Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Electronic supplementary information

Enhanced versions of Figures 1, 2 and 4

- **Fig. S1** Postulated model lithio azaenolates as key intermediates in the SAMP alkylation. The disolvated (THF) structures are shown in the lower half.
- **Fig. S2** Different orientations of the transition states **3_syn** (top) and **3_anti** (bottom) for the reaction of ethyl chloride with the lithiated cyclohexanone-SAMP hydrazone.
- **Fig. S4** Transition states (**3_syn** left, **3_anti** right) for the reaction with phenyl group-bearing carbonyl compounds illustrating the additional π-Li interactions.

Additional tables with absolute energies

- **Table S1** Absolute energies (in a.u. , PM3 in kcal/mol) for the lithiated SAMP-hydrazones 1a-c with varying number of THF solvent molecules.
- **Table S2** Absolute energies (in a.u., PM3 in kcal/mol) for the reaction of EtCl with lithio-SAMP-cyclohexanone-hydrazone · 2 THF.
- **Table S3** Absolute energies (in a.u., PM3 in kcal/mol) for investigated SAMP reactions.

Cartesian coordinates for all calculated structures

- Cartesian coordinates for model compounds **1a-b** (with 0, 1 and 2 THF molecules) at the PM3, B3LYP/6-31G(d) and MP2/6-31G(d) levels of theory
- Cartesian coordinates for complexes **2** and transition states **3** (with 2 THF molecules) for the reaction of cyclohexanone with ethyl chloride at the PM3 and B3LYP/6-31G(d) levels of theory
- Cartesian coordinates for transition states **3** (with 2 THF molecules) for the remaining reactions at the PM3 level of theory

Enhanced versions of Figures 1, 2 and 4:

Fig. S1 Postulated model lithio azaenolates as key intermediates in the SAMP alkylation. The disolvated (THF) structures are shown in the lower half.

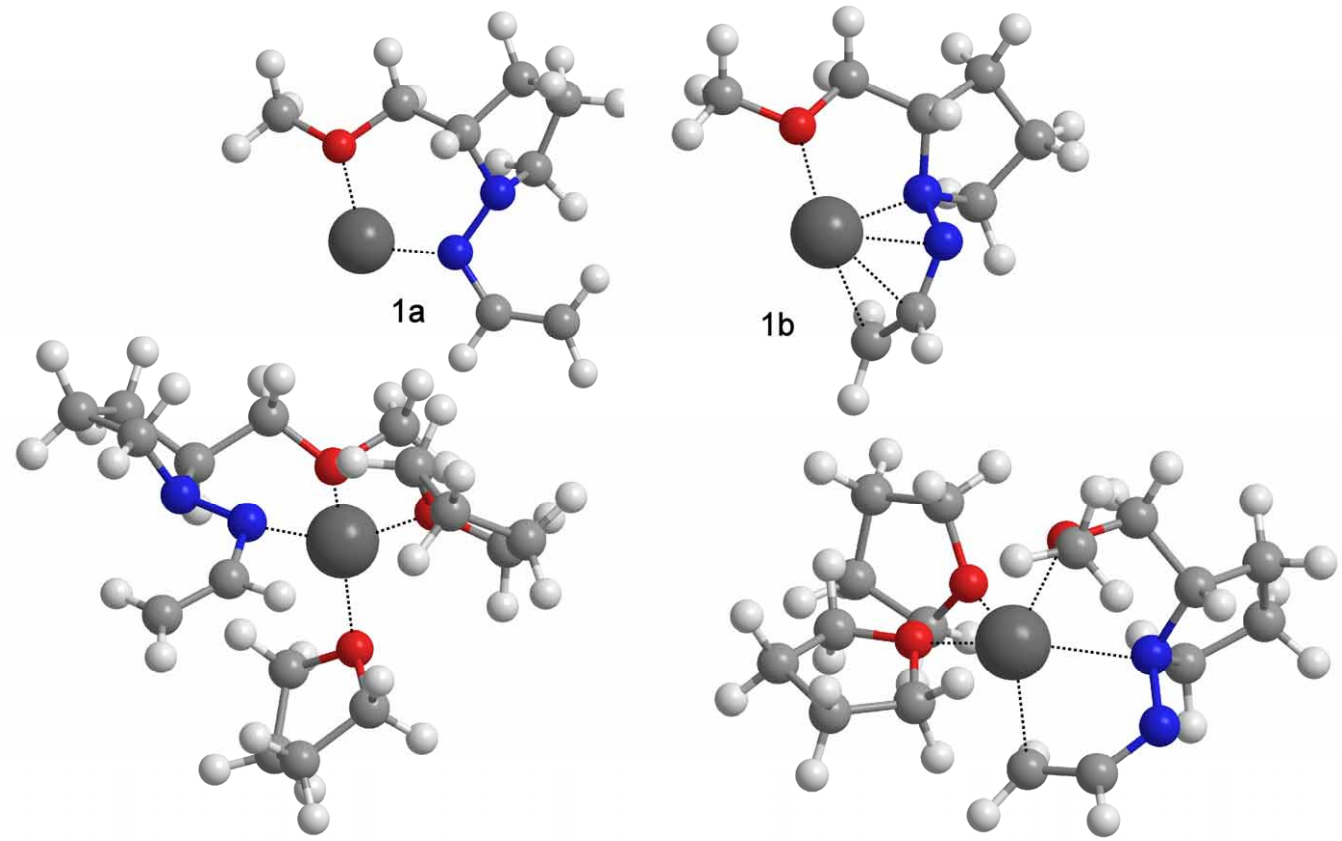

Fig. S2 Different orientations of the transition states **3_syn** (top) and **3_anti** (bottom) for the reaction of ethyl chloride with the lithiated cyclohexanone-SAMP hydrazone.

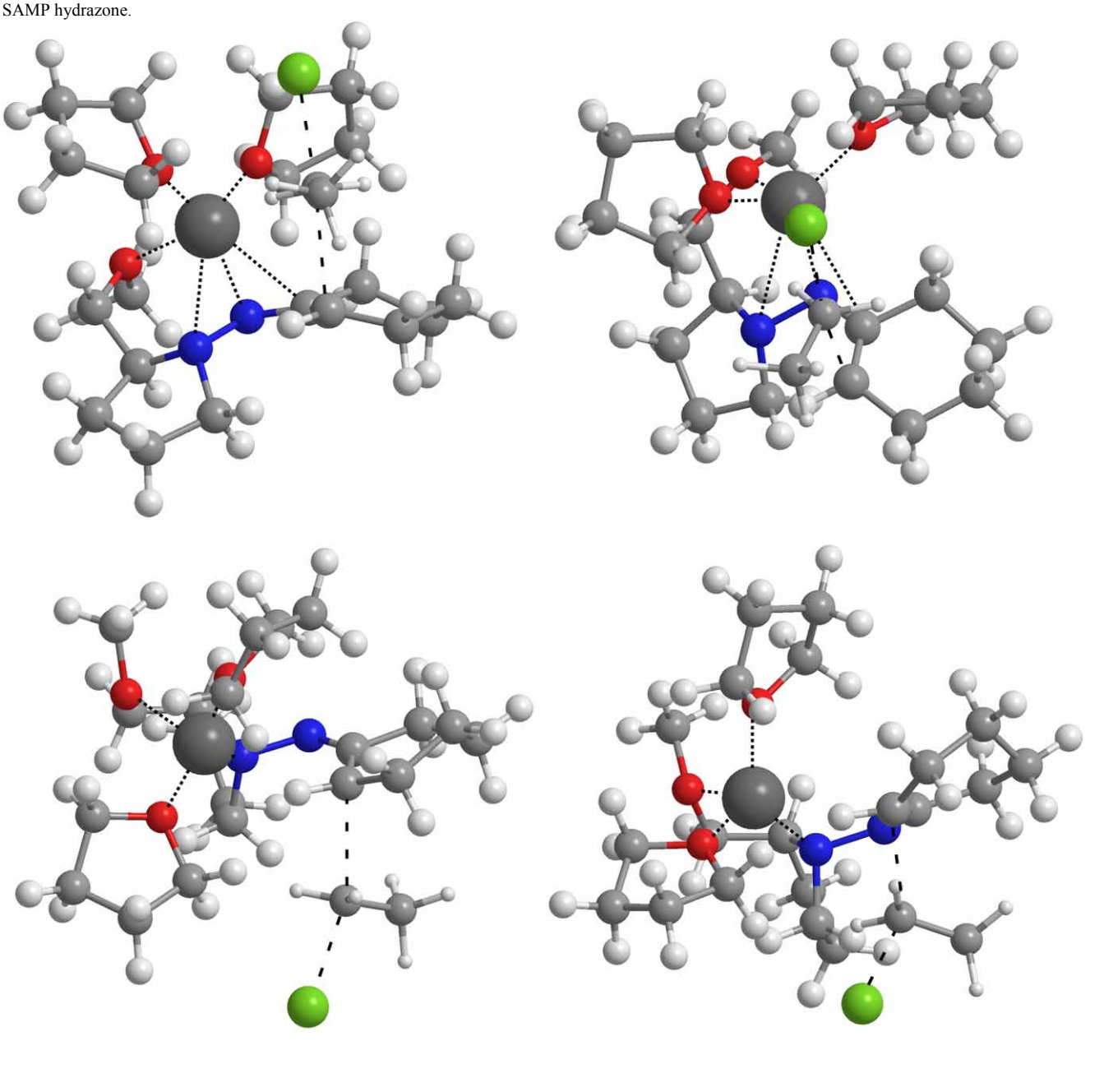

Fig. S4 Transition states (**3_syn** left, **3_anti** right) for the reaction with phenyl group-bearing carbonyl compounds illustrating the additional π-Li interactions.

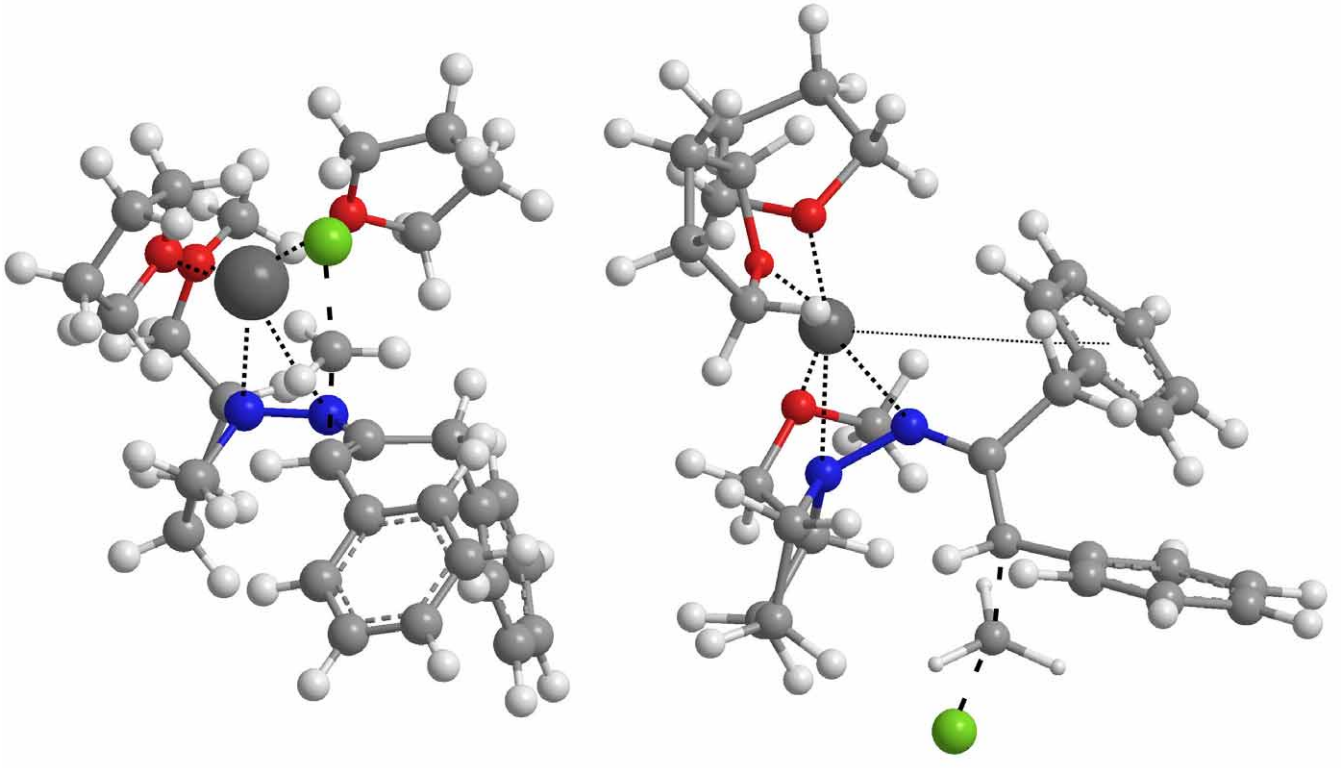

Table S1 Absolute energies (in a.u. , PM3 in kcal/mol) for the lithiated SAMP-hydrazones 1a-c with varying number of THF solvent molecules.

Compound	PM3	B3LYP/6-31G(d)//PM3	B3LYP/6-31G(d)	MP2/6-31G(d)	MP2/6-311++G(d,p)//MP2/6-31G(d)
0 THF					
1a	5.90	-506.0685094	-506.089911	-504.383160	-504.708765
1b	-3.20	-506.0892218	-506.113378	-504.413402	-504.732428
1 THF					
1a	-56.79	-738.5490011	-738.5730438		
1b	-62.31	-738.5503838	-738.5841064		
2 THF					
1a	-111.50	-970.9998805	-971.044462		
1b	-110.24	-971.0087264	-971.0414618		

Table S2 Absolute energies (in a.u., PM3 in kcal/mol) for the reaction of EtCl with lithio-SAMP-cyclohexanone-hydrazone · 2 THF.

Compound	PM3	B3LYP/6-31G(d)//PM3	B3LYP/6-31G(d)	MP2/6-31+G(d)//B3LYP/6-31G(d)
lithiated hydrazone	-126.23	-1127.038679	-1127.100473	-1123.374522
EtCl	-22.09	-539.424867	-539.426271	-538.528540
sum	-148.32	-1666.463546	-1666.526744	-1661.903062
2_syn	-153.63	-1666.461283	-1666.520741	-1661.908720
2_anti	-152.61	-1666.461365	-1666.529708	-1661.915356
3_syn	-114.36	-1666.423115	-1666.481828	-1661.865764
3_anti	-122.49	-1666.442841	-1666.500639	-1661.880971

Table S3 Absolute energies (in a.u., PM3 in kcal/mol) for investigated SAMP reactions.

