Electronic Supplementary Information

Binuclear Cu(II) complex as an efficient Photocatalyst for N-alkylation of aromatic amines

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Section 01. Materials and Instrumentation

All the chemical reagents required were purchased from Sigma and used without further purification. Infrared spectra (4000 to 500 cm^{-1}) were recorded with a BRUKER alpha-II instrument. NMR spectra were recorded on an AVANCE III 400 Ascend Bruker BioSpin machine at ambient temperature. Mass spectrometric analyses were done on Bruker- Daltonics, microTOF-Q II mass spectrometer and elemental analyses were carried out with a ThermoFlash 2000 elemental analyzer. Spectrophotometric measurements were performed on a Perkin Elmer UV-Vis-NIR spectrophotometer (Model: Lambda 1050) using a quartz cuvette with a path length of 2 cm. All voltammetric experiments were performed using a CHI 104 electrochemical workstation (CH Instruments Model CHI62OD series). Potentials were referenced vs the Ag/AgCl electrode, and ferrocene was added as internal standard. HPLC analysis was done through a Dionex HPLC-Ultimate 3000 (High Performance Liquid Chromatography) pump, which was used to analyze products onto a Dionex Acclaim ® 120 C18 column. GC-MS analysis was performed using GC-Hewlett Packard 6890 equipped with HP-5 column (30 m length, 0.25 mm internal diameter and 1 µm film thickness). The Gaussian 09 D.01 package has been used for the computational study.[1] The Pople diffuse basis set 6-31G(d,p) has been considered for non-metals (C, H, O, and N), whereas the effective core potential (ECP) LANL2DZ has been considered for the Cu atom.[2-4] All the calculations are performed using Becke's three-parameter hybrid exchange functional and Lee–Yang–Parr's correlation functional (B3LYP).[5-7]

Section 02. X-ray crystallography

Single crystal X-ray structural studies of complex 1 and complex **2** were performed on a CCD Agilent Technologies (Oxford Diffraction) SUPER NOVA diffractometer. Data for both the compounds were collected at 293 K using a graphite-monochromated MoKα radiation ($\lambda\alpha$ = 0.71073 Å). The strategy for the data collection was evaluated by using the CrysAlisPro CCD software.[8] The data were collected by the standard 'phi-omega scan techniques and were scaled and reduced using CrysAlisPro RED software. The structures were solved by direct

methods using SHELXS and refined by full matrix least-squares with SHELXL, refining on *F*2.[9] The positions of all the atoms were obtained by direct methods. All non-hydrogen atoms were refined anisotropically. The remaining hydrogen atoms were placed in geometrically constrained positions and refined with isotropic temperature factors, generally 1.2*U*eq of their parent atoms. The crystal and refinement data are summarized in Table S1, and the corresponding bond length(s) and bond angle(s) are summarized in Table S2.

Section 03. Powder X-ray Diffraction (PXRD)

Powder X-ray diffraction (PXRD) spectra were recorded with the help of a Rigaku Smart Lab automated multipurpose X-ray diffractometer with a Cu Kα source (the wavelength of X-rays was 0.154 nm). The tube voltage and current were 40 kV and 30 mA, respectively. The XRD patterns were recorded between 20° and 80° (2θ) with a step size and a scan speed of 2°/min.

Section 04. Procedure of HPLC analysis

A Dionex HPLC-Ultimate 3000 (High Performance Liquid Chromatography) pump was used to analyze products. 20 µL of sample was injected onto a Dionex Acclaim ® 120 C18 column of 250 mm length with an internal diameter of 4.6 mm and 5 µm fused silica particles at a flow rate of 1 mL min-1 (linear gradient of 40 % v/v acetonitrile in water for 35 min, gradually rising to 100 % (v/v) acetonitrile in water at 35 min). This concentration was kept constant until 40 min when the gradient was decreased to 40 % (v/v) acetonitrile in water at 42 min. The sample preparation involved mixing of 100 µL of the reaction mixture in 900 µL acetonitrile-water (50: 50 mixture) solution containing 0.1 % trifluoroacetic acid. The samples were then filtered through a 0.45 µm syringe filter (Whatman, 150 units, 13 mm diameter, 2.7 mm pore size) before injection. The products were identified by using Ultimate 3000 RS Variable Wavelength Detector at 254 nm as well as 280 nm.

Section 05. Formulas for calculation of Yield

Conversion of primary alcohol, selectivity, and yield of aldehyde was calculated from the following formulas

conversion (%) = $(C_0 - C_R/C_0) \times 100\%$ (1)

yield (%) = $C_P/C_0 \times 100\%$ (2)

selectivity (%) = $C_P/(C_0 - C_P) \times 100\%$ (3)

In the equations, C_0 is the initial concentration of reactant; C_R and C_P are the concentrations of the residual alcohol and the product aldehyde at a certain reaction time, respectively.

