Supporting Information

For

N-Heterocyclic Olefins as Ancillary Ligands in Catalysis: A Study of their Behaviour in Transfer Hydrogenation Reactions

A. Iturmendi,[a] N. García,[b] E. A. Jaseer,[b] J. Munárriz,[c] P. J. Sanz Miguel,[a] V. Polo,[c] M. Iglesias,[a] and L. A. Oro*[a,b]*

[a] Departamento de Química Inorgánica – Instituto de Síntesis Química y Catálisis Homogénea-ISQCH, Universidad de Zaragoza – CSIC. C/ Pedro Cerbuna 12, 50009 Zaragoza, Spain.

[c] King Fahd University of Petroleum & Minerals (KFUPM)
Dhahran 31261 (Saudi Arabia)

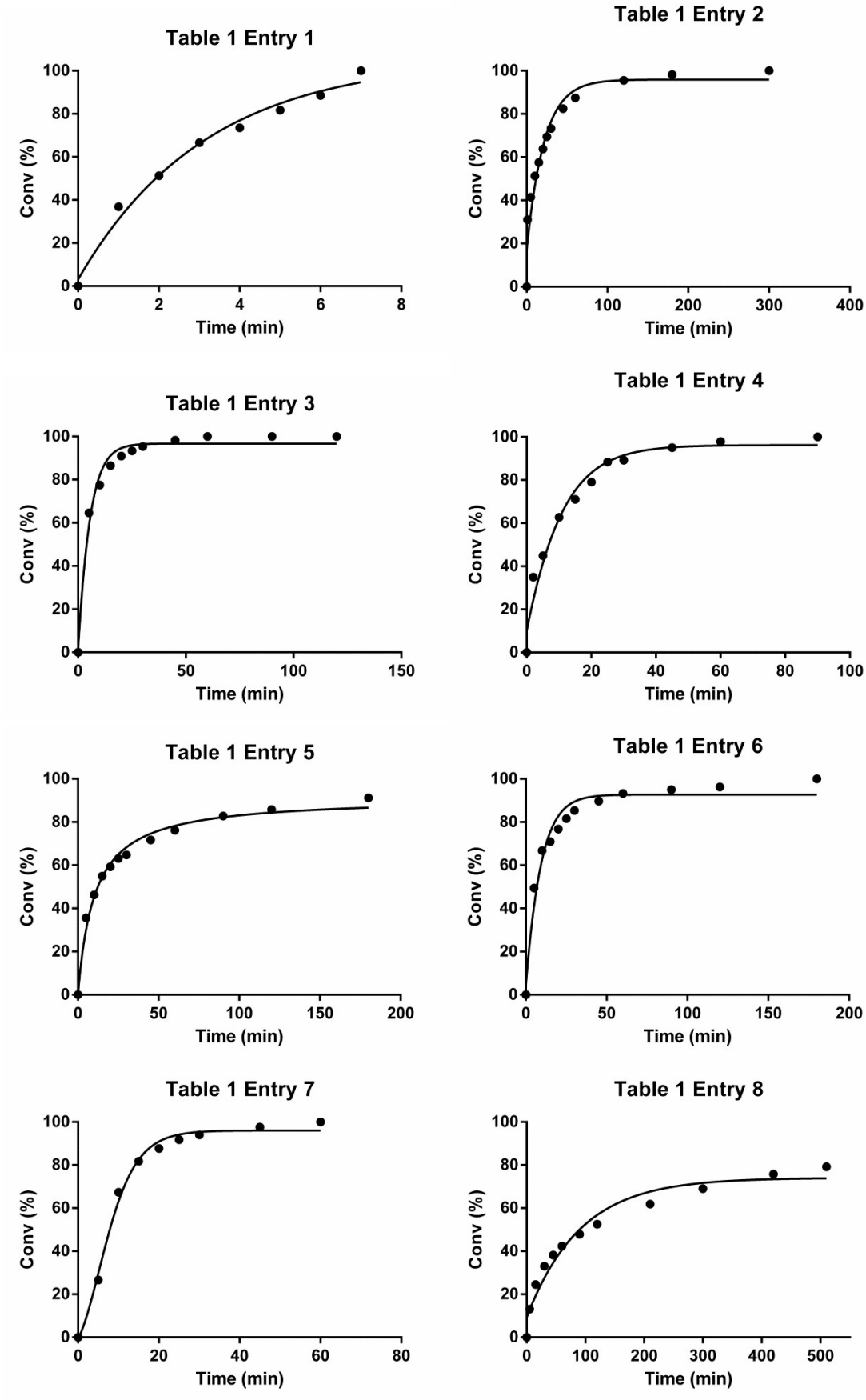
[c] Departmento Química Física - Instituto de Biocomputación y Física de Sistemas Complejos (BIFI)
Universidad de Zaragoza (Spain), C/ Pedro Cerbuna 12, 50009 Zaragoza

E-mail: miglesia@unizar.es and oro@unizar.es

Table of Contents:

Plots of conversion vs. time	S2
NMR spectra	S7
X-ray data complex **3**	S15
Computational details	S16

Plots of conversion vs. time



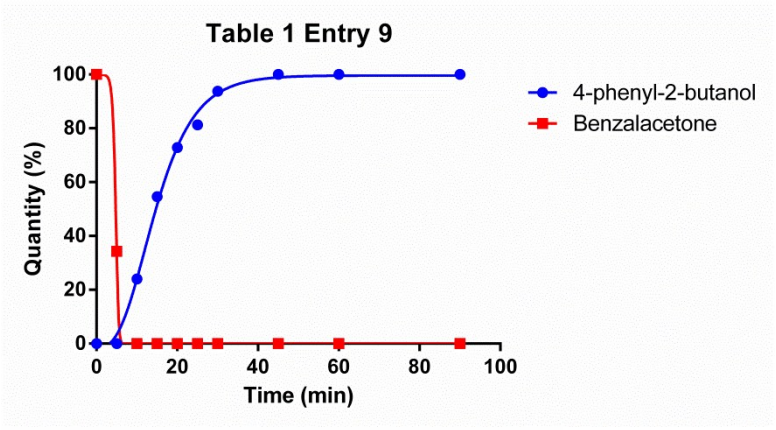


Table 1 Entry 9
Quantity (%)
Time (min)
4-phenyl-2-butanol
Benzalacetone

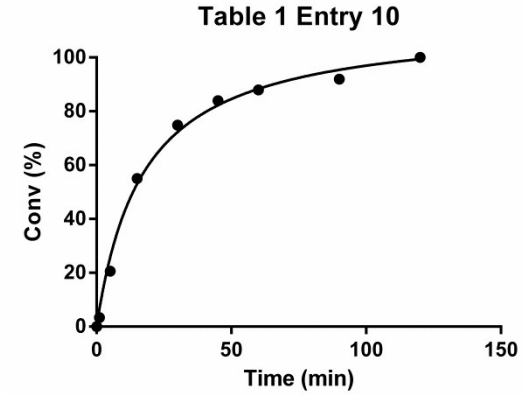


Table 1 Entry 10
Conv (%)
Time (min)

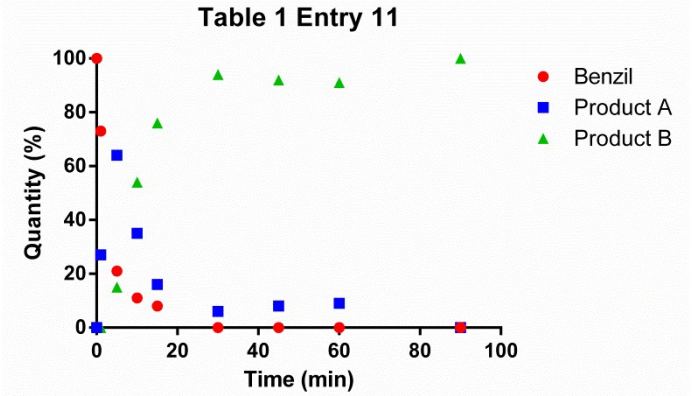


Table 1 Entry 11
Quantity (%)
Time (min)
Benzil
Product A
Product B

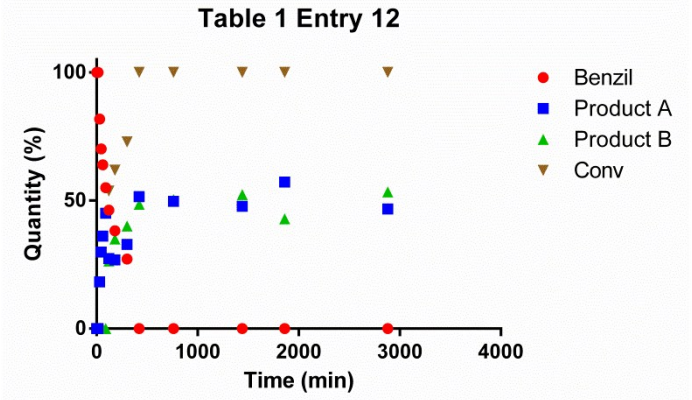


Table 1 Entry 12
Quantity (%)
Time (min)
Benzil
Product A
Product B
Conv

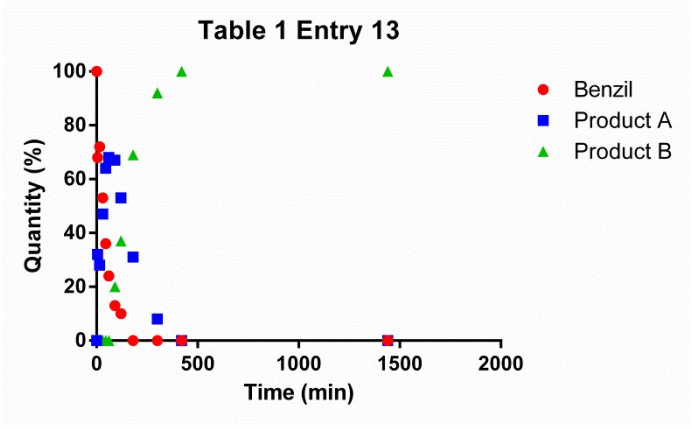


Table 1 Entry 13
Quantity (%)
Time (min)
Benzil
Product A
Product B

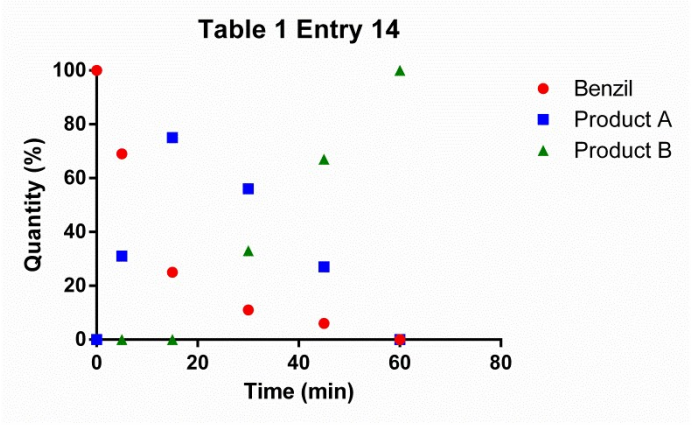


Table 1 Entry 14
Quantity (%)
Time (min)
Benzil
Product A
Product B

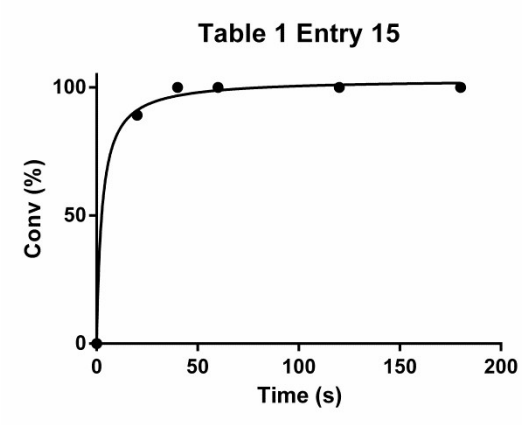


Table 1 Entry 15
Conv (%)
Time (s)

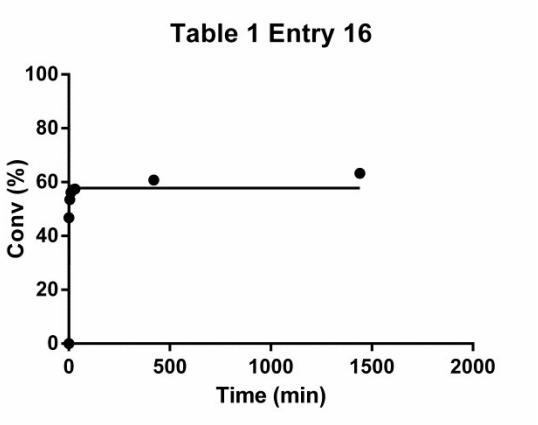


Table 1 Entry 16
Conv (%)
Time (min)

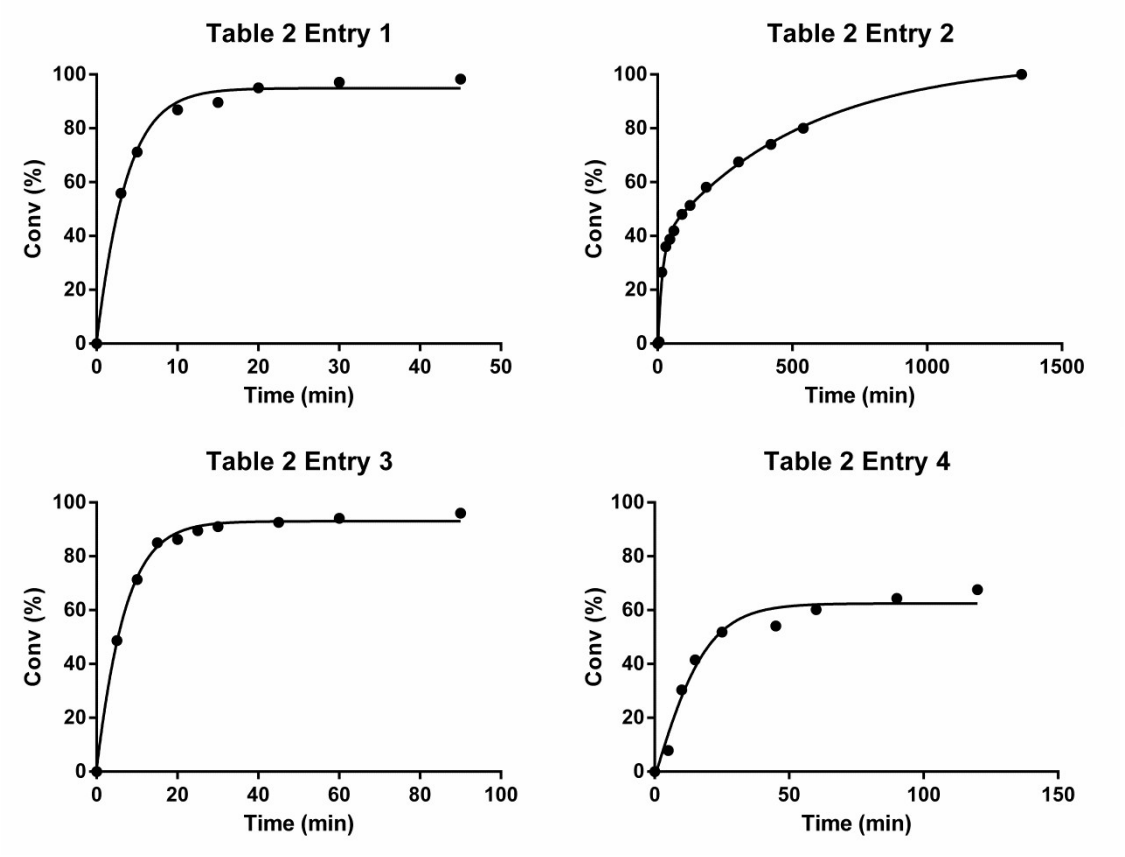


Table 2 Entry 1
Conv (%)
Time (min)
Table 2 Entry 2
Conv (%)
Time (min)
Table 2 Entry 3
Conv (%)
Time (min)
Table 2 Entry 4
Conv (%)
Time (min)