Carbonyl compound	Electrophile	Lith. hydrazone	electrophile	**3_syn**	**3_anti**
PM3					
cyclohexanone	EtCl	-126.23	-22.09	-122.49	-114.36
cyclohexanone	MeCl	-126.23	-14.70	-116.39	-107.99
cyclohexanone	AllylCl	-126.23	3.18	-97.89	-90.44
cyclohexenone	MeCl	-100.79	-14.70	-91.51	-85.41
3-pentanone	EtCl	-128.05	-22.09	-124.25	-119.35
1-phenyl-2-propanone	MeCl	-92.51	-14.70	-82.40	-77.64
1,3-diphenyl-2-propanone	MeCl	-62.21	-14.70	-52.65	-48.42
B3LYP/6-31G(d)//PM3					
cyclohexanone	EtCl			-1666.44284	-1666.42311
cyclohexanone	MeCl			-1627.13671	-1627.11657
cyclohexanone	AllylCl			-1704.52604	-1704.50537
cyclohexenone	MeCl			-1625.91371	-1625.89654
3-pentanone	EtCl			-1628.33174	-1628.30857
1-phenyl-2-propanone	MeCl			-1741.45455	-1741.43495
1,3-diphenyl-2-propanone	MeCl			-1972.49739	-1972.47388

Cartesian coordinates for model compounds **1a-b** (with 0, 1 and 2 THF molecules) at the PM3, B3LYP/6-31G(d) and MP2/6-31G(d) levels of theory

1a

PM3

C	-3.0265	1.0152	1.7755
C	-3.7298	1.1431	2.9104
N	-3.4189	0.4443	0.5528
N	-4.6597	-0.3130	0.5467
Li	-2.0424	0.3370	-0.7199
C	-4.8463	-1.1851	-0.6677
C	-5.9264	0.4766	0.7144
C	-6.3457	-1.5282	-0.6306
C	-4.5070	-0.5570	-2.0413
C	-7.0348	-0.3742	0.0983
O	-3.0747	-0.5749	-2.2149
C	-2.6453	0.0222	-3.4278
H	-2.0005	1.4257	1.6960
H	-4.7483	0.7770	3.0366
H	-3.3157	1.6246	3.7882
H	-4.2182	-2.0998	-0.5161
H	-6.0512	0.6411	1.8071
H	-5.8822	1.4836	0.2497
H	-6.5047	-2.4826	-0.0938
H	-6.7669	-1.6875	-1.6413
H	-4.8944	0.4791	-2.1389
H	-4.9475	-1.1572	-2.8639
H	-7.7330	-0.7501	0.8685
H	-7.6558	0.2239	-0.5949
H	-1.5526	-0.0988	-3.4040
H	-3.0596	-0.5058	-4.2963
H	-2.9125	1.0879	-3.4914

B3LYP/6-31G(d)

C -2.6815097058 -0.3626640676 -0.5751495595
C -3.1819601337 -1.5173925501 -0.0768275582
N -1.4237289725 0.1943955544 -0.4959152679
N -0.5096834065 -0.6493524953 0.2115407436
Li -0.9359519463 1.9232135644 -0.7335409065
C 0.5656320227 0.0224639716 0.9273582216
C 0.109762012 -1.7109361597 -0.5812432469
C 1.4208821003 -1.1793581961 1.4136086242
C 1.489483135 0.9846929057 0.13849454
C 1.1061813048 -2.3313730629 0.4119972546
O 0.8320069726 2.2286959982 -0.2153357046
C 1.7338109643 3.1898742171 -0.7554141792
H -3.3492684934 0.2656270357 -1.1748999111
H -2.5918236973 -2.1835057585 0.5426500576
H -4.2184778077 -1.7811587855 -0.2596193528
H 0.1404495066 0.5960698169 1.7628374063
H -0.6619582913 -2.4037738962 -0.9266750833
H 0.6241113392 -1.3171894939 -1.4815476649
H 1.124252375 -1.4521578871 2.4296735698
H 2.4907459001 -0.940669697 1.4469549168
H 1.8648283918 0.5180126461 -0.7825062158
H 2.348965514 1.2465486649 0.7700013192
H 0.6521168748 -3.1765424213 0.9374527418
H 2.006995409 -2.7029916511 -0.0875510788
H 1.1605831252 4.0939453793 -0.9794194046
H 2.5155854052 3.4346260607 -0.0252900586
H 2.2048909616 2.8168075467 -1.675075795

MP2/6-31G(d)

C -2.6829969723 -0.3733726995 -0.5775618615
C -3.1396559534 -1.5575376361 -0.1014672537
N -1.4395212044 0.2188893667 -0.4604457682
N -0.5420974006 -0.638488004 0.256825017
Li -0.9581778435 1.9714906961 -0.6770694626
C 0.5448171135 0.0360822249 0.9538171891
C 0.0947114404 -1.6538667994 -0.5846639986
C 1.3507765621 -1.1761619721 1.4531220587
C 1.4744844888 0.9451436614 0.1382598033
C 1.1700641875 -2.2414205158 0.3411988185
O 0.850580802 2.2154285678 -0.18264013
C 1.7788487346 3.1041084382 -0.8131031396
H -3.3606295901 0.2379472713 -1.1820155336
H -2.532119994 -2.1945479807 0.5290494977
H -4.1626956097 -1.8565711217 -0.2974444246
H 0.129450695 0.6326126989 1.7778481537
H -0.6611631103 -2.3741811453 -0.9069256728
H 0.5328352003 -1.2092198828 -1.4970739265
H 0.9130791675 -1.5219340988 2.3922033718
H 2.402906394 -0.9399726096 1.6487661068
H 1.7870329025 0.4644263386 -0.7980627727
H 2.370498905 1.1706946425 0.7319902325
H 0.8498860452 -3.1944882969 0.7699428581
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H 1.2486024865 4.035308698 -1.0179469086
H 2.620633902 3.3057117889 -0.1430230894
H 2.1524441756 2.6738094412 -1.7491600925

1b

PM3

C	-3.7476	0.1544	-2.7930
C	-4.5170	1.2863	-2.4221
N	-2.4892	-0.1473	-2.4471
N	-1.8260	0.7535	-1.4856
Li	-3.7954	0.9299	-0.4882
C	-0.9924	-0.0577	-0.5012
C	-0.8927	1.7383	-2.1386
C	0.4848	0.3033	-0.7259
C	-1.4152	0.2865	0.9478
C	0.5325	1.2319	-1.9344
O	-2.8299	0.2722	1.1665
C	-3.4000	-1.0181	1.3627
H	-4.1860	-0.6371	-3.4215
H	-4.0558	2.2875	-2.4135
H	-5.5308	1.3393	-2.8204
H	-1.1440	-1.1557	-0.6742
H	-1.1325	1.8878	-3.2100
H	-1.0459	2.7189	-1.6442
H	1.0936	-0.6039	-0.8919
H	0.9243	0.7902	0.1669
H	-1.1719	1.3321	1.2245
H	-0.9097	-0.3873	1.6679
H	0.8898	0.6923	-2.8320
H	1.2427	2.0652	-1.7860
H	-4.4776	-0.8137	1.4554
H	-3.2096	-1.7106	0.5284
H	-3.0233	-1.4637	2.2925

B3LYP/6-31G(d)

C 0.6459353417 -2.4150704531 -0.6383680973
C 0.7967822546 -2.8459379657 0.6789450414
N 0.1220845357 -1.2767014211 -1.1348072425
N -0.4474250197 -0.4569016339 -0.0512242128
Li 1.4808828961 -0.7671834234 0.3396960208
C -0.4872124945 0.954762578 -0.5145365097
C -1.8330748021 -0.8491670956 0.3181537253
C -1.9522212039 1.4310277802 -0.3851483071
C 0.4885846157 1.8029774538 0.297339451
C -2.7452970423 0.1154843311 -0.4494217589
O 1.7870728355 1.1789424948 0.285462364
C 2.7774246989 1.9403563799 0.9663476378
H 1.1297631147 -3.0010564052 -1.4237562182
H 0.1586248713 -2.4842251978 1.4793874858
H 1.30439575 -3.7874741413 0.861278629
H -0.1718818795 0.9533283215 -1.5641205056
H -1.98406048 -1.9015077835 0.0724272535
H -1.9686270789 -0.7276909511 1.4020971402
H -2.2248789398 2.1432613692 -1.1699968528
H -2.1188892105 1.9255256893 0.5822819651
H 0.1508823683 1.8903333268 1.3414065563
H 0.5758311285 2.8142237103 -0.1265565995
H -2.8402267204 -0.2159445811 -1.4896490624
H -3.7499023171 0.1978053846 -0.0214846123
H 3.7147207125 1.3820919648 0.9081453607
H 2.9112507463 2.9190300979 0.4872208754
H 2.5056217426 2.0909328407 2.0208847031

MP2/6-31G(d)

C -2.3577265746 0.2891671107 -0.9855294897

C -3.003640808 0.1526374026 0.2439935938
N -1.0422348064 0.4409920047 -1.2680962061
N -0.2858486379 0.5424857856 -0.0083477446
Li -1.2389781161 -1.2137448481 0.0060542657
C 1.122003911 0.1902992079 -0.32139796
C -0.2836691949 1.9297670551 0.5191821037
C 1.9785599294 1.4082197368 0.0595592542
C 1.4954076738 -1.072518341 0.4284495387
C 0.9786056945 2.5596990822 -0.0599719983
O 0.5305399857 -2.097110952 0.1106752914
C 0.8422814153 -3.3363098039 0.7532531515
H -2.9461359726 0.1422167052 -1.8946103085
H -2.5707066982 0.5239300912 1.1667821168
H -4.0772293292 -0.0013493224 0.2440379558
H 1.1702124444 0.0024280557 -1.4005654674
H -1.2167110932 2.4174289995 0.2312295546
H -0.2308985909 1.8968978527 1.6161002729
H 2.8544455376 1.5140168933 -0.5873848339
H 2.3341350517 1.3264728236 1.0954968353
H 1.4777783577 -0.892220966 1.5134977884
H 2.4975606003 -1.4245639659 0.1436744306
H 0.8111335237 2.8045125646 -1.1136550795
H 1.2971255872 3.4659304312 0.46500673
H 0.0630700711 -4.0447868033 0.4718663892
H 1.814366502 -3.7073670812 0.4119191811
H 0.8601203023 -3.2155373529 1.8429177972

1a · 1 THF
PM3

C	-3.0265	1.0152	1.7755
C	-3.7304	1.1432	2.9113
N	-3.4019	0.4230	0.5608
N	-4.6556	-0.3145	0.5559
Li	-2.0415	0.1900	-0.7426
C	-4.8602	-1.1942	-0.6494
C	-5.9117	0.4943	0.7187
C	-6.3626	-1.5244	-0.5937
C	-4.5355	-0.5750	-2.0294
C	-7.0344	-0.3538	0.1246
O	-3.1113	-0.6403	-2.2426
C	-2.7073	-0.0560	-3.4702
H	-2.0105	1.4452	1.6990
H	-4.7410	0.7606	3.0473
H	-3.3215	1.6446	3.7805
H	-4.2371	-2.1125	-0.4985
H	-6.0314	0.6783	1.8089
H	-5.8574	1.4925	0.2367
H	-6.5264	-2.4699	-0.0431
H	-6.7931	-1.6924	-1.5990
H	-4.8932	0.4727	-2.1159
H	-5.0171	-1.1594	-2.8409
H	-7.7289	-0.7125	0.9062
H	-7.6561	0.2406	-0.5707
H	-1.6189	-0.2049	-3.4868
H	-3.1667	-0.5742	-4.3222
H	-2.9489	1.0157	-3.5270
O	-0.0564	0.4182	-0.8338
C	0.5314	1.6222	-0.3185
C	1.8730	1.2565	0.3177
C	1.8502	-0.2639	0.4671
C	0.5553	-0.7248	-0.2059
H	0.6164	2.2829	-1.1993
H	2.7201	1.5862	-0.3116
H	2.0093	1.7648	1.2893
H	2.7368	-0.7300	0.0001
H	1.8792	-0.5696	1.5291
H	-0.1702	-1.1724	0.5088
H	0.7156	-1.4382	-1.0351
H	-0.1760	2.0836	0.4019

B3LYP/6-31G(d)
C -2.8268268329 0.6455988176 1.7497138958
C -3.3577023222 0.3423775032 2.9618679677
N -3.2587477528 0.4033103166 0.4685196037
N -4.5371504059 -0.240425042 0.4528810562
Li -2.0682235856 0.1972790058 -0.93910674
C -4.8037340506 -1.058472881 -0.7254776986
C -5.6832634304 0.6566052994 0.6058233663
C -6.3260773472 -1.3553279192 -0.596242453
C -4.5302922397 -0.4245864811 -2.1093326627
C -6.8671849873 -0.2964120663 0.4064427388
O -3.1203881933 -0.3920510694 -2.4173813039
C -2.8603193971 0.0016366069 -3.7580858257
H -1.889044834 1.2149535488 1.7402385317
H -4.2762504214 -0.2246059616 3.0641553871
H -2.8468283096 0.6472185833 3.8697938016
H -4.199021543 -1.9758107724 -0.6744851321
H -5.6508277011 1.12605312 1.5926977288
H -5.6840328393 1.4702042232 -0.1480922934
H -6.4870836929 -2.3727278389 -0.2288727366
H -6.8319431347 -1.286940499 -1.5670085775
H -4.9298254381 0.5977898275 -2.1665888223
H -5.0181510909 -1.0315627223 -2.8852656662
H -7.1318171368 -0.7732786521 1.3551469898
H -7.7605102779 0.2145241571 0.031866737
H -1.7764785565 -0.0172811196 -3.9008021329
H -3.3277558634 -0.697464635 -4.4646410284
H -3.2397772983 1.0145527636 -3.9561406444
O -0.1459561807 0.2433256544 -0.7847501957
C 0.5992349375 1.4878057364 -0.7480228709
C 1.8014241193 1.2222386995 0.1590359419
C 1.2384929141 0.1885587956 1.1472125862
C 0.3358209294 -0.6607902983 0.2538612145
H 0.8716907191 1.7500659572 -1.7746854126
H -0.0514642305 2.2718403673 -0.339775204
H 2.628621279 0.7928661928 -0.4181083519
H 2.1617128435 2.1332643856 0.6453392778
H 2.0143284152 -0.4071299427 1.6366452227
H 0.643191544 0.6804612333 1.9238598896
H -0.5355875067 -1.0658028819 0.7757183681
H 0.8849268997 -1.4746190124 -0.2348565523