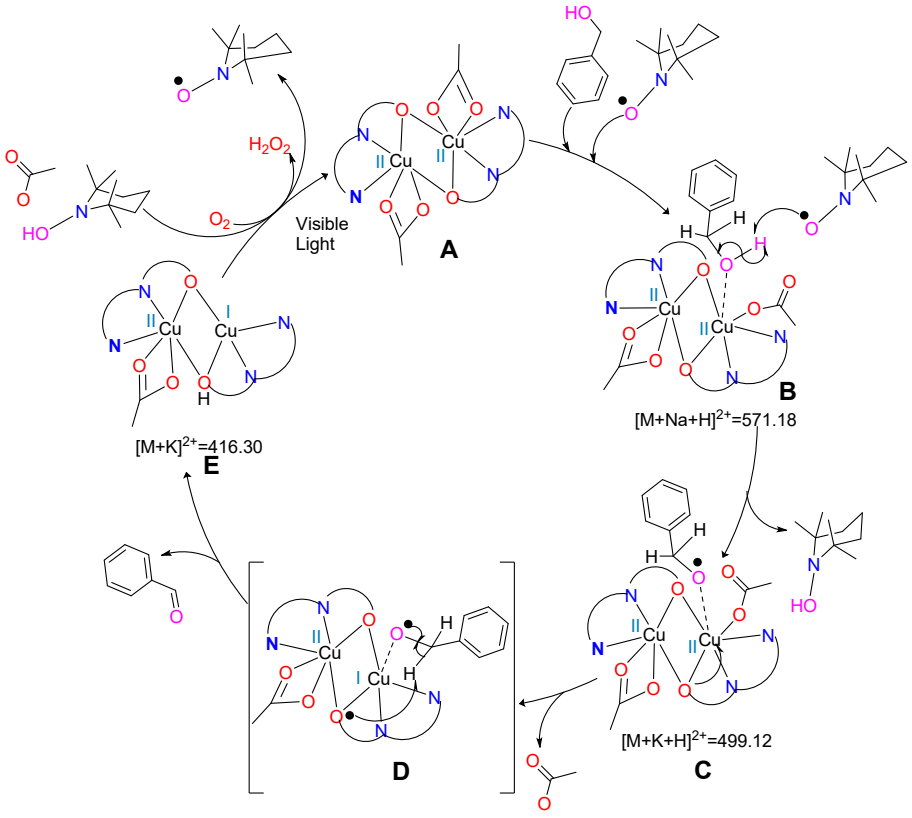
Section 06. Recovery and Reusability of catalyst

The photocatalyst was then further tested for probable reusability for oxidation as well as N-alkylation reactions. The catalyst can be recovered almost quantitatively by extraction using DCM and ethyl acetate. The catalytic reaction mixture was poured into 10 mL of DCM which was further extracted with (2 × 10 mL) ethyl acetate. The product was obtained in the ethyl acetate layer and the photocatalyst was recovered from DCM. After extraction the dichloromethane was evaporated by rotatory evaporator and the solid was washed with ether and dried in vacuum.

The stability of the compound was investigated by the PXRD pattern and it has been found that the pattern remains almost same after the reaction (Fig. S5). The recovered catalyst can be utilized further for four more cycles without much depreciation of its activity (Fig. S16) or significant changes in the structure of the molecule or solid which was further confirmed by LCMS, IR and PXRD pattern (Fig.S1B, S2B and S5).

Section 07. Mechanism for Photocatalytic Oxidation

The plaussible simplified mechanism on the basis of ESI-MS data for the oxidation of benzyl alcohol is depicted in Scheme S1. The reaction begins by the binding of the Benzyl alcohol to complex A through an unshared pair of electrons, forming B. TEMPO is converted into TEMPOH by abstraction of hydrogen from benzyl alcohol to form an intermediate C. In the presence of visible light the phenoxide ion get oxidized to phenoxyl radical by donating a single electron to Cu(II) which gets reduced to Cu(I) and then generate the species D by releasing the acetate ion, which gives the desired product benzaldehyde. After that, the intermediate D gets converted into E. ESI-MS spectrometry of the reaction mixture reveals a molecular ion peak at 571.18, 499.12 and 416.30 indicating formation of intermediate B,C and E respectively (Fig S15). TEMPO is regenerated from TEMPOH which leads to the formation of Cu(II) complex (A) by the oxidation of Cu(I) species in the presence of molecular oxygen under visible light irradiation.



Scheme S1. Proposed Mechanism for the Photocatalytic Oxidation of Benzyl Alcohol.