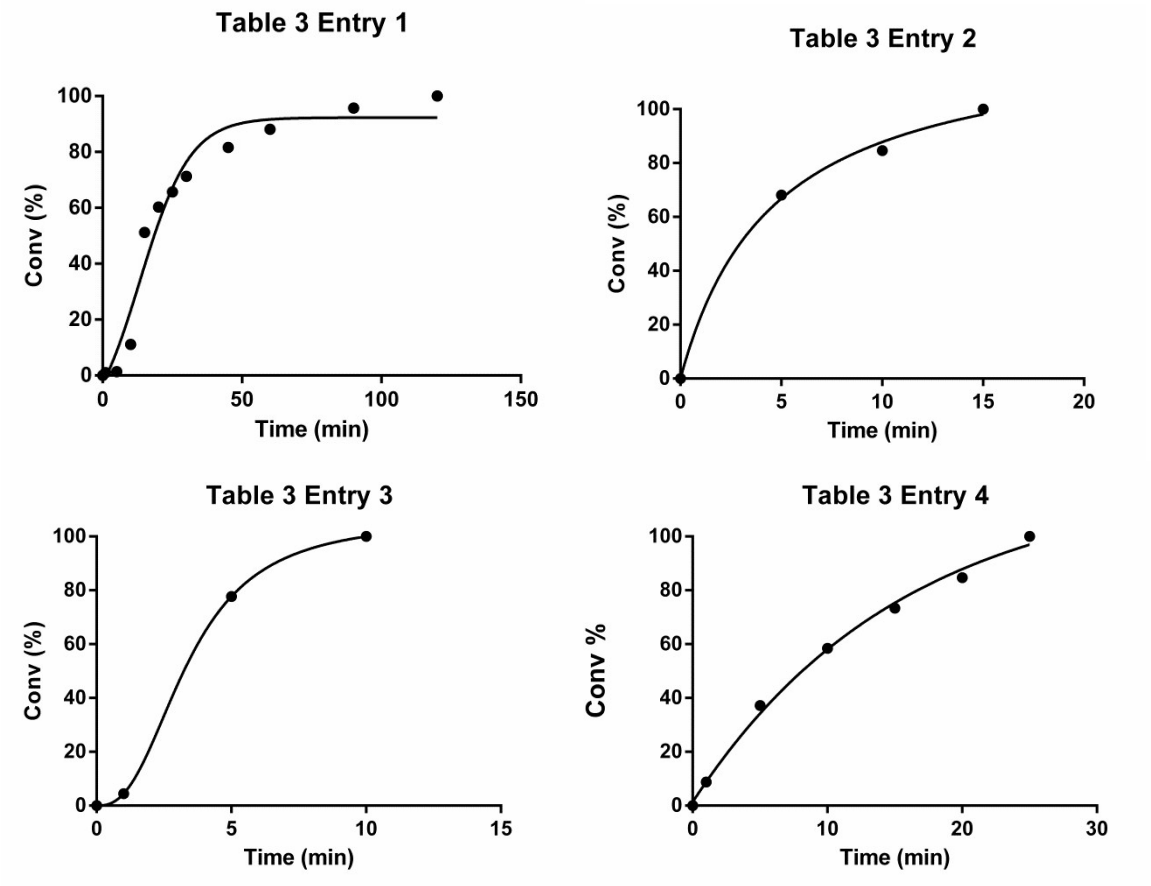


Table 3 Entry 1
Conv (%)
Time (min)
Table 3 Entry 2
Conv (%)
Time (min)
Table 3 Entry 3
Conv (%)
Time (min)
Table 3 Entry 4
Conv %
Time (min)

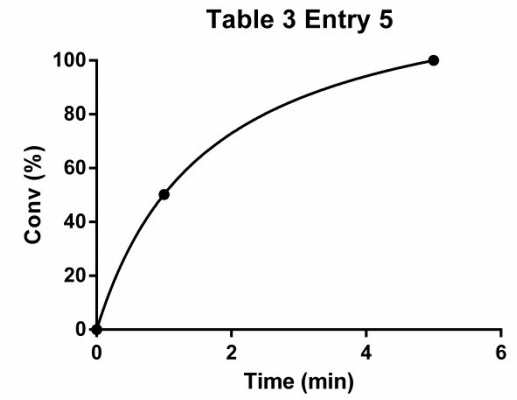


Table 3 Entry 5
Conv (%)
Time (min)
0
20
40
60
80
100
0
2
4
6

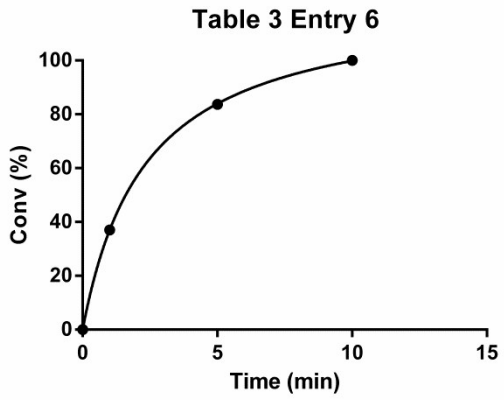


Table 3 Entry 6
Conv (%)
Time (min)
0
20
40
60
80
100
0
5
10
15

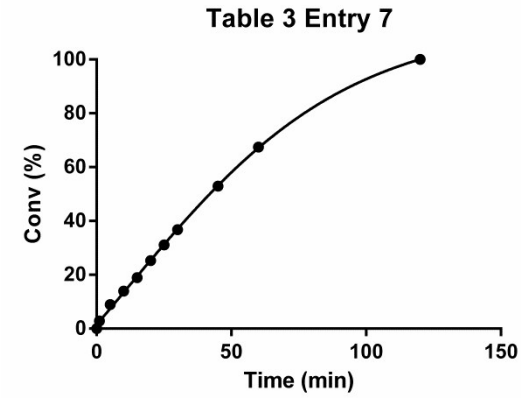


Table 3 Entry 7
Conv (%)
Time (min)
0
20
40
60
80
100
0
50
100
150

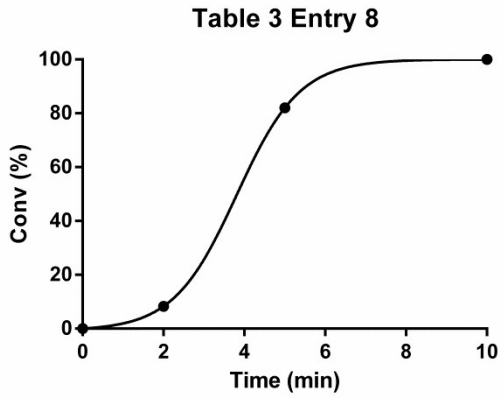


Table 3 Entry 8
Conv (%)
Time (min)
0
20
40
60
80
100
0
2
4
6
8
10

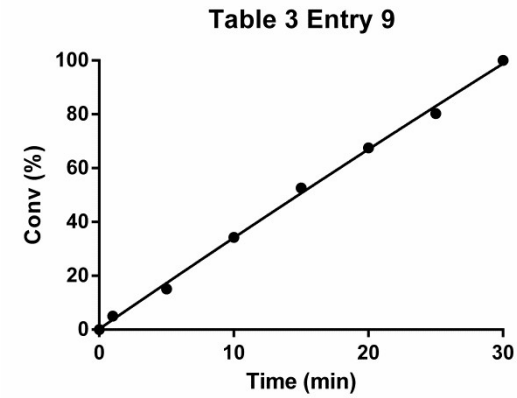


Table 3 Entry 9
Conv (%)
Time (min)
0
20
40
60
80
100
0
10
20
30

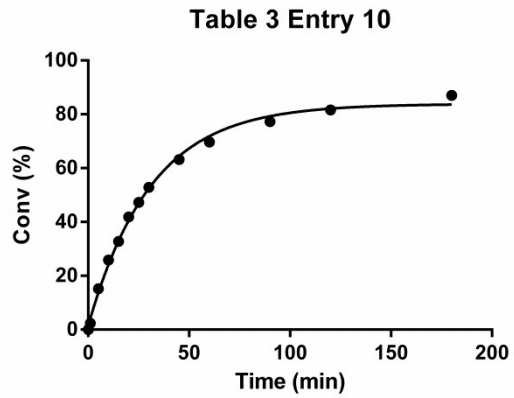


Table 3 Entry 10
Conv (%)
Time (min)
0
20
40
60
80
100
0
50
100
150
200

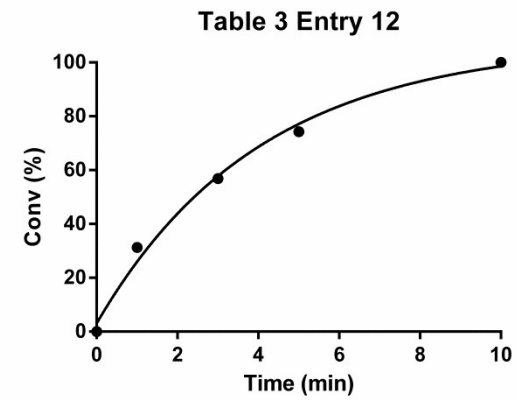


Table 3 Entry 12
Conv (%)
Time (min)
0
20
40
60
80
100
0
2
4
6
8
10

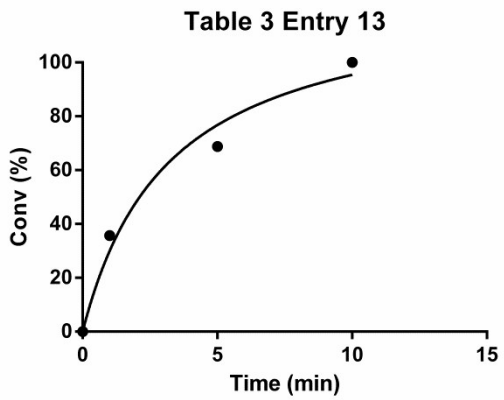
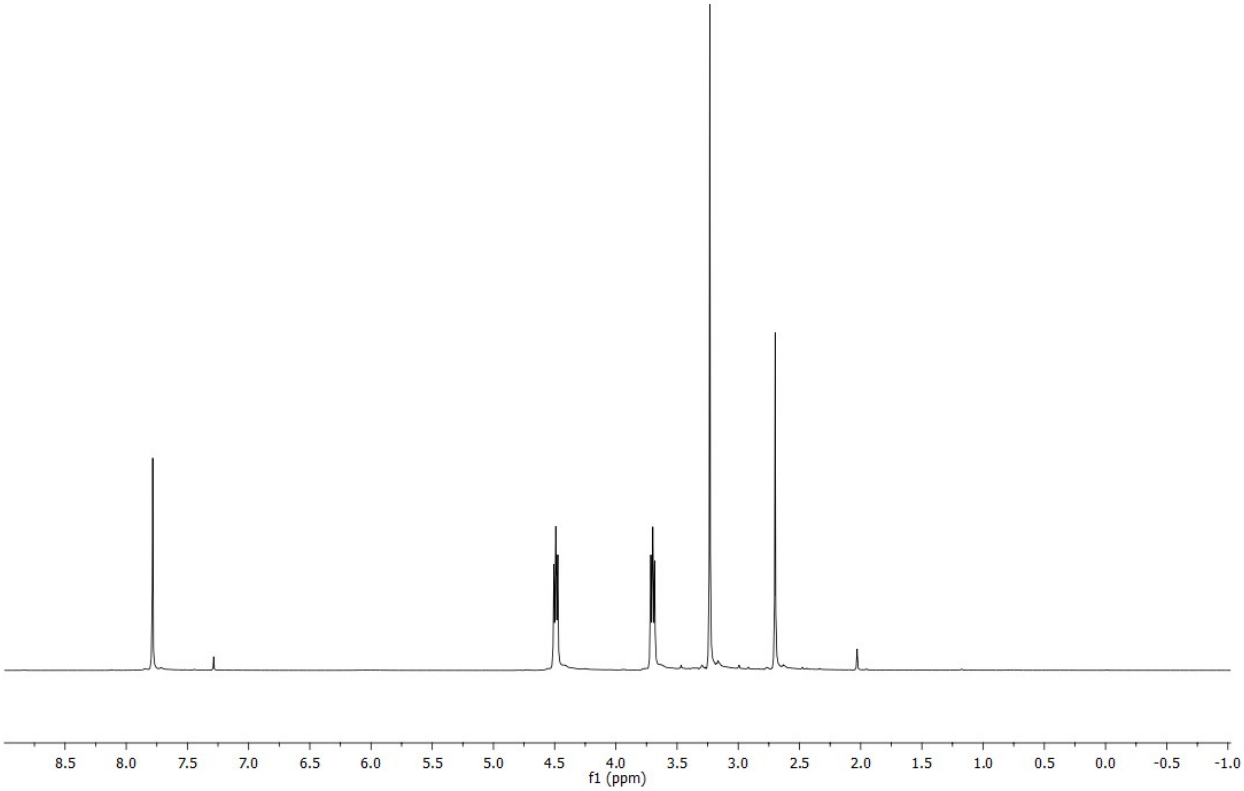
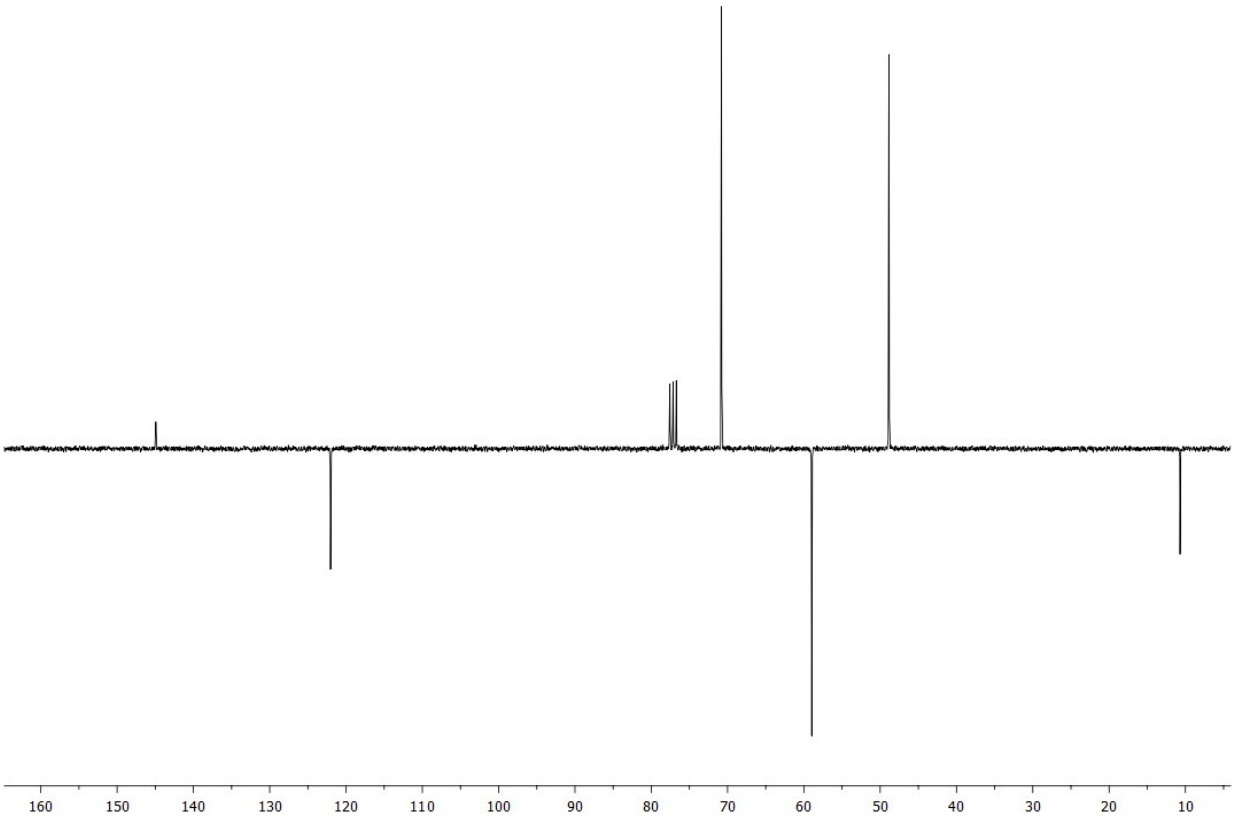