1b · 1 THF
PM3

C	-3.7476	0.1544	-2.7930
C	-4.5225	1.2944	-2.4194
N	-2.4673	-0.0779	-2.5437
N	-1.7906	0.8429	-1.6193
Li	-3.6268	1.5849	-0.5473
C	-1.0054	0.0302	-0.5963
C	-0.8046	1.7450	-2.3155
C	0.4864	0.3447	-0.7882
C	-1.4638	0.4002	0.8327
C	0.5974	1.2083	-2.0397
O	-2.8840	0.4427	0.9927
C	-3.5090	-0.8231	1.1356
H	-4.2086	-0.6770	-3.3485
H	-4.1358	2.2795	-2.7337
H	-5.5867	1.2285	-2.6534
H	-1.1812	-1.0661	-0.7568
H	-1.0103	1.8258	-3.4014
H	-0.9351	2.7663	-1.8984
H	1.0779	-0.5840	-0.8872
H	0.9085	0.8669	0.0930
H	-1.1834	1.4361	1.1162
H	-1.0131	-0.2911	1.5722
H	0.9677	0.6135	-2.8965
H	1.3278	2.0276	-1.9108
H	-4.5794	-0.5796	1.1533
H	-3.2886	-1.5119	0.3087
H	-3.2115	-1.2879	2.0843
O	-3.9006	3.3007	0.4794
C	-5.2896	3.6723	0.4481
C	-5.3714	5.2000	0.4628
C	-3.9484	5.6872	0.1955
C	-3.0952	4.4217	0.0878
H	-5.7592	3.2196	-0.4525
H	-6.0829	5.5705	-0.2971
H	-5.7500	5.5741	1.4317
H	-3.8887	6.2901	-0.7288
H	-3.5890	6.3488	1.0048
H	-2.2391	4.3994	0.7858

H	-2.7112	4.2448	-0.9389
H	-5.7183	3.1934	1.3470

B3LYP/6-31G(d)

C	-3.1830086272	1.2846735648	-2.953786473
C	-2.9553288368	2.6397707356	-3.137095054
N	-2.5756530893	0.3800409302	-2.1560824679
N	-1.4475559725	0.9888268705	-1.4423003106
Li	-3.2486214414	1.8903069991	-0.8654505948
C	-1.0284601285	0.0500092099	-0.3712378091
C	-0.2528427339	1.2489370386	-2.3057082234
C	0.5078083165	-0.0109891731	-0.4216825548
C	-1.5714124015	0.5169399837	0.9776981125
C	0.7890257836	0.1928019507	-1.9164671849
O	-2.9754597847	0.8097632224	0.9413379612
C	-3.8156293116	-0.3475606621	0.9574122748
H	-4.0500505477	0.8461606696	-3.4550516944
H	-2.0330362346	3.125609144	-2.837436453
H	-3.5785382414	3.1834204352	-3.841111688
H	-1.4408324781	-0.9371172528	-0.6195468167
H	-0.5502450497	1.2049118463	-3.3544155195
H	0.1275460454	2.2593676131	-2.1033560114
H	0.8997843178	-0.9529108375	-0.0244099224
H	0.9499326302	0.8074384117	0.1642612465
H	-1.0926218091	1.4608994531	1.2602914367
H	-1.3723730753	-0.224322579	1.7673366503
H	0.5996807748	-0.739729133	-2.4612310847
H	1.8174850116	0.5052500529	-2.1268675344
H	-4.8420970824	0.0165558672	1.0449873282
H	-3.7119425526	-0.9220519902	0.0309246275
H	-3.579727939	-0.9780654553	1.8258072802
O	-4.7311160256	2.9896069607	-0.087425503
C	-4.8040258775	3.4427158771	1.2735622476
C	-4.5186684484	4.9491629912	1.1952048187
C	-5.0320072831	5.3433365693	-0.2181858179
C	-5.4013638328	3.9954893158	-0.8727494442
H	-5.8146106027	3.247695338	1.6635546064
H	-4.081135264	2.8616875145	1.8472748659
H	-5.0150659272	5.5018366218	1.9985266587
H	-3.4430397867	5.1341106446	1.2780540337
H	-5.897616629	6.0111070481	-0.1737538556
H	-4.2498246655	5.8524335972	-0.7883954163
H	-5.0462704299	3.8763741303	-1.8974926732
H	-6.4841797704	3.8112734757	-0.8293420418

1a · 2 THF

PM3

C	-3.0265	1.0152	1.7755
C	-3.7937	1.3034	2.8402
N	-3.4014	0.4238	0.5624
N	-4.6704	-0.2746	0.5804
Li	-2.0876	0.4674	-0.8809
C	-4.8335	-1.3415	-0.4647
C	-5.8967	0.5920	0.5189
C	-6.3523	-1.5922	-0.4903
C	-4.3512	-1.0016	-1.8943
C	-7.0166	-0.3036	-0.0045
O	-2.9139	-1.0997	-1.9292
C	-2.3970	-1.2523	-3.2379
H	-1.9484	1.2799	1.7714
H	-4.8573	1.0744	2.8955
H	-3.3895	1.7772	3.7267
H	-4.2802	-2.2412	-0.0987
H	-6.0698	0.9599	1.5541
H	-5.7673	1.4926	-0.1190
H	-6.6109	-2.4400	0.1716
H	-6.7121	-1.8850	-1.4947
H	-4.6512	0.0255	-2.2184
H	-4.7861	-1.7185	-2.6215
H	-7.7680	-0.5142	0.7786
H	-7.5745	0.1920	-0.8208
H	-1.3096	-1.2669	-3.0892
H	-2.7260	-2.1998	-3.6847
H	-2.6806	-0.4227	-3.9019
O	-0.0803	0.3103	-0.5880
C	0.8795	1.2921	-0.9975
C	2.0793	1.2233	-0.0506
C	1.6971	0.1992	1.0167
C	0.2300	-0.1312	0.7455
H	1.1182	1.0265	-2.0424
H	3.0007	0.9309	-0.5855
H	2.2955	2.2128	0.3924
H	2.3326	-0.7033	0.9530
H	1.8393	0.5916	2.0394
H	-0.4696	0.3754	1.4539
H	0.0007	-1.2123	0.7376
H	0.3829	2.2902	-0.9988
O	-2.2870	2.2063	-2.0450
C	-3.4838	2.4220	-2.8041
C	-3.8517	3.9045	-2.7242
C	-2.7956	4.5381	-1.8206
C	-2.0261	3.3591	-1.2272
H	-3.2262	2.0821	-3.8237
H	-3.8701	4.3736	-3.7240
H	-4.8692	4.0385	-2.3137
H	-2.1292	5.2122	-2.3896
H	-3.2491	5.1628	-1.0303
H	-2.3244	3.1347	-0.1803
H	-0.9204	3.4608	-1.2594
H	-4.2766	1.7452	-2.4083

B3LYP/6-31G(d)

C	-3.2793409467	1.6326687876	1.1437002194
C	-3.3898037834	1.4596508676	2.4914829584
N	-3.6438755059	0.8599337311	0.0745175664
N	-4.3397030593	-0.3251380434	0.4974339349
Li	-2.3084218857	0.8360663423	-1.3251397262
C	-4.231766367	-1.4636982351	-0.4204198623
C	-5.7660340947	-0.115348847	0.7533532566
C	-5.4611186332	-2.3514477994	-0.0566586413
C	-4.2492066193	-1.149285497	-1.9293061994
C	-6.256398289	-1.5415594454	0.9946187908
O	-2.9583204716	-0.7003692474	-2.3779465334
C	-2.8629641995	-0.6319903871	-3.7931182851
H	-2.8272132049	2.5736759483	0.8030536513
H	-3.8252309057	0.5661882985	2.9251689511
H	-3.0653254347	2.2451860578	3.16711322
H	-3.2858929666	-1.9934889393	-0.2340008971
H	-5.8896004351	0.5526882161	1.6105757914
H	-6.2839721439	0.3481765157	-0.1116101452
H	-5.1536955943	-3.3345707878	0.313128188
H	-6.0806852785	-2.5293185869	-0.9450420002
H	-5.005172089	-0.3869291022	-2.1675909127
H	-4.4920368697	-2.0666481095	-2.486135947
H	-5.989158948	-1.8592853262	2.0077448913
H	-7.3397886796	-1.6536121118	0.8787079738
H	-1.8496680497	-0.3021126114	-4.0350342411
H	-3.0386091415	-1.6201699657	-4.2413762357
H	-3.5862285666	0.0831965591	-4.2099935691
O	-0.4316008152	0.5862185047	-0.6560880975
C	0.2086204305	1.6926653753	0.026334775
C	0.4253573112	1.2319935689	1.4679945236
C	0.6326419961	-0.2791554422	1.2876299611
C	-0.3801588925	-0.5999425098	0.189615429
H	1.1573217056	1.909841487	-0.4838704407
H	-0.4455595521	2.5663977906	-0.0522912379
H	1.2728614288	1.7357348981	1.9432069583
H	-0.4814262914	1.4141716118	2.0559664854
H	1.6540789945	-0.4978034645	0.9523906526
H	0.4400132029	-0.848558255	2.2014286909
H	-1.3800092665	-0.7631586811	0.6051762171
H	-0.09957837	-1.4461704146	-0.4440188085
O	-2.3880940795	2.4670885291	-2.4853624311
C	-3.5864557818	3.2583099864	-2.3091072471
C	-3.0578498564	4.6549436885	-2.0007526574
C	-1.8425846967	4.7569578347	-2.944290546
C	-1.3683202345	3.2916963103	-3.0865553987
H	-4.1705181348	3.2482412994	-3.2420270418
H	-4.1535582761	2.7769726093	-1.5080829349
H	-3.8001892326	5.4390234577	-2.1773559442
H	-2.7465437122	4.7095992986	-0.9516732989
H	-2.147125288	5.155257479	-3.9181298693
H	-1.0564081079	5.4093457889	-2.5531477151

H -0.4323089262 3.0907325955 -2.5572647358
H -1.2393983922 3.0023493715 -4.1371084859

1b · 2 THF
PM3

C	-3.7476	0.1544	-2.7930
C	-4.5298	1.2405	-2.3322
N	-2.4639	-0.0785	-2.5430
N	-1.8531	0.7191	-1.4794
Li	-3.8129	1.5076	-0.3095
C	-1.0880	-0.2372	-0.5735
C	-0.8629	1.7312	-1.9893
C	0.3934	0.1646	-0.6047
C	-1.6604	-0.1693	0.8551
C	0.5402	1.1916	-1.7227
O	-3.0865	-0.1312	0.9069
C	-3.7293	-1.3665	0.6444
H	-4.1845	-0.6250	-3.4351
H	-4.1107	2.2501	-2.4864
H	-5.5847	1.2210	-2.6088
H	-1.1937	-1.2891	-0.9497
H	-1.0227	1.9666	-3.0598
H	-1.0417	2.6755	-1.4343
H	1.0363	-0.7176	-0.7768
H	0.7255	0.5841	0.3656
H	-1.3940	0.7854	1.3677
H	-1.2796	-1.0086	1.4687
H	0.9621	0.7234	-2.6327
H	1.2420	2.0001	-1.4503
H	-4.7917	-1.0949	0.5929
H	-3.4094	-1.8316	-0.2973
H	-3.5561	-2.0646	1.4729
O	-5.1162	3.4193	-0.3968
C	-6.2761	3.6334	0.4058
C	-6.5231	5.1374	0.5393
C	-5.3719	5.8071	-0.2044
C	-4.4675	4.6642	-0.6644
H	-7.0894	3.0956	-0.1122
H	-7.5022	5.4243	0.1170
H	-6.5568	5.4418	1.6007
H	-5.7355	6.4036	-1.0603
H	-4.8243	6.5182	0.4398
H	-3.4870	4.6506	-0.1369
H	-4.2711	4.6584	-1.7520
H	-6.0992	3.1368	1.3848
O	-3.4340	2.4819	1.6442
C	-4.0678	2.3381	2.9167
C	-3.3476	3.2246	3.9351
C	-2.2933	3.9801	3.1299
C	-2.2424	3.2586	1.7832
H	-5.1238	2.6290	2.7365
H	-4.0441	3.9109	4.4474
H	-2.8863	2.6189	4.7374
H	-2.5728	5.0424	3.0027
H	-1.3092	3.9909	3.6307
H	-1.3862	2.5542	1.6931
H	-2.2484	3.9365	0.9028
H	-4.0385	1.2651	3.1807

