Supplementary Information

Reactivity of $[K_3(phen)_8][Cu(NPh_2)_2]_3$ — A Possible Intermediate in the Copper(I)-Catalyzed *N*-Arylation of *N*-Phenylaniline

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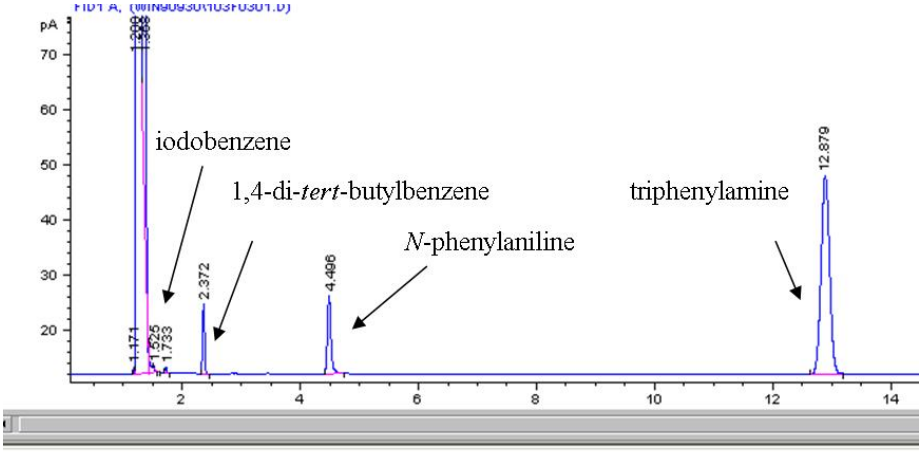
Contents of the supporting information:

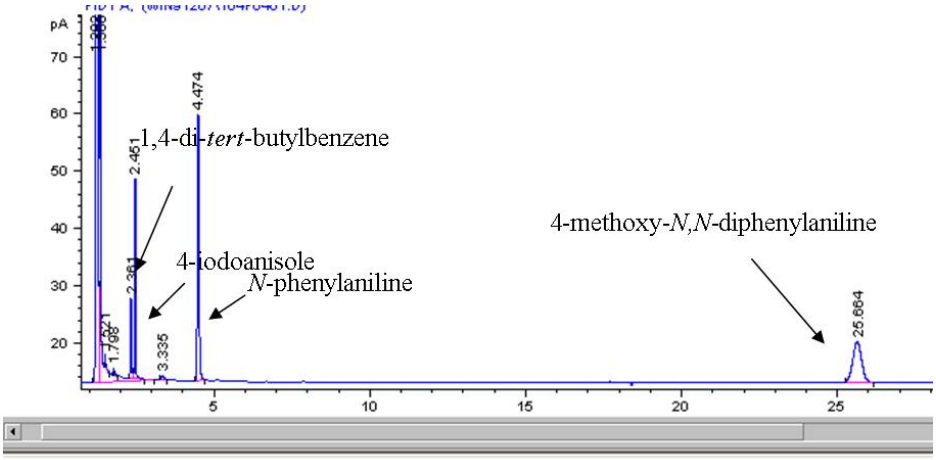
Reaction of Copper(I) Catalyzed C-N Coupling with different base systems.

Reaction between N-phenylaniline and Iodobenzene with tBuOK:



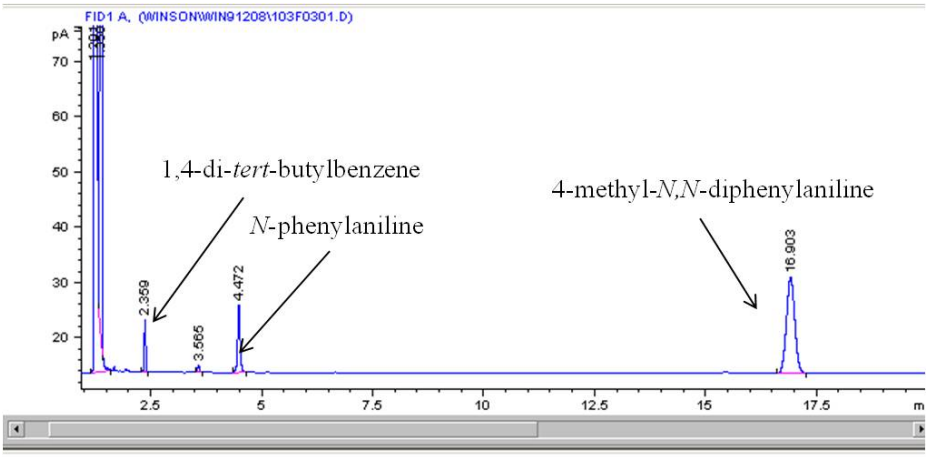
#	Time	Area	Height	Width	Area%	Symmetry
1	1.171	2.1	1.2	0.0251	0.001	0.6
2	1.208	343340.2	165998.3	0.0321	98.376	0.133
3	1.368	5214.3	2397.4	0.0364	1.494	1.164
4	1.525	1	5.1E-1	0.0285	0.000	0.672
5	1.733	2	9.8E-1	0.0317	0.001	1.102
6	2.372	31.2	12.7	0.0392	0.009	1.042
7	4.496	59.5	14.1	0.0637	0.017	0.763
8	12.879	359	35.9	0.1561	0.103	0.909

Reaction between N-phenylaniline and 4-iodoanisole with tBuOK:



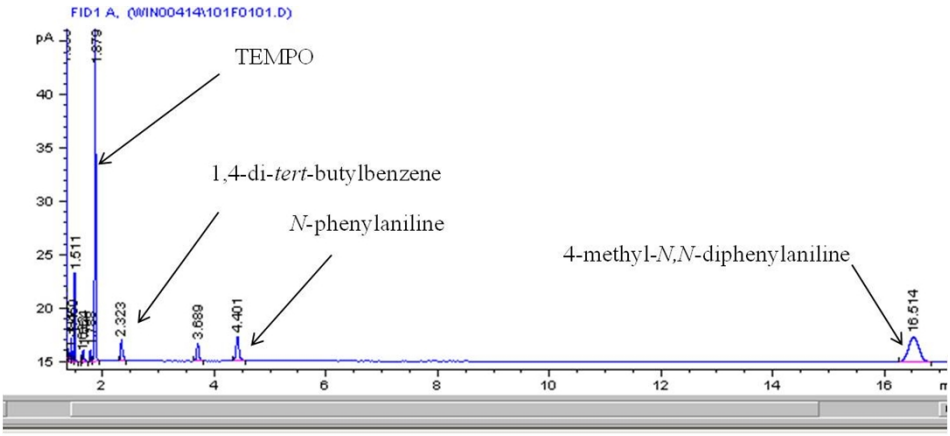
#	Time	Area	Height	Width	Area%	Symmetry
1	1.202	310899.6	158833.8	0.0313	98.012	0.133
2	1.36	5858.7	2819.5	0.0342	1.847	1.084
3	1.521	6.4	2.5	0.0371	0.002	0.427
4	1.798	4.8	1.3	0.0498	0.002	0.403
5	2.361	35.8	14	0.0399	0.011	1.128
6	2.451	84	34.9	0.0376	0.026	0.964
7	3.335	4	6.9E-1	0.0695	0.001	0.601
8	4.474	172.8	46.5	0.0573	0.054	0.902
9	25.664	140.3	7.1	0.2417	0.044	1.019

Reaction between N-phenylaniline and 4-iodotoluene with tBuOK for 6 h



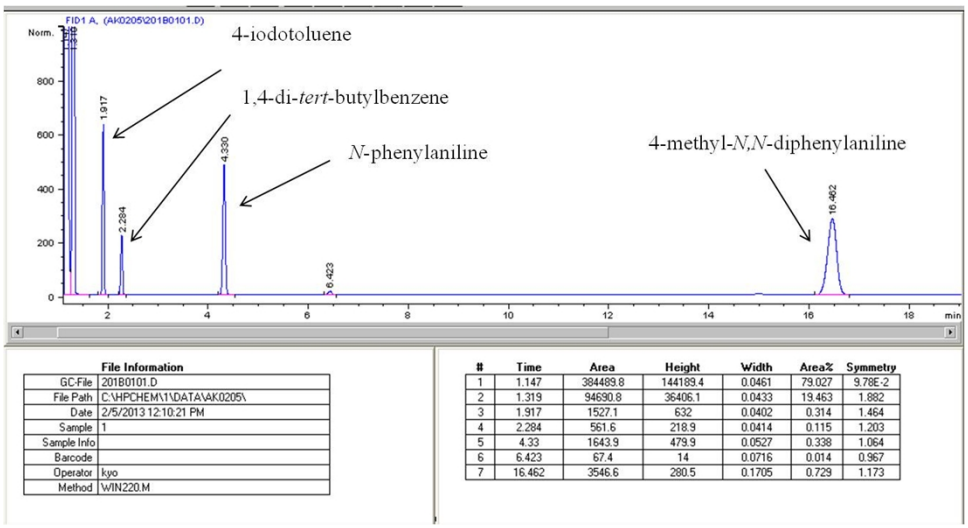
#	Time	Area	Height	Width	Area%	Symmetry
1	1.201	308953.4	162080.2	0.0297	98.647	0.143
2	1.358	3936.9	1986.4	0.0326	1.257	1.017
3	2.359	22.3	9.5	0.0369	0.007	1.052
4	3.565	4	1.3	0.0467	0.001	1.015
5	4.472	49.1	12.2	0.0611	0.016	0.89
6	16.903	226.8	17.4	0.1834	0.072	0.966

Reaction between N-phenylaniline and 4-iodotoluene with tBuOK and 3.0 equiv of TEMPO (488 mg, 3.0 mmol) *for 6 h*:



#	Time	Area	Height	Width	Area%	Symmetry
4	1.398	8.5E-1	6.3E-1	0.0208	0.002	0.606
5	1.45	2.3	2	0.0183	0.006	0.856
6	1.511	9	8.2	0.0168	0.025	0.981
7	1.632	6.3E-1	5.7E-1	0.0178	0.002	1.039
8	1.664	1.6	1	0.0217	0.004	0.678
9	1.788	1.3	1E0	0.0205	0.004	0.983
10	1.879	45.2	31.3	0.0219	0.123	0.988
11	2.323	4.9	1.9	0.0361	0.013	0.615
12	3.689	4.7	1.7	0.0437	0.013	0.922
13	4.401	7.9	2.2	0.0534	0.022	0.823
14	16.514	30	2.4	0.1594	0.082	0.938

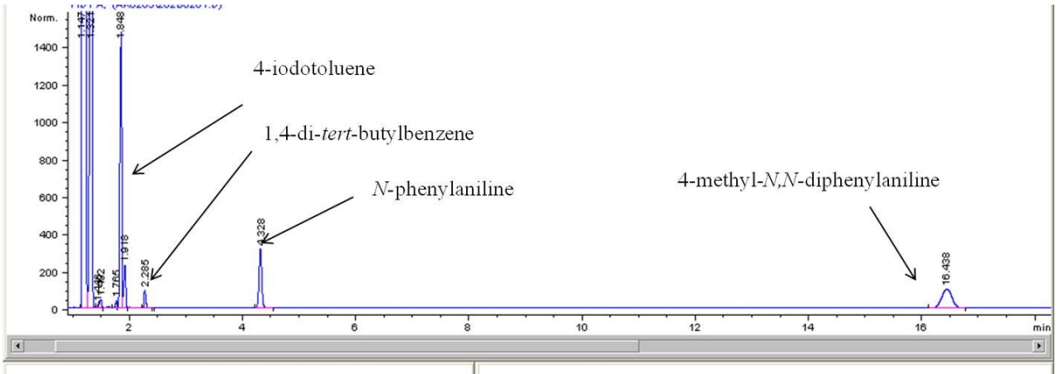
Reaction between N-phenylaniline and 4-iodotoluene with tBuOK for 30 min **:**



File Information	
GC-File	201B0101.D
File Path	C:\HPCHEM\1\DATA\AK0205\
Date	2/5/2013 12:10:21 PM
Sample	1
Sample Info	
Barcode	
Operator	kyo
Method	WIN220.M

#	Time	Area	Height	Width	Area%	Symmetry
1	1.147	384489.8	144189.4	0.0461	79.027	9.78E-2
2	1.319	94690.8	36406.1	0.0433	19.463	1.882
3	1.917	1527.1	632	0.0402	0.314	1.464
4	2.284	561.6	218.9	0.0414	0.115	1.203
5	4.33	1643.9	479.9	0.0527	0.338	1.064
6	6.423	67.4	14	0.0716	0.014	0.967
7	16.462	3546.6	280.5	0.1705	0.729	1.173

Reaction between N-phenylaniline and 4-iodotoluene with tBuOK and 3.0 equiv of TEMPO (488 mg, 3.0 mmol) *for 30 min:*



File Information	
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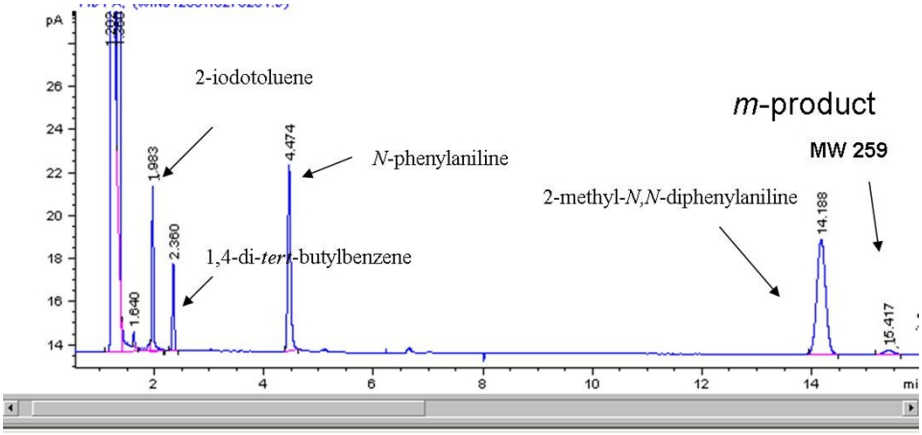
Date	2/5/2013 12:41:24 PM
Sample	2
Sample Info	
Barcode	
Operator	kyo
Method	WIN220.M

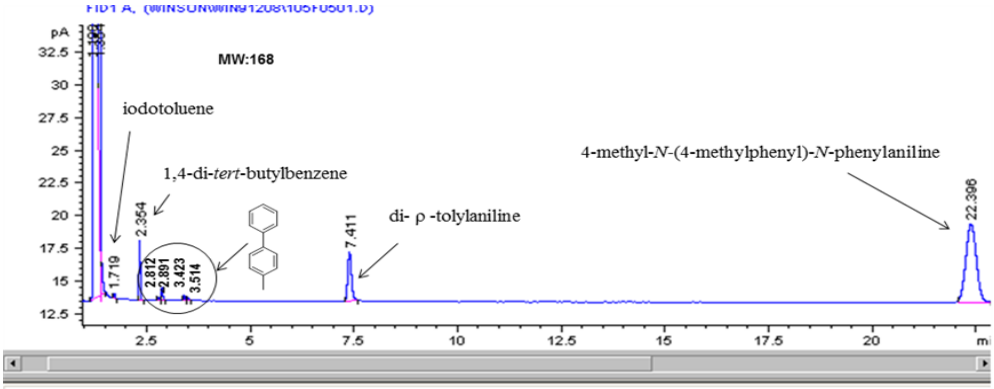
#	Time	Area	Height	Width	Area%	Symmetry
1	1.147	399175.1	146020.1	0.0341	91.009	9.74E-2
2	1.321	32542.8	12413	0.0437	7.420	2.08
3	1.446	21.7	15.1	0.0208	0.005	2.703
4	1.492	112.3	44.4	0.036	0.026	1.775
5	1.765	76.4	37.2	0.0307	0.017	1.331
6	1.848	3524.8	1473.7	0.0402	0.804	1.421
7	1.918	546.8	227.1	0.0398	0.125	1.39
8	2.285	255.9	92.8	0.0437	0.058	1.107
9	4.328	1065.1	312.6	0.0527	0.243	1.029
10	16.438	1290	103.2	0.1603	0.294	1.052

Reaction between N-phenylaniline and 2-iodotoluene with tBuOK:



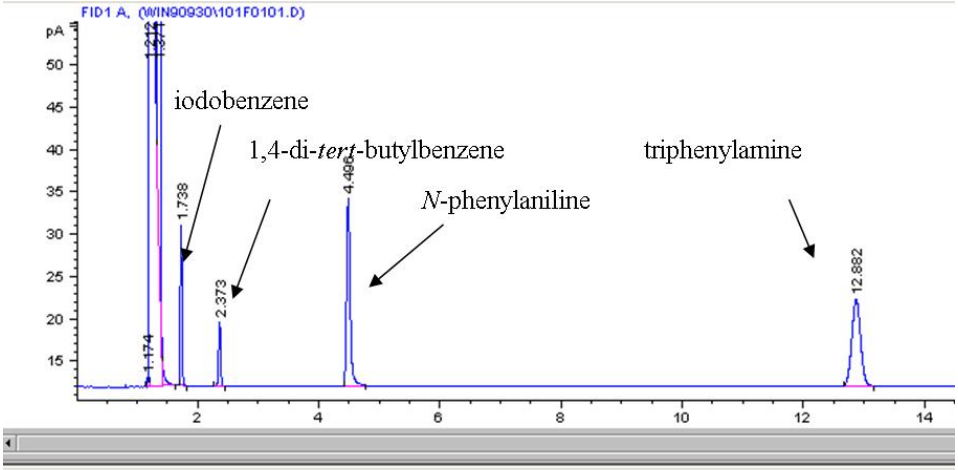
#	Time	Area	Height	Width	Area%	Symmetry
1	1.202	316629.8	159270.5	0.0312	99.423	0
2	1.36	1711.6	843.5	0.0337	0.537	1.094
3	1.64	1.5	7.4E-1	0.0319	0.000	1.136
4	1.983	18.2	7.7	0.0397	0.006	1.046
5	2.36	9.4	4	0.0371	0.003	1.056
6	4.474	33.1	8.7	0.0586	0.010	0.852
7	14.188	59.5	5.3	0.1556	0.019	0.96
8	15.417	3.2	2.4E-1	0.2251	0.001	0.919