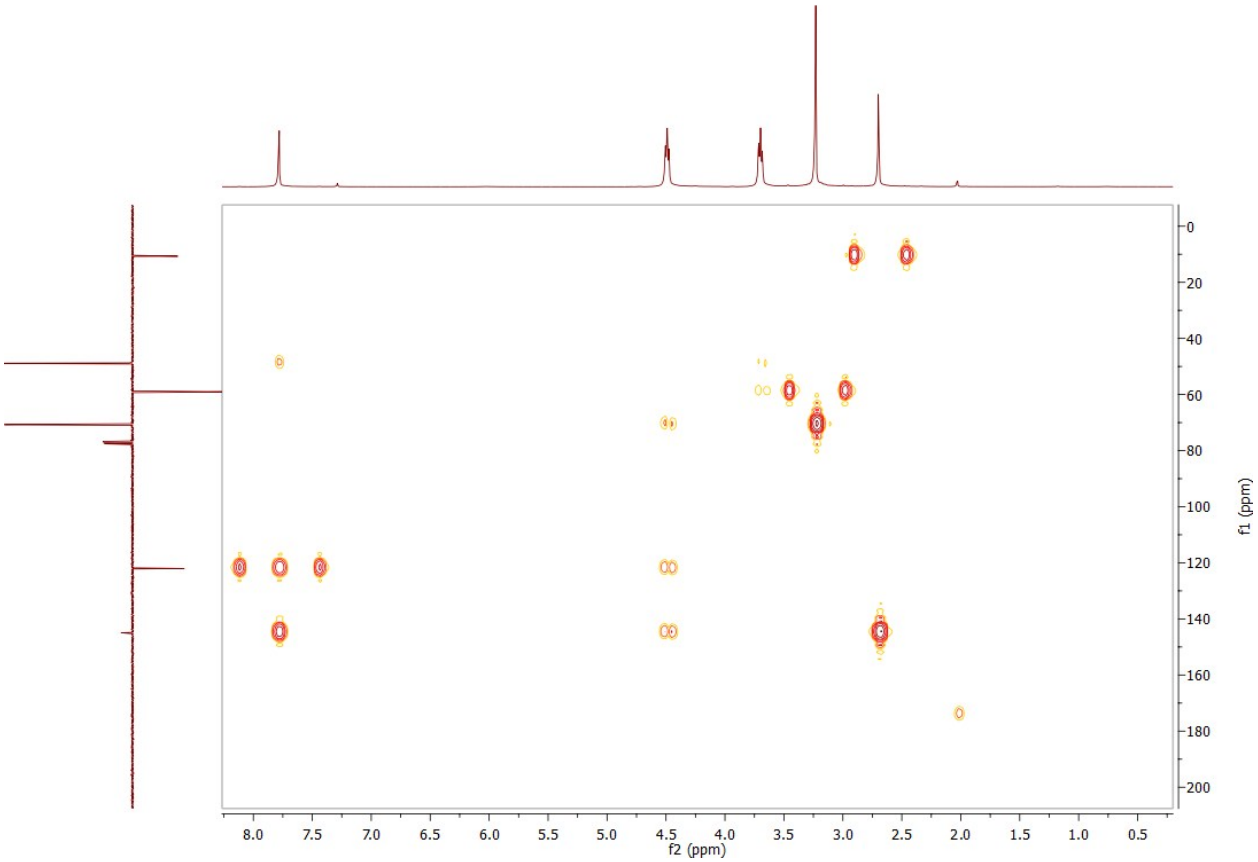
Table 3 Entry 13
Conv (%)
Time (min)
0
20
40
60
80
100
0
5
10
15

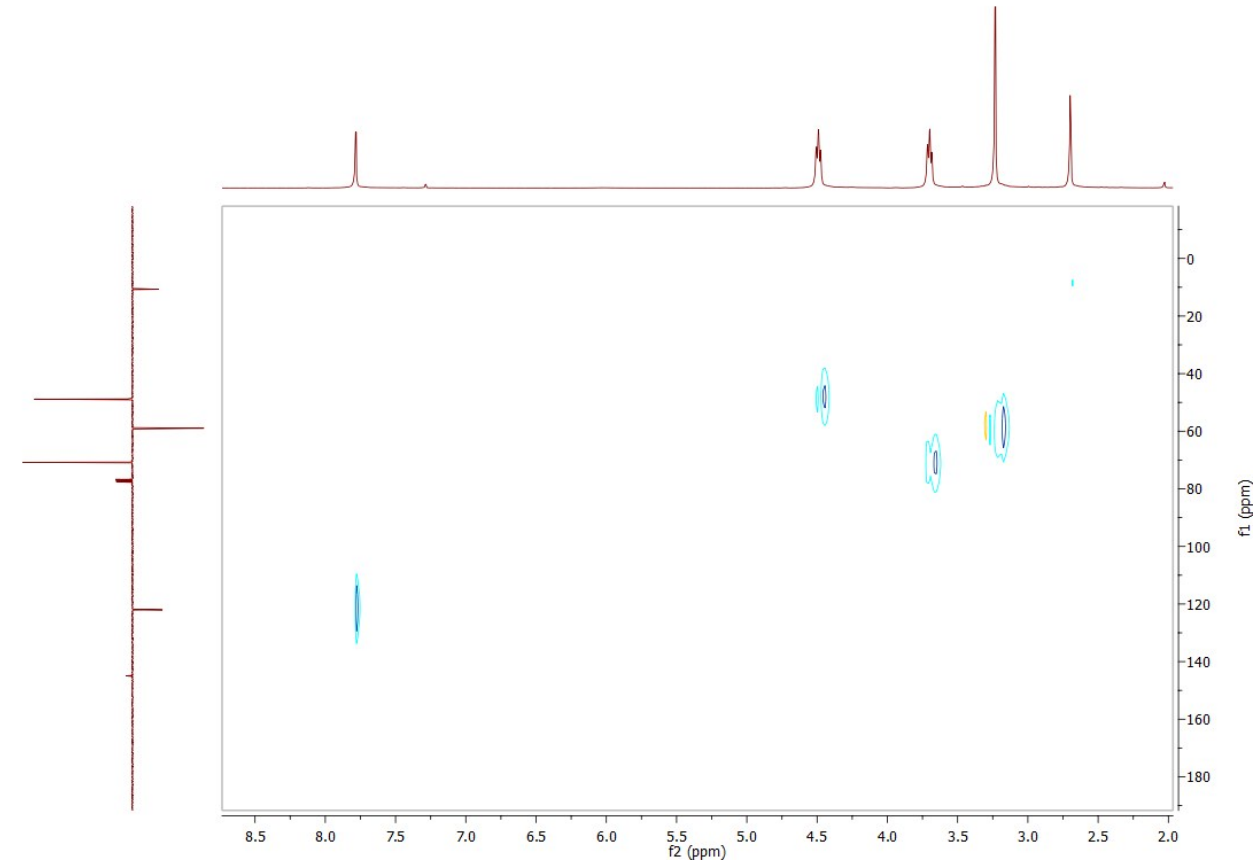
NMR spectra

1,3-bis(2-(methoxyethyl)-2-methylimidazolium chloride (4)