B3LYP/6-31G(d)
C -2.743017824 2.4844901771 -2.3593821095
C -2.0944750318 3.5973380898 -1.8453952365
N -2.6532849445 1.1728499436 -2.0702455022
N -1.6136539323 0.9262317199 -1.0653745177
Li -3.1826752455 2.1481210205 -0.1686089925
C -1.769190159 -0.4676935572 -0.5839086753
C -0.2228454112 1.060207137 -1.5999141258
C -0.3591672598 -1.0836632953 -0.5580963401
C -2.4510055736 -0.491692328 0.782127504
C 0.3280333317 -0.3658442762 -1.726832152
O -3.6745142433 0.2504652859 0.8152040658
C -4.7695381315 -0.4242820313 0.1972828127
H -3.5374259409 2.6664101262 -3.0885588807
H -1.1777091424 3.5254596111 -1.2704757844
H -2.3324977861 4.5763464736 -2.2521722645
H -2.3842787535 -1.0036820054 -1.3195183048
H -0.2514924528 1.60472238 -2.5449572621
H 0.3841658096 1.6432612788 -0.8928339665
H -0.3792680433 -2.1738775825 -0.6597920704
H 0.1518349357 -0.8471259055 0.3865842762
H -1.8027473427 -0.0095312467 1.5213979238
H -2.6390759521 -1.5270503651 1.1105368847
H 0.006289771 -0.8093587314 -2.6767890155
H 1.421895324 -0.4124106912 -1.6846734585
H -5.645408464 0.2088415993 0.3453061102
H -4.5998754596 -0.5538971948 -0.8771019333
H -4.9343719141 -1.4018442875 0.6737538692
O -5.2191566578 2.7590787207 -0.1123506946
C -5.8584349748 3.3329896318 1.0443532239
C -6.8296466993 4.386887849 0.5074883442
C -7.2338752893 3.7797249652 -0.8446877042
C -5.9176605084 3.1562946319 -1.3148166965
H -6.3928987793 2.5390874583 1.5862629652
H -5.0770764845 3.7354032823 1.6924732286
H -7.6757710213 4.5600290152 1.1796925038
H -6.3125203656 5.341922761 0.3560959376
H -8.0004342304 3.0083143496 -0.7024511385
H -7.6225718021 4.5168220578 -1.5538588883
H -5.2938903159 3.8784438618 -1.8532220226
H -6.0449587942 2.2700183517 -1.9427403005
O -2.6284324453 3.0895854343 1.6670540819
C -2.5586224785 2.5412523327 2.9883382193
C -2.5962449163 3.7563783676 3.9396678941
C -2.1588252954 4.9448462121 3.0371495889
C -1.8206201051 4.274981693 1.6946847213
H -3.3921299199 1.8456493354 3.0978587781
H -1.6163560271 1.9839320771 3.1022365124
H -3.6040300368 3.9161570246 4.335053043
H -1.928419158 3.6123890694 4.7944683998
H -2.9799781287 5.6578761741 2.9132476729
H -1.3040831805 5.4931856913 3.4443549802
H -0.7578669695 3.9933189699 1.6468968082
H -2.0686665806 4.8554013372 0.8053406873

Cartesian coordinates for complexes **2** and transition states **3** (with 2 THF molecules) for the reaction of cyclohexanone with ethyl chloride at the PM3 and B3LYP/6-31G(d) levels of theory

2_syn

PM3

C	0.0000	0.0000	0.0000
C	0.0000	1.3572	0.0000
N	-1.1093	-0.8635	0.0000
N	-2.4467	-0.4484	0.4992
C	-3.1217	-1.6513	1.1452
C	-2.5830	0.6902	1.4676
C	-3.8012	-1.1668	2.4335
C	-4.1636	-2.2327	0.1682
C	-3.1178	0.1455	2.7871
O	-3.5802	-2.8192	-1.0007
C	-3.1145	-4.1467	-0.8161
C	1.3043	-0.7641	-0.0555
C	1.2269	2.1917	-0.0080
C	2.4696	1.4157	-0.4137
C	2.5095	0.0856	0.3134
H	-0.9407	1.9217	0.0421
H	-2.3711	-2.4473	1.4008
H	-1.6402	1.2620	1.6018
H	-3.3052	1.3957	1.0078
H	-3.7125	-1.9123	3.2443
H	-4.8887	-1.0169	2.2855
H	-4.8111	-1.4524	-0.2797
H	-4.8169	-2.9668	0.6826
H	-2.2971	-0.0175	3.5116
H	-3.8086	0.8566	3.2751
H	-2.7708	-4.4431	-1.8154
H	-2.2857	-4.2145	-0.0962
H	-3.9293	-4.8078	-0.4927
H	1.4361	-1.1730	-1.0853
H	1.2614	-1.6470	0.6148
H	1.3694	2.6468	0.9931
H	1.0752	3.0414	-0.7134
H	3.3820	2.0042	-0.2015
H	2.4654	1.2469	-1.5167
H	3.4428	-0.4599	0.0737
H	2.5342	0.2591	1.4075
Li	-2.5955	0.0518	-1.4321
C	-0.3175	-2.3543	-1.8125
C	-1.2407	-1.5841	-3.8247
C	0.5412	-2.9601	-2.9209
C	0.0764	-2.2643	-4.1970
O	-1.4639	-1.7373	-2.4180
H	0.2234	-1.5747	-1.2271
H	-0.7402	-3.0947	-1.1077
H	-2.1244	-2.0443	-4.3041
H	-1.2583	-0.4916	-4.0528
H	0.4039	-4.0554	-2.9857
H	1.6182	-2.8050	-2.7307
H	-0.0523	-2.9757	-5.0320
H	0.8182	-1.5222	-4.5476
O	-3.5331	1.4109	-2.6445
C	-3.6682	2.7915	-2.2770
C	-4.4776	3.4827	-3.3762
C	-4.4126	2.5331	-4.5719
C	-3.6441	1.3096	-4.0682
H	-4.1541	2.7727	-1.2840
H	-2.6509	3.2386	-2.1725
H	-5.5206	3.6648	-3.0601
H	-4.0581	4.4773	-3.6143
H	-5.4222	2.2602	-4.9291
H	-3.9054	2.9956	-5.4378
H	-2.6133	1.2407	-4.4907
H	-4.1561	0.3463	-4.2435
C	0.7377	1.2637	-3.4538
C	0.1561	2.6416	-3.3217
H	1.8105	1.2351	-3.1681
H	0.2152	0.5308	-2.8034
H	-0.9461	2.6166	-3.3741
H	0.5204	3.3236	-4.0989
H	0.4216	3.0690	-2.3369
Cl	0.5791	0.7141	-5.1504

B3LYP/6-31G(d)

C -0.3572889675 0.221779626 0.1028644578
C -0.500518678 1.3901121729 0.8009254369
N -1.171244566 -0.893140286 0.1123355469
N -2.1738048909 -0.8171902527 1.1482590519
C -3.2173849001 -1.8240761058 0.9911671776
C -1.6291797487 -1.1057585855 2.4855956244
C -3.958329116 -1.7773720049 2.3453142466
C -4.1479675147 -1.5674500407 -0.1923220184
C -2.8838600618 -1.283808537 3.353169863
O -3.6390974982 -2.064017453 -1.4488085061
C -3.9612899135 -3.4293271598 -1.6902048295
C 0.824973378 0.060866568 -0.8517997602
C 0.4848227342 2.5358199699 0.7775166765
C 1.4628602489 2.459042193 -0.4033517211
C 1.9810044886 1.0275966605 -0.5626743946
Li -1.7554099156 -1.4023032073 -1.694306289
O -2.0607817543 0.0666960477 -3.0865128403
C -2.2637844434 1.4076872906 -2.5639814726
C -3.7183479709 1.7305044255 -2.8859952599
C -3.8856951037 1.0756924181 -4.2667329285
C -3.0143886031 -0.1855868453 -4.1544871637
H -1.3552830621 1.4956349784 1.463039717
H -2.7626939546 -2.8319200072 0.8587734054
H -1.0294440156 -2.0359308607 2.4548607121
H -0.9730499787 -0.2956228479 2.8103603942
H -4.3694478113 -2.7597490266 2.6032206031
H -4.800325284 -1.0763391412 2.296783101
H -4.2803754619 -0.4886980599 -0.3190299403
H -5.133019029 -2.023141934 -0.020084517
H -2.7181460799 -1.9965574527 4.1676649538
H -3.1872779108 -0.3346059536 3.8059476463
H -3.4734059133 -3.7125510287 -2.6245203819
H -3.5959106645 -4.0799519313 -0.88534628
H -5.0488971507 -3.5556221775 -1.7865327451
H 0.4863494393 0.2128748621 -1.890956034
H 1.1829636715 -0.9753126501 -0.7976888074
H 1.0764765015 2.5723199233 1.7125677821
H -0.0472368485 3.499673051 0.7459730811
H 2.2955860552 3.1618081376 -0.2629227478
H 0.9469940099 2.757767078 -1.329328566
H 2.7324040055 0.9670913563 -1.3630653252
H 2.4867176953 0.7240628274 0.3652006425
H -2.0040859809 1.3962784583 -1.5024872814
H -1.5856414013 2.0980353843 -3.0866382135
H -4.3824687847 1.2625497556 -2.1501548276
H -3.9180580905 2.8063158435 -2.891944669
H -4.9250923414 0.8369151115 -4.5108513842
H -3.5012891546 1.7390698935 -5.049914356
H -2.462877576 -0.4036232971 -5.0746467776
H -3.6009307523 -1.063426953 -3.866063391
C -0.0442155953 -3.7553719447 -1.646268625
C -0.1568542441 -2.9778089267 -3.8576084383
C 1.3421260467 -3.9819103393 -2.2911303384
C 1.3318025852 -3.0635467853 -3.5307712636
O -0.8012916164 -2.9309109697 -2.5744635769
H -0.0161413316 -3.2010414357 -0.7044194185
H -0.5821852351 -4.6995349307 -1.495080124
H -0.4977118248 -3.8656040395 -4.4120574598
H -0.4489439494 -2.0821614894 -4.4097447893
H 1.4622328706 -5.0289238299 -2.5893073586
H 2.1563325507 -3.7386360682 -1.6028312674
H 1.9256118373 -3.4570712035 -4.3611628252
H 1.7114051865 -2.0685448078 -3.2757858326
C 0.8396238527 0.9179989872 -5.1109576421
C 1.0486782227 2.4161728445 -5.2337090137
Cl 0.2061681014 0.1967663835 -6.6692582766
H 1.772475928 0.3918152467 -4.9005342481
H 0.1025427928 0.6621514638 -4.3486121291
H 0.1130392983 2.929510412 -5.4752423167
H 1.7835806579 2.6540373976 -6.0084883049
H 1.4172795309 2.8033818016 -4.2756074423

2_anti

PM3

C	0.0000	0.0000	0.0000
C	0.0000	1.4242	0.0000
N	-1.0884	-0.7868	0.0000
N	-2.3732	-0.1443	-0.2083
Li	-1.6203	1.7181	-1.5366
C	-3.2374	-1.0373	-1.0864
C	-3.1273	0.0554	1.0852
C	-4.4813	-1.4395	-0.2805
C	-3.6290	-0.2720	-2.3663
C	-4.2315	-0.9935	1.1554
O	-2.5302	0.3879	-2.9946
C	-1.6713	-0.4724	-3.7238
C	1.2963	-0.7724	0.0310
C	1.2898	2.1900	0.0092
C	2.5639	1.3547	-0.0392
C	2.3970	0.0383	0.6927
H	-0.7559	1.9004	0.6723
H	-2.6693	-1.9590	-1.3793
H	-2.4542	0.0182	1.9741
H	-3.5483	1.0875	1.0739
H	-4.6586	-2.5290	-0.3394
H	-5.3990	-0.9713	-0.6876
H	-4.3103	0.5874	-2.1634
H	-4.1365	-0.9479	-3.0827
H	-3.9231	-1.8494	1.7857
H	-5.1460	-0.5920	1.6283
H	-0.8452	0.1867	-4.0361
H	-1.2802	-1.3049	-3.1236
H	-2.1903	-0.8712	-4.6046
H	1.5856	-1.0296	-1.0087
H	1.1737	-1.7416	0.5554
H	1.3190	2.8366	0.9124
H	1.3027	2.8920	-0.8571
H	3.4079	1.9282	0.3911
H	2.8510	1.1542	-1.0921
H	3.3464	-0.5305	0.6938
H	2.1493	0.2202	1.7634
O	-0.7724	2.8429	-3.1101
C	0.5535	2.4184	-3.4593
C	1.1400	3.4641	-4.4090
C	0.2488	4.6942	-4.2398
C	-0.8503	4.2628	-3.2638
H	1.1468	2.3115	-2.5201
H	0.4024	1.4152	-3.9097
H	2.1958	3.6797	-4.1641
H	1.1427	3.1085	-5.4555
H	0.8132	5.5600	-3.8483
H	-0.1736	5.0262	-5.2056
H	-1.8761	4.4455	-3.6306
H	-0.7446	4.7361	-2.2686
C	-0.7182	1.4894	3.3969
C	0.6272	1.0929	3.9303
Cl	-1.5347	2.5399	4.5870
H	-1.3740	0.6141	3.2018
H	-0.6385	2.0412	2.4328
H	1.2048	0.5473	3.1629
H	0.5422	0.4447	4.8112
H	1.2195	1.9701	4.2222
O	-3.0137	3.2083	-1.0743
C	-3.1731	3.6654	0.2749
C	-4.4377	4.5226	0.3376
C	-5.1877	4.2252	-0.9595
C	-4.2749	3.2842	-1.7485
H	-3.2272	2.7749	0.9417
H	-2.2375	4.2105	0.4949
H	-4.1940	5.5972	0.4258
H	-5.0426	4.2812	1.2299
H	-5.4024	5.1502	-1.5247
H	-6.1718	3.7602	-0.7671
H	-4.6855	2.2529	-1.8367
H	-4.0246	3.6442	-2.7635

B3LYP/6-31G(d)

