18	-4.0591293	0.4444004	-0.3149723
9	C	C19	-1.9394608	-0.7225780	-0.2674805
10	C	C20	-1.9850429	1.6566730	0.1120983
11	C	C21	-3.3702227	1.6287463	-0.0599405
12	C	C22	-3.3234370	-0.7358615	-0.4065835
13	H	H28	-1.3856709	-1.6495293	-0.3627610
14	H	H30	-1.4722421	2.5833396	0.3279167
15	H	H33	-5.1343914	0.4411501	-0.4313642
16	C	C23	3.6490887	1.3944767	-0.0070741
17	C	C24	6.0307823	1.4967964	0.8554797

18	C	C25	5.5076252	2.2557995	-1.5057231
19	C	C26	6.5519716	1.6083247	-0.5845087
20	C	C27	4.1672180	1.5070433	-1.4515880
21	C	C28	4.6921368	0.7433315	0.9151919
22	H	H36	5.8905068	2.5048970	1.2687728
23	H	H37	5.3486534	3.2986839	-1.1992757
24	H	H38	6.7925174	0.6028516	-0.9597954
25	H	H39	4.2967586	0.4965878	-1.8645439
26	H	H40	4.8532592	-0.3016587	0.6106266
27	H	H41	3.4402613	2.4057996	0.3544496
28	H	H42	6.7684484	0.9975785	1.4947389
29	H	H43	5.8759867	2.2893798	-2.5376754
30	H	H44	7.4864250	2.1809629	-0.6053528
31	H	H45	3.4120860	2.0149830	-2.0592718
32	H	H46	4.3094525	0.7201953	1.9423092
33	C	C29	-3.9890580	-2.0548644	-0.6841672
34	C	C30	-4.1151725	2.9351552	0.0475203
35	F	F1	-5.4541487	2.7654965	-0.0240372
36	F	F2	-3.8500760	3.5608646	1.2160605
37	F	F3	-3.7646131	3.7875439	-0.9398024
38	F	F4	-5.3327373	-1.9729156	-0.6611308
39	F	F5	-3.6323375	-2.5501557	-1.8920969
40	F	F6	-3.6250475	-2.9925675	0.2316921
41	N	N1	2.4744326	-2.4736675	-0.7590856
42	C	C1	1.4257689	-2.6453258	-1.7682042
43	H	H4	1.4777839	-3.6292553	-2.2680308
44	H	H5	1.5248856	-1.8680463	-2.5305927
45	C	C13	2.4072905	-3.4928987	0.2970583
46	C	C3	3.7886831	-2.5355159	-1.4060932
47	H	H3	3.8584624	-1.7634978	-2.1766666
48	H	H11	4.5778705	-2.3578008	-0.6696665
49	C	C4	1.1151918	-3.5298157	1.1183454
50	H	H12	1.2566766	-4.3107199	1.8900617
51	H	H13	0.2841926	-3.8723424	0.4923204
52	N	N4	0.7107028	-2.2572025	1.7318656
53	C	C7	1.7242025	-1.7384717	2.6566403
54	H	H17	1.3706376	-0.7971667	3.0857834
55	H	H21	2.6553437	-1.5311150	2.1275283
56	H	H22	1.9358424	-2.4377437	3.4850554
57	C	C8	-0.5607377	-2.4327048	2.4463774
58	H	H18	-0.4708125	-3.1394883	3.2900595
59	H	H23	-1.3335598	-2.8056676	1.7693349
60	H	H24	-0.8937992	-1.4696026	2.8423802
61	H	H48	2.5410912	-4.5074014	-0.1261331
62	H	H49	3.2616450	-3.3258903	0.9616365
63	H	H7	3.9791157	-3.5137009	-1.8831872
64	H	H51	0.4370790	-2.5424611	-1.3193358

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