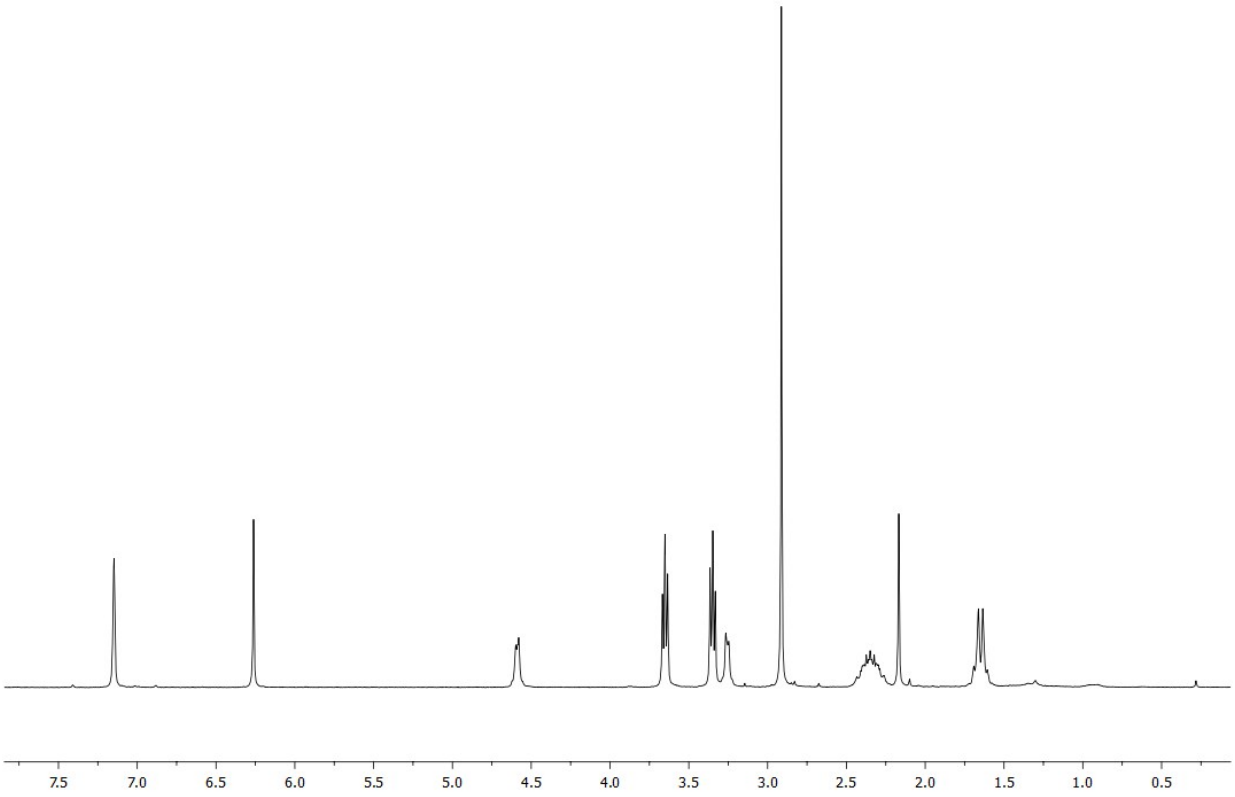


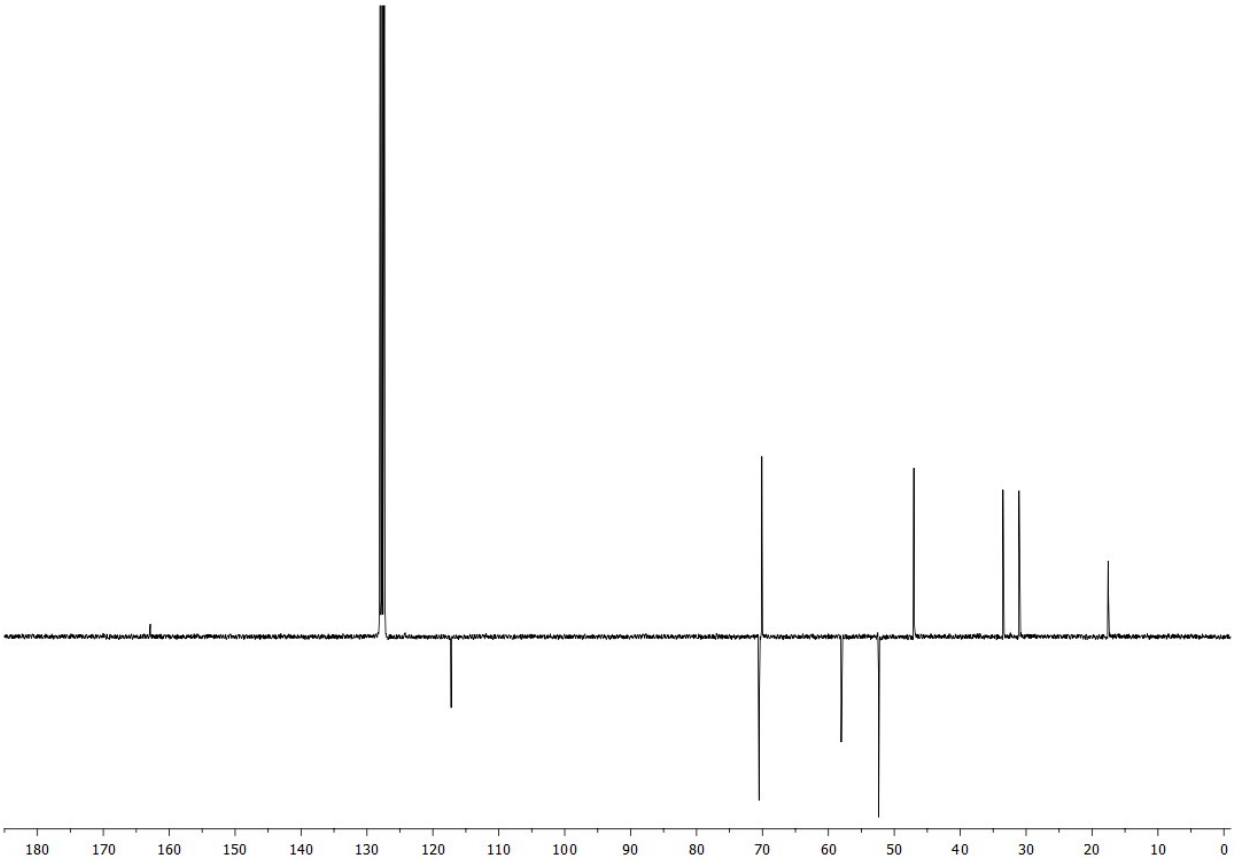


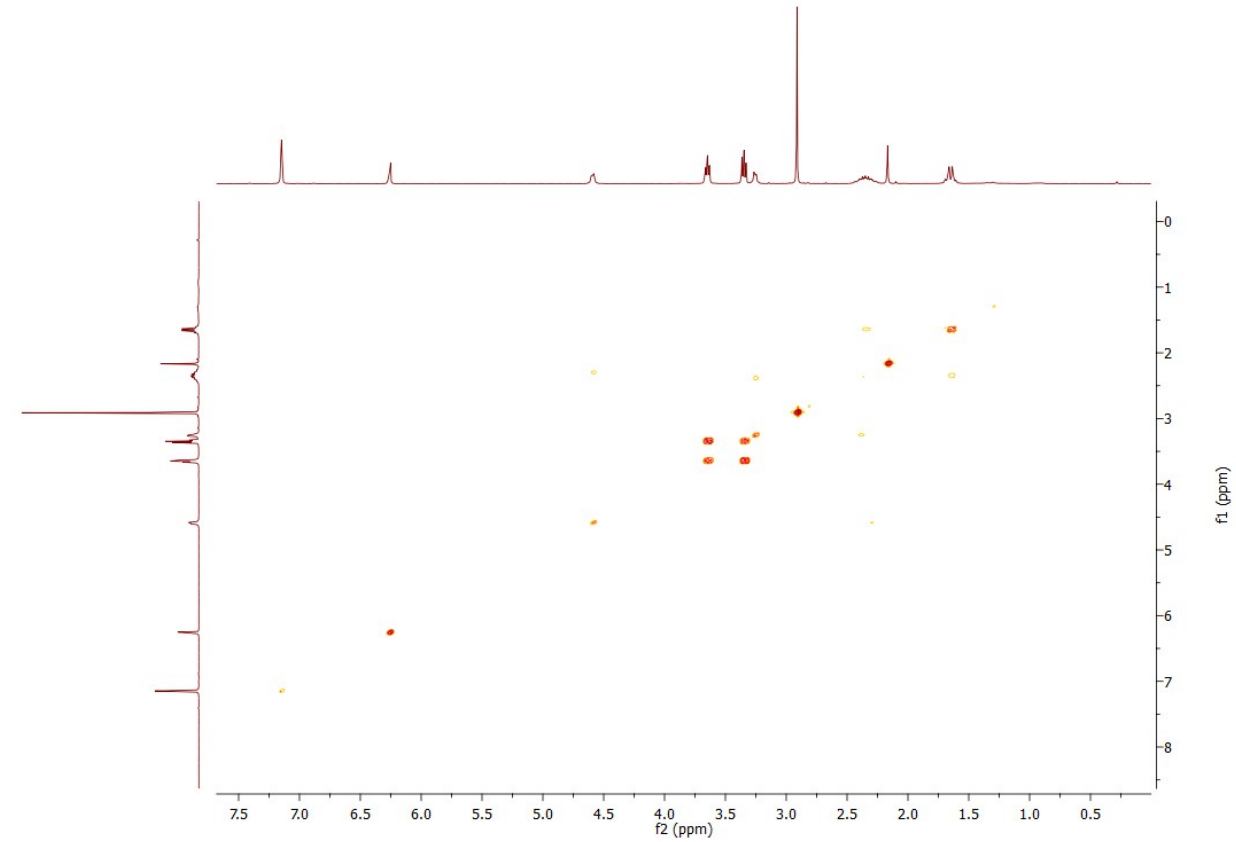

f1 (ppm)
f2 (ppm)

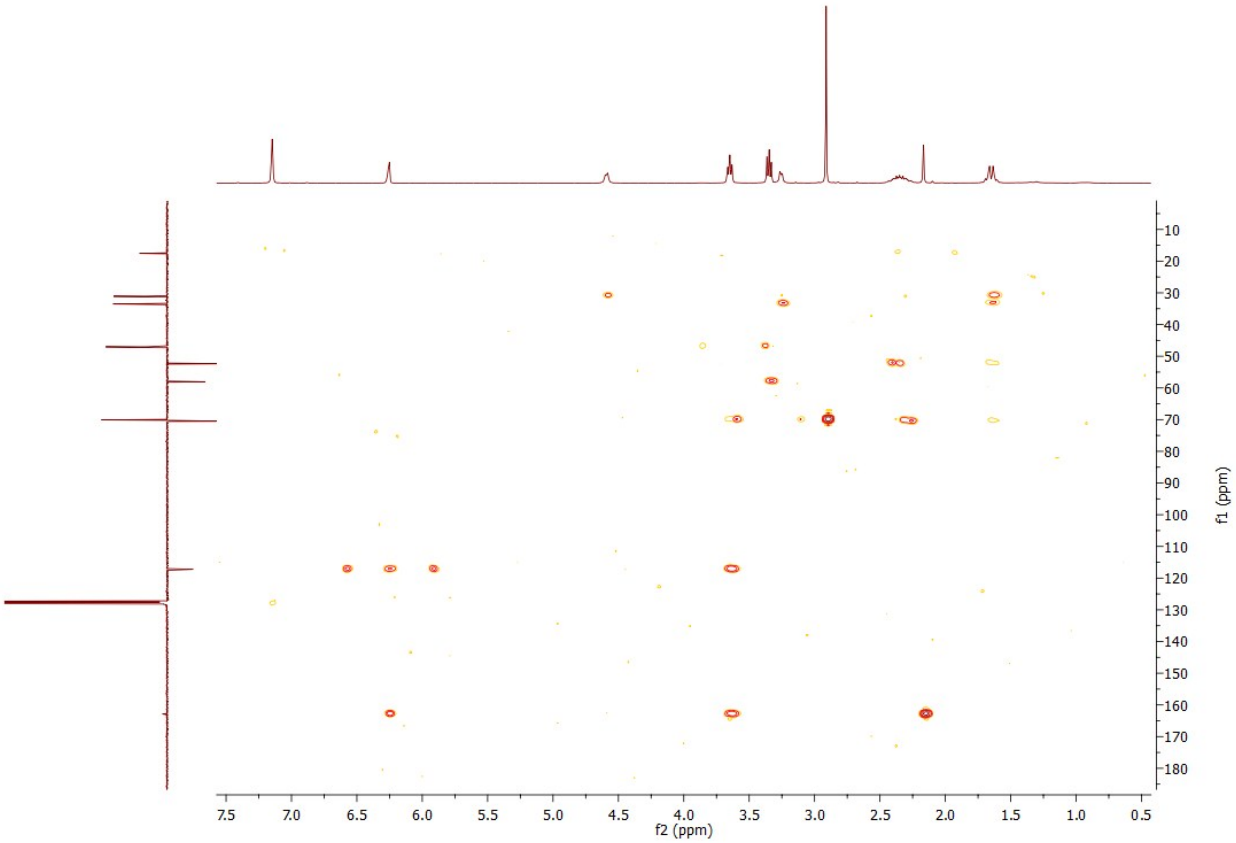

f1 (ppm)
f2 (ppm)