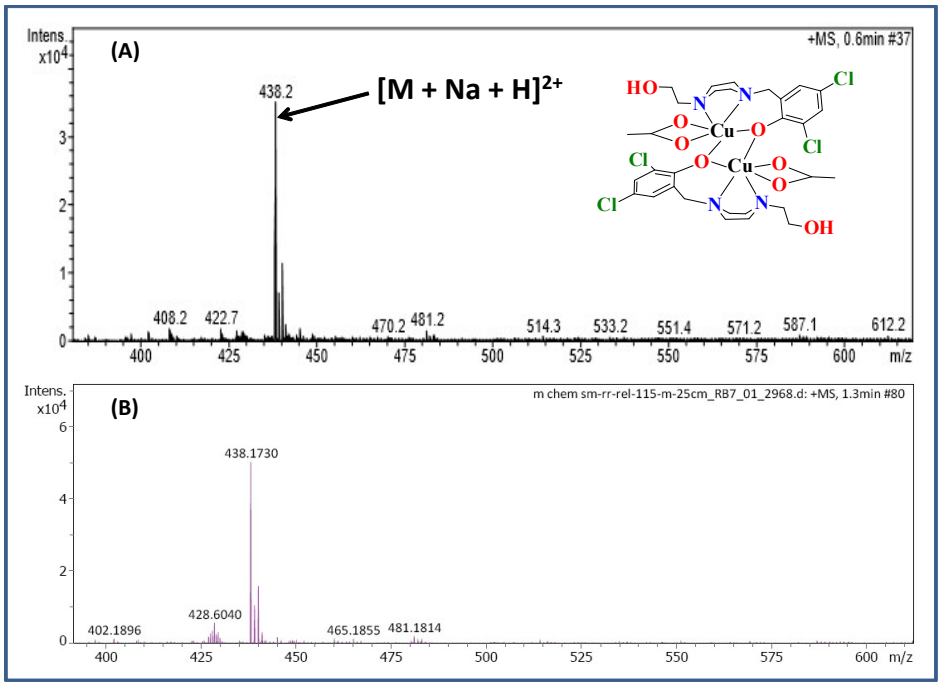


Figure S1. ESI-MS Spectra in MeOH for Complex (A) synthesized and (B) recovered from catalytic reaction.

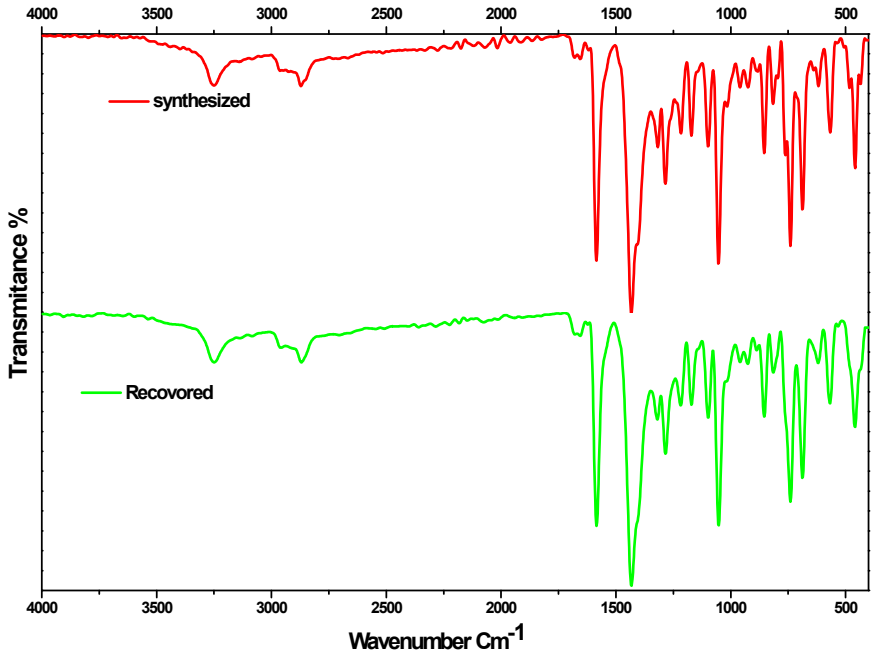


Figure S2. FTIR stretching frequencies of Complex (A) before and (B) after catalytic reaction.

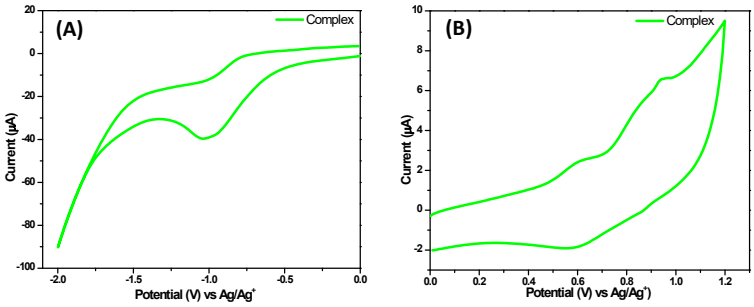


Figure S3. Cyclic voltammograms of (1.0×10^{-4} M) solution of complex in CH_2Cl_2 containing 0.1 M Bu_4NPF_6 as the supporting electrolyte. The data were recorded at a scan speed of 100 mV s^{-1} at 25 °C.

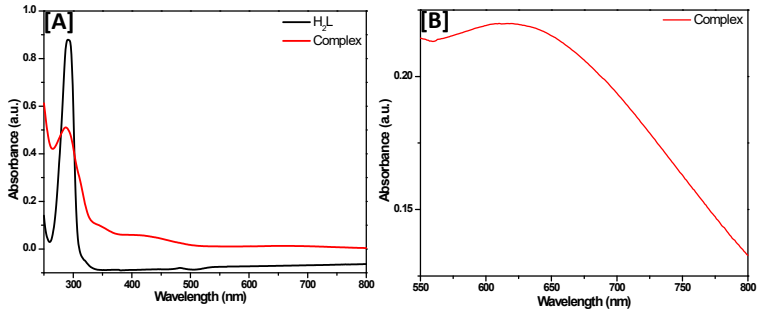


Figure S4. UV-Vis spectra in dichloromethane for (a) Ligand and Complex, and (b) complex.