Reaction between Di-ρ-tolylaniline and Iodobenzene with tBuOK:



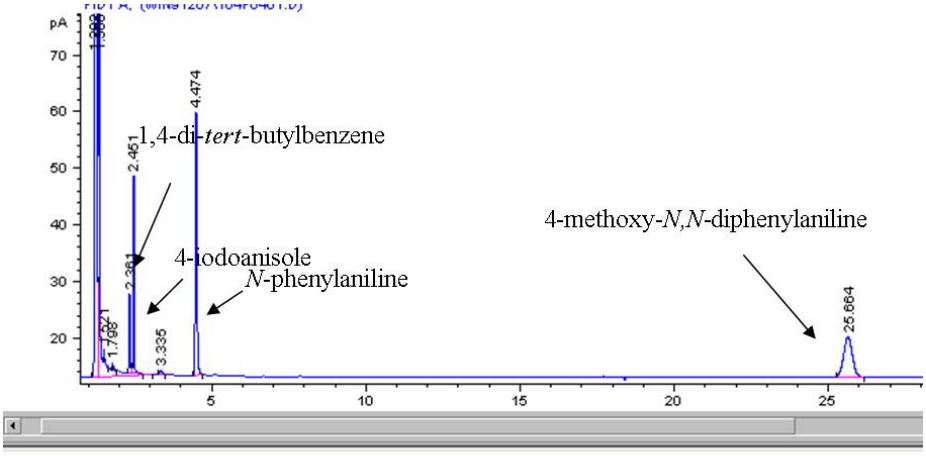
#	Time	Area	Height	Width	Area%	Symmetry
1	1.198	310437	164861.1	0.0295	99.345	0.143
2	1.354	1904.7	1002.4	0.0312	0.610	0.956
3	1.719	7.1E-1	3.8E-1	0.0307	0.000	1.185
4	2.354	10.4	4.5	0.0364	0.003	1.003
5	2.812	5.5E-1	2.2E-1	0.0379	0.000	1.099
6	2.891	2.4	9.4E-1	0.0405	0.001	1.037
7	3.423	1.1	3.8E-1	0.0461	0.000	0.835
8	3.514	6.4E-1	2.2E-1	0.0411	0.000	0.912
9	7.411	23.3	3.7	0.0915	0.007	0.815
10	22.396	104.1	6	0.2105	0.033	0.882

Reaction between N-phenylaniline and Iodobenzene with tBuONa:



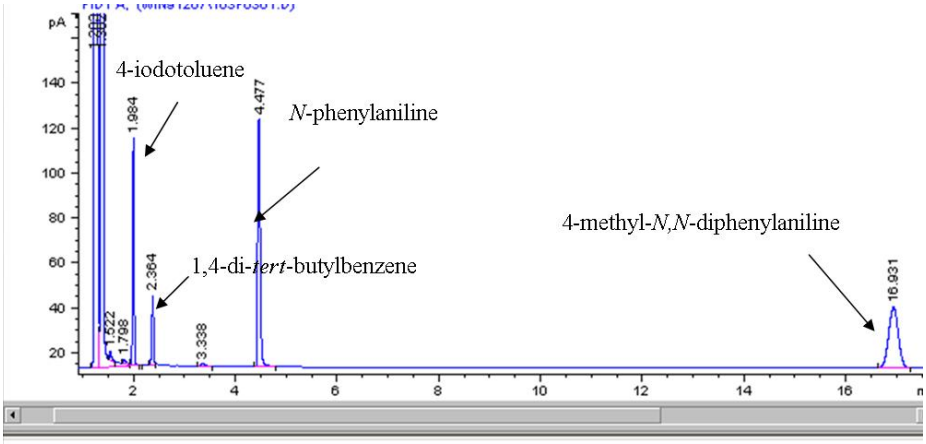
#	Time	Area	Height	Width	Area%	Symmetry
1	1.174	1.9	1.1	0.0264	0.001	0.64
2	1.212	297747.6	152347.3	0.0313	98.949	0.138
3	1.371	2909.2	1415.9	0.0345	0.967	1.164
4	1.738	38.8	19	0.0329	0.013	1.057
5	2.373	18	7.5	0.0369	0.006	1.044
6	4.496	91.7	22.2	0.0632	0.030	0.773
7	12.882	102.5	10.2	0.139	0.034	0.995

Reaction between N-phenylaniline and 4-iodoanisole with tBuONa:



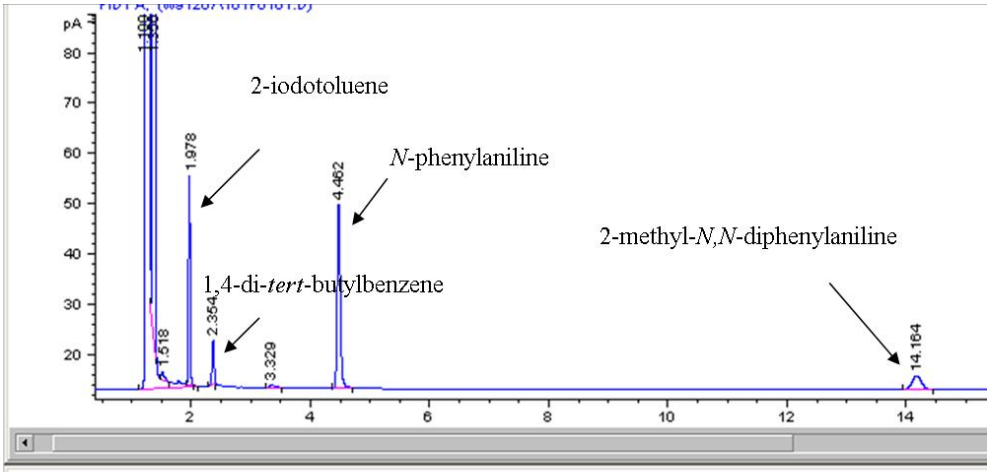
#	Time	Area	Height	Width	Area%	Symmetry
1	1.202	310899.6	158833.8	0.0313	98.012	0.133
2	1.36	5858.7	2819.5	0.0342	1.847	1.084
3	1.521	6.4	2.5	0.0371	0.002	0.427
4	1.798	4.8	1.3	0.0498	0.002	0.403
5	2.361	35.8	14	0.0399	0.011	1.128
6	2.451	84	34.9	0.0376	0.026	0.964
7	3.335	4	6.9E-1	0.0695	0.001	0.601
8	4.474	172.8	46.5	0.0573	0.054	0.902
9	25.664	140.3	7.1	0.2417	0.044	1.019

C-N Coupling Reaction between N-phenylaniline and 4-iodotoluene with tBuONa:



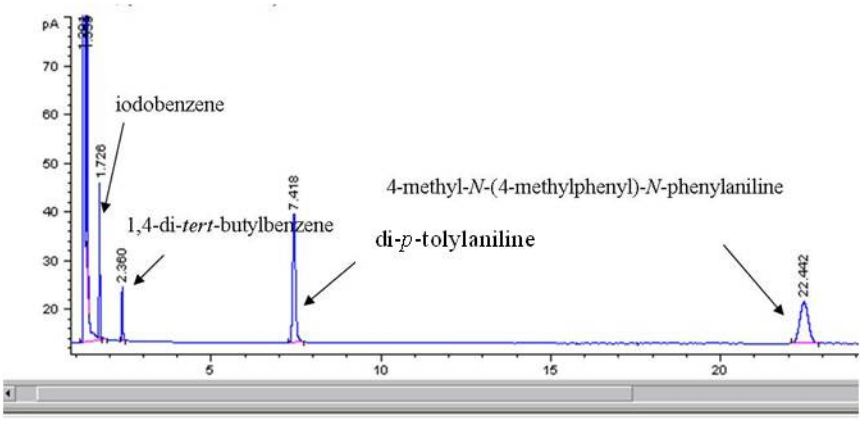
#	Time	Area	Height	Width	Area%	Symmetry
1	1.203	307612.5	158231.6	0.0307	95.503	0.143
2	1.362	13411.8	6657.8	0.0335	4.164	1.146
3	1.522	11.8	4.2	0.0396	0.004	0.365
4	1.798	7.2	2	0.0493	0.002	0.416
5	1.984	207	100.7	0.033	0.064	1.135
6	2.364	77.2	31.1	0.0414	0.024	1.073
7	3.338	7.6	1.2	0.0886	0.002	0.575
8	4.477	404.2	110.6	0.0561	0.125	0.919
9	16.931	356.3	27.2	0.1808	0.111	1.033

Reaction between N-phenylaniline and 2-iodotoluene with tBuONa:



#	Time	Area	Height	Width	Area%	Symmetry
1	1.199	307046.3	161178.6	0.0297	98.784	0.149
2	1.356	3496.9	1811.6	0.032	1.125	1.021
3	1.518	5.2	1.6	0.0444	0.002	0.35
4	1.978	85.2	41.6	0.0324	0.027	1.021
5	2.354	21.8	8.9	0.041	0.007	1.096
6	3.329	3.9	5.8E-1	0.0868	0.001	0.537
7	4.462	135.6	36.5	0.0568	0.044	0.852
8	14.164	30.6	2.8	0.1449	0.010	0.951

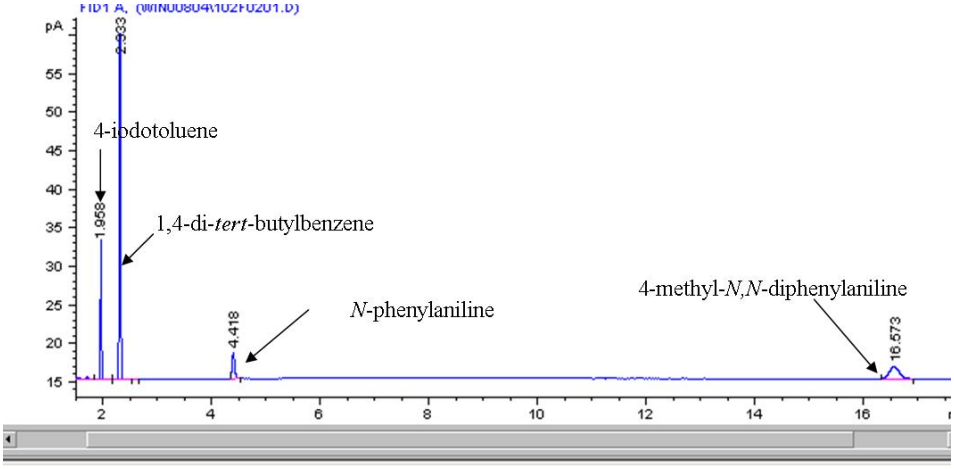
Reaction between Di-ρ-tolylaniline and Iodobenzene with tBuONa:



#	Time	Area	Height	Width	Area%	Symmetry
1	1.201	310717.5	163599.4	0.0307	98.349	0.145
2	1.359	4820.5	2439.8	0.0331	1.526	1.115
3	1.726	61.8	31.7	0.0317	0.020	1.066
4	2.36	26.3	10.9	0.037	0.008	1.012
5	7.418	158	26.4	0.0903	0.050	0.866
6	22.442	149.8	8.5	0.2158	0.047	0.988

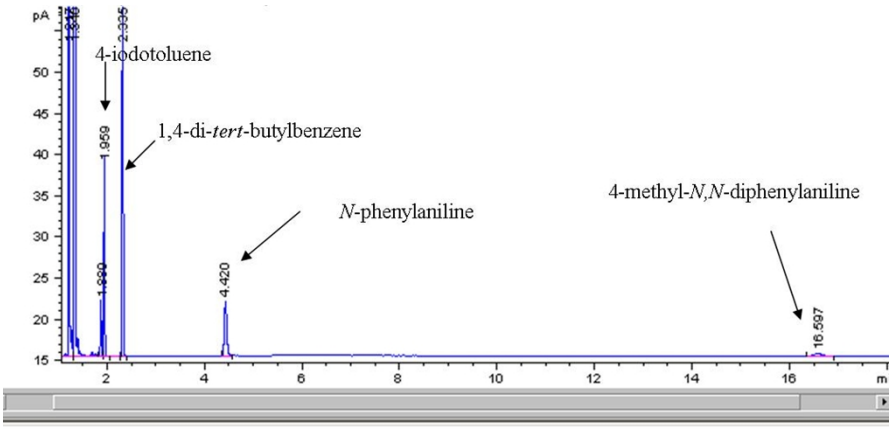
Stoichiometric reaction between complex 1 and 4-iodotoluene.

Without TEMPO:



#	Time	Area	Height	Width	Area%	Symmetry
1	1.216	31134.7	32907.8	0.017	90.398	0.869
2	1.345	3169.4	3356.1	0.0157	9.202	0.991
3	1.958	24.4	17.5	0.0223	0.071	0.944
4	2.333	82	43.9	0.0298	0.238	0.968
5	4.418	11.4	3.3	0.0543	0.033	0.882
6	16.573	19.9	1.6	0.1909	0.058	0.967

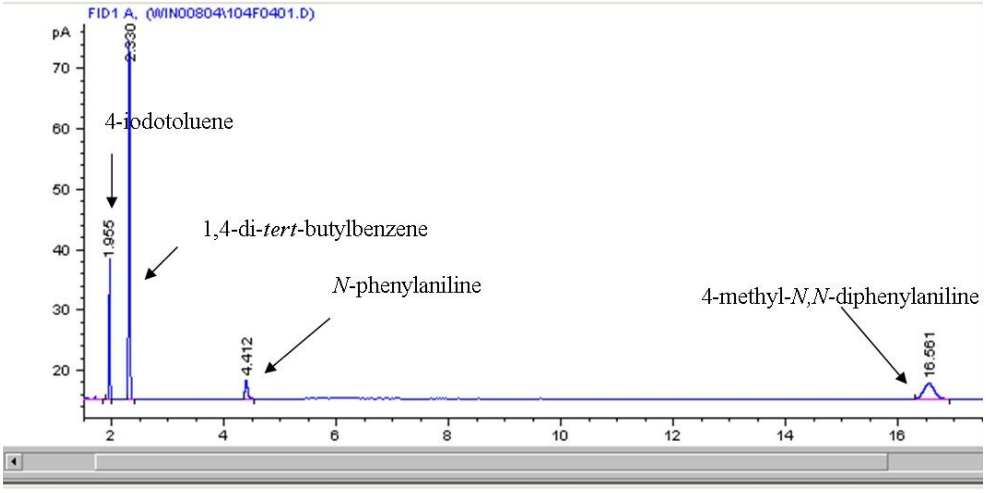
With TEMPO:



#	Time	Area	Height	Width	Area%	Symmetry
1	1.217	30240.3	33453.2	0.0165	86.295	0.878
2	1.346	4646.6	4817.7	0.0161	13.260	1.01
3	1.889	9.9	6.6	0.0236	0.028	1.018
4	1.959	32.5	23.3	0.0243	0.093	0.948
5	2.335	86	46.3	0.0297	0.245	0.972
6	4.42	22.6	6.6	0.052	0.065	0.844
7	16.597	5	4E-1	0.1793	0.014	1.098

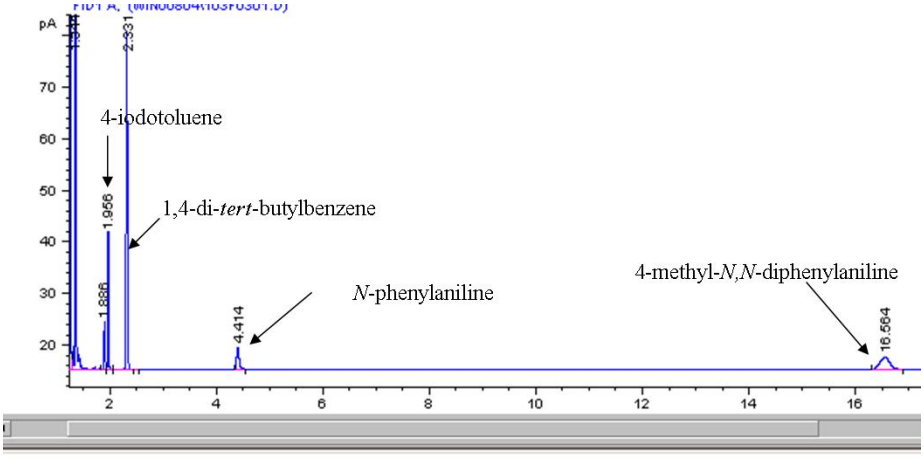
Stoichiometric reaction between complex 2 and 4-iodotoluene.