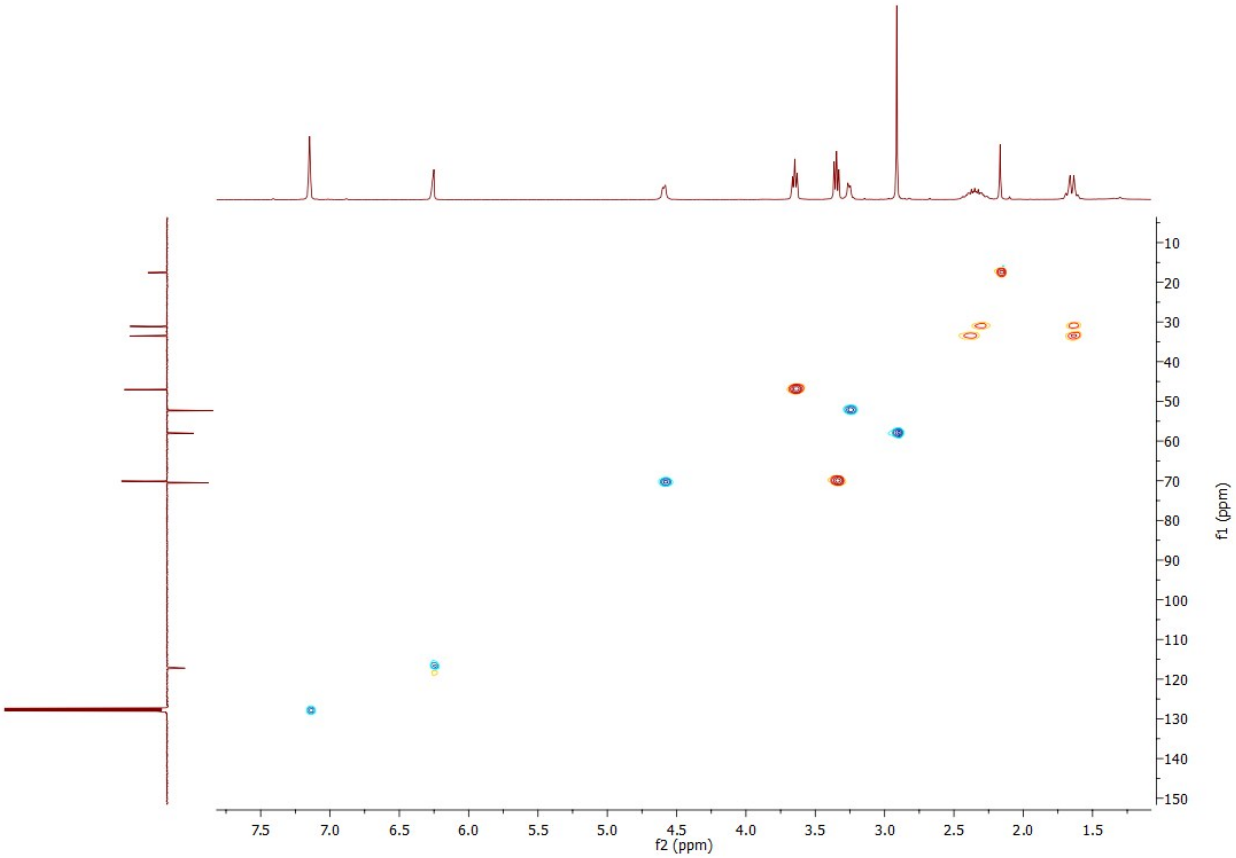
Complex 5

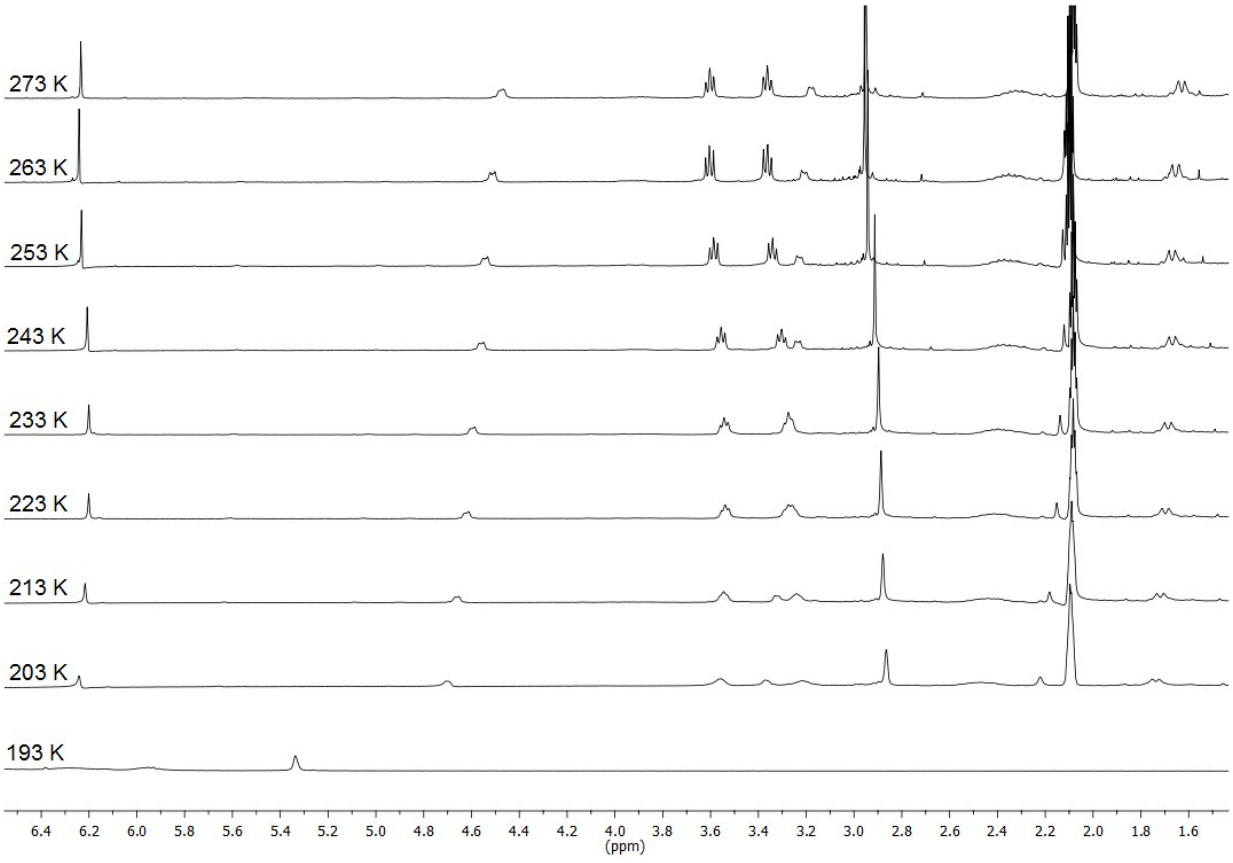

7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

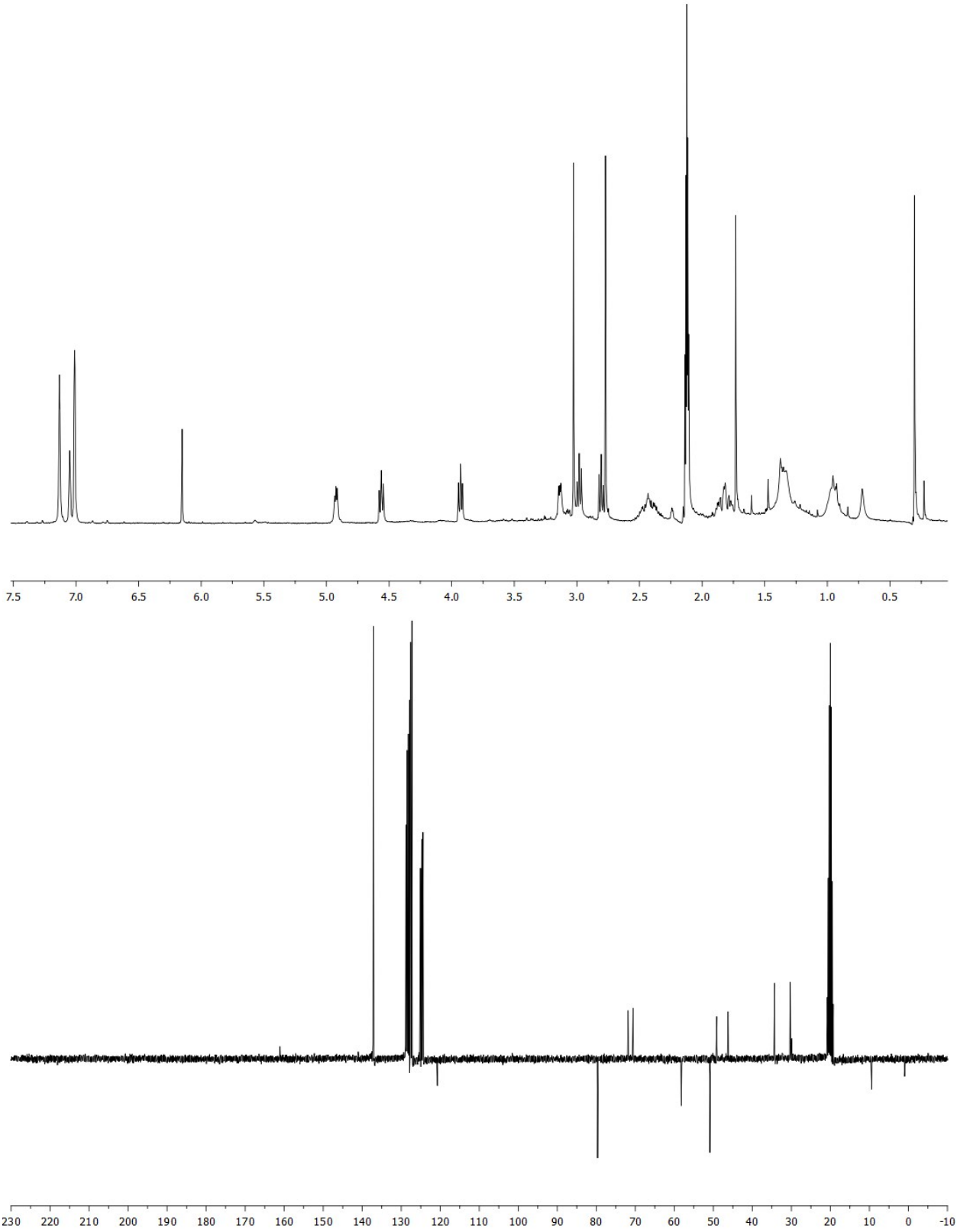

f1 (ppm)
f2 (ppm)

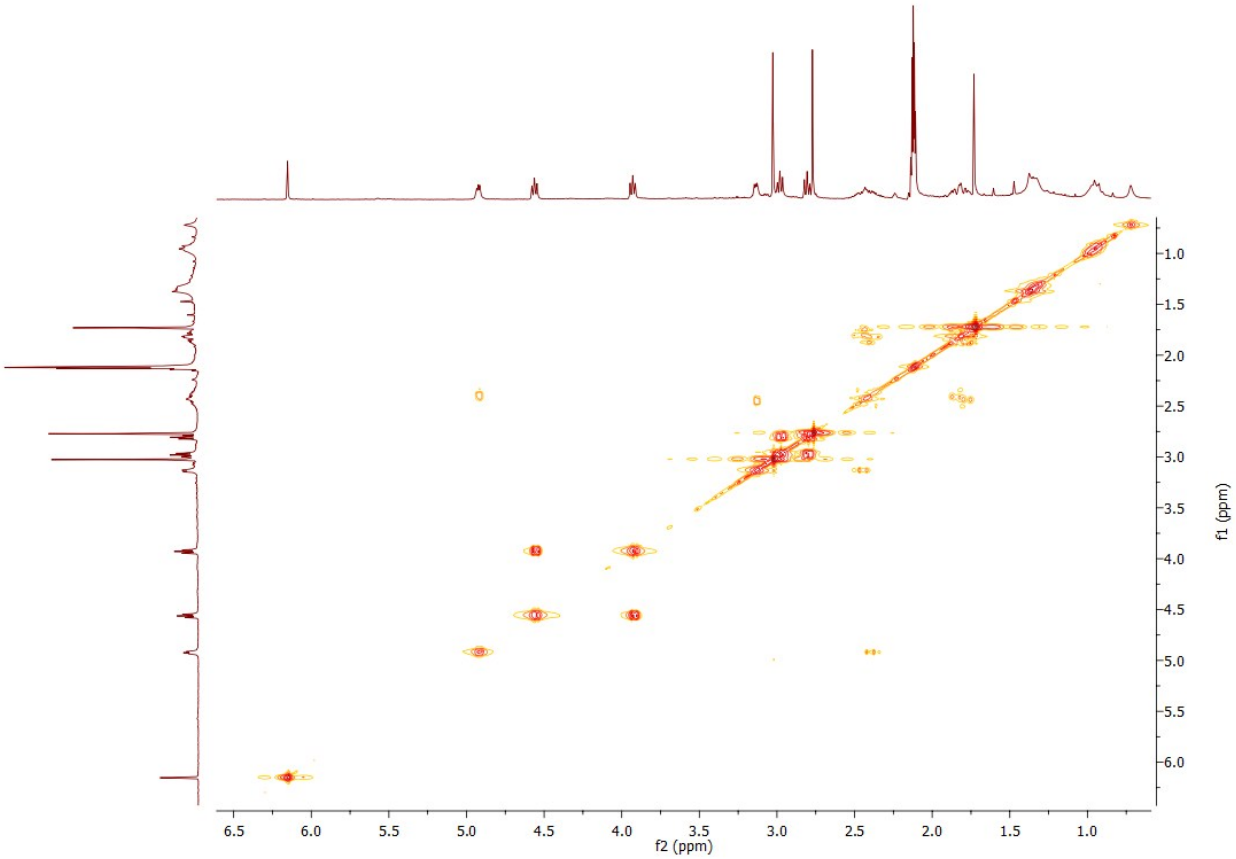

f1 (ppm)
f2 (ppm)

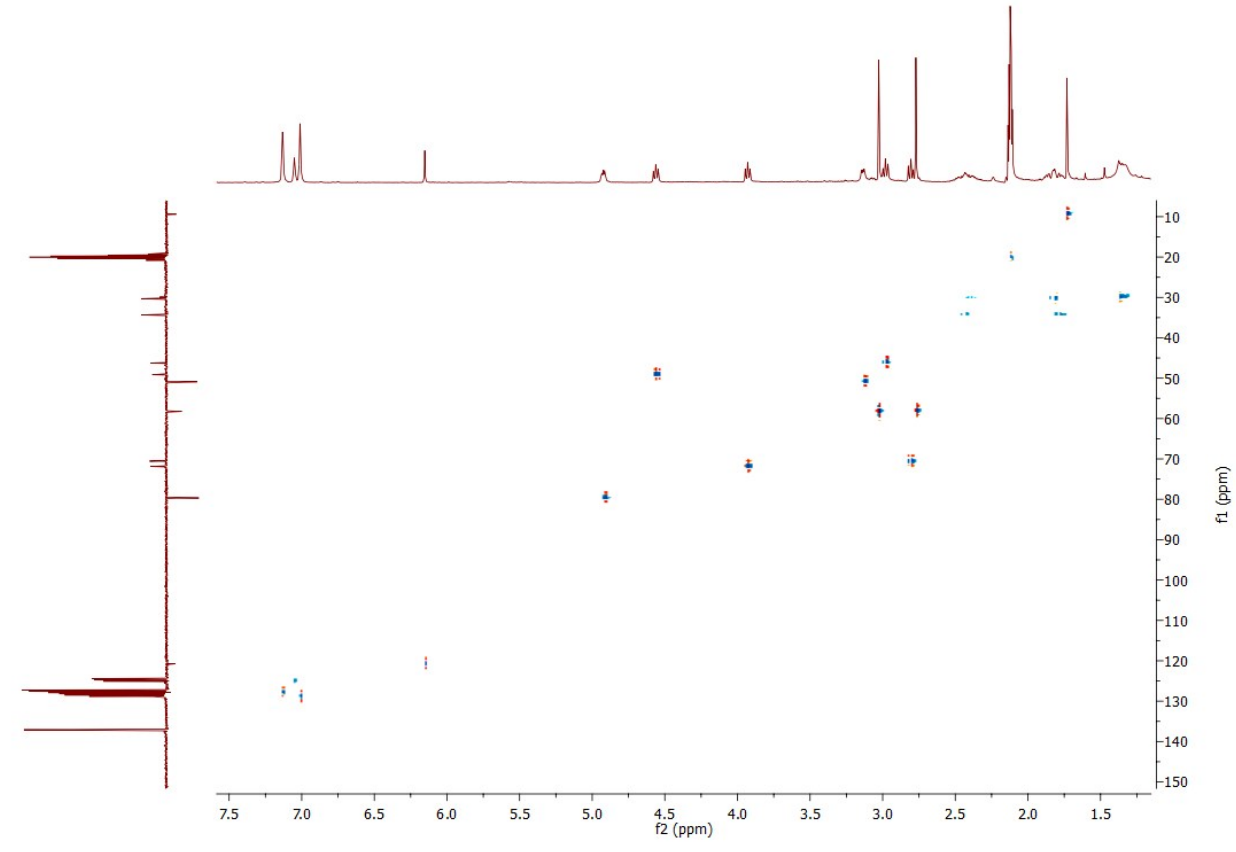

f2 (ppm)
f1 (ppm)

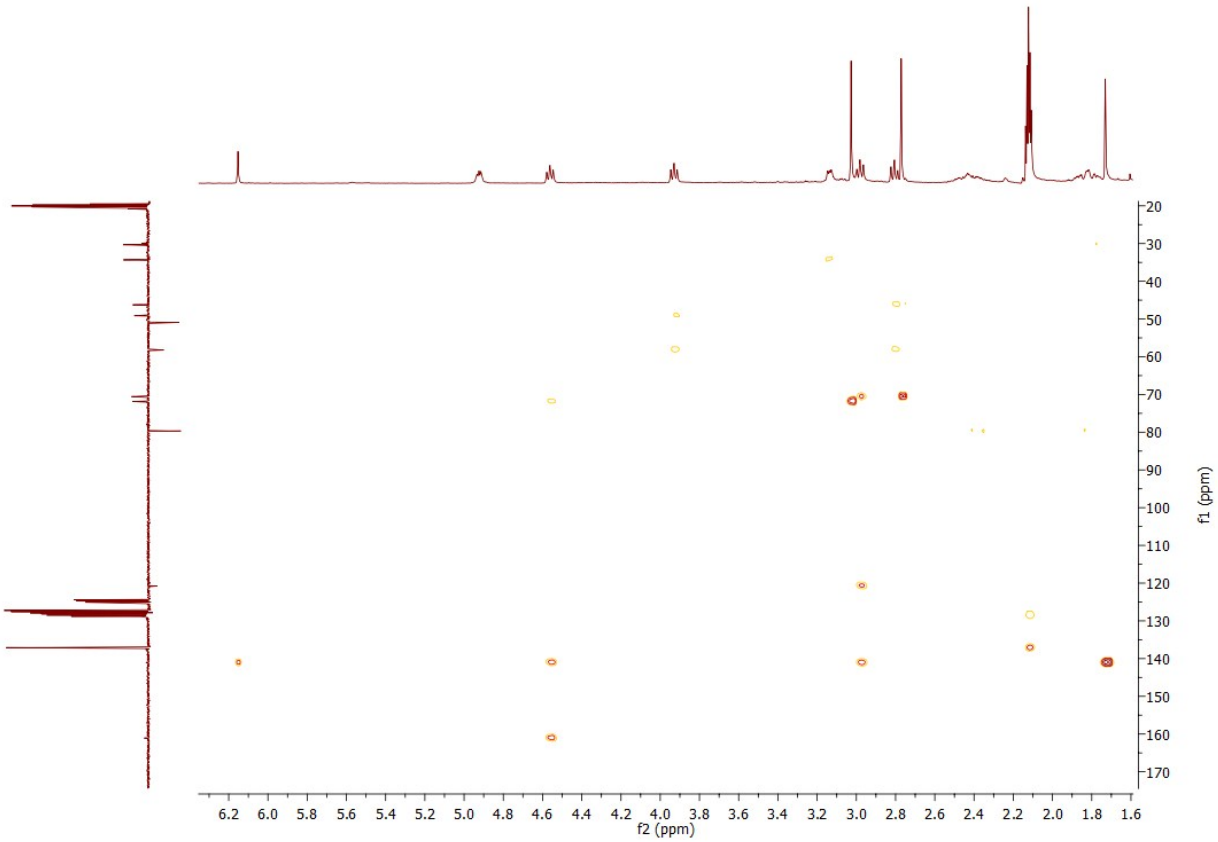

273 K
263 K
253 K
243 K
233 K
223 K
213 K
203 K
193 K
(ppm)

Complex 6


7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


f1 (ppm)
f2 (ppm)


f1 (ppm)
f2 (ppm)


f1 (ppm)
f2 (ppm)

Crystal structure analysis: X-ray diffraction data for compound **3** was recorded on an APEX-II diffractometer equipped with an area detector and graphite monochromated Mo Kα radiation (λ = 0.71073 Å). Data reduction and cell refinement were carried out using the APEX2 software.[S1] Salient structures were found by direct methods and refined by full-matrix least-squares methods based on F^2 using the SHELXL-97 and WinGX software.[S2] All non-hydrogen atoms were refined anisotropically, and all the hydrogen atoms were included in geometrically calculated positions and refined with isotropic displacement parameters according to the riding model. All geometrical calculations were performed using the SHELXL-97 and WinGX programs.[S2]

Crystal data for compound **3**: $[C_{84}H_{100}Cl_{10}Ir_2N_4O_2P_4]$, triclinic, *P–1*, a = 13.9013(7) Å, b = 17.4906(9) Å, c = 20.0339(11) Å, α = 93.6950(10)º, β = 105.6320(10)º, γ = 110.4170(10)º, Z = 2, M_r = 2060.46, V = 4327.9(4) Å^3, D_{calcd} = 1.581 g cm^{-3}, λ(Mo Kα) = 0.71073 Å, T = 100 K, μ = 3.502 mm^{-1}, 52738 reflections collected, 20117 unique (R_{int} = 0.0355), 16485 observed, $R1(F_o)$ = 0.0576 [$I > 2\sigma(I)$], $wR2$ (F_o^2) = 0.1628 (all data), GOF = 1.043.

[S1] APEX2 Bruker AXS Inc., Madison, Wisconsin, USA, 2011.

[S2] a) G. M. Sheldrick, SHELXS-97 and SHELXL-97; University of Göttingen, Germany, 1997; b) L. J. Farrugia, *WinGX*; University of Glasgow, Great Britain, 1998.