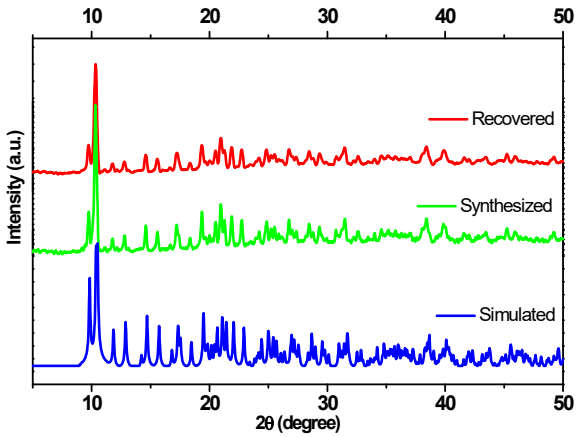


Figure S5. Powder X-ray diffraction patterns of photocatalyst.

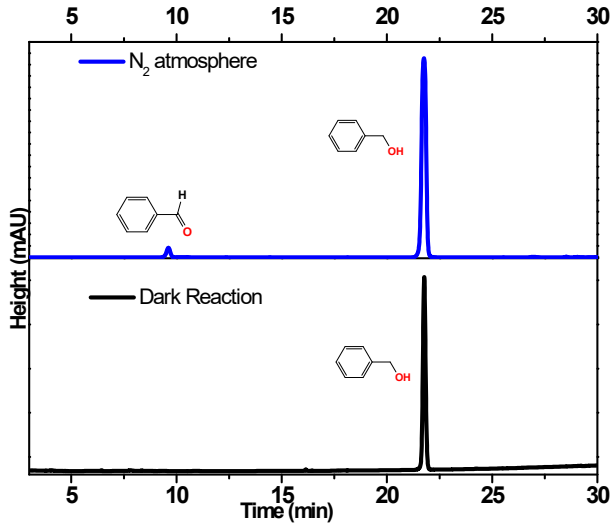


Figure S6. HPLC Chromatogram of benzyl alcohol oxidation reaction in (a) N_2 atmosphere and (b) dark reaction.

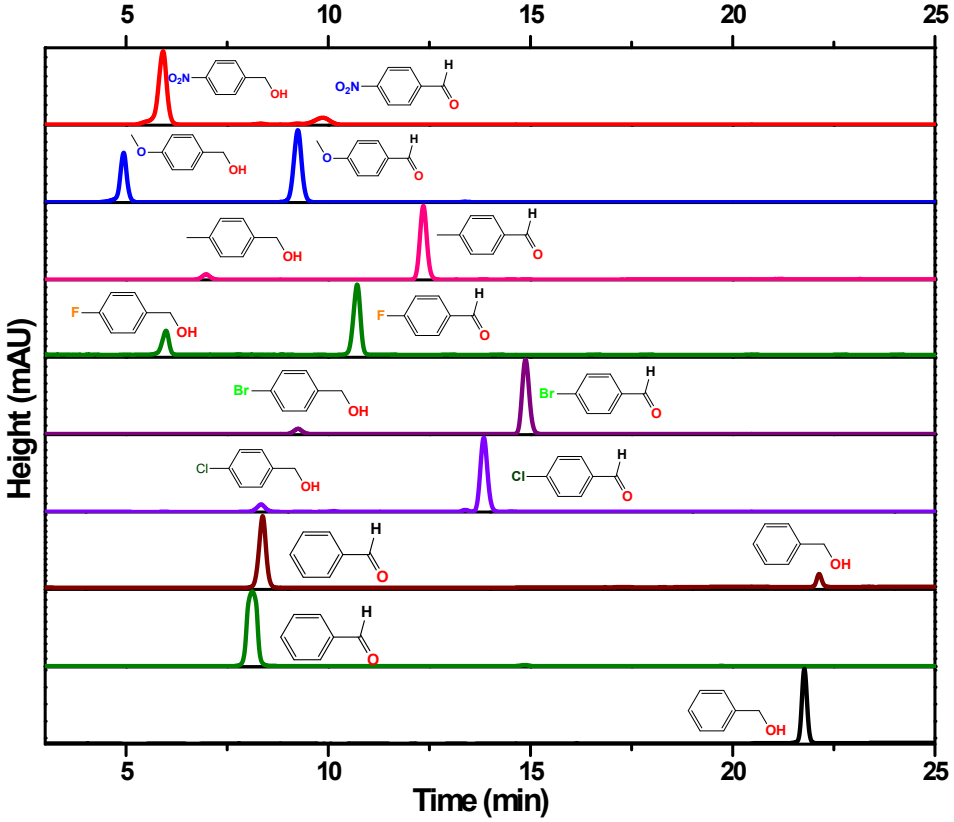


Figure S7. HPLC Chromatogram of oxidation reactions after catalysis ('Ref.' signifies the standard sample).