Without TEMPO:



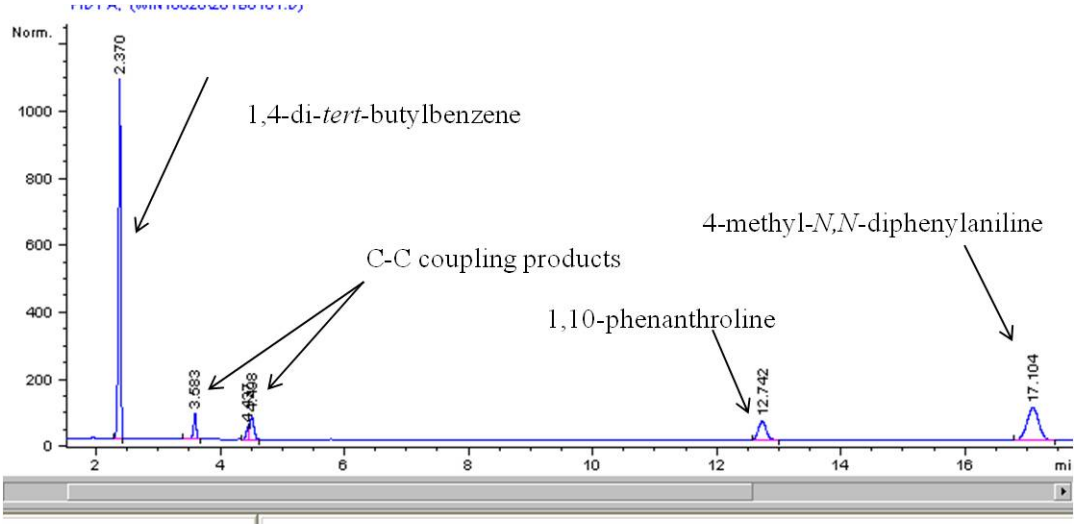
#	Time	Area	Height	Width	Area%	Symmetry
1	1.214	31330.8	28834.6	0.0167	86.596	0.818
2	1.343	4667	5137.9	0.0166	12.899	1.001
3	1.955	31	22.5	0.0221	0.086	0.967
4	2.33	108.8	58.7	0.0296	0.301	0.989
5	4.412	10.5	3	0.0541	0.029	0.872
6	16.561	32.2	2.5	0.1904	0.089	1.083

With TEMPO 100 mol% added:



#	Time	Area	Height	Width	Area%	Symmetry
1	1.215	30710.4	30981.4	0.0176	83.527	0.858
2	1.344	5843.4	6437.2	0.0166	15.893	0.973
3	1.886	13.5	8.9	0.0257	0.037	1.012
4	1.956	35.7	26.1	0.022	0.097	0.951
5	2.331	120.1	64.6	0.0297	0.327	0.957
6	4.414	14.6	4.2	0.052	0.040	0.857
7	16.564	29.3	2.3	0.1743	0.080	0.968

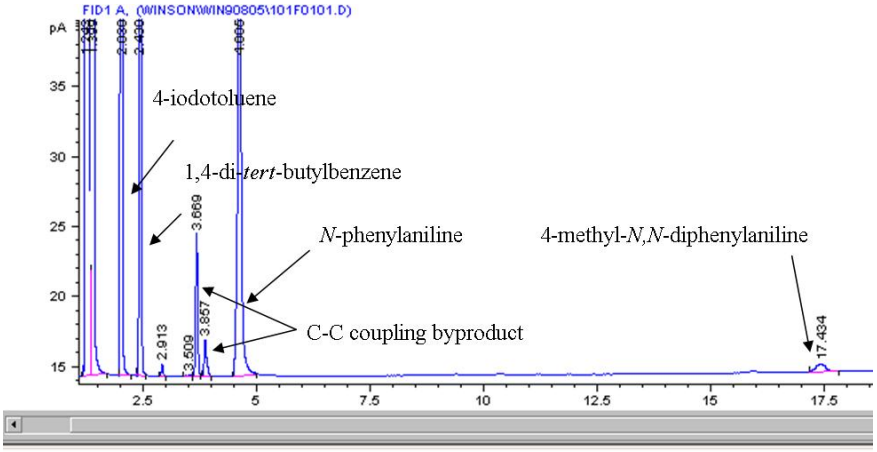
Stoichiometric reaction between complex 1 and 4-iodotoluene plus additional *t*BuOK.



#	Time	Area	Height	Width	Area%	Symmetry
1	1.116	6.8E-1	9.7E-1	0.0104	0.000	0.691
2	1.166	539691.6	143139.3	0.0652	82.355	0.162
3	1.356	110559	38589.7	0.0429	16.871	1.802
4	2.37	2700.9	1073.5	0.0381	0.412	1.292
5	3.583	230.5	75.4	0.0472	0.035	1.178
6	4.437	108.3	36.4	0.0457	0.017	1.971
7	4.498	296.2	69.6	0.0626	0.045	0.768
8	12.742	472.5	56	0.1175	0.072	0.869
9	17.104	1263.7	95.7	0.1591	0.193	0.926

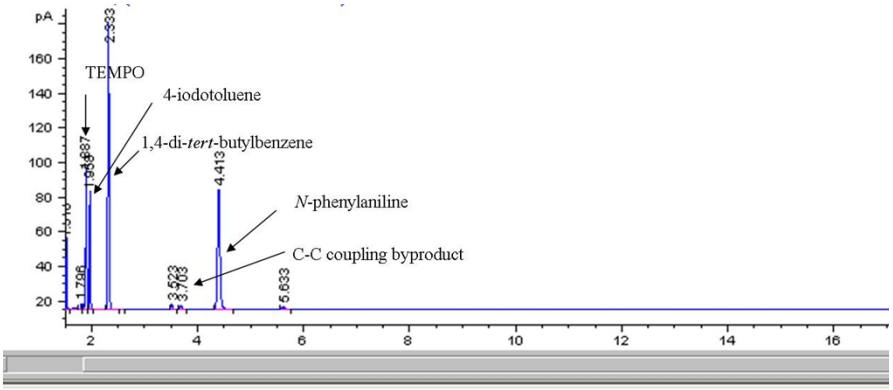
Stoichiometric reaction between (phen)KNPh$_2$ and 4-iodotoluene.

Without TEMPO:



#	Time	Area	Height	Width	Area%	Symmetry
1	1.243	290390.3	125312	0.035	93.791	0.415
2	1.399	18097.3	8176	0.0369	5.845	1.102
3	2.039	582.3	274	0.0328	0.188	1.02
4	2.43	275.3	116.4	0.0376	0.089	1.014
5	2.913	2.2	8.2E-1	0.043	0.001	1.002
6	3.509	5.7E-1	1.2E-1	0.0713	0.000	1.165
7	3.669	31.2	10.1	0.048	0.010	0.968
8	3.857	10.1	2.6	0.058	0.003	0.702
9	4.605	215.8	45.5	0.0714	0.070	0.834
10	17.434	8	5.6E-1	0.1788	0.003	1.093

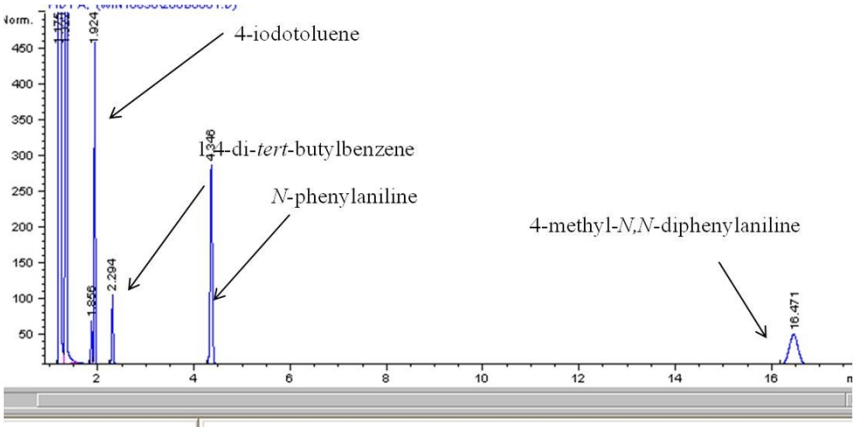
With TEMPO:



#	Time	Area	Height	Width	Area%	Symmetry
3	1.409	7.9	5.9	0.0215	0.018	0.777
4	1.518	43.8	39.4	0.019	0.103	0.939
5	1.796	4.3	3.1	0.0221	0.010	1.001
6	1.887	119.6	78.3	0.0258	0.280	1.049
7	1.958	91.6	66.8	0.022	0.215	0.955
8	2.333	307	163.6	0.0299	0.719	0.942
9	3.523	7.9	3	0.0404	0.018	0.993
10	3.703	6.7	2.4	0.0421	0.016	0.956
11	4.413	234.2	69	0.0516	0.549	0.903
12	5.633	6.6	1.5	0.0703	0.015	0.993

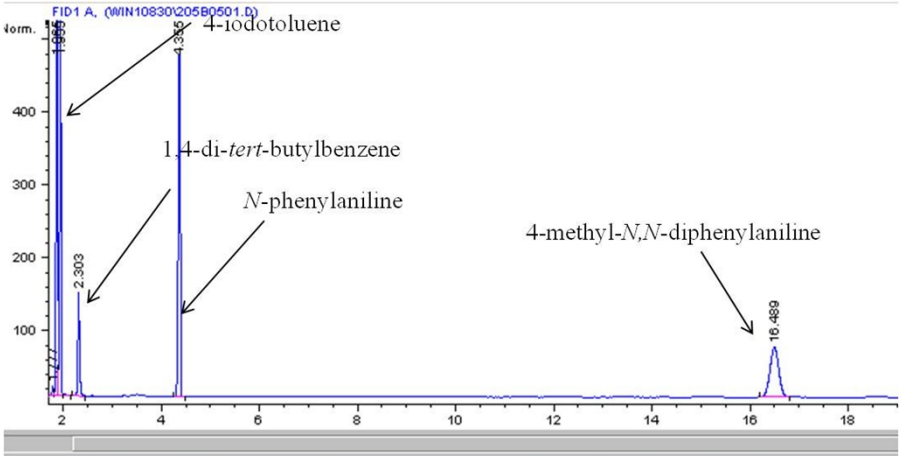
Copper catalyzed C-N cross coupling reaction based on CuI/*t*BuOK.

Without TEMPO:



#	Time	Area	Height	Width	Area%	Symmetry
1	1.175	130806.4	85064	0.0244	77.010	0.174
2	1.322	36652.9	24478.7	0.0242	21.579	1.039
3	1.856	98.3	59	0.0259	0.058	1.07
4	1.924	723	448.5	0.0256	0.426	1.076
5	2.294	189.7	95.8	0.0309	0.112	1.02
6	4.346	863.8	277.7	0.0483	0.509	1.028
7	16.471	522.5	42	0.1557	0.308	0.944

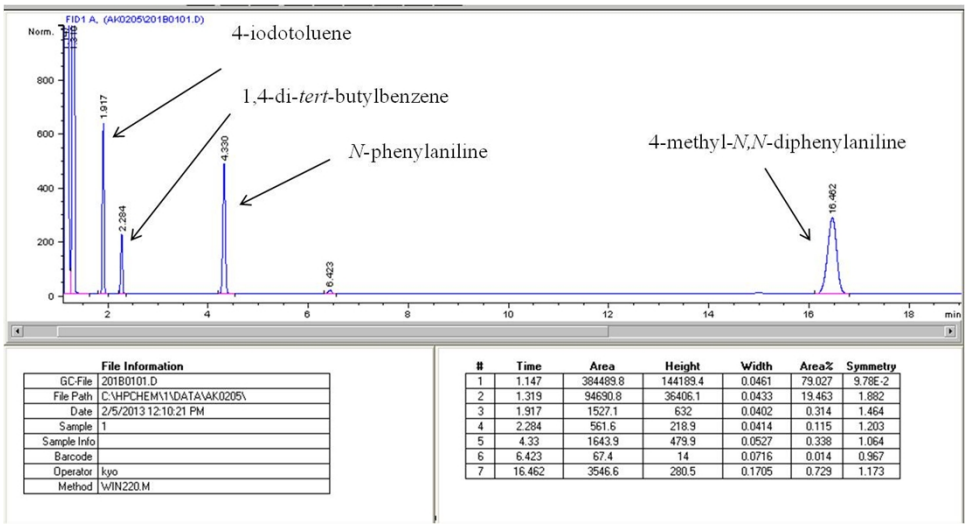
With 200 mol % TEMPO:



#	Time	Area	Height	Width	Area%	Symmetry
1	1.171	204773.1	98992.8	0.0346	79.486	0.131
2	1.331	46056.3	24449.9	0.0315	17.878	1.569
3	1.777	25.9	12.5	0.03	0.010	1.48
4	1.865	3144.6	1736.3	0.0279	1.221	1.198
5	1.933	974.4	549.8	0.0272	0.378	1.217
6	2.303	332.1	140.5	0.0356	0.129	0.903
7	4.355	1467.3	472	0.0488	0.570	1.014
8	16.489	847.7	67.9	0.1537	0.329	1.118

Copper catalyzed C-N cross coupling reaction based on CuI/Phen/*t*BuOK.

Without TEMPO:



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Date	2/5/2013 12:10:21 PM
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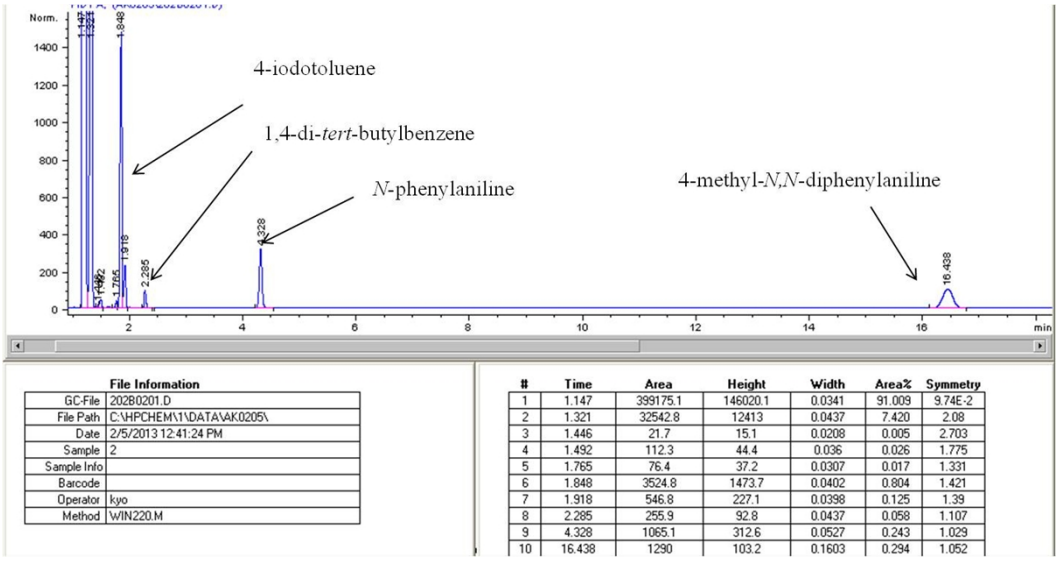
Sample Info	
Barcode	
Operator	kyo
Method	WIN220.M

#	Time	Area	Height	Width	Area%	Symmetry
1	1.147	384489.8	144189.4	0.0461	79.027	9.78E-2
2	1.319	94690.8	36406.1	0.0433	19.463	1.882
3	1.917	1527.1	632	0.0402	0.314	1.464
4	2.284	561.6	218.9	0.0414	0.115	1.203
5	4.33	1643.9	479.9	0.0527	0.338	1.064
6	6.423	67.4	14	0.0716	0.014	0.967
7	16.462	3546.6	280.5	0.1705	0.729	1.173

With TEMPO:



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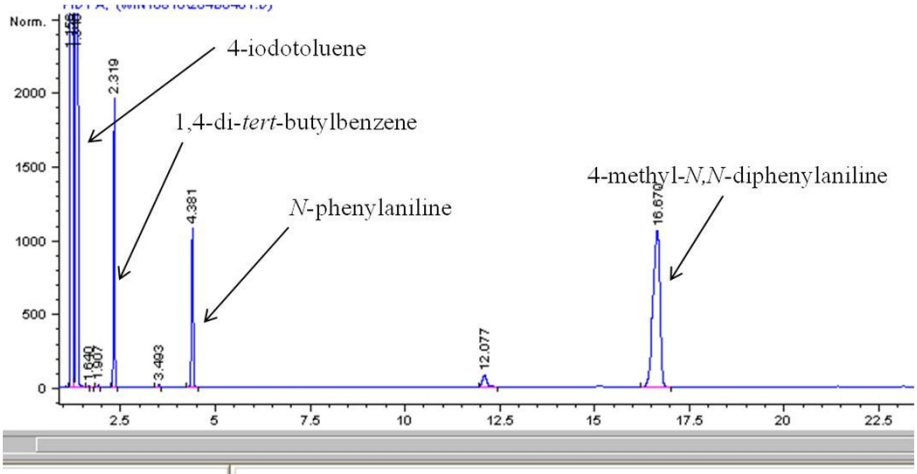
Sample	2
Sample Info	
Barcode	
Operator	kyo
Method	WIN220.M

#	Time	Area	Height	Width	Area%	Symmetry
1	1.147	399175.1	146020.1	0.0341	91.009	9.74E-2
2	1.321	32542.8	12413	0.0437	7.420	2.08
3	1.446	21.7	15.1	0.0208	0.005	2.703
4	1.492	112.3	44.4	0.036	0.026	1.775
5	1.765	76.4	37.2	0.0307	0.017	1.331
6	1.848	3524.8	1473.7	0.0402	0.804	1.421
7	1.918	546.8	227.1	0.0398	0.125	1.39
8	2.285	255.9	92.8	0.0437	0.058	1.107
9	4.328	1065.1	312.6	0.0527	0.243	1.029
10	16.438	1290	103.2	0.1603	0.294	1.052

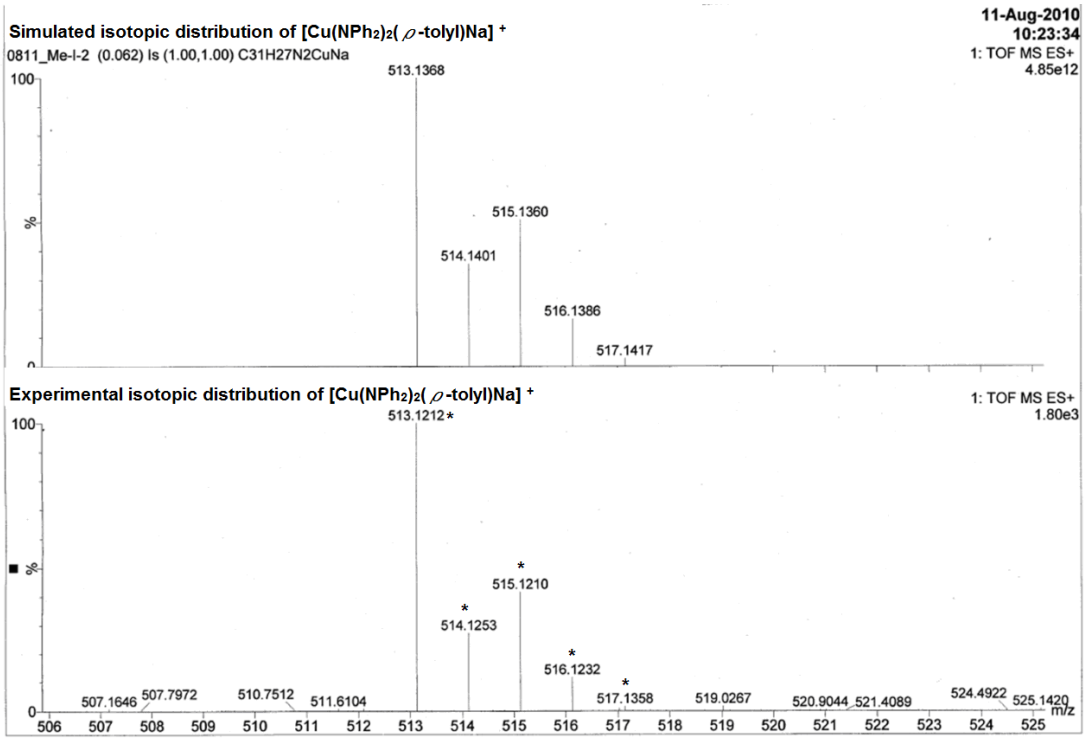
Copper catalyzed C-N cross coupling reaction based on 1.