Computational Details

Table S1. Absolute (a.u.) and relative (kcal/mol, to isolated molecules and **A** or **B** for Figure 3 or Figure 4, respectively) energies of all B3LYP-D3 calculated structures using def2-SVP (DZ) basis set and solvent PCM (2-propanol) for geometry optimization and Gibbs free energy corrections at standard conditions. Basis set corrections using the def2-TZVP (TZ) have been calculated by single point (SP) energy calculations.

	E_PCM_DZ	E_PCM_TZ(SP)	G_PCM_TZ	DE_PCM_DZ	DE_PCM_TZ	DG_PCM_TZ
A	-1873.41739	-1874.86562	-1874.30334	0.0	0.0	0.0
A1	-1873.37465	-1874.81989	-1874.25573	26.8	28.7	29.9
A2	-1873.39238	-1874.83779	-1874.26976	15.7	17.5	21.1
A3	-1873.40803	-1874.85874	-1874.30041	5.9	4.3	1.8
B	-1561.55510	-1562.66835	-1562.27941	0.0	0.0	0.0
TSB/C	-1561.50791	-1562.62694	-1562.24390	29.6	26.0	22.3
C	-1561.55529	-1562.67228	-1562.28932	-0.1	-2.5	-6.2
D	-1753.18277	-1754.50216	-1754.06960	-1.3	-4.9	-9.0
TSD/E	-1753.13375	-1754.45376	-1754.02339	29.4	25.4	20.0
TSB/E	-1946.17956	-1947.71309	-1947.19878	18.6	22.2	34.9
E	-1753.18151	-1754.49581	-1754.05841	-0.5	-1.0	-2.0
TSE/F	-1947.41159	-1948.94689	-1948.40994	0.0	3.9	15.2
F+B	-385.85201	-386.28134	-386.15383	2.8	2.2	0.6
cod	-311.83973	-312.17955	-312.03237			
Acetone	-193.02861	-193.25413	-193.19909			
Phenylacetone	-384.65418	-385.08007	-384.97498			
isopropanol	-194.23093	-194.45884	-194.37891			

Table S2. Absolute (a.u.) and relative (kcal/mol, to **A** and isolated molecules) energies of all B3LYP-D3 calculated structures using def2-SVP (DZ) basis set for geometry optimization and Gibbs free energy corrections and def2-TZVP (TZ) combined with PCM solvent corrections (2-propanol) using single point energy calculations.

	E_DZ	E_TZ_PCM	G_TZ_PCM	DE_DZ	DE_TZ_PCM	DG_TZ_PCM
A	-1873.40216	-1874.86467	-1874.29945	0.0	0.0	0.0
TSA/B'	-1873.34366	-1874.80681	-1874.25018	36.7	36.3	30.9
B'	-1873.40620	-1874.87047	-1874.31506	-2.5	-3.6	-9.8
C'	-2065.03321	-2066.69969	-2066.09561	-3.7	-5.6	-13.5
TSC/D'	-2064.96850	-2066.63468	-2066.02931	36.9	35.2	28.1
D'	-2065.02996	-2066.69515	-2066.08108	-1.6	-2.8	-4.4
TSD/E'	-1947.39768	-1948.94649	-1948.41051	9.7	13.5	5.1
E'+B	-385.84642	-386.28129	-386.15358	1.9	1.0	-1.4
cod	-311.83838	-312.17959	-312.03210			
Acetone	-193.02324	-193.25397	-193.20008			
Phenylacetone	-384.64842	-385.07999	-384.97471			
isopropanol	-194.22685	-194.45875	-194.37852			

Figure S1. DFT calculated Gibbs free energy profile (relative to **A** and isolated molecules, in kcal/mol) for the stepwise and concerted transfer hydrogenation of ketones by 2-propanol catalyzed by **2** without decoordination of cod from the metallic complex.

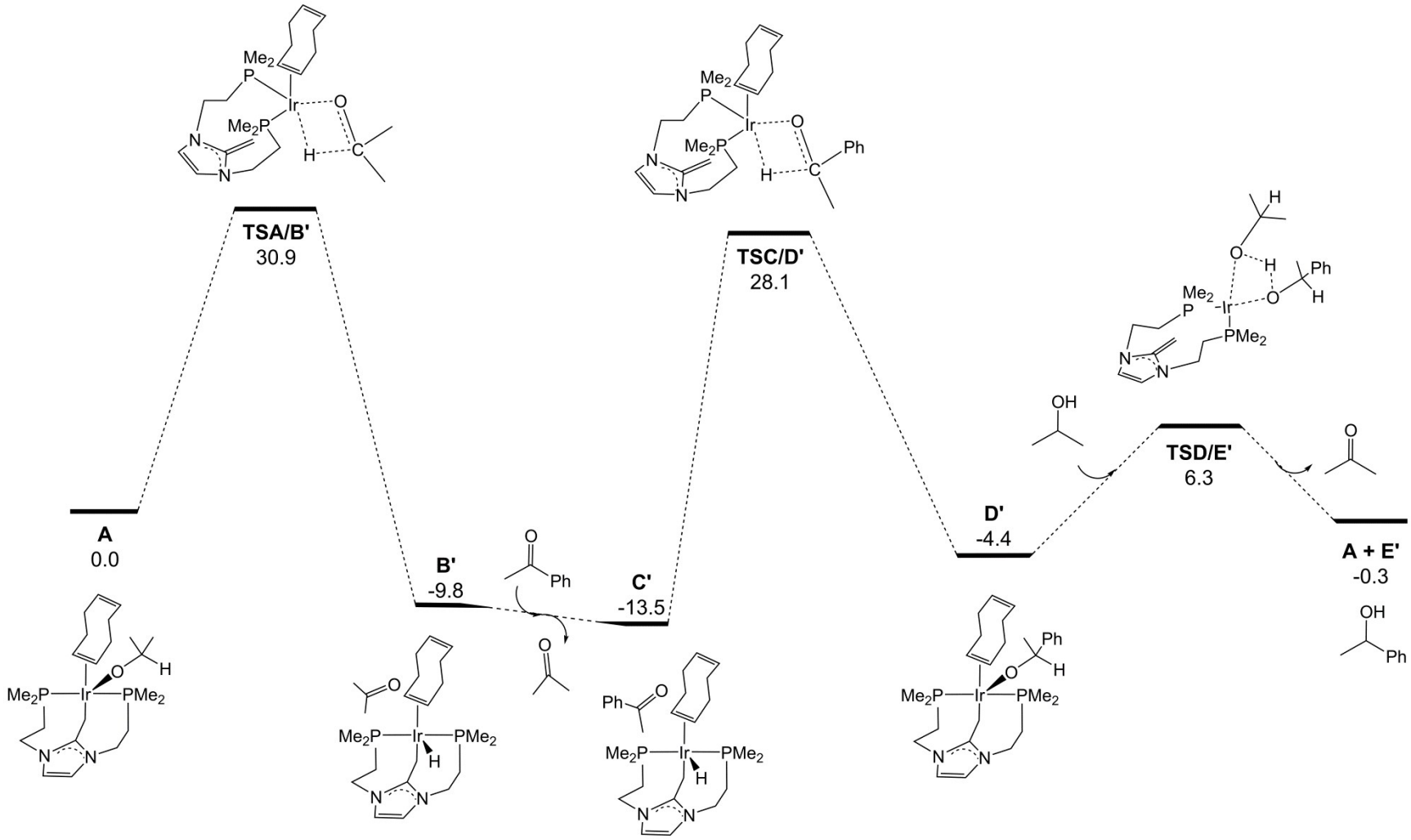


Table S3. Cartesian coordinates (in Å) for all DFT optimized structures.

A
77 0.139852 -0.035290 0.165910
15 -1.086056 -1.861706 0.707908
7 -2.911899 -1.203440 -1.782328
15 -1.084613 1.562773 1.443569
6 -2.393286 0.046180 -1.555335
7 -3.421100 0.790107 -1.038922
6 -4.574743 0.005088 -0.960204
1 -5.513959 0.409960 -0.595710
6 -4.258447 -1.230460 -1.420105
1 -4.862483 -2.125628 -1.531479
6 -2.062454 -2.364409 -2.005750
6 -1.573180 -3.005680 -0.700183
1 -0.683964 -3.614631 -0.923404
1 -2.339862 -3.689843 -0.303255
6 -1.050580 0.441640 -1.751578
6 -3.269166 2.087358 -0.392512
1 -4.230488 2.611616 -0.490139
1 -2.530730 2.673280 -0.957157
6 -2.885513 1.975446 1.090421
1 -3.525419 1.221046 1.572815
1 -3.106540 2.935576 1.584950
6 -2.698271 -1.652273 1.581844
1 -3.350576 -0.950438 1.053321
1 -3.218490 -2.617197 1.674868
1 -2.501125 -1.260788 2.588441
6 -0.342056 -3.136418 1.818861
1 -1.026603 -3.991498 1.922987
1 0.616753 -3.489111 1.417369
1 -0.168221 -2.689643 2.807876
6 -1.190283 1.309692 3.274085
1 -1.784420 2.096875 3.766124
1 -1.627746 0.329683 3.506002
1 -0.164809 1.327735 3.672552
6 -0.389685 3.269015 1.405917
1 -0.824783 3.882116 2.210248
1 0.701026 3.205329 1.493141
1 -0.607387 3.728893 0.434466
6 1.735338 -1.384398 -0.316908
6 1.904892 -0.880652 1.050879
6 5.159187 -0.920790 -0.869620
6 3.045369 0.013367 1.497252
6 5.310170 -0.433602 0.371077
6 4.421445 -0.719780 1.554157
1 3.099685 0.890093 0.840134
1 2.803868 0.392285 2.506800
1 4.957108 -0.428331 2.472349
1 4.237713 -1.806316 1.638079
6 2.681407 -1.122314 -1.470824
1 2.852008 -0.049584 -1.590248
1 2.189719 -1.463028 -2.399313
6 4.059258 -1.841291 -1.332923
1 3.943931 -2.687426 -0.631979
1 4.349840 -2.279720 -2.301450
1 5.857112 -0.571210 -1.640543
1 6.123251 0.284209 0.537065
1 1.693423 -1.623718 1.829817
1 1.417864 -2.439424 -0.355700
1 -2.626735 -3.095835 -2.601223
1 -1.211574 -2.039014 -2.615128
8 1.386135 1.644598 -0.326306
6 1.657767 2.176830 -1.572871
1 1.450018 1.448801 -2.392044
6 0.835986 3.445731 -1.886873
1 1.082807 4.243909 -1.167419
1 1.047036 3.824260 -2.902048
1 -0.245914 3.262997 -1.815385
6 3.151690 2.545852 -1.668273
1 3.789391 1.668883 -1.486658
1 3.411668 2.973449 -2.652372
1 3.391758 3.294712 -0.894069
1 -0.540860 -0.117069 -2.541099
1 -0.938998 1.516849 -1.872821
A1
6 4.271615 -0.739943 -1.285416
6 3.801341 0.397413 -1.812856
6 3.717396 1.768685 -1.200607
1 4.577415 2.367804 -1.561816
1 2.813817 2.237906 -1.609691
6 3.628683 1.951771 0.328488
1 4.625728 1.831533 0.787618
1 3.376120 3.013154 0.474875
6 2.628952 1.152787 1.166986
6 2.691255 -0.213355 1.498045
6 3.762729 -1.242520 1.160842
1 3.283530 -2.192727 0.872974
1 4.295995 -1.460644 2.106131
6 4.822853 -0.902942 0.101970
1 5.376963 -0.005348 0.408157
1 5.556808 -1.726084 0.100290
1 4.209228 -1.651979 -1.891852
1 3.417858 0.345746 -2.840073
1 2.251360 -0.431767 2.474242
1 2.150527 1.781234 1.924318
77 0.961638 0.143678 0.126041
15 0.250645 -1.798678 1.048390

7 -1.465105 -2.421675 -1.554442
15 -4.480400 0.455211 1.001425
6 -1.506298 -1.063851 -1.572945
7 -2.822990 -0.723461 -1.534057
6 -3.604177 -1.875619 -1.496106
1 -4.687172 -1.840560 -1.464600
6 -2.754045 -2.935473 -1.498728
1 -2.946182 -4.003344 -1.465834
6 -0.229115 -3.189481 -1.433148
6 0.200682 -3.369141 0.020675
1 1.219962 -3.786213 0.031217
1 -0.456541 -4.095215 0.526751
6 -0.354297 -0.193406 -1.586997
6 -3.326197 0.650086 -1.627845
1 -3.503808 0.885506 -2.689767
1 -2.519717 1.307438 -1.281870
6 -4.591509 0.906636 -0.816747
1 -5.449824 0.360031 -1.240793
1 -4.826172 1.979350 -0.917615
6 -1.501448 -1.691905 1.637014
1 -2.180077 -1.312160 0.868124
1 -1.862661 -2.674107 1.978999
1 -1.529916 -0.986582 2.479562
6 0.955050 -2.554227 2.586788
1 0.371222 -3.450672 2.843023
1 2.005906 -2.838980 2.457424
1 0.879029 -1.836415 3.415487
6 -5.959190 1.407258 1.596991
1 -5.925853 2.465751 1.290530
1 -6.876021 0.947174 1.196963
1 -6.003894 1.354329 2.695628
6 -3.117789 1.596318 1.534742
1 -3.268686 2.628171 1.178668
1 -3.075721 1.602458 2.634912
1 -2.145459 1.232813 1.168425
1 -0.391277 -4.162532 -1.916908
1 0.546471 -2.662418 -2.001806
8 0.885904 2.064855 -0.776610
6 -0.097157 2.964475 -0.406999
1 -1.119701 2.521284 -0.521561
6 -0.001278 3.428773 1.054597
1 0.974348 3.910496 1.237089
1 -0.798637 4.149790 1.303471
1 -0.086500 2.566032 1.731229
6 -0.046255 4.173271 -1.352555
1 -0.145722 3.843124 -2.399073
1 -0.850071 4.897867 -1.137780
1 0.922817 4.691839 -1.252361
1 0.392392 -0.591257 -2.293383
1 -0.619107 0.820402 -1.896509
A2
77 0.933269 -0.016855 0.052590
15 -0.208433 2.184548 -0.306039
7 -3.418282 1.132582 -0.384256
15 -0.568156 -2.019823 -0.053548
6 -3.797195 -0.205845 -0.255106
7 -3.488039 -0.804733 -1.484728
6 -3.047083 0.189469 -2.370633
1 -2.846786 -0.031784 -3.415559
6 -3.020765 1.364248 -1.707285
1 -2.828777 2.364060 -2.076596
6 -2.952185 1.879441 0.775167
6 -1.796717 2.828959 0.492500
1 -1.486744 3.238907 1.464262
1 -2.128084 3.689418 -0.110077
6 -4.376147 -0.770399 0.839010
6 -3.083627 -2.191451 -1.621903
1 -3.473780 -2.577719 -2.578204
1 -3.574051 -2.772896 -0.830980
6 -1.562315 -2.414586 -1.609929
1 -1.109332 -1.838494 -2.431668
1 -1.387689 -3.478512 -1.837102
6 -0.266623 2.966426 -1.993167
1 -0.709042 2.290438 -2.733834
1 -0.834681 3.908816 -1.971984
1 0.759389 3.196458 -2.307592
6 0.925225 3.393002 0.512977
1 0.513702 4.413725 0.478470
1 1.047765 3.064810 1.553310
1 1.904109 3.378776 0.017187
6 0.526860 -3.520566 -0.065134
1 -0.085073 -4.435486 -0.062978
1 1.184563 -3.536022 -0.941245
1 1.149638 -3.502403 0.839219
6 -1.691061 -2.631533 1.282216
1 -2.158471 -3.577976 0.967951
1 -1.087377 -2.821670 2.177724
1 -2.473373 -1.900367 1.512214
1 -3.778244 2.455782 1.230127
1 -2.637125 1.137238 1.524617
1 -4.589632 -0.168411 1.720059
1 -4.631142 -1.827505 0.856971
6 2.877194 0.694203 0.514267
6 2.776584 -0.712754 0.850797
6 3.490541 -1.788354 0.054253
1 4.587885 -1.711878 0.183541
1 3.208762 -2.768315 0.466259
6 3.124996 -1.733848 -1.440675
1 3.910647 -1.212520 -2.010465
1 3.090398 -2.752744 -1.856110
6 1.785342 -1.045767 -1.706177
6 1.675001 0.335104 -1.974725
6 2.874963 1.270015 -1.966658
1 2.511524 2.299185 -2.092025