C -0.2521062542 0.5105082568 -0.0308358194
C -0.5560434766 1.6457952381 0.7102348724
N -1.0928480885 -0.3990724044 -0.5880528447
N -2.4984673735 -0.1352896893 -0.2509870594
C -3.3393228604 -0.9958739787 -1.1218108912
C -2.8334861898 -0.4882002374 1.166237382
C -4.3942720202 -1.6517636606 -0.2130901055
C -3.9698934019 -0.1786170177 -2.2440807554
C -3.6360434005 -1.7938170138 1.1106870194
O -3.015146805 0.5614082024 -3.0138608073
C -2.2995550816 -0.2348603405 -3.9541634449
C 1.205871035 0.1967749654 -0.369798881
C 0.4803573408 2.6230423262 1.2269263136
C 1.8423295779 2.4597397671 0.5391651153
C 2.2192256743 0.9767188801 0.4765804352
H -1.5737431084 1.7980874223 1.0587671919
H -2.6881850806 -1.7745690387 -1.5421176295
H -1.9099655452 -0.5760024413 1.7389859837
H -3.4343255084 0.3148275285 1.6145372998
H -4.7582483992 -2.6017447434 -0.618527117
H -5.2639280253 -0.9908184377 -0.0846302558
H -4.6375463454 0.5744655987 -1.8138044133
H -4.5606257442 -0.8218227392 -2.9163798384
H -2.9542704782 -2.6511156894 1.0575597853
H -4.29115217 -1.9343208251 1.9772658428
H -1.7577390698 0.4580068585 -4.6010115766
H -1.5901595811 -0.9024737059 -3.4515975093
H -2.9952678672 -0.8254873147 -4.5674552409
H 1.3824830496 0.4049251089 -1.4336024289
H 1.3541782311 -0.8826633984 -0.2520149491
H 0.6367547922 2.5152077046 2.3176991454
H 0.1327589043 3.6620282875 1.1019474566
H 2.6114887764 3.0395065978 1.0672483575
H 1.7885107223 2.8575140066 -0.4858522456
H 3.2303255962 0.8424765931 0.0688036614
H 2.2394087537 0.5714007259 1.4993784532
Li -1.7415704155 1.4723762062 -1.4692065908
O -0.39069638 2.3992249659 -2.9167888927
C 0.6876133403 1.8703215956 -3.6979508731
C 0.7223894717 2.7466367623 -4.9611656905
C 0.1513139054 4.106143428 -4.4692361469
C -0.2510867657 3.8245039906 -3.0062234671
H 1.6267186712 1.9564607442 -3.1323409133
H 0.4844946019 0.8135858883 -3.877769966
H 1.7341346269 2.8319863865 -5.3687585546
H 0.0848517453 2.3202960874 -5.7422345605
H 0.8860439315 4.9146255728 -4.530868756
H -0.7158235657 4.4030793149 -5.0667978798
H -1.2022520852 4.2578316174 -2.6993814931
H 0.5343206676 4.1536842929 -2.3098301128
C -0.3436706557 0.2396783092 4.3046135484
C 1.0307797295 0.5330163375 4.8789683502
Cl -1.6578301336 1.0604910155 5.2746234648
H -0.5781673371 -0.826225807 4.3336387926
H -0.4505272981 0.6025853064 3.2800627899
H 1.7893085617 0.0274563674 4.2679226911
H 1.1189046796 0.1727211177 5.9086425598
H 1.2421649266 1.6063142829 4.8662510316
O -3.0023804268 3.2484034686 -1.3888039198
C -3.1245147621 4.0370410516 -0.1916629157
C -3.889717689 5.318991146 -0.6018201553
C -4.423723183 5.0000469935 -2.0234295793
C -4.1915159076 3.4902618653 -2.1499524658
H -3.6793512278 3.464500705 0.563636127
H -2.1148256011 4.2133971027 0.1819193411
H -3.2344797647 6.1947970417 -0.6111168747
H -4.7020963351 5.5271506018 0.1009334517
H -3.8431944776 5.5339729326 -2.7831655757
H -5.4753298162 5.2720654254 -2.1555341972
H -5.0318480837 2.9253747041 -1.7166364182
H -4.0122285264 3.1303927869 -3.1640006514

3_syn

PM3

C	0.0000	0.0000	0.0000
C	1.4111	-0.0000	-0.0000
N	-0.8436	1.0570	0.0000
N	-0.4737	2.4403	0.3307
C	-1.7241	3.1711	0.8196

C	0.5958	2.7011	1.3563
C	-1.3796	3.8655	2.1456
C	-2.1590	4.2123	-0.2330
C	-0.0621	3.2639	2.6101
O	-2.5487	3.6222	-1.4762
C	-3.8925	3.1703	-1.5159
C	-0.7222	-1.3235	-0.1491
C	2.1582	-1.2060	0.4699
C	1.4836	-2.4908	0.0226
C	0.0343	-2.4878	0.4708
H	1.9324	0.9424	0.2405
H	-2.5674	2.4483	0.9877
H	1.2089	1.8021	1.5805
H	1.2875	3.4386	0.8993
H	-2.1813	3.7239	2.8932
H	-1.2877	4.9621	2.0166
H	-1.3258	4.8730	-0.5496
H	-2.9713	4.8517	0.1679
H	-0.2310	2.4689	3.3616
H	0.5825	4.0103	3.1085
H	-4.0048	2.7870	-2.5378
H	-4.0967	2.3728	-0.7878
H	-4.5891	4.0022	-1.3491
H	-0.8781	-1.5077	-1.2393
H	-1.7397	-1.2777	0.2915
H	2.2592	-1.1890	1.5743
H	3.1972	-1.1521	0.0691
H	2.0157	-3.3739	0.4216
H	1.5393	-2.5624	-1.0877
H	-0.4580	-3.4403	0.1942
H	-0.0182	-2.4314	1.5762
Li	-1.1246	2.1481	-1.9680
C	-2.7560	-0.2262	-2.9370
C	-1.5704	0.7713	-4.6983
C	-3.0891	-1.0492	-4.1797
C	-2.1398	-0.5309	-5.2560
O	-2.0448	0.9481	-3.3519
H	-2.1122	-0.7847	-2.2194
H	-3.6401	0.1573	-2.3950
H	-1.9227	1.6704	-5.2373
H	-0.4505	0.7893	-4.6657
H	-4.1465	-0.9222	-4.4769
H	-2.9579	-2.1305	-3.9961
H	-2.6553	-0.3727	-6.2198
H	-1.3275	-1.2533	-5.4639
O	0.3402	3.3293	-2.8461
C	1.5349	3.7752	-2.1909
C	2.3997	4.4915	-3.2284
C	1.8486	4.0431	-4.5800
C	0.6006	3.2226	-4.2563
H	1.1795	4.4211	-1.3678
H	2.0590	2.8917	-1.7551
H	2.3467	5.5894	-3.1129
H	3.4662	4.2281	-3.1091
H	1.6146	4.9048	-5.2306
H	2.5833	3.4347	-5.1394
H	0.7136	2.1356	-4.5049
H	-0.3207	3.6032	-4.7343
C	1.8392	0.0013	-2.1329
C	3.2323	0.5073	-2.0095
H	1.6432	-1.0805	-2.1048
H	0.9941	0.6962	-2.2287
H	3.2522	1.5931	-1.8136
H	3.8113	0.3245	-2.9272
H	3.7620	-0.0038	-1.1852
Cl	1.7708	-0.1052	-4.3379

B3LYP/6-31G(d)
C 0.0245423614 0.0983788052 -0.151498322
C 1.3796908691 -0.113246696 0.1563366868
N -0.711390033 1.2230684145 -0.1342018071
N -0.1735609485 2.3667090685 0.5702908875
C -1.2442065819 3.3794429299 0.7112281978
C 0.1689809289 2.0957429845 1.9898093066
C -0.6851745466 4.3591921193 1.7615750297
C -1.6335172419 4.1285038305 -0.5597754217
C 0.2638598629 3.4894599489 2.623352207
O -2.3441537088 3.365222484 -1.547984071
C -3.6988238292 3.0873011812 -1.2094648847
C -0.7547198091 -1.1019395377 -0.6884970328
C 1.8893956728 -1.4725563601 0.6024132193
C 1.1096122442 -2.6509408651 0.0003070287
C -0.3995534639 -2.3954082021 0.0591405675
H 1.9544519039 0.7327735718 0.5209638502
H -2.1437732723 2.88405435 1.1220628934
H -0.6393603891 1.5004182444 2.4512745301
H 1.0897880402 1.5235726392 2.081292538
H -1.4944067872 4.8148437462 2.3411385919
H -0.1367816362 5.1746634557 1.2744316532
H -0.7386447233 4.4917347099 -1.0695495173
H -2.2529051355 4.9959373297 -0.2855968572
H -0.0279019465 3.4689014533 3.6780399937
H 1.2888165954 3.8702068955 2.5762450836
H -4.1613471791 2.6492704042 -2.0967613817
H -3.7724729254 2.3821611855 -0.3733985812
H -4.227849099 4.0154852439 -0.9523474349
H -0.5326704294 -1.2398366852 -1.757717489
H -1.8263401376 -0.892154475 -0.6056904093
H 1.8361285415 -1.5520065653 1.703981666
H 2.9580383533 -1.5827433565 0.3645065217
H 1.3659639343 -3.5795574955 0.526781706
H 1.4040355086 -2.7972081651 -1.0487266473
H -0.9527629403 -3.2416631613 -0.3701049507
H -0.7184868223 -2.3087599689 1.1079790189
Li -1.0943814607 1.879487689 -2.0462834379
C -3.1454319241 0.0352072633 -3.3527350862
C -1.3102785524 0.3474131027 -4.7129854204
C -2.906225876 -1.3482702004 -3.9852557598
C -1.6505577673 -1.141246815 -4.8767359281
O -1.8891330182 0.7249038803 -3.4423522474
H -3.42784595 0.001097527 -2.2982230767
H -3.9074955105 0.6009855039 -3.9099039126
H -1.7745818848 0.9554370199 -5.5034398028
H -0.2388727163 0.5508060219 -4.6688317913
H -3.7791619933 -1.6764227834 -4.5574759565
H -2.7153253928 -2.0983971353 -3.2129584458
H -1.8327731329 -1.3952588034 -5.9248361461
H -0.8171899613 -1.7570691521 -4.528148223
O 0.286614319 3.0263237794 -2.9502638099
C 1.5577098422 3.5274244922 -2.4847104532
C 1.6129316713 4.9758049761 -2.9950726954
C 0.7113193291 4.9559156875 -4.2611456037
C 0.1546858603 3.5187270942 -4.2978873755
H 1.564361799 3.4191586361 -1.3978485996
H 2.3546296864 2.9211412396 -2.9315030427
H 1.2129962362 5.668763232 -2.2474444122
H 2.6396811088 5.2828851793 -3.2142288147
H -0.0960629139 5.6893176663 -4.1748805439
H 1.2698934776 5.1830040312 -5.1737564265
H 0.7431405265 2.8749829574 -4.9621362941
H -0.9026278092 3.4581937343 -4.5659679444
C 2.2757076787 0.1028409557 -2.1538893044
C 3.7279595484 0.2387872664 -1.7912510531
H 1.8446448544 -0.8751651667 -2.2850042779
H 1.6040108134 0.9372699592 -2.1042323295
H 4.0732188602 1.2653056091 -1.9435776288
H 4.3369013113 -0.4168540968 -2.4195368578
H 3.9101686882 -0.0323455044 -0.7454208344
Cl 2.4297290222 0.3932066917 -4.4301668333

3_anti
PM3

C	2.0289	-0.2902	-0.1744
C	1.4396	-1.3206	0.6057
N	1.4287	0.5120	-1.0580
N	-0.0064	0.4659	-1.3025
Li	-1.4744	-0.1228	0.3826
C	-0.4416	1.8767	-1.6988
C	-0.3061	-0.4134	-2.5089
C	-0.5068	1.9227	-3.2306
C	-1.8261	2.2078	-1.1006
C	-0.6226	0.4793	-3.7067
O	-1.9219	1.9219	0.2986

C	-1.3010	2.8795	1.1400
C	3.5169	-0.0407	-0.0990
H	0.3353	-1.2870	0.7498
C	2.1308	-1.8222	1.8365
H	0.2999	2.6287	-1.3223
H	0.5395	-1.1101	-2.7248
H	-1.1613	-1.0886	-2.2571
H	0.4056	2.3987	-3.6377
H	-1.3487	2.5448	-3.5891
H	-2.6426	1.5656	-1.5138
H	-2.0913	3.2656	-1.2956
H	0.0658	0.2798	-4.5490
H	-1.6350	0.2666	-4.1001
H	-1.2431	2.3800	2.1207
H	-0.2937	3.1634	0.8073
H	-1.9323	3.7739	1.2032
C	3.5479	-1.3062	2.0379
O	-1.6828	-0.4434	2.3781
C	-0.7360	0.0061	3.3579
C	-1.2447	-0.4068	4.7377
C	-2.3699	-1.4048	4.4711
C	-2.5158	-1.4605	2.9496
H	0.2543	-0.4443	3.1112
H	-0.4352	-0.8514	5.3449
H	-1.6052	0.4643	5.3147
H	-2.1390	-2.4026	4.8865
H	-3.3122	-1.0923	4.9565
H	-3.5342	-1.2281	2.5878
H	-2.2043	-2.4329	2.5197
H	-0.6830	1.1042	3.1975
C	4.2438	-1.1010	0.7079
H	3.6871	0.9573	0.3555
H	3.9531	0.0151	-1.1168
H	2.1376	-2.9325	1.8166
H	1.5250	-1.5539	2.7354
H	4.1222	-2.0111	2.6692
H	3.5338	-0.3499	2.5984
H	5.2996	-0.8054	0.8600
H	4.2734	-2.0609	0.1455
C	1.1342	-3.0003	-0.7576
C	2.3184	-3.8770	-0.6081
H	1.1331	-2.2522	-1.5596
H	0.2678	-3.1129	-0.0980
H	3.2359	-3.2861	-0.4409
H	2.4717	-4.4701	-1.5222
H	2.2192	-4.5842	0.2256
Cl	-0.0521	-4.2425	-2.1603
O	-2.9920	-1.3031	-0.3039
C	-2.6974	-2.6110	-0.8382
C	-3.9075	-3.0695	-1.6455
C	-4.7016	-1.7961	-1.9285
C	-4.0962	-0.7285	-1.0164
H	-3.7119	0.1606	-1.5674
H	-4.7878	-0.3730	-0.2307
H	-5.7805	-1.9322	-1.7335
H	-4.6260	-1.5006	-2.9914
H	-4.5132	-3.8061	-1.0861
H	-3.5929	-3.5841	-2.5722
H	-1.7651	-2.5478	-1.4586
H	-2.4806	-3.2305	0.0516

B3LYP/6-31G(d)