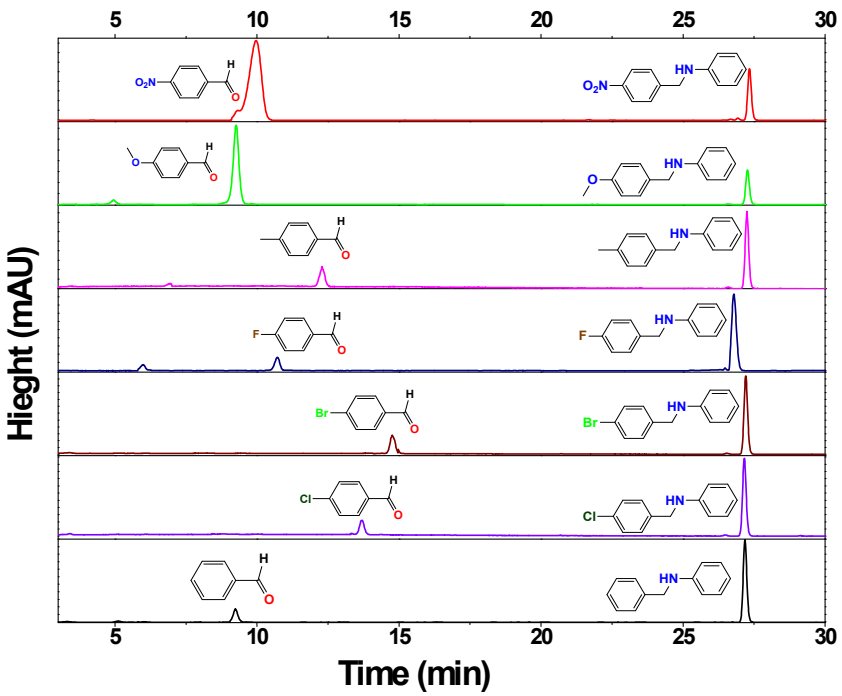


Figure S8. HPLC Chromatogram of N-alkylation reactions of substituted benzyl alcohols with aniline after catalysis.