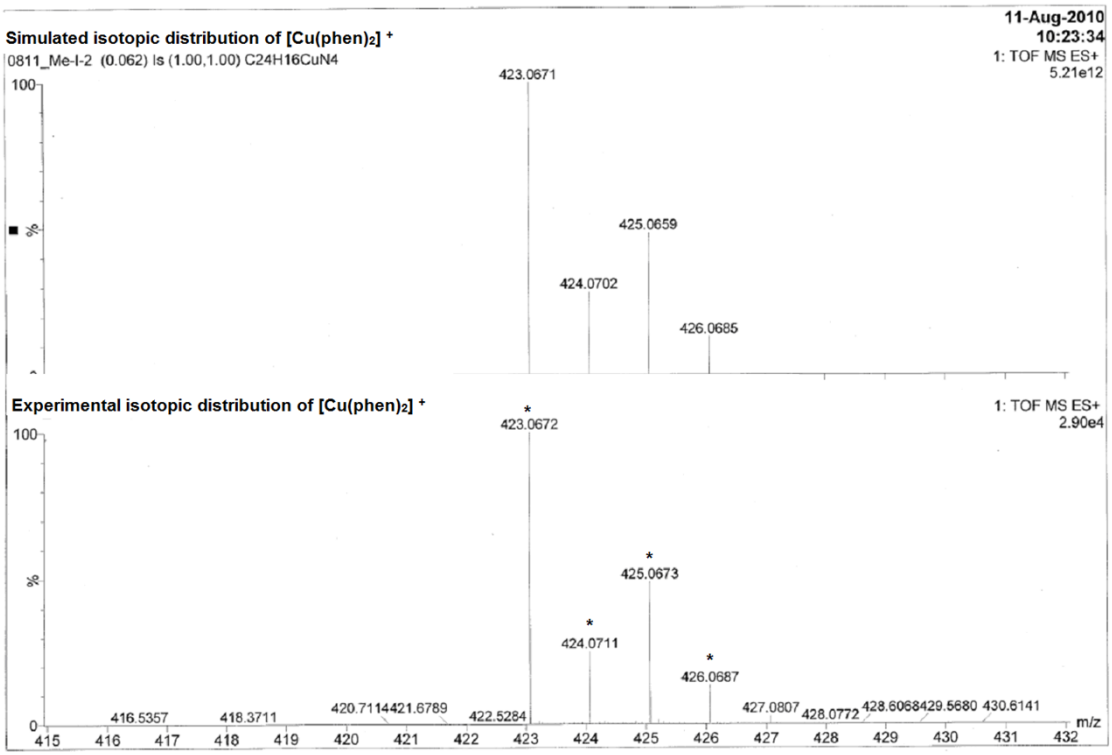


10 mol%

#	Time	Area	Height	Width	Area%	Symmetry
1	1.156	453786.7	137516	0.0575	68.907	9.47E-2
2	1.34	182051	84298.1	0.0304	27.644	1.783
3	1.64	14.4	9.5	0.0224	0.002	1.309
4	1.907	36.3	17.5	0.0302	0.006	1.698
5	2.319	4233	1958.6	0.033	0.643	1.234
6	3.493	40.7	14.5	0.0433	0.006	1.151
7	4.381	3445.7	1076.8	0.0493	0.523	1.104
8	12.077	643.4	78.1	0.1182	0.098	0.747
9	16.67	14301	1055.3	0.1876	2.172	1.606

In situ ESI-MS isotopic patterns and simulated patterns of Intermediates




Simulated isotopic distribution of [Cu(phen)2] +
0811_Me-I-2 (0.062) Is (1.00,1.00) C24H16CuN4
11-Aug-2010
10:23:34
1: TOF MS ES+
5.21e12
423.0671
425.0659
424.0702
426.0685
Experimental isotopic distribution of [Cu(phen)2] +
1: TOF MS ES+
2.90e4
423.0672
425.0673
424.0711
426.0687
416.5357
418.3711
420.7114
421.6789
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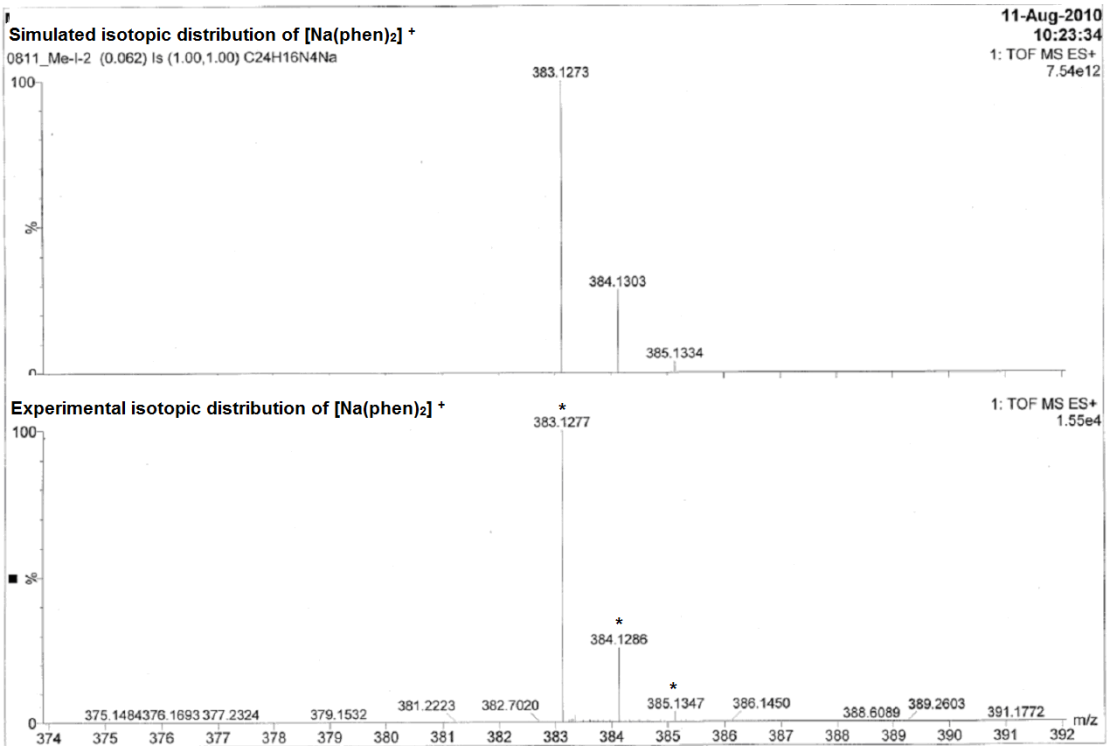
428.0772
428.6068
429.5680
430.6141
m/z


Simulated isotopic distribution of [Na(phen)2] +
0811_Me-I-2 (0.062) Is (1.00,1.00) C24H16N4Na
11-Aug-2010
10:23:34
1: TOF MS ES+
7.54e12
383.1273
384.1303
385.1334
Experimental isotopic distribution of [Na(phen)2] +
1: TOF MS ES+
1.55e4
383.1277
384.1286
385.1347
375.1484
376.1693
377.2324
379.1532
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388.6089
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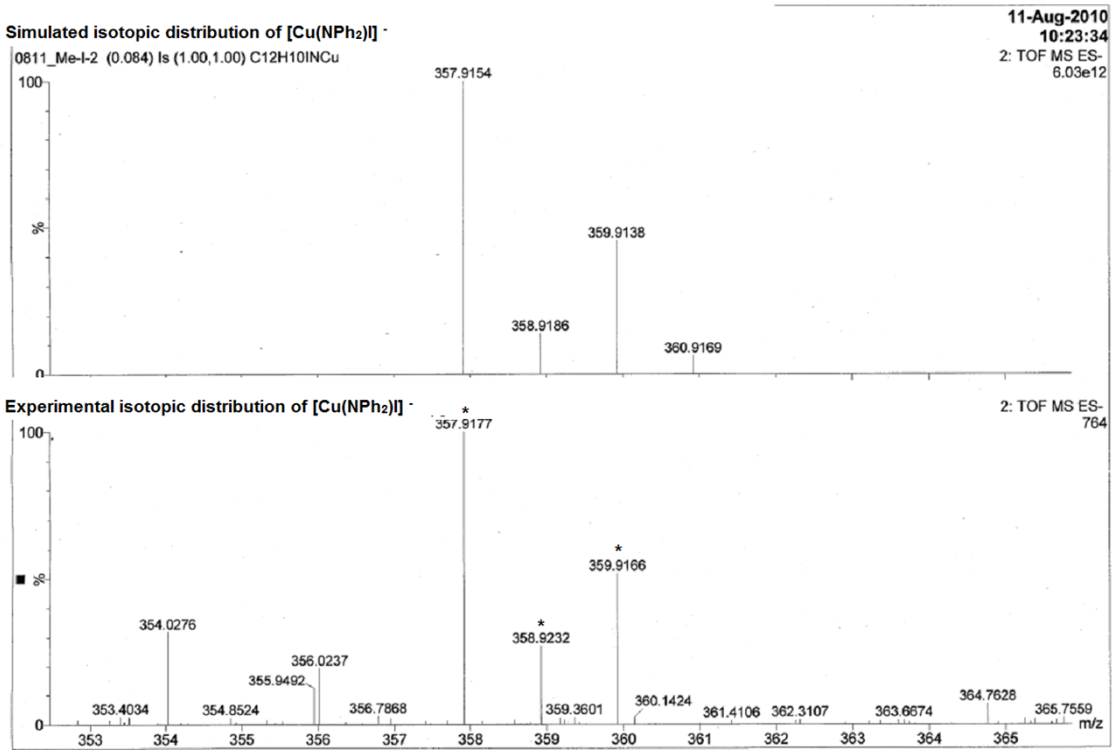
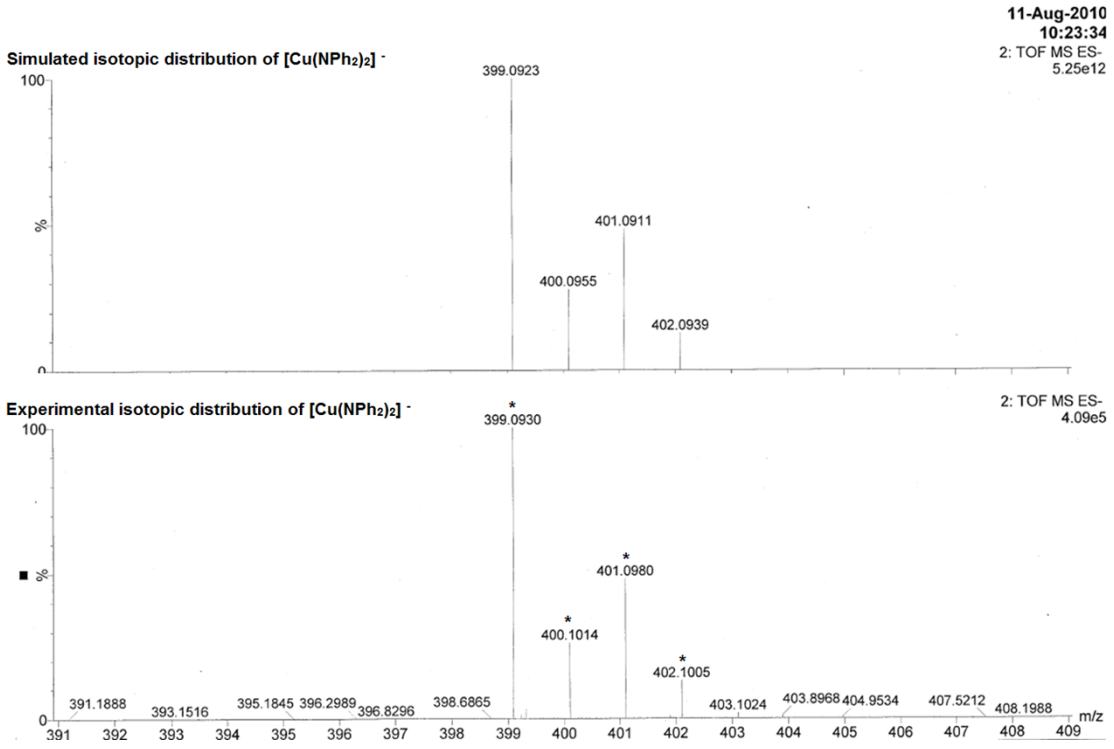
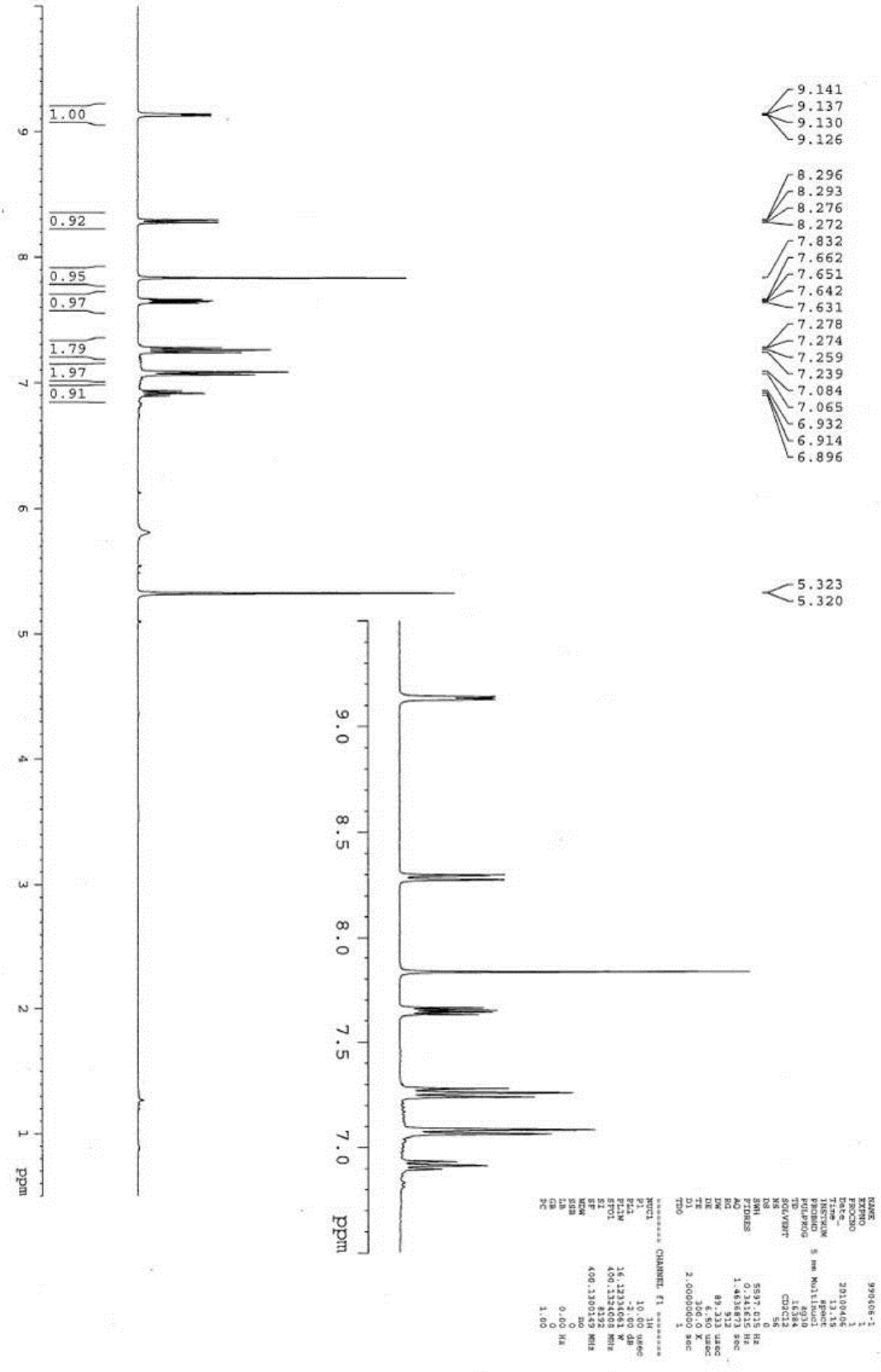
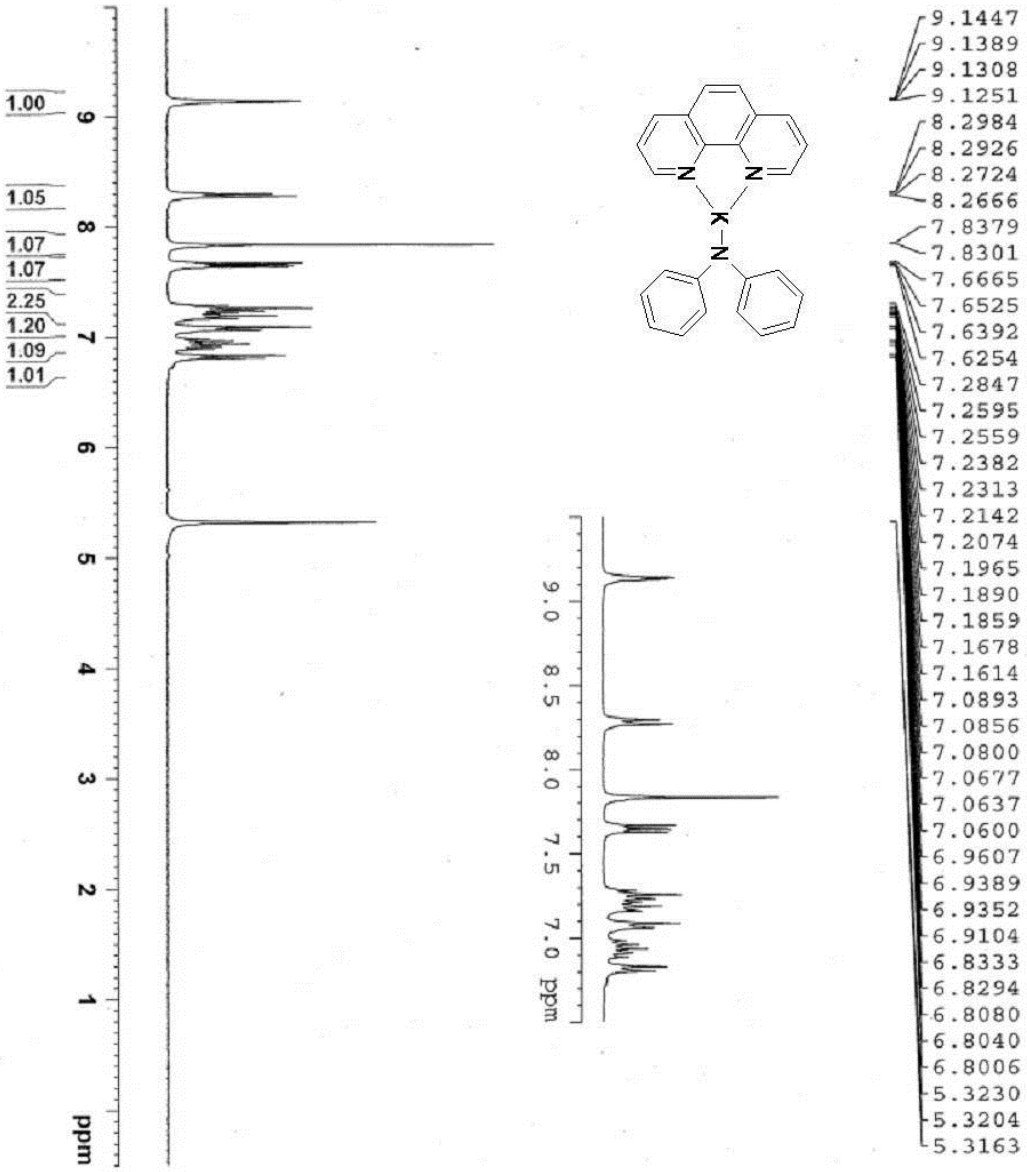