1 3.500532 1.068399 -2.857315
6 3.707337 1.183574 -0.671732
1 4.581639 0.528247 -0.820437
1 4.121815 2.178011 -0.444219
1 2.821839 1.384543 1.360508
1 2.672192 -0.938058 1.916848
1 0.864947 0.633572 -2.645537
1 1.043078 -1.675195 -2.202078
8 0.503235 0.650440 1.977742
6 -0.326536 0.027998 2.902840
1 -1.245032 -0.364053 2.419288
6 -0.779086 1.071135 3.931371
1 -1.317545 1.893375 3.435281
1 -1.443994 0.631230 4.693183
1 0.098226 1.502433 4.442096
6 0.377436 -1.143271 3.601692
1 0.757820 -1.859132 2.858553
1 1.242015 -0.769878 4.176103
1 -0.293882 -1.679126 4.293719
A3
77 0.811507 0.387201 -0.070569
15 1.228328 -0.187057 -2.259012
7 1.868803 -2.930896 -0.302517
15 0.813973 0.885582 2.176523
6 1.073747 -2.269175 0.592449
7 1.673372 -2.425312 1.811479
6 2.891626 -3.084748 1.655328
1 3.542011 -3.289673 2.500160
6 3.012919 -3.399182 0.342204
1 3.790369 -3.935133 -0.193381
6 1.653672 -2.986792 -1.739308
6 2.191442 -1.763882 -2.489910
1 2.223585 -1.997317 -3.566782
1 3.225650 -1.565829 -2.167101
6 -0.123847 -1.528237 0.303726
6 1.213585 -1.829258 3.054929
1 1.608313 -2.450511 3.871147
1 0.118187 -1.913417 3.097281
6 1.667925 -0.378488 3.246487
1 2.748462 -0.306263 3.045652
1 1.512155 -0.097713 4.301109
6 2.265458 0.973523 -3.236647
1 3.224068 1.112540 -2.717978
1 2.441621 0.590026 -4.253454
1 1.760515 1.946270 -3.276899
6 -0.188262 -0.476283 -3.413411
1 0.156375 -0.788968 -4.411676
1 -0.854745 -1.248886 -3.003821
1 -0.762374 0.456973 -3.504492
6 1.704548 2.402797 2.723167
1 1.685943 2.496127 3.820008
1 2.745446 2.356120 2.374699
1 1.227958 3.282468 2.270751
6 -0.792659 1.063956 3.075689
1 -0.643847 1.200429 4.158398
1 -1.324058 1.936820 2.669972
1 -1.419524 0.178255 2.900244
6 -5.953690 -1.532423 -0.412462
6 -5.006829 -1.698986 -1.346528
6 -3.978038 0.867863 1.160804
6 -3.540351 -1.372199 -1.206720
6 -3.032497 0.699639 0.226148
6 -3.230122 0.153311 -1.165067
1 -3.127467 -1.836965 -0.295639
1 -2.999475 -1.822693 -2.053197
1 -2.309475 0.341944 -1.732589
1 -4.040312 0.692367 -1.686262
6 -5.757517 -0.982875 0.980174
1 -4.940520 -1.520083 1.493190
1 -6.670127 -1.177895 1.563710
6 -5.447000 0.544443 1.024610
1 -5.862864 1.013095 0.115444
1 -5.984618 0.990527 1.875199
1 -3.659556 1.244710 2.139396
1 -1.991611 0.930444 0.483553
1 -5.324646 -2.080820 -2.324043
1 -6.983750 -1.789144 -0.686909
1 2.158290 -3.893394 -2.102022
1 0.579406 -3.129405 -1.924997
8 1.535644 2.318423 -0.529329
6 0.614633 3.349125 -0.499070
1 0.044368 3.364047 0.467468
6 1.356551 4.688921 -0.596575
1 1.915714 4.737366 -1.546934
1 0.668963 5.550767 -0.553451
1 2.084214 4.781137 0.225638
6 -0.451787 3.242368 -1.604483
1 -0.966509 2.273051 -1.525696
1 -1.204219 4.047167 -1.534624
1 0.019682 3.297756 -2.601024
1 -0.654511 -1.920351 -0.573757
1 -0.819031 -1.502720 1.153520
B
77 -0.333902 0.013095 0.194258
15 -0.335570 -2.285482 0.118826
7 2.892476 -1.168946 -0.167635
15 -0.204119 2.304630 0.029061
6 2.374443 -0.052622 0.429534
7 2.948811 1.013303 -0.207534
6 3.729871 0.559498 -1.269549
1 4.256057 1.246439 -1.925056
6 3.694455 -0.795608 -1.244908
1 4.183148 -1.532383 -1.875059
6 2.538507 -2.539244 0.164559

6 1.252612 -3.031490 -0.507594
1 1.192291 -4.125833 -0.387966
1 1.303976 -2.823613 -1.588110
6 1.403716 -0.009045 1.490930
6 2.673186 2.412284 0.077625
1 3.551214 2.983893 -0.254790
1 2.611482 2.538423 1.168186
6 1.417802 2.953892 -0.614087
1 1.460466 2.713383 -1.688212
1 1.414585 4.052699 -0.524170
6 -1.528713 -3.122572 -1.006649
1 -1.446260 -2.675012 -2.006015
1 -1.330151 -4.204015 -1.060951
1 -2.550427 -2.955711 -0.641011
6 -0.577147 -3.220713 1.694811
1 -0.496586 -4.308958 1.544653
1 0.170610 -2.900719 2.435362
1 -1.573243 -2.980301 2.094479
6 -1.368430 3.157253 -1.109103
1 -1.140712 4.232223 -1.176661
1 -1.301177 2.694804 -2.103056
1 -2.390982 3.014427 -0.739161
6 -0.402429 3.289134 1.580398
1 -0.270030 4.368207 1.403220
1 -1.410243 3.106968 1.981507
1 0.326921 2.952973 2.331964
1 3.381459 -3.170373 -0.150270
1 2.473815 -2.625770 1.258811
8 -2.100862 0.073367 -0.960802
6 -3.287826 -0.224682 -0.316656
1 -3.219849 -1.192088 0.245605
6 -3.694990 0.825520 0.733318
1 -3.886872 1.801069 0.254625
1 -4.606420 0.528977 1.281179
1 -2.874038 0.954929 1.456420
6 -4.399112 -0.397713 -1.360584
1 -4.134716 -1.197262 -2.071187
1 -5.369068 -0.649045 -0.898546
1 -4.519673 0.537148 -1.934689
1 1.457855 -0.893186 2.140661
1 1.504554 0.891394 2.112383
TSB/C
77 0.971688 0.015284 0.123219
8 2.457593 1.073277 -1.005664
6 2.953992 -0.137197 -1.018893
1 2.014848 -1.237746 -0.264479
6 2.948243 -0.854395 -2.363825
1 3.721899 -0.392003 -3.001473
1 3.176448 -1.925325 -2.263237
1 1.974775 -0.733040 -2.855898
6 4.201073 -0.371020 -0.174893
1 4.423441 -1.441000 -0.053091
1 5.055505 0.105230 -0.687407
1 4.080912 0.091307 0.813633
15 -0.222536 -1.510965 1.222167
7 -2.355715 -1.429074 -1.286231
15 -0.221470 1.929131 0.675256
6 -2.067033 -0.123230 -1.702120
7 -3.045632 0.678061 -1.097195
6 -3.936381 -0.141200 -0.386371
1 -4.808707 0.273313 0.111761
6 -3.523934 -1.419800 -0.512565
1 -3.966721 -2.339970 -0.142134
6 -1.378959 -2.503610 -1.250068
6 -0.931427 -2.888186 0.165327
1 -0.130429 -3.639284 0.072179
1 -1.751248 -3.369566 0.723205
6 -1.085928 0.290468 -2.548022
6 -2.811493 2.058220 -0.723528
1 -3.792575 2.549937 -0.632764
1 -2.288107 2.568417 -1.543884
6 -2.065496 2.224958 0.610568
1 -2.536233 1.582829 1.370238
1 -2.198240 3.264442 0.954574
6 -1.634566 -1.034771 2.305424
1 -2.423347 -0.555127 1.714668
1 -2.056248 -1.919024 2.807283
1 -1.268324 -0.331640 3.067208
6 0.753076 -2.528099 2.417785
1 0.140701 -3.335700 2.849924
1 1.620574 -2.959908 1.898877
1 1.118148 -1.876500 3.224987
6 0.099609 2.524689 2.393298
1 -0.353952 3.511876 2.575742
1 -0.303573 1.800738 3.115746
1 1.187408 2.586189 2.539580
6 0.381633 3.352424 -0.328121
1 -0.067433 4.298946 0.009196
1 1.475326 3.399724 -0.240368
1 0.136271 3.182577 -1.385802
1 -1.784769 -3.396207 -1.756562
1 -0.507910 -2.171294 -1.827132
1 -0.366103 -0.413851 -2.956330
1 -0.948024 1.347690 -2.762093
C
77 0.192158 -0.195899 -0.242783
15 1.026610 1.942368 -0.347346
7 -2.316031 2.043826 0.361071
15 -0.748148 -2.279024 -0.260554
6 -2.088176 0.784536 0.856075
7 -3.155692 0.025395 0.448053
6 -3.982180 0.784611 -0.380543
1 -4.874621 0.364743 -0.834450
6 -3.461892 2.034442 -0.434561

1 -3.808141 2.928089 -0.944758
6 -1.420939 3.180664 0.502801
6 -0.295857 3.240100 -0.540050
1 0.177080 4.234839 -0.485220
1 -0.724869 3.134428 -1.549123
6 -0.968924 0.349745 1.628556
6 -3.317432 -1.397382 0.695860
1 -4.397049 -1.604439 0.678634
1 -2.974107 -1.611522 1.718268
6 -2.610649 -2.299459 -0.323971
1 -2.905428 -1.998506 -1.341825
1 -2.957721 -3.335504 -0.175447
6 2.182385 2.396972 -1.706287
1 1.725195 2.140803 -2.672365
1 2.438529 3.468190 -1.686799
1 3.096879 1.799410 -1.577669
6 1.953397 2.581145 1.119123
1 2.176546 3.655141 1.018534
1 1.373129 2.414646 2.037878
1 2.893682 2.015655 1.190552
6 -0.361774 -3.441984 -1.636791
1 -0.909560 -4.392603 -1.539024
1 -0.620785 -2.962248 -2.591610
1 0.720145 -3.640061 -1.633913
6 -0.422933 -3.348699 1.214105
1 -0.741595 -2.828304 2.129073
1 -0.944007 -4.316576 1.145318
1 0.660963 -3.522476 1.286271
1 -2.040786 4.084933 0.421670
1 -1.010981 3.173338 1.523217
1 -0.492774 1.148864 2.206352
1 -1.181251 -0.515041 2.266181
1 1.066483 -0.595911 -1.575508
8 4.448751 0.410461 0.399601
6 3.929096 -0.686525 0.539334
6 2.995358 -0.987057 1.675947
1 3.042460 -2.037516 1.997001
1 3.163155 -0.307020 2.521392
1 1.963358 -0.803497 1.266337
6 4.108618 -1.782887 -0.483923
1 4.497296 -2.698660 -0.010575
1 3.116934 -2.021777 -0.903782
1 4.782230 -1.454957 -1.286529
D
77 -0.448691 -0.215454 -0.475280
15 0.634482 1.809036 -0.573584
7 -2.517335 2.278876 0.702289
15 -1.703255 -2.131881 -0.504973
6 -2.396974 0.962361 1.065643
7 -3.611698 0.389404 0.792530
6 -4.444195 1.322021 0.174113
1 -5.449726 1.065362 -0.144762
6 -3.765956 2.493514 0.119109
1 -4.058213 3.468752 -0.257915
6 -1.454546 3.269227 0.752930
6 -0.529030 3.261693 -0.470866
1 0.070426 4.187085 -0.460966
1 -1.136667 3.271886 -1.389353
6 -1.237096 0.312200 1.586662
6 -3.929561 -1.020172 0.947641
1 -5.015324 -1.088489 1.106013
1 -3.454643 -1.383360 1.870198
6 -3.534347 -1.883035 -0.256531
1 -3.934766 -1.429119 -1.176945
1 -4.006428 -2.873566 -0.148831
6 1.603668 2.248128 -2.076393
1 0.953904 2.158866 -2.958718
1 2.013382 3.268774 -2.017361
1 2.428035 1.526905 -2.176581
6 1.839864 2.246015 0.759238
1 2.139713 3.304033 0.701122
1 1.406640 2.043319 1.748939
1 2.729923 1.613591 0.648121
6 -1.729337 -3.179250 -2.021245
1 -2.402947 -4.043767 -1.911167
1 -2.054185 -2.564664 -2.873042
1 -0.707745 -3.533668 -2.221650
6 -1.345988 -3.399777 0.794677
1 -1.378059 -2.933644 1.789924
1 -2.062318 -4.235360 0.757874
1 -0.329116 -3.786790 0.637711
1 -1.939733 4.251918 0.837730
1 -0.884767 3.120422 1.681519
1 -0.562416 0.982454 2.129751
1 -1.462140 -0.575973 2.186616
1 0.173875 -0.606170 -1.944860
8 3.207833 -0.540871 3.072673
6 2.935613 -1.020566 1.979889
6 1.719110 -1.873279 1.773636
1 1.968875 -2.823257 1.278385
1 1.230891 -2.064432 2.737476
1 0.999929 -1.339821 1.097362
6 3.797223 -0.721941 0.788180
6 3.419948 -1.082064 -0.515842
6 4.991153 -0.006204 0.984325
6 4.219535 -0.721796 -1.603704
1 2.481133 -1.606890 -0.692639
6 5.792831 0.344962 -0.099737
1 5.263500 0.275187 2.002905
6 5.405131 -0.009979 -1.398713
1 3.910220 -0.992412 -2.615739
1 6.719336 0.901066 0.061608
1 6.028487 0.271078 -2.251018
TSD/E