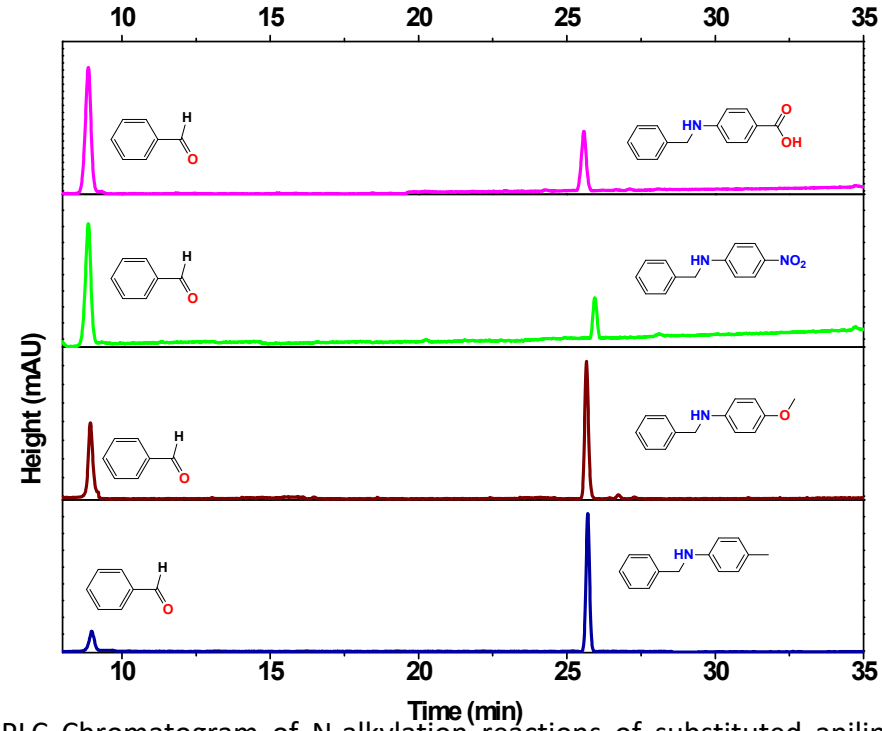
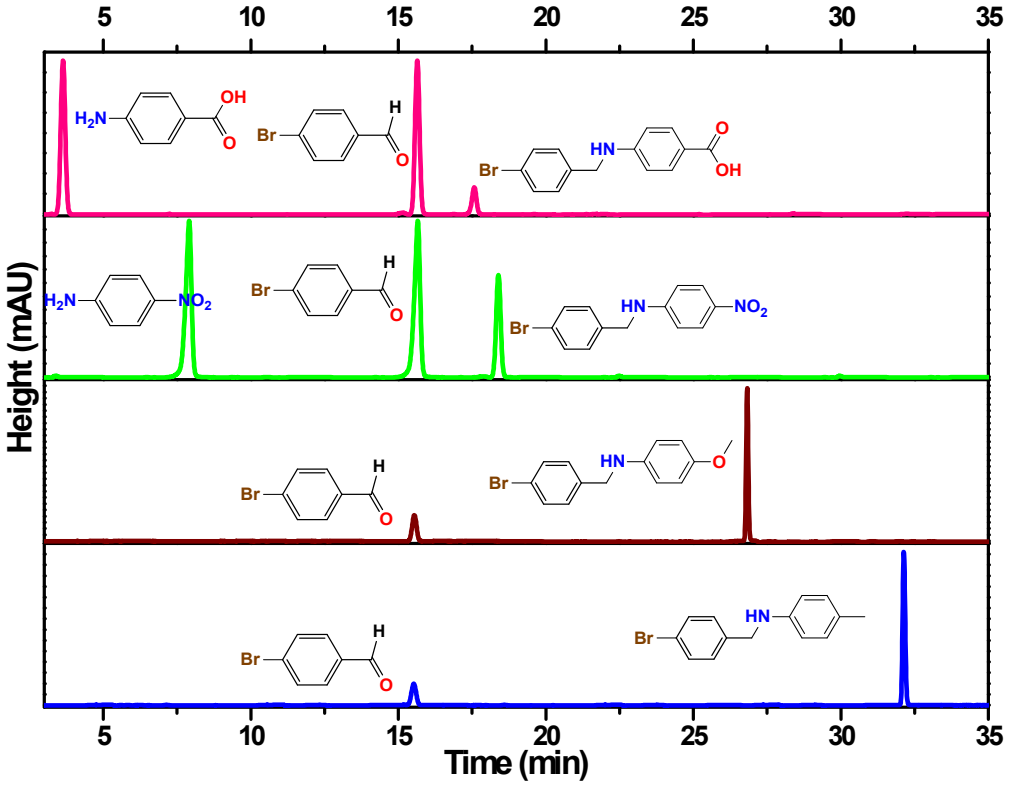
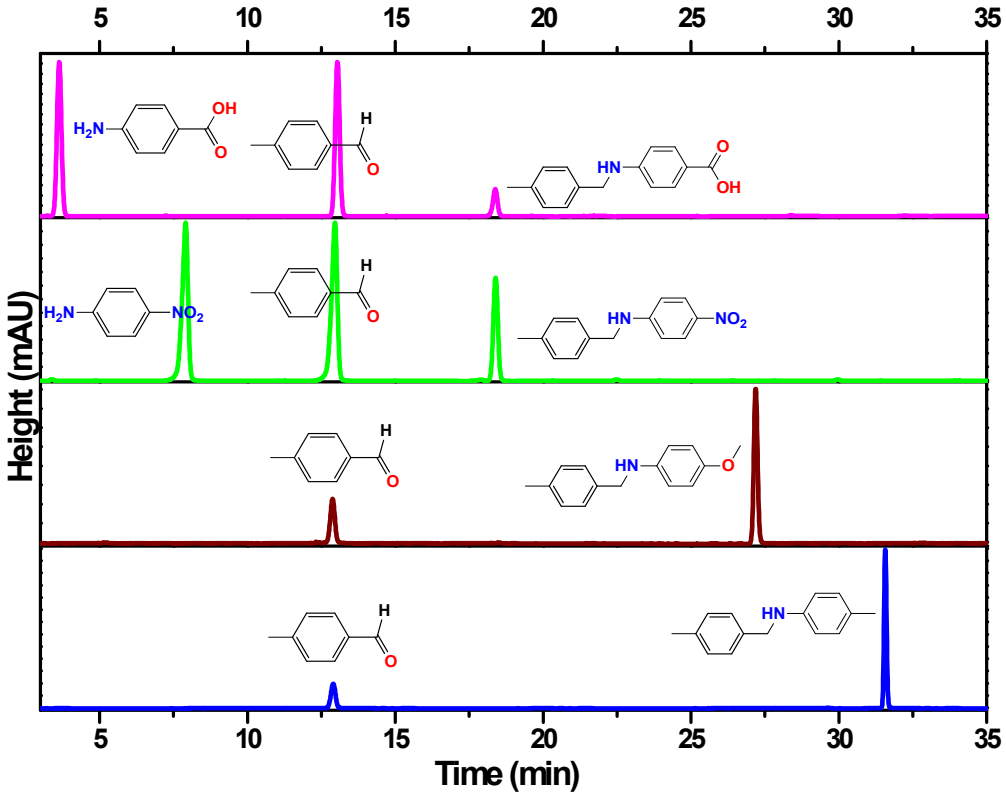