Simulated isotopic distribution of [Cu(NPh2)I] -
11-Aug-2010
10:23:34
0811_Me-I-2 (0.084) Is (1.00,1.00) C12H10INCu
2: TOF MS ES-
6.03e12
357.9154
359.9138
358.9186
360.9169
Experimental isotopic distribution of [Cu(NPh2)I] -
2: TOF MS ES-
764
357.9177
359.9166
354.0276
358.9232
356.0237
355.9492
353.4034
354.8524
356.7868
359.3601
360.1424
361.4106
362.3107
363.6674
364.7628
365.7559
m/z


11-Aug-2010
10:23:34
Simulated isotopic distribution of [Cu(NPh2)2] -
2: TOF MS ES-
5.25e12
399.0923
401.0911
400.0955
402.0939
Experimental isotopic distribution of [Cu(NPh2)2] -
2: TOF MS ES-
4.09e5
399.0930
401.0980
400.1014
402.1005
391.1888
393.1516
395.1845
396.2989
396.8296
398.6865
403.1024
403.8968
404.9534
407.5212
408.1988
m/z

^{1}H NMR Spectrum of 1


9.141
9.137
9.130
9.126
8.296
8.293
8.276
8.272
7.832
7.662
7.651
7.642
7.631
7.278
7.274
7.259
7.239
7.084
7.065
6.932
6.914
6.896
5.323
5.320
1.00
0.92
0.95
0.97
1.79
1.97
0.91
ppm

^{1}H NMR Spectrum of (phen)KNPh$_2$

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PROCNO                                       1
Date_                             20100721
Time                                   14.33
INSTRUM                                 spect
PROBHD                  5 mm QNP 1H/13    2930
PULPROG                                 zg30
TD                                      16384
SOLVENT                                 CD2Cl2
NS                                          64
DS                                           0
SWH                                   4807.692 Hz
FIDRES                                0.293438 Hz
AQ                                    1.7039860 sec
RG                                        1290
DW                                     104.000 usec
DE                                       6.50 usec
TE                                      300.0 K
D1                                    2.00000000 sec
TD0                                          1

======== CHANNEL f1 ========
NUC1                                      1H
P1                                      9.10 usec
PL1                                    -4.00 dB
PL1W                                26.37401772 W
SFO1                                300.1319508 MHz
SI                                       8192
SF                                  300.1300106 MHz
WDW                                        no
SSB                                         0
LB                                       0.00 Hz
GB                                          0
PC                                       1.00
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Crystal Data for Compound $[K_3(phen)_8][Cu(NPh)_2]_3$

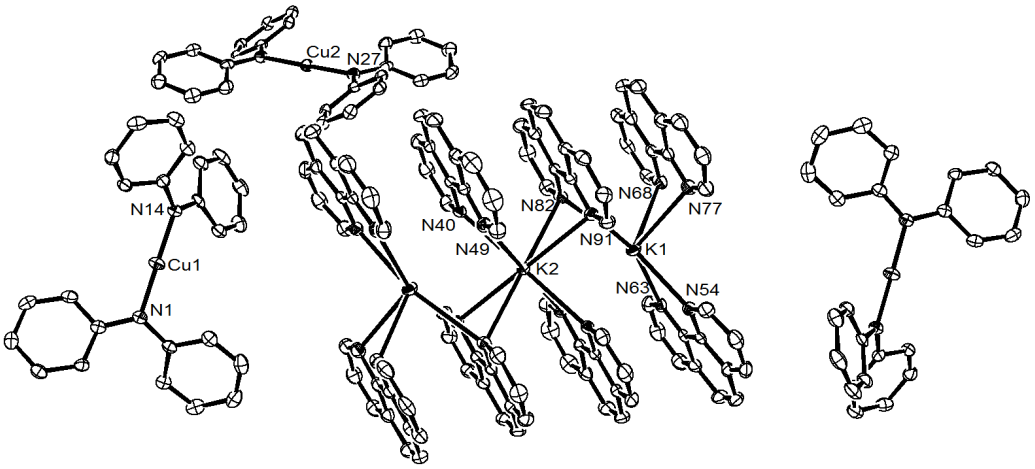

Table 1. Crystal data and structure refinement for i11702.

Identification code	i11702	
Empirical formula	C168 H124 Cu3 K3 N22	
Formula weight	2758.81	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 14.0666(3) Å	α= 90°.
	b = 17.4108(4) Å	β= 93.7670(10)°.
	c = 26.8525(7) Å	γ = 90°.
Volume	6562.3(3) $Å^3$	
Z	2	
Density (calculated)	1.396 Mg/m^3	
Absorption coefficient	0.644 mm^{-1}	
F(000)	2860	
Crystal size	0.28 x 0.24 x 0.2 mm^3	
Theta range for data collection	1.39 to 25.03°.	

Index ranges	-12<=h<=16, -19<=k<=20, -27<=l<=31
Reflections collected	47735
Independent reflections	11597 [R(int) = 0.0545]
Completeness to theta = 25.03°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.7011
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11597 / 0 / 886
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.0943
R indices (all data)	R1 = 0.0683, wR2 = 0.1182
Largest diff. peak and hole	0.367 and -0.445 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for i11702. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	6901(1)	468(1)	2541(1)	23(1)
Cu(2)	0	0	0	21(1)
K(1)	-2673(1)	-26(1)	5328(1)	23(1)
K(2)	0	0	5000	21(1)
N(1)	7703(2)	1181(1)	2873(1)	21(1)
N(14)	6082(2)	-242(1)	2218(1)	21(1)
N(27)	-708(2)	-128(1)	562(1)	21(1)
N(40)	619(2)	-602(1)	4073(1)	21(1)
N(49)	1149(2)	-1359(1)	4949(1)	22(1)
N(54)	-2931(2)	434(1)	6320(1)	22(1)
N(63)	-3418(2)	1403(1)	5530(1)	21(1)
N(68)	-4262(2)	-571(1)	4695(1)	27(1)
N(77)	-3747(2)	-1438(1)	5522(1)	27(1)
N(82)	-1783(2)	-604(1)	4409(1)	21(1)
N(91)	-1312(2)	-1273(1)	5313(1)	20(1)
C(2)	7283(2)	1692(2)	3192(1)	19(1)
C(3)	6519(2)	1433(2)	3456(1)	25(1)
C(4)	6002(2)	1920(2)	3739(1)	31(1)
C(5)	6228(2)	2688(2)	3778(1)	30(1)
C(6)	6985(2)	2958(2)	3525(1)	28(1)
C(7)	7508(2)	2473(2)	3239(1)	22(1)
C(8)	8641(2)	1262(2)	2751(1)	18(1)
C(9)	8919(2)	918(2)	2312(1)	22(1)
C(10)	9839(2)	938(2)	2170(1)	26(1)
C(11)	10544(2)	1314(2)	2463(1)	27(1)
C(12)	10294(2)	1653(2)	2899(1)	23(1)
C(13)	9369(2)	1632(2)	3046(1)	21(1)
C(15)	6346(2)	-1009(2)	2203(1)	21(1)
C(16)	7317(2)	-1205(2)	2209(1)	24(1)

C(17)	7621(2)	-1956(2)	2226(1)	26(1)
C(18)	6976(2)	-2554(2)	2228(1)	29(1)
C(19)	6013(2)	-2378(2)	2217(1)	28(1)
C(20)	5708(2)	-1627(2)	2207(1)	25(1)
C(21)	5227(2)	12(2)	1991(1)	21(1)
C(22)	4843(2)	712(2)	2140(1)	24(1)
C(23)	4045(2)	1033(2)	1899(1)	30(1)
C(24)	3569(2)	653(2)	1503(1)	31(1)
C(25)	3920(2)	-41(2)	1353(1)	31(1)
C(26)	4730(2)	-359(2)	1588(1)	26(1)
C(28)	-204(2)	-356(2)	1004(1)	20(1)
C(29)	736(2)	-95(2)	1102(1)	23(1)
C(30)	1294(2)	-341(2)	1512(1)	26(1)
C(31)	944(2)	-850(2)	1849(1)	24(1)
C(32)	22(2)	-1111(2)	1763(1)	22(1)
C(33)	-543(2)	-875(2)	1352(1)	20(1)
C(34)	-1700(2)	-67(2)	549(1)	20(1)
C(35)	-2228(2)	39(2)	970(1)	23(1)
C(36)	-3205(2)	109(2)	936(1)	26(1)
C(37)	-3715(2)	81(2)	477(1)	29(1)
C(38)	-3212(2)	0(2)	56(1)	29(1)
C(39)	-2237(2)	-76(2)	90(1)	26(1)
C(41)	368(2)	-258(2)	3642(1)	27(1)
C(42)	392(2)	-606(2)	3174(1)	32(1)
C(43)	672(2)	-1353(2)	3155(1)	30(1)
C(44)	1204(2)	-2540(2)	3593(1)	29(1)
C(45)	1422(2)	-2916(2)	4020(1)	33(1)
C(46)	1607(2)	-2924(2)	4947(1)	36(1)
C(47)	1586(2)	-2526(2)	5383(1)	37(1)
C(48)	1365(2)	-1749(2)	5365(1)	30(1)
C(50)	897(2)	-1352(2)	4051(1)	18(1)
C(51)	928(2)	-1752(2)	3596(1)	23(1)
C(52)	1155(2)	-1753(2)	4511(1)	19(1)
C(53)	1396(2)	-2540(2)	4488(1)	26(1)
C(55)	-2758(2)	-30(2)	6704(1)	27(1)

C(56)	-2878(2)	166(2)	7199(1)	33(1)
C(57)	-3165(2)	892(2)	7302(1)	32(1)
C(58)	-3622(2)	2200(2)	6993(1)	33(1)
C(59)	-3817(2)	2676(2)	6608(1)	33(1)
C(60)	-4009(2)	2905(2)	5697(1)	33(1)
C(61)	-3969(2)	2629(2)	5224(1)	34(1)
C(62)	-3671(2)	1876(2)	5161(1)	27(1)
C(64)	-3230(2)	1160(2)	6419(1)	21(1)
C(65)	-3336(2)	1421(2)	6910(1)	24(1)
C(66)	-3467(2)	1672(2)	6003(1)	19(1)
C(67)	-3763(2)	2428(2)	6105(1)	26(1)
C(69)	-4564(2)	-177(2)	4294(1)	30(1)
C(70)	-4594(2)	-468(2)	3806(1)	31(1)
C(71)	-4301(2)	-1209(2)	3736(1)	30(1)
C(72)	-3740(2)	-2448(2)	4111(1)	29(1)
C(73)	-3511(2)	-2873(2)	4517(1)	31(1)
C(74)	-3325(2)	-2999(2)	5441(1)	30(1)
C(75)	-3356(2)	-2666(2)	5897(1)	31(1)
C(76)	-3559(2)	-1882(2)	5919(1)	30(1)
C(78)	-4009(2)	-1318(2)	4628(1)	23(1)
C(79)	-4010(2)	-1658(2)	4152(1)	26(1)
C(80)	-3750(2)	-1775(2)	5068(1)	23(1)
C(81)	-3521(2)	-2557(2)	5005(1)	25(1)
C(83)	-2026(2)	-299(2)	3967(1)	26(1)
C(84)	-2017(2)	-695(2)	3516(1)	30(1)
C(85)	-1741(2)	-1447(2)	3521(1)	28(1)
C(86)	-1174(2)	-2582(2)	4015(1)	27(1)
C(87)	-939(2)	-2913(2)	4460(1)	26(1)
C(88)	-767(2)	-2820(2)	5382(1)	26(1)
C(89)	-819(2)	-2381(2)	5800(1)	27(1)
C(90)	-1094(2)	-1618(2)	5747(1)	25(1)
C(92)	-1516(2)	-1355(2)	4417(1)	18(1)
C(93)	-1478(2)	-1798(2)	3982(1)	22(1)
C(94)	-1262(2)	-1710(2)	4893(1)	19(1)
C(95)	-988(2)	-2489(2)	4912(1)	22(1)

Table 3. Bond lengths [Å] and angles [°] for i11702.