77 0.285552 0.129973 -0.156653
8 1.502866 1.211770 -1.558557
6 2.102430 0.043634 -1.506211
1 1.189311 -1.070928 -0.909922
6 2.200411 -0.694076 -2.841942
1 2.916659 -0.145662 -3.476398
1 2.554724 -1.728324 -2.735326
1 1.219683 -0.695999 -3.336456
15 -0.504372 -1.468928 1.181113
7 -3.023958 -1.646312 -0.910518
15 -0.852003 1.961268 0.671497
6 -2.873467 -0.330088 -1.366176
7 -3.785518 0.422981 -0.615503
6 -4.500190 -0.432620 0.236117
1 -5.302180 -0.059388 0.867325
6 -4.044177 -1.688967 0.049206
1 -4.367434 -2.626574 0.492421
6 -1.985251 -2.657253 -1.014618
6 -1.262780 -2.945239 0.307499
1 -0.429657 -3.634105 0.093666
1 -1.928089 -3.465549 1.015531
6 -2.053271 0.124936 -2.352322
6 -3.610858 1.830910 -0.323212
1 -4.604949 2.252998 -0.108429
1 -3.250726 2.341758 -1.226918
6 -2.699043 2.109190 0.883619
1 -2.993851 1.454175 1.717735
1 -2.871809 3.144629 1.221978
6 -1.715147 -1.108508 2.521705
1 -2.647498 -0.720914 2.093621
1 -1.939879 -2.017266 3.100881
1 -1.279762 -0.355168 3.193575
6 0.808780 -2.329045 2.154681
1 0.404800 -3.201267 2.693251
1 1.607428 -2.651860 1.471654
1 1.237863 -1.620118 2.877466
6 -0.310323 2.560245 2.329256
1 -0.800352 3.509384 2.598454
1 -0.544756 1.802527 3.089980
1 0.779725 2.700891 2.306869
6 -0.505311 3.427175 -0.389418
1 -0.930486 4.346093 0.042098
1 0.583131 3.527165 -0.497474
1 -0.926882 3.259248 -1.390455
1 -2.417020 -3.595016 -1.403615
1 -1.258717 -2.303823 -1.755477
1 -1.382269 -0.549140 -2.877918
1 -2.004789 1.185130 -2.588365
6 3.328038 -0.059140 -0.619984
6 3.930672 1.115652 -0.147963
6 3.904942 -1.296604 -0.292067
6 5.078674 1.055606 0.645704
1 3.474916 2.071686 -0.408823
6 5.049819 -1.357869 0.504276
1 3.439780 -2.222017 -0.640824
6 5.642625 -0.180980 0.977298
1 5.536329 1.979690 1.008496
1 5.480539 -2.328991 0.761129
1 6.538296 -0.228907 1.601328
TSB/E
77 -0.172901 -0.748624 0.546760
15 -1.921449 -1.652401 -0.455443
7 -2.308404 1.050780 -2.325248
15 -1.227842 0.674408 1.919651
6 -1.740693 1.994298 -1.460559
7 -2.819491 2.533741 -0.741616
6 -4.014272 1.980030 -1.231796
1 -4.981654 2.306677 -0.859448
6 -3.703198 1.093031 -2.199702
1 -4.348622 0.494977 -2.836870
6 -1.581224 -0.074990 -2.883015
6 -2.004789 -1.434132 -2.316829
1 -1.323171 -2.194752 -2.730382
1 -3.019501 -1.707162 -2.650595
6 -0.438482 2.365128 -1.357519
6 -2.688928 2.930728 0.647718
1 -3.526334 3.607445 0.879298
1 -1.773570 3.526446 0.765791
6 -2.731894 1.759217 1.642418
1 -3.581209 1.105600 1.396224
1 -2.942297 2.175012 2.641795
6 -3.653137 -1.382025 0.103408
1 -3.957197 -0.342901 -0.063423
1 -4.338705 -2.043878 -0.447648
1 -3.712954 -1.616797 1.175859
6 -1.848569 -3.498626 -0.395884
1 -2.606871 -3.952131 -1.053675
1 -0.841515 -3.808214 -0.706207
1 -2.016875 -3.830373 0.638977
6 -1.830162 -0.187188 3.444679
1 -2.215005 0.521628 4.195005
1 -2.626621 -0.894600 3.172199
1 -0.995089 -0.759737 3.872753
6 -0.075397 1.922177 2.641353
1 -0.532098 2.428332 3.505180
1 0.848361 1.407452 2.934087
1 0.180342 2.669622 1.877900
1 -1.691682 -0.091683 -3.981346
1 -0.520278 0.087655 -2.666486
1 0.338452 1.870506 -1.933314
1 -0.135495 3.103741 -0.619320
8 1.065052 -2.223587 -0.378672
6 2.185318 -1.933587 -0.967767
1 2.865198 -1.192888 -0.090113

8 1.752904 -0.245223 1.441737
6 2.946012 -0.367128 0.945080
6 3.148170 -3.100166 -1.132182
1 2.774574 -3.761614 -1.932597
1 4.157275 -2.761280 -1.408740
1 3.198202 -3.681969 -0.201024
6 2.151168 -0.937732 -2.117692
1 3.158371 -0.665789 -2.461666
1 1.602717 -1.399882 -2.955601
1 1.617410 -0.028603 -1.811076
6 3.917945 -1.163923 1.811660
1 4.862639 -1.401111 1.304613
1 4.145534 -0.575077 2.715477
1 3.433874 -2.100242 2.123176
6 3.513388 0.816702 0.188083
6 4.803601 0.806445 -0.367733
6 2.702531 1.942510 -0.003983
6 5.269209 1.901790 -1.097975
1 5.446978 -0.067362 -0.248561
6 3.165346 3.037966 -0.736333
1 1.698897 1.928879 0.414529
6 4.450905 3.022102 -1.285855
1 6.273976 1.879744 -1.527010
1 2.516097 3.904453 -0.884337
1 4.815104 3.876894 -1.860958
E
77 0.438216 -0.097460 -0.388429
15 -0.038733 2.157390 -0.400552
15 0.980882 -2.314328 -0.107079
6 2.659364 2.985837 0.193957
6 1.182855 3.199295 0.543900
1 0.934286 4.260492 0.377430
1 1.028044 2.991993 1.614623
6 2.382212 0.288207 -1.254894
6 3.754332 -1.836619 0.500687
1 4.627968 -2.221516 1.045387
1 3.969185 -1.967431 -0.569611
6 2.505580 -2.621842 0.915809
1 2.251431 -2.378207 1.959518
1 2.739669 -3.698496 0.878332
6 -1.603779 2.732882 0.382057
1 -1.669858 2.317768 1.396539
1 -1.639892 3.832340 0.423999
1 -2.462160 2.361537 -0.192712
6 -0.081537 3.033920 -2.027081
1 -0.247872 4.116215 -1.907919
1 0.864499 2.869274 -2.563567
1 -0.892749 2.605081 -2.633494
6 -0.227056 -3.381804 0.774321
1 0.169055 -4.399619 0.912489
1 -0.452173 -2.931452 1.750470
1 -1.157714 -3.415311 0.195137
6 1.346531 -3.315174 -1.616937
1 1.644025 -4.345260 -1.364669
1 0.444668 -3.340658 -2.246008
1 2.149744 -2.837357 -2.196908
1 3.265182 3.772261 0.665492
1 2.827352 3.067806 -0.889477
8 -1.507418 -0.526688 0.325241
6 -2.531063 -0.405251 -0.586909
1 -2.397352 0.484045 -1.251700
6 -2.626224 -1.614785 -1.544509
1 -2.840131 -2.533744 -0.974583
1 -3.417662 -1.487812 -2.301653
1 -1.660366 -1.737100 -2.059529
1 2.406333 1.169880 -1.910032
1 2.800797 -0.566974 -1.803472
6 -3.874856 -0.199050 0.112876
6 -4.989314 0.291714 -0.585861
6 -4.021769 -0.505951 1.471766
6 -6.220359 0.465048 0.052984
1 -4.888209 0.549212 -1.644876
6 -5.252210 -0.337457 2.116095
1 -3.142403 -0.865766 2.007672
6 -6.357604 0.147903 1.409771
1 -7.075222 0.853862 -0.507181
1 -5.348898 -0.581943 3.177836
1 -7.318371 0.284705 1.912813
6 3.062917 0.520377 -0.006694
6 4.094506 0.183229 1.972448
6 3.795871 1.503149 1.888459
1 4.586468 -0.387457 2.753934
1 3.973577 2.319421 2.581810
7 3.677447 -0.411720 0.782760
7 3.197245 1.713214 0.647534
TSE/F
77 -0.498157 0.579818 0.221813
8 -0.561756 2.408216 -0.969645
6 -0.815514 3.725544 -0.520924
6 -0.112933 4.054213 0.798020
1 0.982469 4.039505 0.680121
1 -0.400857 5.055897 1.156485
1 -0.378383 3.307912 1.562726
6 -0.437479 4.706901 -1.631078
1 -0.695013 5.742479 -1.356226
1 0.645886 4.665769 -1.832857
1 -0.965918 4.451195 -2.562479
15 0.201965 -1.185752 1.382499
7 -0.247897 -2.820533 -1.417865
15 -2.660693 0.367774 0.674981
6 -1.200527 -1.905169 -1.888680
7 -2.445705 -2.460694 -1.553532
6 -2.237531 -3.713111 -0.951595
1 -3.072792 -4.349519 -0.671354

6 -0.907775 -3.931581 -0.877941
1 -0.357977 -4.795858 -0.515350
6 1.110124 -2.442526 -1.062378
6 1.354372 -2.329962 0.446577
1 2.372622 -1.943847 0.596480
1 1.314160 -3.320464 0.927877
6 -0.979655 -0.744784 -2.560904
6 -3.609295 -1.655051 -1.230800
1 -4.501514 -2.276943 -1.404163
1 -3.673920 -0.821171 -1.943020
6 -3.644752 -1.156487 0.225864
1 -3.344382 -1.974953 0.895099
1 -4.687336 -0.909199 0.485701
6 -0.932502 -2.384403 2.205066
1 -1.529821 -2.918032 1.456502
1 -0.345349 -3.118163 2.777902
1 -1.597433 -1.849111 2.895980
6 1.264354 -0.751980 2.830387
1 1.743603 -1.649085 3.254384
1 2.039509 -0.042003 2.518278
1 0.636564 -0.275026 3.596826
6 -3.251448 0.611703 2.407781
1 -4.350290 0.566938 2.468905
1 -2.822457 -0.154739 3.067331
1 -2.904604 1.596260 2.752804
6 -3.653488 1.648033 -0.208273
1 -4.730941 1.457817 -0.091508
1 -3.415089 2.634127 0.210955
1 -3.387657 1.654753 -1.273868
1 1.824808 -3.165292 -1.490788
1 1.312837 -1.473730 -1.529105
1 0.028974 -0.376897 -2.728461
1 -1.813000 -0.108187 -2.847904
1 -1.903513 3.819888 -0.349108
8 1.402783 1.192408 -0.710987
6 2.619782 1.589783 -0.107032
1 2.440448 1.911529 0.936352
6 3.223043 2.767425 -0.878808
1 3.401561 2.482014 -1.927234
1 2.542668 3.631993 -0.866168
1 4.181357 3.075123 -0.433445
6 3.586151 0.419958 -0.081309
6 4.327023 0.112166 1.065967
6 3.765870 -0.364000 -1.230377
6 5.210569 -0.972960 1.078360
1 4.205201 0.722595 1.964794
6 4.646589 -1.446850 -1.224424
1 3.190508 -0.128253 -2.127319
6 5.367883 -1.759894 -0.065846
1 5.771426 -1.207183 1.986510
1 4.766389 -2.055633 -2.124102
1 6.050486 -2.613045 -0.056911
1 0.635627 2.035963 -0.983480
F (phenyletanol)
6 1.654968 -0.225744 -0.330104
1 1.855303 -0.909495 -1.179524
6 0.150948 -0.086051 -0.195636
6 -0.675455 -1.204272 -0.381280
6 -0.434023 1.137167 0.157013
6 -2.058350 -1.105395 -0.210567
1 -0.231184 -2.162366 -0.666340
6 -1.818922 1.239109 0.324742
1 0.207360 2.009018 0.290095
6 -2.635618 0.119061 0.143990
1 -2.688756 -1.985414 -0.360664
1 -2.262195 2.200497 0.596945
1 -3.717604 0.199458 0.273947
6 2.270636 -0.837863 0.931944
1 3.361315 -0.952023 0.814081
1 2.075293 -0.188024 1.799272
1 1.846142 -1.832163 1.137068
8 2.207402 1.054185 -0.596247
1 3.170011 0.970956 -0.575517
COD
6 1.737448 -0.670796 -0.117924
6 1.737897 0.669695 -0.117979
6 -1.738009 -0.669707 0.117199
6 0.654892 1.571258 0.423850
6 -1.737555 0.670793 0.117172
6 -0.653679 1.572186 -0.423281
1 0.401554 1.287781 1.460407
1 1.047199 2.598320 0.472039
1 -1.045301 2.599560 -0.470261
1 -0.400468 1.289832 -1.460193
6 0.653865 -1.571592 0.424019
1 0.400664 -1.287791 1.460519
1 1.045527 -2.598893 0.472371
6 -0.654684 -1.571840 -0.423147
1 -0.401300 -1.289789 -1.460103
1 -1.046921 -2.598983 -0.469996
1 -2.594079 -1.172920 0.582057
1 -2.593258 1.174602 0.582063
1 2.593072 1.173164 -0.584202
1 2.592259 -1.174872 -0.584159
Acetone
6 0.000040 0.184696 -0.000069
6 1.286140 -0.613290 0.001882
1 1.366295 -1.187430 -0.936360
1 2.149076 0.058872 0.095568
1 1.286025 -1.347039 0.823930
6 -1.286139 -0.613332 -0.001896
1 -1.285943 -1.347639 -0.823419
1 -1.366528 -1.186793 0.936761
1 -2.148944 0.058923 -0.096074

8 -0.000029 1.400332 0.000012
Phenylacetone
6 -1.701201 -0.203406 -0.000103
6 -2.550913 1.048114 0.000024
1 -2.336453 1.666112 0.886165
1 -2.336605 1.666186 -0.886100
1 -3.610239 0.763296 0.000104
8 -2.216058 -1.309903 0.000050
6 -0.208897 -0.056354 -0.000057
6 0.427505 1.196527 -0.000021
6 0.576025 -1.222806 -0.000013
6 1.821895 1.278752 0.000010
1 -0.159299 2.116017 -0.000038
6 1.966837 -1.140829 0.000023
1 0.067143 -2.188049 -0.000026
6 2.592707 0.112187 0.000031
1 2.308342 2.256709 0.000022
1 2.568519 -2.052659 0.000041
1 3.683310 0.178506 0.000061
Isopropanol
6 -1.269370 -0.665450 0.098774
1 -1.298680 -0.712442 1.201343
1 -1.317892 -1.697239 -0.283681
1 -2.162608 -0.122224 -0.245829
6 0.000000 0.041866 -0.370542
1 -0.000001 0.069260 -1.474238
6 1.269366 -0.665457 0.098773
1 2.162606 -0.122235 -0.245830
1 1.298676 -0.712450 1.201342
1 1.317882 -1.697247 -0.283683
8 0.000003 1.411737 0.022245
1 0.000018 1.434932 0.990593