Figure S9. HPLC Chromatogram of N-alkylation reactions of substituted anilines with benzyl alcohol after catalysis.


5
10
15
20
25
30
35
Height (mAU)
Time (min)
H2N
OH
O
Br
H
HN
NO2


5
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Height (mAU)
Time (min)
H2N
OH
O
Br
H
HN
NO2

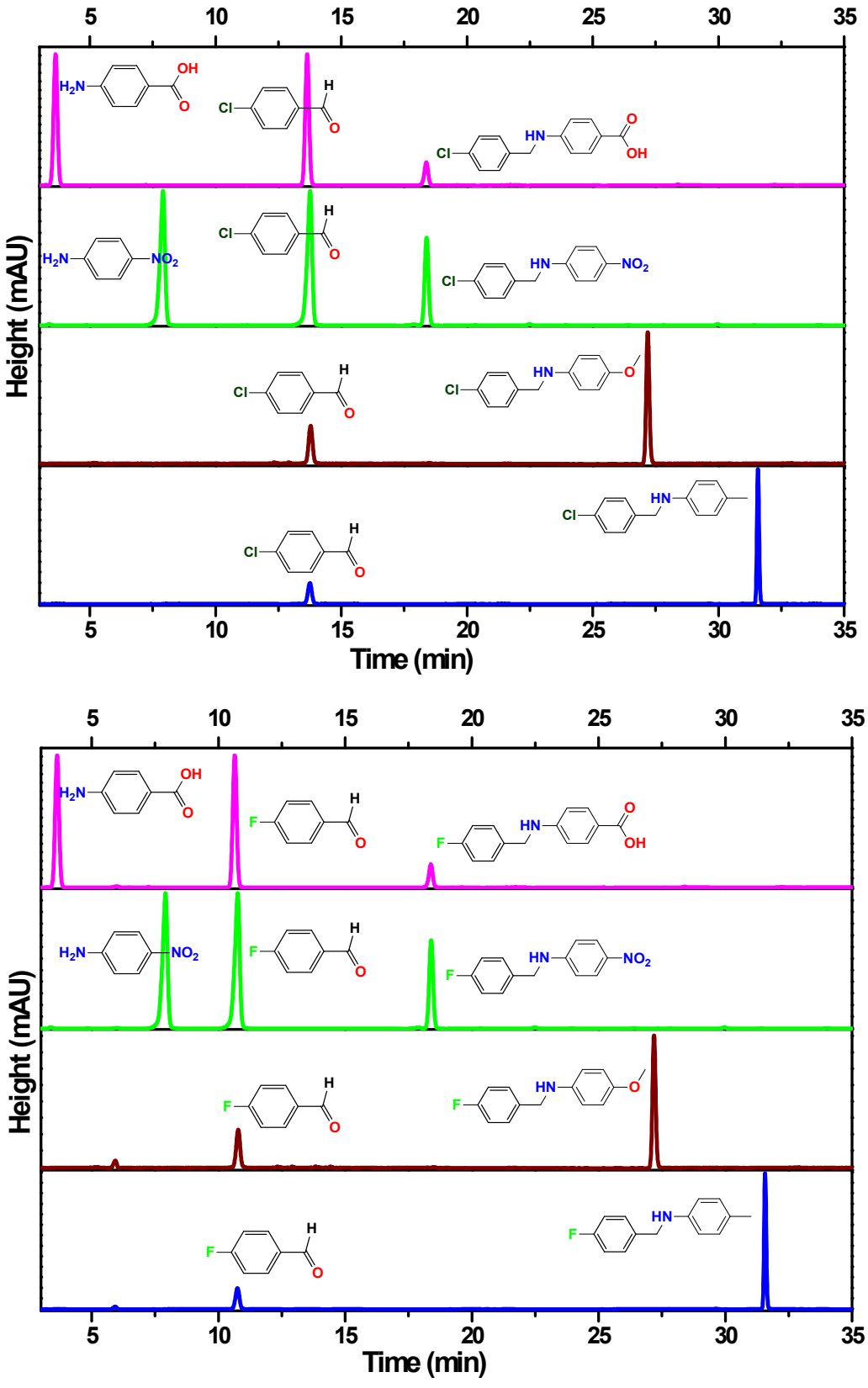

Figure S10. HPLC Chromatogram of N-alkylation reactions of substituted anilines with substituted benzyl alcohol after catalysis.

Peak Report TIC							
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	14.614	2568693	24.87	612570	25.50	4.19	Benzenamine, N-(phenylmethylene)-
2	14.886	2302317	22.29	693810	28.88	3.32	Benzenemethanamine, N-phenyl-
3	14.950	1247037	12.07	526348	21.91	2.37	Benzenemethanamine, N-phenyl-
4	15.057	4212249	40.78	569576	23.71	7.40	Benzenemethanamine, N-phenyl-
		0330296	100.00	2402304	100.00		

Peak Report TIC							
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	14.621	408419	100.00	112914	100.00	3.62	Benzenamine, N-[(4-chlorophenyl)methyl]-
		408419	100.00	112914	100.00		

Peak Report TIC							
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	11.584	3823812	62.13	688456	57.24	5.55	Benzaldehyde, 4-methoxy-
2	16.356	2330575	37.87	514292	42.76	4.53	Benzenamine, N-[(4-methoxyphenyl)methyl]-
		6154387	100.00	1202748	100.00		

Peak Report TIC							
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	16.209	1022833	100.00	370934	100.00	2.76	Benzenamine, N-[(4-bromophenyl)methyl]-
		1022833	100.00	370934	100.00		

Peak Report TIC							
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	12.300	3421917	54.44	718886	56.24	4.76	Benzaldehyde, 4-nitro-
2	17.238	2863906	45.56	559358	43.76	5.12	Benzenamine, N-[(4-nitrophenyl)methyl]-
		6285823	100.00	1278244	100.00		

Peak Report TIC							
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	10.484	1314983	51.85	526409	58.39	2.50	Benzenemethanol, 4-methyl-
2	15.548	1221023	48.15	375138	41.61	3.25	Benzenamine, N-[(4-methylphenyl)methyl]-
		2536006	100.00	901547	100.00		

Figure S11. Product identification by GCMS of N-alkylation reactions of substituted benzyl alcohol with aniline during catalysis.