C 1.7846784804 -0.4975768652 -0.0142767883
C 1.0829002102 -1.6431270883 0.4395936113
N 1.4026807991 0.517900775 -0.7772778796
N -0.0025581527 0.4999672257 -1.2155626322
Li -1.4940387627 -0.0792111479 0.1781309492
C -0.3363598733 1.9382511543 -1.4552719258
C -0.0337883478 -0.0705285714 -2.5964109909
C 0.3046259597 2.3390474313 -2.8114337973
C -1.8529549953 2.1245909927 -1.486118154
C 0.5835799913 0.9940997166 -3.5264770352
O -2.4693576633 1.6760752061 -0.2645134415
C -2.6205314897 2.7022510431 0.7126368629
C 3.2599124941 -0.3314393697 0.3788417823
C 1.5621341829 -2.4464559013 1.6463121374
C 2.8148967633 -1.863513074 2.3171788637
C 3.8296064509 -1.460407163 1.2461710727
H 0.0042747191 -1.6372231123 0.3036556596
H 0.0841740166 2.5059960901 -0.6214301458
H 0.5112045223 -1.0107799481 -2.6116708473
H -1.0766934222 -0.280168579 -2.8696361109
H 1.2304552243 2.8918019157 -2.6405706652
H -0.3631028874 2.9871392128 -3.3931690716
H -2.3084820874 1.5344549548 -2.2882234725
H -2.1080023168 3.1778181925 -1.662375304
H 1.6594244217 0.8297058991 -3.6126948486
H 0.1532507353 0.9504593615 -4.5321614119
H -3.0021564942 2.2258879752 1.6166820849
H -1.662484392 3.1882024302 0.9399966427
H -3.3338087653 3.4611456822 0.3646683665
H 3.349342653 0.6219110269 0.9172991303
H 3.8516477997 -0.208333547 -0.5358748688
H 1.7930699939 -3.4911661991 1.3734511473
H 0.754869775 -2.5273446359 2.3919902698
H 3.2454748156 -2.5931368421 3.0156861825
H 2.5509584138 -0.9736925773 2.9097377288
H 4.7756992179 -1.1360413099 1.6985421765
H 4.0646917655 -2.3373930369 0.6281160718
O -1.4830183665 0.044903434 2.1724309396
C -0.4031024709 0.6794147416 2.9098958802
C -0.3425661469 -0.0332533493 4.2645694341
C -1.7848675521 -0.5332142384 4.4446759429
C -2.1654653828 -0.9121550128 3.0145971744
H 0.512333421 0.5815897225 2.3216337584
H -0.6520170948 1.7422229815 3.0200118646
H 0.3512979662 -0.8790485927 4.2191741902
H -0.0132304445 0.6326883665 5.0673937973
H -1.8665178834 -1.3774611564 5.1354310513
H -2.4312499206 0.2727139714 4.8122534319
H -3.2363796371 -0.8410946785 2.804798335
H -1.8218407778 -1.9230575885 2.7609718602
C 0.9571582371 -3.3450938037 -1.2660462897
C 2.3629000174 -3.344757243 -1.7941591542
Cl -0.1215394486 -5.0063673628 -2.501244695
H 0.2245616852 -2.6811712817 -1.6770235521
H 0.6962035645 -3.9100369566 -0.3892649209
H 3.0731398173 -3.6426905395 -1.0160550382
H 2.643426264 -2.3503648654 -2.1579448528
H 2.4574983378 -4.0518258788 -2.6234419945
O -2.8277041075 -1.4800110271 -0.2715386274
C -2.5940124253 -2.8804830318 -0.6285430737
C -3.977623453 -3.4877805357 -0.870555168
C -4.8079973905 -2.2653113859 -1.2912464106
C -4.2362446975 -1.176354523 -0.3868174231
H -1.9768253661 -2.9158040188 -1.5287457407
H -2.0446963138 -3.3578317543 0.1870770575
H -4.381827243 -3.9219835059 0.0516088103
H -3.9388320624 -4.2739898791 -1.6284751971
H -5.8848690615 -2.401542558 -1.1528714334
H -4.6255366706 -2.0199172638 -2.3440015872
H -4.3277922096 -0.1606917888 -0.7785461291
H -4.6947409391 -1.2101407147 0.6127494108

Cartesian coordinates for transition states **3** (with 2 THF molecules) for the remaining reactions at the PM3 level of theory

Cyclohexanone + methyl chloride

3_syn

C	0.0000	0.0000	0.0000
C	1.4095	0.0131	-0.1184
N	-0.8528	1.0439	0.0663
N	-0.4730	2.4367	0.3303
C	-1.6987	3.1705	0.8779
C	0.6478	2.7223	1.2946
C	-1.3114	3.8146	2.2179
C	-2.1447	4.2519	-0.1288
C	0.0439	3.2352	2.5958
O	-2.5288	3.7097	-1.3954
C	-3.8706	3.2539	-1.4566
C	-0.7232	-1.3284	-0.0937
C	2.1939	-1.1892	0.3031
C	1.4966	-2.4781	-0.0971
C	0.0865	-2.4890	0.4621
H	1.9401	0.9577	0.0938
H	-2.5482	2.4540	1.0411
H	1.3066	1.8426	1.4600
H	1.2830	3.4955	0.8140
H	-2.0725	3.6130	2.9939
H	-1.2597	4.9185	2.1371
H	-1.3181	4.9336	-0.4177
H	-2.9621	4.8663	0.2998
H	-0.0649	2.4170	3.3335
H	0.6960	3.9850	3.0795
H	-3.9812	2.9232	-2.4970
H	-4.0688	2.4183	-0.7705
H	-4.5720	4.0717	-1.2470
H	-0.9604	-1.5112	-1.1694
H	-1.7046	-1.2900	0.4224
H	2.3580	-1.1702	1.4007
H	3.2045	-1.1470	-0.1505
H	2.0648	-3.3585	0.2553
H	1.4664	-2.5440	-1.2086
H	-0.4187	-3.4443	0.2212
H	0.1187	-2.4362	1.5685
Li	-1.0877	2.2542	-1.9244
C	-2.7559	-0.1175	-2.8704
C	-1.5781	0.8641	-4.6461
C	-3.1355	-0.9210	-4.1125
C	-2.2101	-0.4057	-5.2111
O	-2.0230	1.0415	-3.2903
H	-2.1138	-0.6980	-2.1690
H	-3.6190	0.2845	-2.3080
H	-1.9006	1.7845	-5.1676
H	-0.4585	0.8386	-4.6332
H	-4.1989	-0.7759	-4.3779
H	-3.0155	-2.0062	-3.9442
H	-2.7570	-0.2065	-6.1498
H	-1.4326	-1.1489	-5.4696
O	0.3120	3.4589	-2.8665
C	1.4642	3.9229	-2.1495
C	2.4477	4.5164	-3.1573
C	1.9931	3.9856	-4.5138
C	0.6507	3.3039	-4.2552
H	1.0670	4.6535	-1.4206
H	1.8940	3.0648	-1.5917
H	2.4356	5.6215	-3.1302
H	3.4875	4.2230	-2.9261
H	1.9046	4.7941	-5.2613
H	2.7198	3.2641	-4.9332
H	0.6717	2.2073	-4.4814
H	-0.1955	3.7631	-4.7978
C	1.6453	0.0114	-2.2353
H	2.6698	0.3325	-2.0948
H	1.4164	-1.0536	-2.2322
H	0.8523	0.7540	-2.3089
Cl	1.8510	0.0343	-4.3744

3_anti

C	2.0289	-0.2902	-0.1744
C	1.4368	-1.3584	0.5628
N	1.4305	0.5440	-1.0252
N	0.0013	0.4631	-1.2982
Li	-1.4108	-0.2247	0.4069
C	-0.4919	1.8667	-1.6439
C	-0.2385	-0.3666	-2.5487
C	-0.5305	1.9867	-3.1745
C	-1.9019	2.0959	-1.0568
C	-0.3768	0.5781	-3.7392
O	-1.9852	1.7895	0.3390
C	-1.4421	2.7824	1.1934
C	3.5178	-0.0635	-0.0802
H	0.3337	-1.3138	0.7226
C	2.1288	-1.8903	1.7845
H	0.2049	2.6343	-1.2164
H	0.5733	-1.1171	-2.7015
H	-1.1635	-0.9726	-2.3947
H	0.2855	2.6439	-3.5300
H	-1.4651	2.4664	-3.5233
H	-2.6695	1.4015	-1.4803
H	-2.2386	3.1345	-1.2440
H	0.5072	0.5127	-4.4014
H	-1.2384	0.2965	-4.3727
H	-1.3554	2.2799	2.1701
H	-0.4556	3.1406	0.8702
H	-2.1368	3.6284	1.2585
C	3.6091	-1.5537	1.9017
O	-1.6379	-0.5502	2.4058
C	-0.7028	-0.0655	3.3808
C	-1.1689	-0.5334	4.7581
C	-2.2226	-1.6048	4.4839
C	-2.3832	-1.6407	2.9632
H	0.3081	-0.4545	3.1138
H	-0.3249	-0.9279	5.3526
H	-1.5860	0.3014	5.3507
H	-1.9148	-2.5914	4.8758
H	-3.1788	-1.3713	4.9866
H	-3.4202	-1.4783	2.6171
H	-2.0043	-2.5779	2.5103
H	-0.7154	1.0362	3.2401
C	4.2228	-1.2516	0.5497
H	3.7020	0.8511	0.5209
H	3.9509	0.1421	-1.0801
H	1.9954	-2.9920	1.8135
H	1.6058	-1.5157	2.6975
H	4.1499	-2.3889	2.3876
H	3.7514	-0.6818	2.5725
H	5.3047	-1.0409	0.6524
H	4.1429	-2.1400	-0.1104
C	1.3594	-2.9883	-0.7614
H	2.3964	-3.2508	-0.5917
H	1.1093	-2.3176	-1.5793
H	0.5872	-3.3950	-0.1167
Cl	1.0084	-4.6469	-2.0961
O	-2.8141	-1.5329	-0.3050
C	-2.3935	-2.7519	-0.9482
C	-3.5746	-3.2818	-1.7563
C	-4.5132	-2.0870	-1.9179
C	-3.9706	-1.0113	-0.9758
H	-3.6632	-0.0758	-1.4992
H	-4.6675	-0.7384	-0.1626
H	-5.5576	-2.3513	-1.6731
H	-4.5351	-1.7269	-2.9630
H	-4.0748	-4.1207	-1.2380
H	-3.2437	-3.6889	-2.7293
H	-1.5062	-2.5187	-1.5842
H	-2.0692	-3.4076	-0.1192

Cyclohexanone + allyl chloride

3_syn

C	0.0000	0.0000	0.0000
C	1.4122	-0.0138	0.0083
N	-0.8374	1.0622	-0.0069
N	-0.4743	2.4433	0.3312
C	-1.7221	3.1576	0.8491

C	0.6168	2.7119	1.3314
C	-1.3377	3.9023	2.1357
C	-2.2320	4.1544	-0.2122
C	-0.0092	3.3131	2.5837
O	-2.6566	3.5217	-1.4223
C	-3.9834	3.0217	-1.3896
C	-0.7370	-1.3150	-0.1616
C	2.1370	-1.2358	0.4721
C	1.4570	-2.5048	-0.0101
C	0.0065	-2.5006	0.4322
H	1.9471	0.9172	0.2615
H	-2.5375	2.4197	1.0776
H	1.2211	1.8103	1.5683
H	1.3096	3.4277	0.8425
H	-2.1179	3.7945	2.9112
H	-1.2453	4.9926	1.9603
H	-1.4334	4.8306	-0.5817
H	-3.0457	4.7808	0.2064
H	-0.1595	2.5410	3.3626
H	0.6483	4.0732	3.0433
H	-4.1279	2.6094	-2.3963
H	-4.1255	2.2360	-0.6345
H	-4.7015	3.8322	-1.2103
H	-0.9047	-1.4823	-1.2526
H	-1.7501	-1.2632	0.2891
H	2.2104	-1.2371	1.5792
H	3.1838	-1.1998	0.1021
H	1.9802	-3.4015	0.3704
H	1.5208	-2.5491	-1.1216
H	-0.4935	-3.4415	0.1311
H	-0.0494	-2.4710	1.5385
Li	-1.2067	2.1017	-1.9742
C	-2.8129	-0.2941	-2.9516
C	-1.5494	0.6568	-4.6857
C	-3.0677	-1.1655	-4.1798
C	-2.0586	-0.6810	-5.2164
O	-2.0773	0.8660	-3.3636
H	-2.2119	-0.8213	-2.1759
H	-3.7301	0.1035	-2.4793
H	-1.9099	1.5230	-5.2714
H	-0.4322	0.7147	-4.6149
H	-4.1061	-1.0567	-4.5436
H	-2.9428	-2.2383	-3.9485
H	-2.5119	-0.5777	-6.2183
H	-1.2234	-1.3972	-5.3371
O	0.1716	3.3573	-2.8938
C	1.3263	3.8943	-2.2354
C	2.1639	4.6316	-3.2802
C	1.6647	4.1109	-4.6254
C	0.4602	3.2294	-4.2968
H	0.9211	4.5401	-1.4356
H	1.8919	3.0548	-1.7678
H	2.0420	5.7269	-3.1986
H	3.2421	4.4378	-3.1368
H	1.3939	4.9367	-5.3071
H	2.4430	3.5283	-5.1522
H	0.6400	2.1446	-4.5137
H	-0.4735	3.5442	-4.7978
C	1.8173	0.0392	-2.1198
C	3.1132	0.6955	-1.9859
H	1.7296	-1.0574	-2.1146
H	0.9056	0.6429	-2.2310
H	5.2272	0.5255	-1.8694
C	4.2666	0.0278	-1.9562
H	3.0908	1.7966	-1.9296
Cl	1.8691	0.0058	-4.3270
H	4.3264	-1.0549	-2.0395