Cu(1)-N(14)	1.863(2)
Cu(1)-N(1)	1.864(2)
Cu(2)-N(27)#1	1.875(2)
Cu(2)-N(27)	1.875(2)
K(1)-N(63)	2.768(2)
K(1)-N(54)	2.830(2)
K(1)-N(68)	2.878(2)
K(1)-N(91)	2.896(2)
K(1)-N(77)	2.949(2)
K(1)-N(82)	3.011(2)
K(1)-N(49)#2	3.343(2)
K(1)-N(40)#2	3.395(2)
K(1)-C(78)	3.413(3)
K(1)-C(80)	3.451(3)
K(1)-K(2)	3.9183(6)
K(2)-N(49)	2.873(2)
K(2)-N(49)#2	2.873(2)
K(2)-N(40)#2	2.887(2)
K(2)-N(40)	2.887(2)
K(2)-N(91)	3.037(2)
K(2)-N(91)#2	3.037(2)
K(2)-N(82)	3.064(2)
K(2)-N(82)#2	3.064(2)
K(2)-C(94)	3.468(3)
K(2)-C(94)#2	3.468(3)
K(2)-C(92)	3.482(3)
K(2)-C(92)#2	3.482(3)
N(1)-C(8)	1.387(3)
N(1)-C(2)	1.393(3)
N(14)-C(21)	1.385(3)
N(14)-C(15)	1.388(3)
N(27)-C(28)	1.399(3)
N(27)-C(34)	1.399(4)
N(40)-C(41)	1.331(4)
N(40)-C(50)	1.365(3)
N(40)-K(1)#2	3.395(2)
N(49)-C(48)	1.325(4)
N(49)-C(52)	1.363(3)
N(49)-K(1)#2	3.343(2)
N(54)-C(55)	1.319(3)
N(54)-C(64)	1.363(3)
N(63)-C(62)	1.320(3)
N(63)-C(66)	1.359(3)
N(68)-C(69)	1.323(4)
N(68)-C(78)	1.363(3)
N(77)-C(76)	1.329(4)
N(77)-C(80)	1.354(4)
N(82)-C(83)	1.326(4)
N(82)-C(92)	1.360(3)
N(91)-C(90)	1.329(3)
N(91)-C(94)	1.366(3)
C(2)-C(3)	1.400(4)
C(2)-C(7)	1.401(4)
C(3)-C(4)	1.378(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.375(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.383(4)
C(5)-H(5)	0.9300
C(6)-C(7)	1.386(4)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-C(9)	1.402(4)
C(8)-C(13)	1.409(4)
C(9)-C(10)	1.373(4)

C(9)-H(9)	0.9300	C(30)-H(30)	0.9300
C(10)-C(11)	1.389(4)	C(31)-C(32)	1.379(4)
C(10)-H(10)	0.9300	C(31)-H(31)	0.9300
C(11)-C(12)	1.379(4)	C(32)-C(33)	1.381(4)
C(11)-H(11)	0.9300	C(32)-H(32)	0.9300
C(12)-C(13)	1.383(4)	C(33)-H(33)	0.9300
C(12)-H(12)	0.9300	C(34)-C(35)	1.403(4)
C(13)-H(13)	0.9300	C(34)-C(39)	1.405(4)
C(15)-C(20)	1.401(4)	C(35)-C(36)	1.376(4)
C(15)-C(16)	1.407(4)	C(35)-H(35)	0.9300
C(16)-C(17)	1.374(4)	C(36)-C(37)	1.386(4)
C(16)-H(16)	0.9300	C(36)-H(36)	0.9300
C(17)-C(18)	1.382(4)	C(37)-C(38)	1.378(4)
C(17)-H(17)	0.9300	C(37)-H(37)	0.9300
C(18)-C(19)	1.388(4)	C(38)-C(39)	1.375(4)
C(18)-H(18)	0.9300	C(38)-H(38)	0.9300
C(19)-C(20)	1.376(4)	C(39)-H(39)	0.9300
C(19)-H(19)	0.9300	C(41)-C(42)	1.398(4)
C(20)-H(20)	0.9300	C(41)-H(41)	0.9300
C(21)-C(22)	1.401(4)	C(42)-C(43)	1.362(4)
C(21)-C(26)	1.407(4)	C(42)-H(42)	0.9300
C(22)-C(23)	1.376(4)	C(43)-C(51)	1.398(4)
C(22)-H(22)	0.9300	C(43)-H(43)	0.9300
C(23)-C(24)	1.386(4)	C(44)-C(45)	1.337(4)
C(23)-H(23)	0.9300	C(44)-C(51)	1.426(4)
C(24)-C(25)	1.376(4)	C(44)-H(44)	0.9300
C(24)-H(24)	0.9300	C(45)-C(53)	1.421(4)
C(25)-C(26)	1.381(4)	C(45)-H(45)	0.9300
C(25)-H(25)	0.9300	C(46)-C(47)	1.363(4)
C(26)-H(26)	0.9300	C(46)-C(53)	1.415(4)
C(28)-C(33)	1.405(4)	C(46)-H(46)	0.9300
C(28)-C(29)	1.407(4)	C(47)-C(48)	1.388(4)
C(29)-C(30)	1.379(4)	C(47)-H(47)	0.9300
C(29)-H(29)	0.9300	C(48)-H(48)	0.9300
C(30)-C(31)	1.381(4)	C(50)-C(51)	1.409(4)

C(50)-C(52)	1.445(4)	C(73)-C(81)	1.422(4)
C(52)-C(53)	1.413(4)	C(73)-H(73)	0.9300
C(55)-C(56)	1.393(4)	C(74)-C(75)	1.358(4)
C(55)-H(55)	0.9300	C(74)-C(81)	1.412(4)
C(56)-C(57)	1.359(4)	C(74)-H(74)	0.9300
C(56)-H(56)	0.9300	C(75)-C(76)	1.395(4)
C(57)-C(65)	1.409(4)	C(75)-H(75)	0.9300
C(57)-H(57)	0.9300	C(76)-H(76)	0.9300
C(58)-C(59)	1.338(4)	C(78)-C(79)	1.410(4)
C(58)-C(65)	1.436(4)	C(78)-C(80)	1.449(4)
C(58)-H(58)	0.9300	C(80)-C(81)	1.412(4)
C(59)-C(67)	1.425(4)	C(83)-C(84)	1.394(4)
C(59)-H(59)	0.9300	C(83)-H(83)	0.9300
C(60)-C(61)	1.363(4)	C(84)-C(85)	1.365(4)
C(60)-C(67)	1.400(4)	C(84)-H(84)	0.9300
C(60)-H(60)	0.9300	C(85)-C(93)	1.407(4)
C(61)-C(62)	1.389(4)	C(85)-H(85)	0.9300
C(61)-H(61)	0.9300	C(86)-C(87)	1.349(4)
C(62)-H(62)	0.9300	C(86)-C(93)	1.431(4)
C(64)-C(65)	1.412(4)	C(86)-H(86)	0.9300
C(64)-C(66)	1.450(4)	C(87)-C(95)	1.427(4)
C(66)-C(67)	1.412(4)	C(87)-H(87)	0.9300
C(69)-C(70)	1.402(4)	C(88)-C(89)	1.363(4)
C(69)-H(69)	0.9300	C(88)-C(95)	1.403(4)
C(70)-C(71)	1.370(4)	C(88)-H(88)	0.9300
C(70)-H(70)	0.9300	C(89)-C(90)	1.388(4)
C(71)-C(79)	1.402(4)	C(89)-H(89)	0.9300
C(71)-H(71)	0.9300	C(90)-H(90)	0.9300
C(72)-C(73)	1.342(4)	C(92)-C(93)	1.405(4)
C(72)-C(79)	1.433(4)	C(92)-C(94)	1.442(4)
C(72)-H(72)	0.9300	C(94)-C(95)	1.410(4)

N(14)-Cu(1)-N(1)	178.99(10)	N(63)-K(1)-N(68)	97.07(7)
N(27)#1-Cu(2)-N(27)	180.00(19)	N(54)-K(1)-N(68)	120.45(7)
N(63)-K(1)-N(54)	59.10(7)	N(63)-K(1)-N(91)	159.32(7)

N(54)-K(1)-N(91)	110.56(7)	N(91)-K(1)-C(80)	67.53(6)
N(68)-K(1)-N(91)	103.49(7)	N(77)-K(1)-C(80)	22.73(6)
N(63)-K(1)-N(77)	120.63(7)	N(82)-K(1)-C(80)	74.94(6)
N(54)-K(1)-N(77)	88.30(7)	N(49)#2-K(1)-C(80)	150.53(7)
N(68)-K(1)-N(77)	56.14(7)	N(40)#2-K(1)-C(80)	136.77(6)
N(91)-K(1)-N(77)	74.03(6)	C(78)-K(1)-C(80)	24.37(7)
N(63)-K(1)-N(82)	130.14(7)	N(63)-K(1)-K(2)	114.51(5)
N(54)-K(1)-N(82)	162.18(6)	N(54)-K(1)-K(2)	113.11(5)
N(68)-K(1)-N(82)	75.84(6)	N(68)-K(1)-K(2)	126.23(5)
N(91)-K(1)-N(82)	55.05(6)	N(91)-K(1)-K(2)	50.24(4)
N(77)-K(1)-N(82)	96.43(7)	N(77)-K(1)-K(2)	124.04(5)
N(63)-K(1)-N(49)#2	69.63(6)	N(82)-K(1)-K(2)	50.43(4)
N(54)-K(1)-N(49)#2	97.42(6)	N(49)#2-K(1)-K(2)	45.77(4)
N(68)-K(1)-N(49)#2	126.24(6)	N(40)#2-K(1)-K(2)	45.80(4)
N(91)-K(1)-N(49)#2	95.91(6)	C(78)-K(1)-K(2)	112.70(5)
N(77)-K(1)-N(49)#2	169.72(6)	C(80)-K(1)-K(2)	112.32(5)
N(82)-K(1)-N(49)#2	75.60(6)	N(49)-K(2)-N(49)#2	180.00(9)
N(63)-K(1)-N(40)#2	86.48(6)	N(49)-K(2)-N(40)#2	122.82(6)
N(54)-K(1)-N(40)#2	67.68(6)	N(49)#2-K(2)-N(40)#2	57.18(6)
N(68)-K(1)-N(40)#2	171.83(6)	N(49)-K(2)-N(40)	57.18(6)
N(91)-K(1)-N(40)#2	72.85(6)	N(49)#2-K(2)-N(40)	122.82(6)
N(77)-K(1)-N(40)#2	127.92(6)	N(40)#2-K(2)-N(40)	180.00(4)
N(82)-K(1)-N(40)#2	96.23(6)	N(49)-K(2)-N(91)	76.48(6)
N(49)#2-K(1)-N(40)#2	48.28(6)	N(49)#2-K(2)-N(91)	103.52(6)
N(63)-K(1)-C(78)	119.92(7)	N(40)#2-K(2)-N(91)	78.68(6)
N(54)-K(1)-C(78)	127.22(7)	N(40)-K(2)-N(91)	101.32(6)
N(68)-K(1)-C(78)	23.07(6)	N(49)-K(2)-N(91)#2	103.52(6)
N(91)-K(1)-C(78)	80.74(6)	N(49)#2-K(2)-N(91)#2	76.48(6)
N(77)-K(1)-C(78)	43.82(7)	N(40)#2-K(2)-N(91)#2	101.32(6)
N(82)-K(1)-C(78)	64.72(6)	N(40)-K(2)-N(91)#2	78.68(6)
N(49)#2-K(1)-C(78)	133.69(6)	N(91)-K(2)-N(91)#2	180.00(6)
N(40)#2-K(1)-C(78)	153.34(6)	N(49)-K(2)-N(82)	97.85(6)
N(63)-K(1)-C(80)	131.77(7)	N(49)#2-K(2)-N(82)	82.15(6)
N(54)-K(1)-C(80)	111.02(7)	N(40)#2-K(2)-N(82)	106.75(6)
N(68)-K(1)-C(80)	43.65(7)	N(40)-K(2)-N(82)	73.25(6)

N(91)-K(2)-N(82)	53.20(6)	C(94)#2-K(2)-C(92)	156.05(6)
N(91)#2-K(2)-N(82)	126.80(6)	N(49)-K(2)-C(92)#2	104.45(6)
N(49)-K(2)-N(82)#2	82.15(6)	N(49)#2-K(2)-C(92)#2	75.55(6)
N(49)#2-K(2)-N(82)#2	97.85(6)	N(40)#2-K(2)-C(92)#2	64.96(6)
N(40)#2-K(2)-N(82)#2	73.25(6)	N(40)-K(2)-C(92)#2	115.04(6)
N(40)-K(2)-N(82)#2	106.75(6)	N(91)-K(2)-C(92)#2	137.35(6)
N(91)-K(2)-N(82)#2	126.80(6)	N(91)#2-K(2)-C(92)#2	42.65(6)
N(91)#2-K(2)-N(82)#2	53.20(6)	N(82)-K(2)-C(92)#2	157.15(6)
N(82)-K(2)-N(82)#2	180.0	N(82)#2-K(2)-C(92)#2	22.85(6)
N(49)-K(2)-C(94)	64.89(6)	C(94)-K(2)-C(92)#2	156.05(6)
N(49)#2-K(2)-C(94)	115.11(6)	C(94)#2-K(2)-C(92)#2	23.95(6)
N(40)#2-K(2)-C(94)	101.64(6)	C(92)-K(2)-C(92)#2	180.0
N(40)-K(2)-C(94)	78.36(6)	C(8)-N(1)-C(2)	121.9(2)
N(91)-K(2)-C(94)	23.03(6)	C(8)-N(1)-Cu(1)	120.70(18)
N(91)#2-K(2)-C(94)	156.97(6)	C(2)-N(1)-Cu(1)	116.82(17)
N(82)-K(2)-C(94)	42.72(6)	C(21)-N(14)-C(15)	121.4(2)
N(82)#2-K(2)-C(94)	137.28(6)	C(21)-N(14)-Cu(1)	119.03(18)
N(49)-K(2)-C(94)#2	115.11(6)	C(15)-N(14)-Cu(1)	119.55(17)
N(49)#2-K(2)-C(94)#2	64.89(6)	C(28)-N(27)-C(34)	119.4(2)
N(40)#2-K(2)-C(94)#2	78.36(6)	C(28)-N(27)-Cu(2)	116.79(18)
N(40)-K(2)-C(94)#2	101.64(6)	C(34)-N(27)-Cu(2)	123.56(18)
N(91)-K(2)-C(94)#2	156.97(6)	C(41)-N(40)-C(50)	116.9(2)
N(91)#2-K(2)-C(94)#2	23.03(6)	C(41)-N(40)-K(2)	120.62(19)
N(82)-K(2)-C(94)#2	137.28(6)	C(50)-N(40)-K(2)	119.27(17)
N(82)#2-K(2)-C(94)#2	42.72(6)	C(41)-N(40)-K(1)#2	115.81(17)
C(94)-K(2)-C(94)#2	180.00(10)	C(50)-N(40)-K(1)#2	95.25(15)
N(49)-K(2)-C(92)	75.55(6)	K(2)-N(40)-K(1)#2	76.70(5)
N(49)#2-K(2)-C(92)	104.45(6)	C(48)-N(49)-C(52)	117.0(3)
N(40)#2-K(2)-C(92)	115.04(6)	C(48)-N(49)-K(2)	118.77(19)
N(40)-K(2)-C(92)	64.96(6)	C(52)-N(49)-K(2)	119.41(16)
N(91)-K(2)-C(92)	42.65(6)	C(48)-N(49)-K(1)#2	116.25(17)
N(91)#2-K(2)-C(92)	137.35(6)	C(52)-N(49)-K(1)#2	97.51(16)
N(82)-K(2)-C(92)	22.85(6)	K(2)-N(49)-K(1)#2	77.74(6)
N(82)#2-K(2)-C(92)	157.15(6)	C(55)-N(54)-C(64)	117.4(2)
C(94)-K(2)-C(92)	23.95(6)	C(55)-N(54)-K(1)	122.30(19)

C(64)-N(54)-K(1)	120.33(17)	C(5)-C(6)-H(6)	119.3
C(62)-N(63)-C(66)	117.2(2)	C(7)-C(6)-H(6)	119.3
C(62)-N(63)-K(1)	120.07(19)	C(6)-C(7)-C(2)	121.1(3)
C(66)-N(63)-K(1)	122.46(17)	C(6)-C(7)-H(7)	119.5
C(69)-N(68)-C(78)	117.4(3)	C(2)-C(7)-H(7)	119.5
C(69)-N(68)-K(1)	120.30(18)	N(1)-C(8)-C(9)	118.5(2)
C(78)-N(68)-K(1)	101.09(16)	N(1)-C(8)-C(13)	125.6(2)
C(76)-N(77)-C(80)	117.3(3)	C(9)-C(8)-C(13)	115.8(2)
C(76)-N(77)-K(1)	123.36(18)	C(10)-C(9)-C(8)	122.9(3)
C(80)-N(77)-K(1)	99.95(17)	C(10)-C(9)-H(9)	118.5
C(83)-N(82)-C(92)	117.0(2)	C(8)-C(9)-H(9)	118.5
C(83)-N(82)-K(1)	120.20(18)	C(9)-C(10)-C(11)	120.4(3)
C(92)-N(82)-K(1)	115.98(17)	C(9)-C(10)-H(10)	119.8
C(83)-N(82)-K(2)	118.70(17)	C(11)-C(10)-H(10)	119.8
C(92)-N(82)-K(2)	96.10(15)	C(12)-C(11)-C(10)	118.1(3)
K(1)-N(82)-K(2)	80.32(6)	C(12)-C(11)-H(11)	121.0
C(90)-N(91)-C(94)	116.7(2)	C(10)-C(11)-H(11)	121.0
C(90)-N(91)-K(1)	116.18(18)	C(11)-C(12)-C(13)	121.8(3)
C(94)-N(91)-K(1)	119.96(16)	C(11)-C(12)-H(12)	119.1
C(90)-N(91)-K(2)	117.59(17)	C(13)-C(12)-H(12)	119.1
C(94)-N(91)-K(2)	96.49(16)	C(12)-C(13)-C(8)	121.0(3)
K(1)-N(91)-K(2)	82.62(6)	C(12)-C(13)-H(13)	119.5
N(1)-C(2)-C(3)	118.5(2)	C(8)-C(13)-H(13)	119.5
N(1)-C(2)-C(7)	124.9(3)	N(14)-C(15)-C(20)	124.5(2)
C(3)-C(2)-C(7)	116.3(3)	N(14)-C(15)-C(16)	119.7(2)
C(4)-C(3)-C(2)	122.1(3)	C(20)-C(15)-C(16)	115.8(3)
C(4)-C(3)-H(3)	118.9	C(17)-C(16)-C(15)	122.1(3)
C(2)-C(3)-H(3)	118.9	C(17)-C(16)-H(16)	119.0
C(5)-C(4)-C(3)	120.8(3)	C(15)-C(16)-H(16)	119.0
C(5)-C(4)-H(4)	119.6	C(16)-C(17)-C(18)	121.0(3)
C(3)-C(4)-H(4)	119.6	C(16)-C(17)-H(17)	119.5
C(4)-C(5)-C(6)	118.3(3)	C(18)-C(17)-H(17)	119.5
C(4)-C(5)-H(5)	120.8	C(17)-C(18)-C(19)	118.2(3)
C(6)-C(5)-H(5)	120.8	C(17)-C(18)-H(18)	120.9
C(5)-C(6)-C(7)	121.3(3)	C(19)-C(18)-H(18)	120.9