3_anti

C	1.9970	-0.3208	-0.1744
C	1.3843	-1.3590	0.5823
N	1.4072	0.5282	-1.0217
N	-0.0181	0.4705	-1.3091
Li	-1.4072	0.1683	0.5360
C	-0.4378	1.8326	-1.8678
C	-0.2811	-0.5423	-2.4184
C	-0.7337	1.6449	-3.3634
C	-1.7089	2.3554	-1.1628
C	-1.0193	0.1613	-3.5494
O	-1.6893	2.2167	0.2599
C	-0.9008	3.1839	0.9338
C	3.4890	-0.0992	-0.0923
H	0.3027	-1.2277	0.8138
C	2.1142	-2.0041	1.7230
H	0.3848	2.5809	-1.7259
H	0.6678	-1.0036	-2.7924
H	-0.8582	-1.3987	-1.9904
H	0.1389	1.9550	-3.9700
H	-1.5736	2.2772	-3.7071
H	-2.6186	1.7638	-1.4283
H	-1.8976	3.4109	-1.4435
H	-0.6906	-0.2010	-4.5401
H	-2.1102	-0.0640	-3.5005
H	-0.9654	2.8834	1.9863
H	0.1457	3.1883	0.6017
H	-1.3320	4.1841	0.8003
C	3.5553	-1.5605	1.9132
O	-1.4488	0.0621	2.5620
C	-0.3393	0.1339	3.4685
C	-0.8710	-0.0128	4.8929
C	-2.3199	-0.4699	4.7414
C	-2.5861	-0.4947	3.2361
H	0.3854	-0.6672	3.1904
H	-0.2689	-0.7371	5.4712
H	-0.8046	0.9398	5.4501
H	-2.4835	-1.4659	5.1922
H	-3.0174	0.2097	5.2645
H	-3.4398	0.1339	2.9218
H	-2.7414	-1.5193	2.8430
H	0.1277	1.1143	3.2610
C	4.2072	-1.2545	0.5806
H	3.6751	0.8392	0.4702
H	3.9177	0.0658	-1.1016
H	2.0739	-3.1081	1.5685
H	1.5561	-1.8245	2.6723
H	4.1245	-2.3434	2.4507
H	3.5998	-0.6629	2.5626
H	5.2774	-1.0081	0.7170
H	4.1787	-2.1540	-0.0710
C	0.9009	-3.0544	-0.6746
C	1.9528	-3.0105	-1.6807
H	-0.0383	-2.4927	-0.8158
H	1.0254	-3.6766	0.2213
H	3.8295	-3.7340	-2.3646
C	3.0551	-3.7565	-1.6046
H	1.7791	-2.3328	-2.5328
Cl	-0.2553	-4.6693	-1.6421
O	-2.9823	-1.0492	-0.0096
C	-2.7017	-2.4624	-0.1077
C	-3.2235	-2.9735	-1.4499
C	-3.8121	-1.7480	-2.1457
C	-3.8988	-0.6847	-1.0520
H	-3.5965	0.3335	-1.3816
H	-4.9021	-0.6170	-0.5926
H	-4.7977	-1.9545	-2.5969
H	-3.1610	-1.3948	-2.9782
H	-3.9827	-3.7640	-1.3087
H	-2.4001	-3.4541	-2.0285
H	-1.5958	-2.5793	-0.0042
H	-3.1897	-2.9328	0.7654
H	3.2440	-4.4499	-0.7887

Cyclohexenone + methyl chloride

3_syn

C	0.0000	-0.0000	0.0000
C	1.4119	-0.0488	0.0883
N	-0.8266	1.0700	-0.0477
N	-0.4735	2.4395	0.3306
C	-1.7391	3.1495	0.8061
C	0.5811	2.6884	1.3734
C	-1.3708	3.9576	2.0578
C	-2.2679	4.0850	-0.2996

C	-0.0757	3.3530	2.5779
O	-2.6781	3.3895	-1.4800
C	-4.0043	2.8899	-1.4354
C	-0.7128	-1.2852	-0.1538
C	2.0371	-1.3264	0.5543
C	1.4190	-2.5394	-0.1252
C	-0.0626	-2.4542	-0.1807
H	1.9547	0.8481	0.4291
H	-2.5403	2.4070	1.0679
H	1.1334	1.7688	1.6631
H	1.3274	3.3590	0.9002
H	-2.1766	3.9206	2.8136
H	-1.2368	5.0320	1.8209
H	-1.4838	4.7609	-0.6992
H	-3.0942	4.7129	0.0912
H	-0.2762	2.6154	3.3788
H	0.5835	4.1139	3.0341
H	-4.1313	2.4059	-2.4124
H	-4.1596	2.1621	-0.6274
H	-4.7259	3.7101	-1.3282
H	-1.8112	-1.2536	-0.2539
H	1.9390	-1.4153	1.6558
H	3.1261	-1.3004	0.3518
H	1.7407	-3.4731	0.3718
H	1.7788	-2.5950	-1.1790
H	-0.6093	-3.3980	-0.2842
Li	-1.2341	1.9540	-2.0277
C	-2.9151	-0.4852	-2.7519
C	-1.2764	-0.0535	-4.3802
C	-2.8290	-1.7443	-3.6137
C	-1.5992	-1.5401	-4.4930
O	-1.9881	0.4884	-3.2543
H	-2.6444	-0.6729	-1.6869
H	-3.9070	0.0034	-2.7809
H	-1.6211	0.5247	-5.2583
H	-0.1913	0.1689	-4.2184
H	-3.7436	-1.8795	-4.2199
H	-2.7448	-2.6545	-2.9931
H	-1.7809	-1.8389	-5.5407
H	-0.7480	-2.1582	-4.1494
O	0.0089	3.2195	-3.0900
C	0.9735	4.0595	-2.4382
C	2.0606	4.4377	-3.4430
C	1.8602	3.4839	-4.6149
C	0.4692	2.8925	-4.4120
H	0.3992	4.9256	-2.0605
H	1.3691	3.4950	-1.5702
H	1.9667	5.4937	-3.7582
H	3.0697	4.3449	-3.0041
H	1.9536	3.9931	-5.5894
H	2.6162	2.6680	-4.6165
H	0.4709	1.7782	-4.4853
H	-0.2922	3.3016	-5.1002
C	1.9289	0.0583	-1.9716
H	2.9440	0.3148	-1.6977
H	1.6610	-0.9926	-2.0656
H	1.1930	0.8493	-2.1011
Cl	2.3635	0.1504	-4.0821

3_anti

C	2.0289	-0.2902	-0.1744
C	1.5076	-1.5195	0.3483
N	1.4117	0.6135	-0.9352
N	0.0089	0.4603	-1.2940
Li	-1.2775	-0.3114	0.4446
C	-0.5564	1.8473	-1.5969
C	-0.1457	-0.3340	-2.5778
C	-0.6527	2.0011	-3.1219
C	-1.9524	2.0014	-0.9544
C	-0.3273	0.6434	-3.7343
O	-1.9646	1.6715	0.4386
C	-1.4414	2.6811	1.2865
C	3.4437	0.0355	0.0902
H	0.4032	-1.6135	0.4657
C	2.2579	-2.0980	1.5128
H	0.1209	2.6373	-1.1772
H	0.7197	-1.0181	-2.7459
H	-1.0300	-1.0049	-2.4626
H	0.0535	2.7742	-3.4786
H	-1.6542	2.3560	-3.4330
H	-2.7033	1.2781	-1.3587
H	-2.3440	3.0256	-1.1122
H	0.5900	0.6989	-4.3513
H	-1.1227	0.3037	-4.4232
H	-1.2385	2.1620	2.2370
H	-0.5151	3.1323	0.9060
H	-2.1984	3.4612	1.4291
C	3.7547	-2.1262	1.2439
O	-1.2829	-0.6583	2.4417
C	-0.2627	-0.1351	3.3063
C	-0.5401	-0.6411	4.7207
C	-1.5504	-1.7746	4.5508
C	-1.8847	-1.8038	3.0583
H	0.7285	-0.4702	2.9175
H	0.3886	-0.9862	5.2104
H	-0.9383	0.1612	5.3686
H	-1.1383	-2.7438	4.8860
H	-2.4539	-1.6080	5.1652
H	-2.9632	-1.7075	2.8369
H	-1.4996	-2.7081	2.5473
H	-0.3497	0.9656	3.1846
C	4.2426	-0.8151	0.7443
H	3.8289	0.9913	-0.2865
H	1.8943	-3.1239	1.7208
H	2.0414	-1.5119	2.4386
H	3.9681	-2.8915	0.4612
H	4.3102	-2.4326	2.1494
H	5.2997	-0.5814	0.9096
C	1.7103	-2.9893	-1.1182
H	2.7302	-3.2138	-0.8165
H	1.5315	-2.2589	-1.9011
H	0.8820	-3.5038	-0.6434
Cl	1.7153	-4.5441	-2.6211
O	-2.6558	-1.6630	-0.2276
C	-2.2031	-2.8261	-0.9459
C	-3.4006	-3.4031	-1.6963
C	-4.4251	-2.2703	-1.7413
C	-3.8768	-1.1862	-0.8120
H	-3.6501	-0.2275	-1.3342
H	-4.5313	-0.9636	0.0500
H	-5.4255	-2.6120	-1.4198
H	-4.5593	-1.8843	-2.7685
H	-3.8070	-4.2946	-1.1839
H	-3.1132	-3.7467	-2.7067
H	-1.3782	-2.5126	-1.6287
H	-1.7820	-3.4881	-0.1669

3-pentanone + ethyl chloride

3_syn

C	-0.0000	-0.0000	-0.0000
C	1.4069	0.0010	0.1253
N	-0.8262	1.0691	-0.0640
N	-0.4737	2.4402	0.3307
C	-1.7513	3.1809	0.7199
C	0.5087	2.6732	1.4450
C	-1.5047	3.8675	2.0714
C	-2.0874	4.2278	-0.3628
C	-0.2464	3.2327	2.6442
O	-2.4226	3.6362	-1.6216
C	-3.7862	3.2692	-1.7504
C	-0.7242	-1.3128	-0.2268
C	2.1492	-1.1366	0.7300
H	1.6350	-2.1039	0.6153
C	-0.9117	-2.0779	1.0661
H	1.8945	0.9679	0.3452
H	-2.6136	2.4674	0.8185
H	1.0911	1.7637	1.7058
H	1.2436	3.4072	1.0547
H	-2.3703	3.7471	2.7478
H	-1.3737	4.9612	1.9518
H	-1.2147	4.8566	-0.6341
H	-2.8994	4.8983	-0.0157

H	-0.4978	2.4314	3.3653
H	0.3655	3.9589	3.2091
H	-3.8461	2.8435	-2.7602
H	-4.1004	2.5248	-1.0057
H	-4.4348	4.1518	-1.6770
H	-0.1466	-1.9255	-0.9516
H	-1.7167	-1.1510	-0.7107
H	2.3012	-0.9845	1.8089
H	3.1495	-1.2197	0.2691
H	0.0628	-2.3912	1.4769
H	-1.5094	-2.9841	0.9054
H	-1.4197	-1.4778	1.8311
Li	-1.0551	2.0851	-2.0324
C	-2.8578	-0.1599	-3.0203
C	-1.2775	0.4592	-4.6414
C	-2.7416	-1.3516	-3.9704
C	-1.5923	-1.0075	-4.9135
O	-1.9093	0.8437	-3.4092
H	-2.6268	-0.4191	-1.9630
H	-3.8496	0.3292	-3.0514
H	-1.6769	1.1395	-5.4159
H	-0.1841	0.6612	-4.5135
H	-3.6856	-1.5175	-4.5215
H	-2.5501	-2.2897	-3.4193
H	-1.8570	-1.1768	-5.9721
H	-0.6991	-1.6351	-4.7222
O	0.4815	3.2069	-2.8495
C	1.6410	3.6723	-2.1456
C	2.5416	4.3884	-3.1529
C	2.0488	3.9271	-4.5231
C	0.8172	3.0671	-4.2405
H	1.2421	4.3208	-1.3448
H	2.1561	2.7993	-1.6785
H	2.4764	5.4866	-3.0473
H	3.6041	4.1333	-2.9890
H	1.8081	4.7836	-5.1782
H	2.8194	3.3447	-5.0612
H	0.9878	1.9795	-4.4472
H	-0.0922	3.3944	-4.7767
C	1.9749	-0.0855	-1.9777
C	3.3586	0.4230	-1.7870
H	1.7744	-1.1591	-1.9210
H	1.1409	0.6070	-2.1529
H	3.3679	1.5138	-1.6195
H	3.9894	0.2158	-2.6644
H	3.8370	-0.0669	-0.9200
Cl	2.0315	-0.2796	-4.1752

3_anti

C	2.0289	-0.2902	-0.1744
C	1.4331	-1.3390	0.5830
N	1.4251	0.5322	-1.0347
N	-0.0057	0.4657	-1.3021
Li	-1.4436	-0.1481	0.3915
C	-0.4637	1.8715	-1.6889
C	-0.2743	-0.4008	-2.5226
C	-0.5218	1.9396	-3.2215
C	-1.8556	2.1706	-1.0908
C	-0.4589	0.5059	-3.7367
O	-1.9398	1.8898	0.3102
C	-1.3412	2.8677	1.1441
C	3.5224	-0.0546	-0.1068
H	0.3264	-1.3155	0.7123
C	2.1111	-1.8518	1.8053
H	0.2631	2.6318	-1.2997
H	0.5410	-1.1468	-2.6836
H	-1.1842	-1.0194	-2.3261
H	0.3255	2.5350	-3.6116
H	-1.4323	2.4611	-3.5738
H	-2.6577	1.5058	-1.4970
H	-2.1479	3.2203	-1.2909
H	0.3719	0.3803	-4.4561
H	-1.3732	0.2356	-4.2971
H	-1.2697	2.3763	2.1278
H	-0.3416	3.1732	0.8074
H	-1.9934	3.7473	1.2025
H	3.1877	-1.6190	1.8307
O	-1.6331	-0.4526	2.3923
C	-0.6798	0.0192	3.3555
C	-1.1470	-0.4222	4.7411
C	-2.2320	-1.4669	4.4866
C	-2.4070	-1.5130	2.9677
H	0.3200	-0.3963	3.0856
H	-0.3090	-0.8339	5.3326
H	-1.5359	0.4294	5.3288
H	-1.9479	-2.4578	4.8857
H	-3.1769	-1.2023	4.9953
H	-3.4419	-1.3219	2.6292
H	-2.0621	-2.4660	2.5207
H	-0.6666	1.1195	3.2034
C	4.2499	-0.8741	-1.1522
H	3.8947	-0.3230	0.9067
H	3.7628	1.0197	-0.2367
H	2.0197	-2.9501	1.8771
H	1.6677	-1.4256	2.7242
H	4.0372	-1.9517	-1.0433
H	5.3361	-0.7419	-1.0699
H	3.9594	-0.5870	-2.1710
C	1.1546	-3.0230	-0.7842
C	2.3062	-3.9096	-0.4993
H	1.2320	-2.2808	-1.5874
H	0.2421	-3.0996	-0.1824
H	3.2536	-3.4733	-0.8579
H	2.1805	-4.8867	-0.9883
H	2.4133	-4.0879	0.5844
Cl	0.0456	-4.2460	-2.2478
O	-2.9244	-1.3752	-0.2925
C	-2.6258	-2.6472	-0.9039
C	-3.8715	-3.1086	-1.6536
C	-4.7301	-1.8554	-1.8119
C	-4.0777	-0.7985	-0.9201
H	-3.7394	0.1050	-1.4783
H	-4.7188	-0.4657	-0.0833
H	-5.7801	-2.0387	-1.5214
H	-4.7673	-1.5199	-2.8647
H	-4.4098	-3.8984	-1.0979
H	-3.6037	-3.5597	-2.6268
H	-1.7368	-2.5268	-1.5758
H	-2.3335	-3.2976	-0.0588

1-phenyl-2-propanone + methyl chloride

3_syn

C	0.0000	-0.0000	-0.0000
C	1.4177	-0.0264	0.1189
N	-0.8128	1.0725	-0.0404
N	-0.4748	2.4461	0.3315
C	-1.7570	3.1522	0.7703
C	0.5506	2.7095	1.4009
C	-1.4278	3.9642	2.0304
C	-2.2615	4.0843	-0.3495
C	-0.1436	3.3692	2.5864
O	-2.6366	3.3853	-1.5393
C	-3.9598	2.8765	-1.5283
C	-0.7481	-1.2916	-0.1825
C	2.1452	-1.1846	0.6427
C	3.0453	-0.9796	1.6996
H	-0.2586	-1.9352	-0.9354
H	1.8993	0.9177	0.4379
H	-2.5613	2.4062	1.0116
H	1.1060	1.7971	1.7090
H	1.3009	3.3872	0.9446
H	-2.2536	3.9229	2.7638
H	-1.2945	5.0390	1.7955
H	-1.4713	4.7652	-0.7285
H	-3.1017	4.7069	0.0192
H	-0.3601	2.6305	3.3819
H	0.4976	4.1348	3.0598
H	-4.0522	2.3742	-2.5002
H	-4.1355	2.1609	-0.7133
H	-4.6890	3.6939	-1.4577
H	-1.7980	-1.1578	-0.5012
H	-0.7542	-1.8470	0.7661

C	2.0290	-2.4731	0.1102
C	2.7812	-3.5237	0.6211
C	3.7965	-2.0307	2.2069
C	3.6664	-3.3078	1.6706
H	3.1580	0.0229	2.1289
H	1.3357	-2.6561	-0.7240
Li	-1.1461	1.9977	-2.0564
C	-2.8221	-0.4124	-2.8581
C	-1.0190	-0.1050	-4.3222
C	-2.5080	-1.7909	-3.4427
C	-1.1858	-1.6151	-4.1846
O	-1.8376	0.5253	-3.3212
H	-2.7716	-0.3965	-1.7456
H	-3.8038	-0.0146	-3.1744
H	-1.3704	0.2737	-5.3002
H	0.0267	0.2582	-4.1581
H	-3.3127	-2.1350	-4.1174
H	-2.4321	-2.5566	-2.6486
H	-1.1818	-2.1185	-5.1670
H	-0.3425	-2.0543	-3.6151
O	0.0998	3.2854	-3.0662
C	1.0446	4.1304	-2.3911
C	2.1410	4.5334	-3.3759
C	1.9648	3.5950	-4.5641
C	0.5728	2.9959	-4.3930
H	0.4551	4.9851	-2.0106
H	1.4344	3.5598	-1.5243
H	2.0409	5.5928	-3.6761
H	3.1455	4.4434	-2.9250
H	2.0730	4.1175	-5.5300
H	2.7248	2.7824	-4.5623
H	0.5770	1.8844	-4.4943
H	-0.1817	3.4228	-5.0780
C	1.9906	0.1047	-1.9124
H	3.0323	0.0591	-1.6231
H	1.4578	-0.8169	-2.1225
H	1.4855	1.0666	-1.9711
Cl	2.4988	0.2800	-4.0110
H	4.4945	-1.8538	3.0313
H	2.6793	-4.5246	0.1893
H	4.2600	-4.1356	2.0699

3_anti

C	2.0289	-0.2902	-0.1744
C	1.3852	-1.1609	0.7735
N	1.4338	0.4764	-1.0777
N	-0.0080	0.4665	-1.3034
Li	-1.5692	-0.3537	0.2313
C	-0.4315	1.8973	-1.6284
C	-0.2919	-0.3230	-2.5707
C	-0.4228	2.0458	-3.1601
C	-1.8415	2.1816	-1.0710
C	-0.2209	0.6491	-3.7450
O	-2.0110	1.7609	0.2845
C	-1.4709	2.6475	1.2480
C	3.5249	-0.1891	-0.2207
H	0.4635	-0.7195	1.2162
C	2.1769	-1.8739	1.7750
H	0.2873	2.6221	-1.1664
H	0.4072	-1.1871	-2.6655
H	-1.3089	-0.7809	-2.4896
H	0.3866	2.7285	-3.4797
H	-1.3587	2.5086	-3.5285
H	-2.6429	1.5937	-1.5811
H	-2.0897	3.2561	-1.1804
H	0.7540	0.5751	-4.2632
H	-0.9812	0.4100	-4.5112
H	-1.6704	2.1374	2.2033
H	-0.3929	2.8096	1.1205
H	-1.9934	3.6115	1.2195
H	3.9539	-1.1750	-0.4702
O	-2.1065	-0.8904	2.1487
C	-1.6457	-0.2907	3.3660
C	-2.3221	-1.0120	4.5306
C	-2.8530	-2.3149	3.9349
C	-2.5735	-2.2196	2.4335
H	-0.5361	-0.3790	3.3999
H	-1.6108	-1.1939	5.3563
H	-3.1369	-0.4050	4.9658
H	-2.3570	-3.1987	4.3764
H	-3.9311	-2.4455	4.1400
H	-3.4712	-2.3444	1.8000
H	-1.7986	-2.9354	2.0924
H	-1.9095	0.7825	3.2678
C	1.8064	-1.8235	3.1269
H	3.9180	0.0993	0.7639
H	3.9001	0.5348	-0.9565
C	3.2687	-2.6812	1.4203
C	3.9562	-3.4113	2.3794
C	2.4965	-2.5552	4.0841
C	3.5727	-3.3538	3.7157
H	0.9578	-1.1965	3.4372
H	3.5876	-2.7158	0.3677
C	0.4691	-2.7699	-0.3170
H	1.1696	-3.4704	0.1216
H	0.7237	-2.2800	-1.2556
H	-0.4508	-2.5277	0.2175
Cl	-0.5853	-4.3074	-1.3735
O	-3.2394	-1.2149	-0.6521
C	-3.1499	-2.3621	-1.5170
C	-4.5267	-2.5905	-2.1338
C	-5.2892	-1.2860	-1.9088
C	-4.3815	-0.4325	-1.0218
H	-4.0098	0.4847	-1.5321
H	-4.8434	-0.1332	-0.0637
H	-6.2698	-1.4643	-1.4317
H	-5.5126	-0.7729	-2.8620
H	-5.0424	-3.4463	-1.6604
H	-4.4484	-2.8481	-3.2054
H	-2.3609	-2.1540	-2.2759
H	-2.7794	-3.1893	-0.8739
H	2.1923	-2.5014	5.1344
H	4.8023	-4.0388	2.0810
H	4.1136	-3.9330	4.4694

1,3-diphenyl-2-propanone + methyl chloride

3_syn

C	0.0000	0.0000	-0.0000
C	1.4112	0.0693	-0.1940
N	-0.8594	1.0171	0.1208
N	-0.5244	2.4293	0.2458
C	-1.7627	3.1626	0.7729
C	0.5816	2.8160	1.1997
C	-1.5064	3.5261	2.2440
C	-1.9957	4.4412	-0.0623
C	-0.0476	3.1953	2.5359
O	-2.2303	4.1526	-1.4442
C	-3.5929	3.9419	-1.7742
C	-0.7255	-1.3329	-0.0342
C	2.3360	-0.9819	0.2318
C	3.3546	-0.6416	1.1367
H	-0.0789	-2.1078	-0.5034
H	1.8639	1.0660	-0.0227
H	-2.6710	2.5071	0.6929
H	1.3451	2.0154	1.3142
H	1.1079	3.6804	0.7431
H	-2.1832	2.9591	2.9103
H	-1.7258	4.5926	2.4446
H	-1.0968	5.0893	-0.1104
H	-2.8250	5.0400	0.3661
H	0.0328	2.3646	3.2629
H	0.4835	4.0458	3.0011
H	-3.5678	3.7410	-2.8522
H	-4.0326	3.0891	-1.2378
H	-4.1861	4.8434	-1.5739
H	-1.6201	-1.2620	-0.6985
C	-1.1346	-1.7773	1.3347
C	2.3013	-2.2912	-0.2616
C	3.2448	-3.2292	0.1402
C	4.2971	-1.5795	1.5344
C	4.2450	-2.8782	1.0389
H	3.4056	0.3788	1.5349

H	1.5185	-2.5817	-0.9771
Li	-0.8937	2.6055	-1.9911
C	-2.8668	0.3209	-2.6872
C	-1.6358	1.0843	-4.5403
C	-3.2361	-0.5991	-3.8490
C	-2.2627	-0.2395	-4.9670
O	-1.9738	1.3374	-3.1663
H	-2.3474	-0.2159	-1.8607
H	-3.7290	0.8667	-2.2603
H	-2.0285	1.9498	-5.1065
H	-0.5187	1.0927	-4.6016
H	-4.2861	-0.4495	-4.1623
H	-3.1601	-1.6631	-3.5614
H	-2.7670	-0.1549	-5.9459
H	-1.4873	-1.0186	-5.0960
O	0.5741	3.7034	-2.8920
C	1.7712	4.0175	-2.1615
C	2.8988	4.2683	-3.1610
C	2.3989	3.6604	-4.4674
C	0.8914	3.5154	-4.2837
H	1.5107	4.8962	-1.5433
H	1.9847	3.1631	-1.4851
H	3.1067	5.3490	-3.2692
H	3.8478	3.8113	-2.8279
H	2.6504	4.2833	-5.3427
H	2.8513	2.6616	-4.6548
H	0.5247	2.4989	-4.5667
H	0.3019	4.2785	-4.8228
C	1.6056	0.1254	-2.3271
H	2.6693	0.2663	-2.1824
H	1.2072	-0.8808	-2.3803
H	0.9331	0.9820	-2.3176
Cl	1.7894	0.2762	-4.4543
H	5.0839	-1.2960	2.2408
H	3.2017	-4.2475	-0.2594
H	4.9887	-3.6170	1.3518
C	-0.2043	-2.3827	2.1824
C	-0.5870	-2.8100	3.4480
C	-1.8992	-2.6380	3.8770
C	-2.8287	-2.0359	3.0365
C	-2.4500	-1.6066	1.7692
H	0.8325	-2.5128	1.8389
H	0.1477	-3.2833	4.1074
H	-2.1992	-2.9766	4.8736
H	-3.8616	-1.8987	3.3720
H	-3.1840	-1.1263	1.1123

3_anti

C	-3.3034	-2.3241	-3.2530
C	-4.3657	-3.2700	-3.0967
N	-3.3141	-1.0374	-2.8808
N	-4.4044	-0.3016	-2.2318
Li	-2.3895	0.8780	-2.6560
C	-5.4347	0.2844	-3.1867
C	-5.1456	-0.9379	-1.0898
C	-6.8121	0.1028	-2.5449
C	-5.1114	1.7693	-3.4211
C	-6.6319	-0.9267	-1.4363
O	-3.8333	1.9392	-4.0373
C	-3.8133	1.5360	-5.3977
C	-1.9899	-2.7562	-3.8782
C	-4.1619	-4.7019	-3.3472
C	-4.2799	-5.6015	-2.2794
C	-4.1537	-6.9689	-2.4866
C	-5.9129	-2.6984	-4.3399
H	-5.2981	-1.9074	-4.7622
Cl	-7.5632	-1.7528	-5.4324
H	-4.8400	-3.1334	-2.1033
H	-5.3957	-0.2920	-4.1667
H	-4.8031	-1.9889	-0.9644
H	-4.9775	-0.3457	-0.1616
H	-7.5249	-0.2917	-3.3040
H	-7.1422	1.0627	-2.1051
H	-5.0674	2.2952	-2.4461
H	-5.8591	2.2041	-4.1137
H	-6.9321	-1.9318	-1.8120
H	-7.2127	-0.6172	-0.5505
H	-2.7576	1.4186	-5.6765
H	-4.3085	0.5514	-5.4438
H	-4.2459	2.3600	-5.9769
C	-1.7178	-2.0776	-5.1845
H	-1.9949	-3.8572	-4.0280
C	-3.9092	-7.4635	-3.7634
C	-3.7961	-6.5816	-4.8322
C	-3.9229	-5.2128	-4.6282
H	-4.4832	-5.2227	-1.2717
H	-4.2562	-7.6602	-1.6442
H	-3.8158	-8.5413	-3.9273
H	-6.5102	-2.5406	-3.4415
H	-5.9988	-3.6357	-4.8717
O	-1.6885	0.9274	-0.6623
C	-0.4762	1.5450	-0.2138
C	-0.3465	1.3459	1.2967
C	-1.5400	0.4801	1.6925
C	-2.1840	0.0649	0.3706
H	0.3894	1.0747	-0.7232
H	-0.5074	2.6314	-0.4414
H	0.5905	0.8024	1.5164
H	-1.1566	-2.5472	-3.1727
H	-0.4189	2.3249	1.8037
H	-1.1808	-0.4191	2.2243
H	-2.2568	1.0869	2.2758
H	-3.2877	0.1736	0.4471
H	-1.9094	-0.9829	0.1405
H	-3.5969	-6.9665	-5.8375
H	-3.8256	-4.5258	-5.4775
C	-1.0272	-0.8628	-5.2081
C	-0.7569	-0.2392	-6.4210
C	-1.1604	-0.8231	-7.6178
C	-1.8515	-2.0295	-7.5961
C	-2.1349	-2.6532	-6.3864
H	-0.6899	-0.4058	-4.2697
H	-0.2153	0.7124	-6.4350
H	-0.9266	-0.3400	-8.5718
H	-2.1842	-2.4883	-8.5412
H	-2.7015	-3.6048	-6.3751
O	-1.0464	2.3751	-3.3108
C	0.1478	2.3272	-4.0973
C	-1.2734	3.7147	-2.8554
C	-0.3577	4.6570	-3.6341
C	0.6753	3.7480	-4.2946
H	-0.1345	1.9003	-5.0784
H	0.8896	1.7348	-3.5166
H	-0.9972	3.7373	-1.7780
H	-2.3288	3.9542	-3.0856
H	0.1509	5.3398	-2.9300
H	-0.9433	5.1763	-4.4153
H	0.7260	3.9741	-5.3749
H	1.6451	3.8554	-3.7747