C(20)-C(19)-C(18)	120.8(3)	C(30)-C(31)-H(31)	120.9
C(20)-C(19)-H(19)	119.6	C(31)-C(32)-C(33)	121.4(3)
C(18)-C(19)-H(19)	119.6	C(31)-C(32)-H(32)	119.3
C(19)-C(20)-C(15)	122.1(3)	C(33)-C(32)-H(32)	119.3
C(19)-C(20)-H(20)	119.0	C(32)-C(33)-C(28)	121.3(3)
C(15)-C(20)-H(20)	119.0	C(32)-C(33)-H(33)	119.3
N(14)-C(21)-C(22)	119.5(2)	C(28)-C(33)-H(33)	119.3
N(14)-C(21)-C(26)	124.4(3)	N(27)-C(34)-C(35)	124.8(2)
C(22)-C(21)-C(26)	115.9(3)	N(27)-C(34)-C(39)	119.9(3)
C(23)-C(22)-C(21)	122.5(3)	C(35)-C(34)-C(39)	115.3(3)
C(23)-C(22)-H(22)	118.8	C(36)-C(35)-C(34)	122.5(3)
C(21)-C(22)-H(22)	118.8	C(36)-C(35)-H(35)	118.7
C(22)-C(23)-C(24)	120.3(3)	C(34)-C(35)-H(35)	118.7
C(22)-C(23)-H(23)	119.9	C(35)-C(36)-C(37)	120.8(3)
C(24)-C(23)-H(23)	119.9	C(35)-C(36)-H(36)	119.6
C(25)-C(24)-C(23)	118.7(3)	C(37)-C(36)-H(36)	119.6
C(25)-C(24)-H(24)	120.7	C(38)-C(37)-C(36)	117.9(3)
C(23)-C(24)-H(24)	120.7	C(38)-C(37)-H(37)	121.0
C(24)-C(25)-C(26)	121.2(3)	C(36)-C(37)-H(37)	121.0
C(24)-C(25)-H(25)	119.4	C(39)-C(38)-C(37)	121.4(3)
C(26)-C(25)-H(25)	119.4	C(39)-C(38)-H(38)	119.3
C(25)-C(26)-C(21)	121.4(3)	C(37)-C(38)-H(38)	119.3
C(25)-C(26)-H(26)	119.3	C(38)-C(39)-C(34)	122.1(3)
C(21)-C(26)-H(26)	119.3	C(38)-C(39)-H(39)	118.9
N(27)-C(28)-C(33)	124.8(2)	C(34)-C(39)-H(39)	118.9
N(27)-C(28)-C(29)	118.9(2)	N(40)-C(41)-C(42)	124.5(3)
C(33)-C(28)-C(29)	116.1(2)	N(40)-C(41)-H(41)	117.7
C(30)-C(29)-C(28)	121.8(3)	C(42)-C(41)-H(41)	117.7
C(30)-C(29)-H(29)	119.1	C(43)-C(42)-C(41)	118.1(3)
C(28)-C(29)-H(29)	119.1	C(43)-C(42)-H(42)	120.9
C(29)-C(30)-C(31)	121.0(3)	C(41)-C(42)-H(42)	120.9
C(29)-C(30)-H(30)	119.5	C(42)-C(43)-C(51)	120.1(3)
C(31)-C(30)-H(30)	119.5	C(42)-C(43)-H(43)	119.9
C(32)-C(31)-C(30)	118.3(3)	C(51)-C(43)-H(43)	119.9
C(32)-C(31)-H(31)	120.9	C(45)-C(44)-C(51)	120.9(3)

C(45)-C(44)-H(44)	119.5	C(59)-C(58)-C(65)	120.7(3)
C(51)-C(44)-H(44)	119.5	C(59)-C(58)-H(58)	119.7
C(44)-C(45)-C(53)	121.0(3)	C(65)-C(58)-H(58)	119.7
C(44)-C(45)-H(45)	119.5	C(58)-C(59)-C(67)	121.5(3)
C(53)-C(45)-H(45)	119.5	C(58)-C(59)-H(59)	119.2
C(47)-C(46)-C(53)	119.5(3)	C(67)-C(59)-H(59)	119.2
C(47)-C(46)-H(46)	120.3	C(61)-C(60)-C(67)	119.7(3)
C(53)-C(46)-H(46)	120.3	C(61)-C(60)-H(60)	120.1
C(46)-C(47)-C(48)	118.9(3)	C(67)-C(60)-H(60)	120.1
C(46)-C(47)-H(47)	120.6	C(60)-C(61)-C(62)	118.5(3)
C(48)-C(47)-H(47)	120.6	C(60)-C(61)-H(61)	120.8
N(49)-C(48)-C(47)	124.6(3)	C(62)-C(61)-H(61)	120.8
N(49)-C(48)-H(48)	117.7	N(63)-C(62)-C(61)	124.6(3)
C(47)-C(48)-H(48)	117.7	N(63)-C(62)-H(62)	117.7
N(40)-C(50)-C(51)	122.4(3)	C(61)-C(62)-H(62)	117.7
N(40)-C(50)-C(52)	118.7(2)	N(54)-C(64)-C(65)	122.1(3)
C(51)-C(50)-C(52)	118.8(2)	N(54)-C(64)-C(66)	118.6(2)
C(43)-C(51)-C(50)	117.9(3)	C(65)-C(64)-C(66)	119.2(3)
C(43)-C(51)-C(44)	121.9(3)	C(57)-C(65)-C(64)	117.7(3)
C(50)-C(51)-C(44)	120.2(3)	C(57)-C(65)-C(58)	122.5(3)
N(49)-C(52)-C(53)	122.7(3)	C(64)-C(65)-C(58)	119.8(3)
N(49)-C(52)-C(50)	118.6(2)	N(63)-C(66)-C(67)	122.4(3)
C(53)-C(52)-C(50)	118.6(2)	N(63)-C(66)-C(64)	118.9(2)
C(52)-C(53)-C(46)	117.2(3)	C(67)-C(66)-C(64)	118.7(3)
C(52)-C(53)-C(45)	120.3(3)	C(60)-C(67)-C(66)	117.6(3)
C(46)-C(53)-C(45)	122.5(3)	C(60)-C(67)-C(59)	122.4(3)
N(54)-C(55)-C(56)	124.6(3)	C(66)-C(67)-C(59)	120.0(3)
N(54)-C(55)-H(55)	117.7	N(68)-C(69)-C(70)	124.1(3)
C(56)-C(55)-H(55)	117.7	N(68)-C(69)-H(69)	117.9
C(57)-C(56)-C(55)	118.5(3)	C(70)-C(69)-H(69)	117.9
C(57)-C(56)-H(56)	120.7	C(71)-C(70)-C(69)	118.5(3)
C(55)-C(56)-H(56)	120.7	C(71)-C(70)-H(70)	120.7
C(56)-C(57)-C(65)	119.6(3)	C(69)-C(70)-H(70)	120.7
C(56)-C(57)-H(57)	120.2	C(70)-C(71)-C(79)	119.3(3)
C(65)-C(57)-H(57)	120.2	C(70)-C(71)-H(71)	120.3

C(79)-C(71)-H(71)	120.3	N(82)-C(83)-H(83)	117.8
C(73)-C(72)-C(79)	121.2(3)	C(84)-C(83)-H(83)	117.8
C(73)-C(72)-H(72)	119.4	C(85)-C(84)-C(83)	118.9(3)
C(79)-C(72)-H(72)	119.4	C(85)-C(84)-H(84)	120.5
C(72)-C(73)-C(81)	121.3(3)	C(83)-C(84)-H(84)	120.5
C(72)-C(73)-H(73)	119.3	C(84)-C(85)-C(93)	119.0(3)
C(81)-C(73)-H(73)	119.3	C(84)-C(85)-H(85)	120.5
C(75)-C(74)-C(81)	119.9(3)	C(93)-C(85)-H(85)	120.5
C(75)-C(74)-H(74)	120.1	C(87)-C(86)-C(93)	121.2(3)
C(81)-C(74)-H(74)	120.1	C(87)-C(86)-H(86)	119.4
C(74)-C(75)-C(76)	118.3(3)	C(93)-C(86)-H(86)	119.4
C(74)-C(75)-H(75)	120.8	C(86)-C(87)-C(95)	120.7(3)
C(76)-C(75)-H(75)	120.8	C(86)-C(87)-H(87)	119.7
N(77)-C(76)-C(75)	124.5(3)	C(95)-C(87)-H(87)	119.7
N(77)-C(76)-H(76)	117.8	C(89)-C(88)-C(95)	119.3(3)
C(75)-C(76)-H(76)	117.8	C(89)-C(88)-H(88)	120.4
N(68)-C(78)-C(79)	122.3(3)	C(95)-C(88)-H(88)	120.4
N(68)-C(78)-C(80)	118.1(3)	C(88)-C(89)-C(90)	118.8(3)
C(79)-C(78)-C(80)	119.6(3)	C(88)-C(89)-H(89)	120.6
N(68)-C(78)-K(1)	55.84(14)	C(90)-C(89)-H(89)	120.6
C(79)-C(78)-K(1)	138.00(18)	N(91)-C(90)-C(89)	124.7(3)
C(80)-C(78)-K(1)	79.27(15)	N(91)-C(90)-H(90)	117.6
C(71)-C(79)-C(78)	118.2(3)	C(89)-C(90)-H(90)	117.6
C(71)-C(79)-C(72)	122.6(3)	N(82)-C(92)-C(93)	122.7(2)
C(78)-C(79)-C(72)	119.2(3)	N(82)-C(92)-C(94)	118.5(2)
N(77)-C(80)-C(81)	122.5(3)	C(93)-C(92)-C(94)	118.8(2)
N(77)-C(80)-C(78)	118.8(3)	N(82)-C(92)-K(2)	61.05(13)
C(81)-C(80)-C(78)	118.7(3)	C(93)-C(92)-K(2)	133.69(18)
N(77)-C(80)-K(1)	57.33(14)	C(94)-C(92)-K(2)	77.50(14)
C(81)-C(80)-K(1)	140.76(18)	C(92)-C(93)-C(85)	118.0(3)
C(78)-C(80)-K(1)	76.36(15)	C(92)-C(93)-C(86)	120.0(3)
C(74)-C(81)-C(80)	117.4(3)	C(85)-C(93)-C(86)	122.0(3)
C(74)-C(81)-C(73)	122.6(3)	N(91)-C(94)-C(95)	122.3(2)
C(80)-C(81)-C(73)	119.9(3)	N(91)-C(94)-C(92)	118.0(2)
N(82)-C(83)-C(84)	124.3(3)	C(95)-C(94)-C(92)	119.7(2)

N(91)-C(94)-K(2)	60.47(13)
C(95)-C(94)-K(2)	133.28(17)
C(92)-C(94)-K(2)	78.55(15)
C(88)-C(95)-C(94)	118.2(3)
C(88)-C(95)-C(87)	122.2(3)
C(94)-C(95)-C(87)	119.7(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x,-y,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for i11702. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	22(1)	20(1)	27(1)	-1(1)	-4(1)	-4(1)
Cu(2)	27(1)	21(1)	15(1)	1(1)	4(1)	-5(1)
K(1)	27(1)	20(1)	24(1)	-5(1)	3(1)	2(1)
K(2)	21(1)	18(1)	23(1)	-5(1)	5(1)	0(1)
N(1)	20(1)	19(1)	22(1)	-1(1)	-1(1)	-3(1)
N(14)	21(1)	20(1)	24(1)	-2(1)	1(1)	-4(1)
N(27)	27(1)	21(1)	16(1)	1(1)	3(1)	-3(1)
N(40)	19(1)	16(1)	29(2)	-2(1)	4(1)	-2(1)
N(49)	20(1)	26(1)	21(1)	0(1)	2(1)	0(1)
N(54)	20(1)	23(1)	22(1)	-1(1)	0(1)	-3(1)
N(63)	15(1)	26(1)	22(1)	1(1)	3(1)	-2(1)
N(68)	21(1)	24(2)	35(2)	2(1)	2(1)	-1(1)
N(77)	23(1)	24(2)	34(2)	-2(1)	4(1)	-2(1)
N(82)	18(1)	20(1)	25(1)	-1(1)	-1(1)	-1(1)
N(91)	22(1)	17(1)	21(1)	-1(1)	2(1)	-2(1)
C(2)	16(2)	21(2)	20(2)	2(1)	-6(1)	-1(1)
C(3)	23(2)	26(2)	24(2)	4(1)	-3(1)	-1(1)
C(4)	20(2)	43(2)	28(2)	12(2)	0(1)	3(2)
C(5)	28(2)	40(2)	22(2)	1(2)	0(1)	15(2)
C(6)	37(2)	23(2)	23(2)	3(1)	-5(1)	7(1)
C(7)	24(2)	22(2)	19(2)	3(1)	-1(1)	0(1)
C(8)	23(2)	12(2)	19(2)	5(1)	-3(1)	0(1)
C(9)	25(2)	16(2)	24(2)	-1(1)	-5(1)	-1(1)
C(10)	37(2)	21(2)	20(2)	-4(1)	2(1)	4(1)
C(11)	23(2)	28(2)	30(2)	3(2)	7(1)	2(1)
C(12)	22(2)	22(2)	24(2)	4(1)	-4(1)	-3(1)
C(13)	22(2)	22(2)	17(2)	-2(1)	-2(1)	-2(1)
C(15)	22(2)	26(2)	15(2)	-3(1)	2(1)	-4(1)
C(16)	22(2)	28(2)	21(2)	-3(1)	2(1)	-8(1)
C(17)	21(2)	32(2)	23(2)	-4(1)	2(1)	1(1)
C(18)	37(2)	21(2)	29(2)	-4(1)	-2(1)	1(1)
C(19)	29(2)	25(2)	28(2)	2(1)	-2(1)	-8(1)

C(20)	21(2)	25(2)	28(2)	2(1)	0(1)	-2(1)
C(21)	18(2)	24(2)	20(2)	5(1)	2(1)	-10(1)
C(22)	23(2)	25(2)	25(2)	1(1)	1(1)	-6(1)
C(23)	29(2)	26(2)	34(2)	8(2)	5(1)	-3(1)
C(24)	24(2)	31(2)	38(2)	16(2)	-3(1)	-5(1)
C(25)	30(2)	36(2)	26(2)	10(2)	-5(1)	-17(2)
C(26)	26(2)	23(2)	27(2)	2(1)	2(1)	-8(1)
C(28)	24(2)	16(2)	18(2)	-4(1)	3(1)	-2(1)
C(29)	26(2)	28(2)	17(2)	-3(1)	9(1)	-6(1)
C(30)	22(2)	31(2)	26(2)	-6(2)	4(1)	-1(1)
C(31)	22(2)	29(2)	19(2)	0(1)	0(1)	5(1)
C(32)	28(2)	20(2)	17(2)	1(1)	5(1)	2(1)
C(33)	23(2)	17(2)	19(2)	-2(1)	4(1)	-2(1)
C(34)	29(2)	11(2)	19(2)	1(1)	2(1)	-1(1)
C(35)	33(2)	19(2)	19(2)	1(1)	-1(1)	2(1)
C(36)	32(2)	23(2)	24(2)	-2(1)	6(1)	5(1)
C(37)	25(2)	28(2)	33(2)	-2(2)	-1(1)	5(1)
C(38)	36(2)	29(2)	22(2)	2(1)	-4(1)	3(1)
C(39)	34(2)	29(2)	16(2)	0(1)	4(1)	-1(1)
C(41)	26(2)	27(2)	30(2)	6(2)	2(1)	-1(1)
C(42)	31(2)	44(2)	21(2)	9(2)	0(1)	-8(2)
C(43)	29(2)	43(2)	19(2)	-7(2)	6(1)	-10(2)
C(44)	26(2)	27(2)	34(2)	-15(2)	5(1)	-2(1)
C(45)	26(2)	20(2)	53(2)	-11(2)	5(2)	2(1)
C(46)	27(2)	27(2)	54(2)	12(2)	-4(2)	7(1)
C(47)	30(2)	44(2)	36(2)	13(2)	-8(2)	5(2)
C(48)	27(2)	41(2)	23(2)	-1(2)	-2(1)	-2(2)
C(50)	15(1)	17(2)	24(2)	-4(1)	4(1)	-4(1)
C(51)	15(2)	30(2)	23(2)	-7(1)	5(1)	-6(1)
C(52)	14(1)	20(2)	22(2)	-5(1)	2(1)	-1(1)
C(53)	15(2)	23(2)	39(2)	0(2)	1(1)	2(1)
C(55)	26(2)	30(2)	25(2)	2(2)	-2(1)	-1(1)
C(56)	29(2)	45(2)	26(2)	11(2)	-2(1)	-9(2)
C(57)	20(2)	56(2)	20(2)	-7(2)	4(1)	-8(2)
C(58)	23(2)	45(2)	30(2)	-18(2)	5(1)	-2(2)
C(59)	28(2)	30(2)	41(2)	-17(2)	6(2)	1(1)
C(60)	28(2)	23(2)	49(2)	1(2)	5(2)	1(1)

C(61)	31(2)	31(2)	39(2)	13(2)	4(2)	3(2)
C(62)	22(2)	34(2)	25(2)	3(2)	2(1)	2(1)
C(64)	11(1)	25(2)	26(2)	-6(1)	2(1)	-5(1)
C(65)	14(2)	37(2)	22(2)	-5(2)	3(1)	-4(1)
C(66)	15(1)	20(2)	22(2)	0(1)	3(1)	-6(1)
C(67)	19(2)	24(2)	35(2)	-7(2)	4(1)	-3(1)
C(69)	20(2)	20(2)	50(2)	5(2)	0(2)	-2(1)
C(70)	21(2)	34(2)	39(2)	11(2)	-2(1)	-10(1)
C(71)	23(2)	35(2)	33(2)	-4(2)	3(1)	-9(1)
C(72)	32(2)	26(2)	31(2)	-11(2)	7(1)	-4(1)
C(73)	30(2)	22(2)	42(2)	-7(2)	6(2)	1(1)
C(74)	25(2)	21(2)	45(2)	3(2)	2(1)	1(1)
C(75)	29(2)	31(2)	34(2)	8(2)	2(1)	-1(1)
C(76)	27(2)	32(2)	31(2)	0(2)	3(1)	-4(1)
C(78)	14(1)	19(2)	35(2)	-3(1)	4(1)	-3(1)
C(79)	18(2)	32(2)	29(2)	-2(2)	4(1)	-5(1)
C(80)	15(2)	20(2)	34(2)	-1(1)	5(1)	-2(1)
C(81)	18(2)	22(2)	36(2)	0(2)	5(1)	1(1)
C(83)	22(2)	26(2)	30(2)	4(2)	0(1)	3(1)
C(84)	28(2)	39(2)	22(2)	8(2)	-5(1)	1(2)
C(85)	25(2)	35(2)	24(2)	-7(2)	-2(1)	-1(1)
C(86)	22(2)	26(2)	32(2)	-15(2)	0(1)	-2(1)
C(87)	27(2)	19(2)	33(2)	-5(1)	-1(1)	-1(1)
C(88)	26(2)	19(2)	32(2)	2(1)	0(1)	-2(1)
C(89)	32(2)	25(2)	24(2)	3(1)	1(1)	-3(1)
C(90)	31(2)	21(2)	23(2)	-3(1)	3(1)	-2(1)
C(92)	14(1)	18(2)	24(2)	-1(1)	1(1)	-3(1)
C(93)	17(2)	25(2)	24(2)	-2(1)	0(1)	-3(1)
C(94)	15(1)	20(2)	22(2)	-3(1)	1(1)	-2(1)
C(95)	17(2)	18(2)	29(2)	-2(1)	0(1)	-2(1)

Crystal Data for Compound (phen)$KNPh_2$

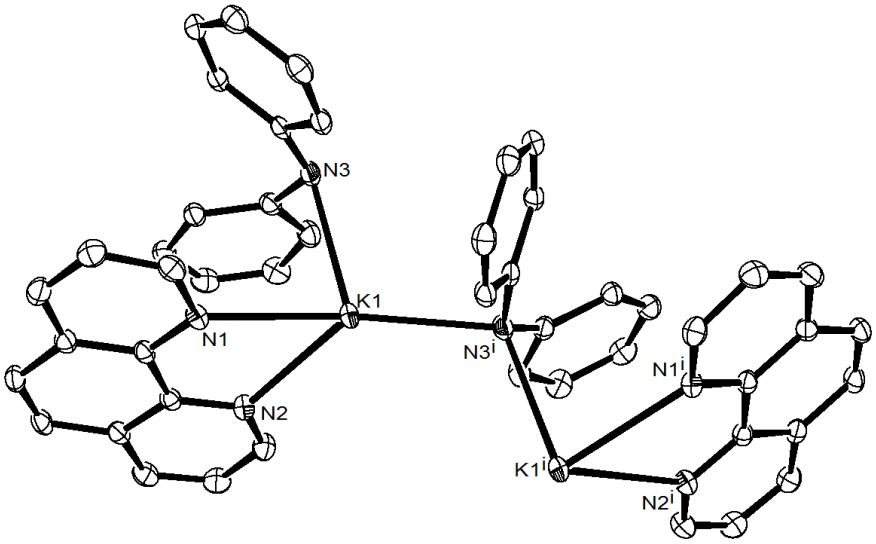

Table 1. Crystal data and structure refinement for sgy023_1.

Identification code	sgy023_1	
Empirical formula	C24 H18 K N3	
Formula weight	387.51	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 7.5630(2) Å	α= 90°.
	b = 18.4368(6) Å	β= 90°.
	c = 27.0336(8) Å	γ = 90°.
Volume	3769.50(19) $Å^3$	
Z	8	
Density (calculated)	1.366 Mg/m^3	
Absorption coefficient	0.296 mm^{-1}	
F(000)	1616	
Crystal size	0.4 x 0.3 x 0.3 mm^3	
Theta range for data collection	2.67 to 32.75°.	

Index ranges	-9<=h<=11, -27<=k<=25, -40<=l<=27
Reflections collected	34110
Independent reflections	6532 [R(int) = 0.0480]
Completeness to theta = 32.75°	93.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1 and 0.45815
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6532 / 0 / 253
Goodness-of-fit on F^2	0.928
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.0957
R indices (all data)	R1 = 0.0702, wR2 = 0.1025
Largest diff. peak and hole	0.401 and -0.282 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sgy023_1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(23)	10738(2)	6469(1)	2118(1)	22(1)
C(19)	10488(2)	5168(1)	1932(1)	16(1)
C(20)	12019(2)	5250(1)	1633(1)	18(1)
C(24)	9893(2)	5807(1)	2173(1)	19(1)
C(21)	12854(2)	5917(1)	1584(1)	20(1)
C(22)	12238(2)	6534(1)	1822(1)	22(1)
K(1)	5958(1)	4627(1)	2001(1)	21(1)
N(2)	4973(1)	3843(1)	1156(1)	19(1)
N(3)	9625(2)	4534(1)	2047(1)	19(1)
N(1)	6739(1)	5138(1)	1040(1)	18(1)
C(5)	6551(2)	4696(1)	640(1)	16(1)
C(6)	5623(2)	4015(1)	701(1)	16(1)
C(18)	8988(2)	3276(1)	1950(1)	24(1)
C(7)	5440(2)	3546(1)	289(1)	18(1)
C(4)	7260(2)	4872(1)	171(1)	18(1)
C(11)	7034(2)	4383(1)	-237(1)	21(1)
C(13)	9593(2)	3939(1)	1742(1)	18(1)
C(12)	6163(2)	3751(1)	-180(1)	21(1)
C(9)	3932(2)	2711(1)	821(1)	24(1)
C(1)	7641(2)	5746(1)	979(1)	21(1)
C(8)	4553(2)	2884(1)	362(1)	22(1)
C(14)	9901(2)	3927(1)	1225(1)	18(1)
C(10)	4175(2)	3210(1)	1205(1)	23(1)
C(3)	8185(2)	5529(1)	125(1)	23(1)
C(16)	8989(2)	2672(1)	1158(1)	25(1)
C(2)	8389(2)	5966(1)	529(1)	23(1)
C(15)	9592(2)	3310(1)	946(1)	22(1)
C(17)	8689(2)	2662(1)	1665(1)	26(1)

Table 3. Bond lengths [Å] and angles [°] for sgy023_1.

C(23)-C(24)	1.3854(18)	C(18)-C(13)	1.4209(18)
C(23)-C(22)	1.3928(19)	C(7)-C(8)	1.4065(18)
C(19)-N(3)	1.3743(16)	C(7)-C(12)	1.4319(17)
C(19)-C(24)	1.4191(17)	C(4)-C(3)	1.4040(18)
C(19)-C(20)	1.4199(17)	C(4)-C(11)	1.4335(18)
C(19)-K(1)#1	3.0729(12)	C(11)-C(12)	1.3474(19)
C(20)-C(21)	1.3898(17)	C(13)-C(14)	1.4176(17)
C(20)-K(1)#2	3.3448(12)	C(9)-C(8)	1.3635(19)
C(24)-K(1)#1	3.2204(13)	C(9)-C(10)	1.3987(19)
C(21)-C(22)	1.3873(18)	C(1)-C(2)	1.4030(18)
C(21)-K(1)#2	3.5278(13)	C(14)-C(15)	1.3832(17)
K(1)-N(3)#3	2.7695(10)	C(3)-C(2)	1.3657(19)
K(1)-N(3)	2.7813(12)	C(16)-C(17)	1.387(2)
K(1)-N(2)	2.8057(11)	C(16)-C(15)	1.3870(19)
K(1)-N(1)	2.8276(11)	C(24)-C(23)-C(22)	120.85(12)
K(1)-C(19)#3	3.0729(12)	N(3)-C(19)-C(24)	116.85(11)
K(1)-C(13)	3.1075(12)	N(3)-C(19)-C(20)	127.34(11)
K(1)-C(24)#3	3.2204(13)	C(24)-C(19)-C(20)	115.54(12)
K(1)-C(20)#4	3.3448(12)	N(3)-C(19)-K(1)#1	64.31(6)
K(1)-C(18)	3.3873(14)	C(24)-C(19)-K(1)#1	82.85(7)
K(1)-C(21)#4	3.5278(13)	C(20)-C(19)-K(1)#1	118.34(8)
K(1)-K(1)#1	4.6449(3)	C(21)-C(20)-C(19)	121.30(11)
K(1)-K(1)#3	4.6449(3)	C(21)-C(20)-K(1)#2	85.84(7)
N(2)-C(10)	1.3210(16)	C(19)-C(20)-K(1)#2	121.34(8)
N(2)-C(6)	1.3617(16)	C(23)-C(24)-C(19)	122.41(12)
N(3)-C(13)	1.3730(15)	C(23)-C(24)-K(1)#1	123.66(8)
N(3)-K(1)#1	2.7695(10)	C(19)-C(24)-K(1)#1	71.22(7)
N(1)-C(1)	1.3212(17)	C(20)-C(21)-C(22)	121.87(12)
N(1)-C(5)	1.3620(15)	C(20)-C(21)-K(1)#2	71.02(7)
C(5)-C(4)	1.4143(17)	C(22)-C(21)-K(1)#2	128.87(8)
C(5)-C(6)	1.4473(17)	C(21)-C(22)-C(23)	118.02(12)
C(6)-C(7)	1.4155(16)	N(3)#3-K(1)-N(3)	108.53(3)
C(18)-C(17)	1.3881(19)	N(3)#3-K(1)-N(2)	128.95(3)
		N(3)-K(1)-N(2)	105.62(3)
		N(3)#3-K(1)-N(1)	162.00(3)
		N(3)-K(1)-N(1)	81.55(3)

N(2)-K(1)-N(1)	58.55(3)	C(24)#3-K(1)-C(21)#4	66.42(3)
N(3)#3-K(1)-C(19)#3	26.56(3)	C(20)#4-K(1)-C(21)#4	23.14(3)
N(3)-K(1)-C(19)#3	95.37(3)	C(18)-K(1)-C(21)#4	158.89(3)
N(2)-K(1)-C(19)#3	154.35(3)	N(3)#3-K(1)-K(1)#1	75.92(2)
N(1)-K(1)-C(19)#3	141.17(3)	N(3)-K(1)-K(1)#1	33.12(2)
N(3)#3-K(1)-C(13)	120.43(3)	N(2)-K(1)-K(1)#1	133.58(2)
N(3)-K(1)-C(13)	26.22(3)	N(1)-K(1)-K(1)#1	111.33(2)
N(2)-K(1)-C(13)	80.82(3)	C(19)#3-K(1)-K(1)#1	63.19(2)
N(1)-K(1)-C(13)	75.16(3)	C(13)-K(1)-K(1)#1	53.91(2)
C(19)#3-K(1)-C(13)	116.53(3)	C(24)#3-K(1)-K(1)#1	78.51(2)
N(3)#3-K(1)-C(24)#3	46.06(3)	C(20)#4-K(1)-K(1)#1	153.90(2)
N(3)-K(1)-C(24)#3	105.08(3)	C(18)-K(1)-K(1)#1	58.21(2)
N(2)-K(1)-C(24)#3	147.88(3)	C(21)#4-K(1)-K(1)#1	136.68(2)
N(1)-K(1)-C(24)#3	117.69(3)	N(3)#3-K(1)-K(1)#3	33.28(2)
C(19)#3-K(1)-C(24)#3	25.93(3)	N(3)-K(1)-K(1)#3	141.81(2)
C(13)-K(1)-C(24)#3	130.81(3)	N(2)-K(1)-K(1)#3	104.89(2)
N(3)#3-K(1)-C(20)#4	88.49(3)	N(1)-K(1)-K(1)#3	134.74(2)
N(3)-K(1)-C(20)#4	157.31(3)	C(19)#3-K(1)-K(1)#3	50.26(2)
N(2)-K(1)-C(20)#4	72.42(3)	C(13)-K(1)-K(1)#3	148.34(2)
N(1)-K(1)-C(20)#4	78.34(3)	C(24)#3-K(1)-K(1)#3	52.67(2)
C(19)#3-K(1)-C(20)#4	93.72(3)	C(20)#4-K(1)-K(1)#3	56.47(2)
C(13)-K(1)-C(20)#4	149.42(3)	C(18)-K(1)-K(1)#3	125.07(2)
C(24)#3-K(1)-C(20)#4	75.63(3)	C(21)#4-K(1)-K(1)#3	69.15(2)
N(3)#3-K(1)-C(18)	103.82(3)	K(1)#1-K(1)-K(1)#3	108.999(10)
N(3)-K(1)-C(18)	44.11(3)	C(10)-N(2)-C(6)	117.52(11)
N(2)-K(1)-C(18)	76.53(3)	C(10)-N(2)-K(1)	119.66(8)
N(1)-K(1)-C(18)	93.79(3)	C(6)-N(2)-K(1)	121.31(8)
C(19)#3-K(1)-C(18)	110.82(3)	C(13)-N(3)-C(19)	123.52(10)
C(13)-K(1)-C(18)	24.80(3)	C(13)-N(3)-K(1)#1	127.91(8)
C(24)#3-K(1)-C(18)	133.98(3)	C(19)-N(3)-K(1)#1	89.12(7)
C(20)#4-K(1)-C(18)	147.44(3)	C(13)-N(3)-K(1)	90.26(7)
N(3)#3-K(1)-C(21)#4	95.56(3)	C(19)-N(3)-K(1)	114.27(8)
N(3)-K(1)-C(21)#4	136.00(3)	K(1)#1-N(3)-K(1)	113.61(4)
N(2)-K(1)-C(21)#4	84.85(3)	C(1)-N(1)-C(5)	117.62(11)
N(1)-K(1)-C(21)#4	67.67(3)	C(1)-N(1)-K(1)	120.27(8)
C(19)#3-K(1)-C(21)#4	90.26(3)	C(5)-N(1)-K(1)	120.54(8)
C(13)-K(1)-C(21)#4	142.35(3)	N(1)-C(5)-C(4)	122.29(11)

N(1)-C(5)-C(6)	118.67(11)	C(14)-C(13)-K(1)	111.99(8)
C(4)-C(5)-C(6)	119.03(11)	C(18)-C(13)-K(1)	88.69(8)
N(2)-C(6)-C(7)	122.11(11)	C(11)-C(12)-C(7)	121.11(11)
N(2)-C(6)-C(5)	118.70(11)	C(8)-C(9)-C(10)	118.38(12)
C(7)-C(6)-C(5)	119.18(11)	N(1)-C(1)-C(2)	124.14(12)
C(17)-C(18)-C(13)	122.30(12)	C(9)-C(8)-C(7)	119.66(12)
C(17)-C(18)-K(1)	120.82(9)	C(15)-C(14)-C(13)	121.48(12)
C(13)-C(18)-K(1)	66.51(7)	N(2)-C(10)-C(9)	124.49(12)
C(8)-C(7)-C(6)	117.82(11)	C(2)-C(3)-C(4)	119.72(12)
C(8)-C(7)-C(12)	122.38(11)	C(17)-C(16)-C(15)	118.25(12)
C(6)-C(7)-C(12)	119.80(11)	C(3)-C(2)-C(1)	118.46(12)
C(3)-C(4)-C(5)	117.76(11)	C(14)-C(15)-C(16)	121.84(12)
C(3)-C(4)-C(11)	122.28(12)	C(16)-C(17)-C(18)	120.69(13)
C(5)-C(4)-C(11)	119.96(11)		
C(12)-C(11)-C(4)	120.92(11)		
N(3)-C(13)-C(14)	127.04(11)		
N(3)-C(13)-C(18)	117.09(11)		
C(14)-C(13)-C(18)	115.43(11)		
N(3)-C(13)-K(1)	63.51(6)		

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,y,-z+1/2 #2 x+1,y,z #3 x-1/2,y,-z+1/2

#4 x-1,y,z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sgy023_1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(23)	28(1)	19(1)	19(1)	-3(1)	-4(1)	5(1)
C(19)	19(1)	19(1)	11(1)	0(1)	-3(1)	2(1)
C(20)	20(1)	21(1)	13(1)	-2(1)	-2(1)	4(1)
C(24)	21(1)	24(1)	13(1)	-3(1)	0(1)	3(1)
C(21)	20(1)	27(1)	13(1)	2(1)	0(1)	-1(1)
C(22)	28(1)	20(1)	19(1)	3(1)	-5(1)	-1(1)
K(1)	22(1)	29(1)	11(1)	-2(1)	1(1)	0(1)
N(2)	22(1)	18(1)	15(1)	0(1)	2(1)	1(1)
N(3)	22(1)	22(1)	12(1)	-2(1)	0(1)	-1(1)
N(1)	21(1)	17(1)	14(1)	0(1)	-2(1)	2(1)
C(5)	16(1)	18(1)	14(1)	-1(1)	-1(1)	4(1)
C(6)	17(1)	17(1)	14(1)	-1(1)	-2(1)	4(1)
C(18)	29(1)	25(1)	18(1)	3(1)	-2(1)	-2(1)
C(7)	18(1)	19(1)	16(1)	-3(1)	-2(1)	5(1)
C(4)	18(1)	21(1)	15(1)	0(1)	-1(1)	3(1)
C(11)	22(1)	29(1)	13(1)	0(1)	2(1)	4(1)
C(13)	16(1)	20(1)	16(1)	-1(1)	-2(1)	2(1)
C(12)	23(1)	25(1)	14(1)	-6(1)	-1(1)	6(1)
C(9)	25(1)	18(1)	28(1)	0(1)	-1(1)	-2(1)
C(1)	24(1)	18(1)	20(1)	-2(1)	-4(1)	2(1)
C(8)	25(1)	19(1)	23(1)	-7(1)	-4(1)	2(1)
C(14)	19(1)	20(1)	16(1)	-1(1)	-1(1)	0(1)
C(10)	25(1)	22(1)	20(1)	1(1)	3(1)	-2(1)
C(3)	22(1)	26(1)	20(1)	5(1)	4(1)	2(1)
C(16)	25(1)	20(1)	31(1)	-7(1)	-2(1)	0(1)
C(2)	23(1)	19(1)	27(1)	2(1)	1(1)	-2(1)
C(15)	22(1)	27(1)	19(1)	-6(1)	1(1)	2(1)
C(17)	31(1)	19(1)	30(1)	3(1)	-4(1)	-1(1)