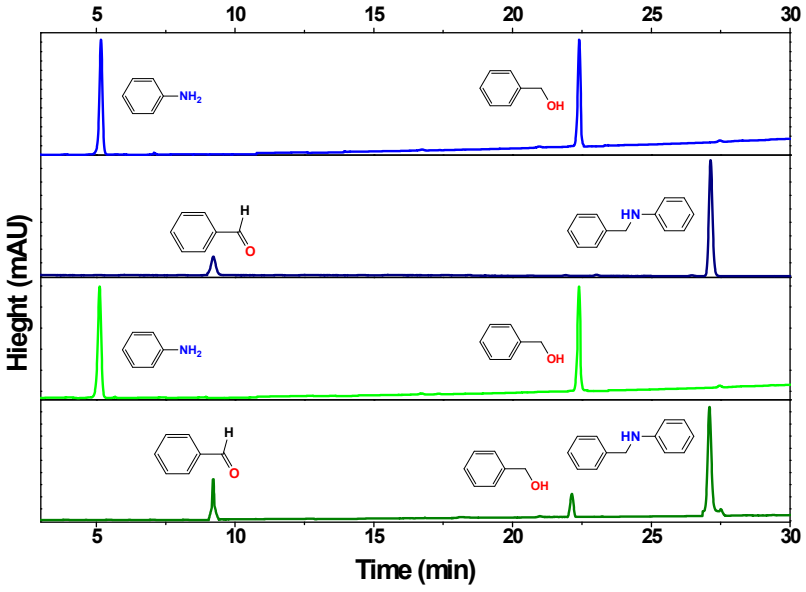

Figure S12. HPLC Chromatogram of N-alkylation reactions in presence of (a) $Cu(OAC)_2$ in DCM (b) Complex-1 in DCM (c) $Cu(OAC)_2$ in ACN (d) Complex in ACN.

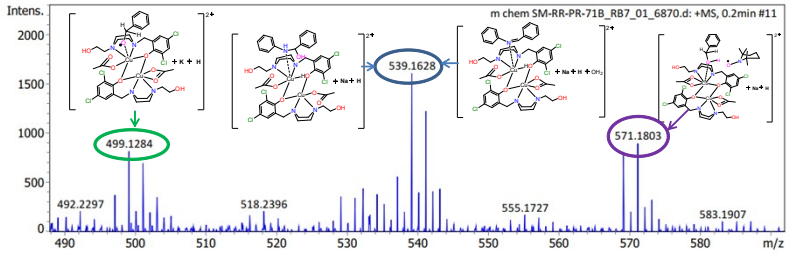

Figure S13. ESI-MS Spectrum in MeOH of the borrowing hydrogen reaction intermediates.

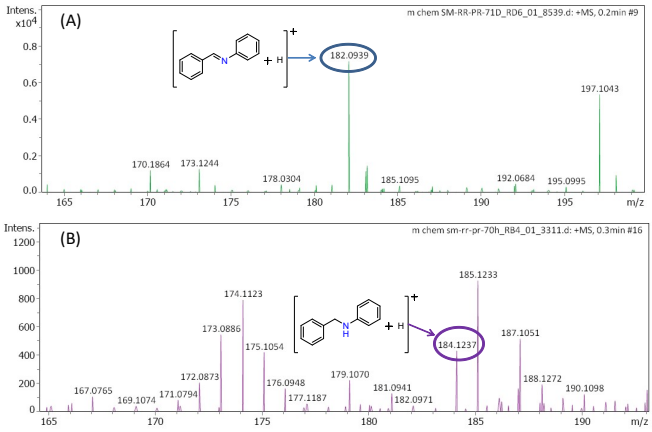

Figure S14. ESI-MS Spectrum in MeOH of (A) free Schiff base intermediate and (B) N-alkyl amine product.

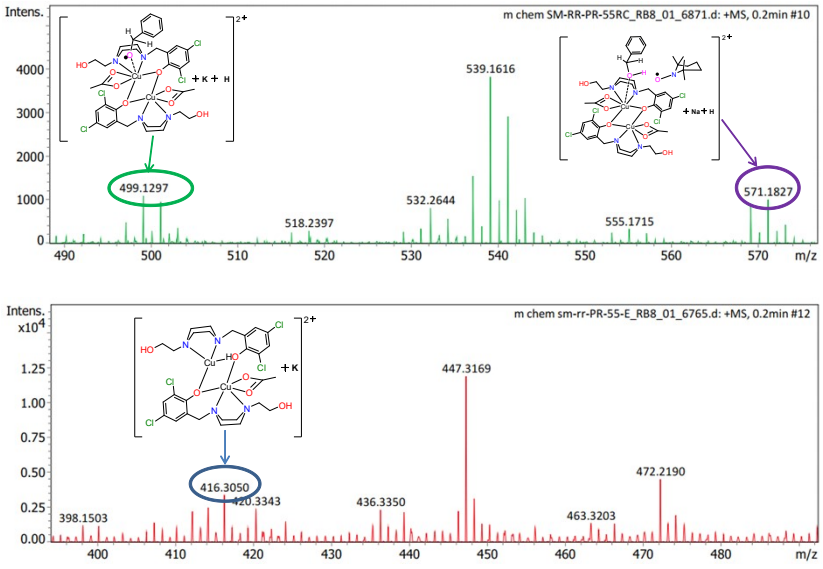

Figure S15. ESI-MS Spectrum in MeOH of the photocatalytic alcohol oxidation reaction intermediates.

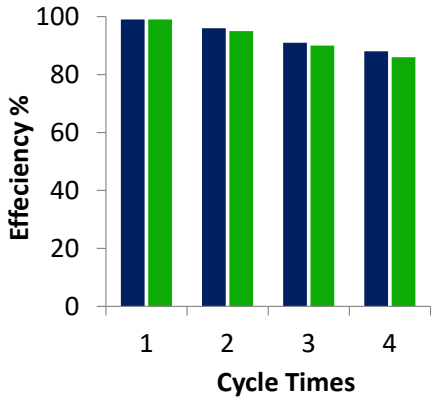

Figure S16. Reusability of the photocatalyst. The blue and green bar indicates the yield of benzaldehyde and N-benzylamine in the presence of catalyst for separate run, respectively.

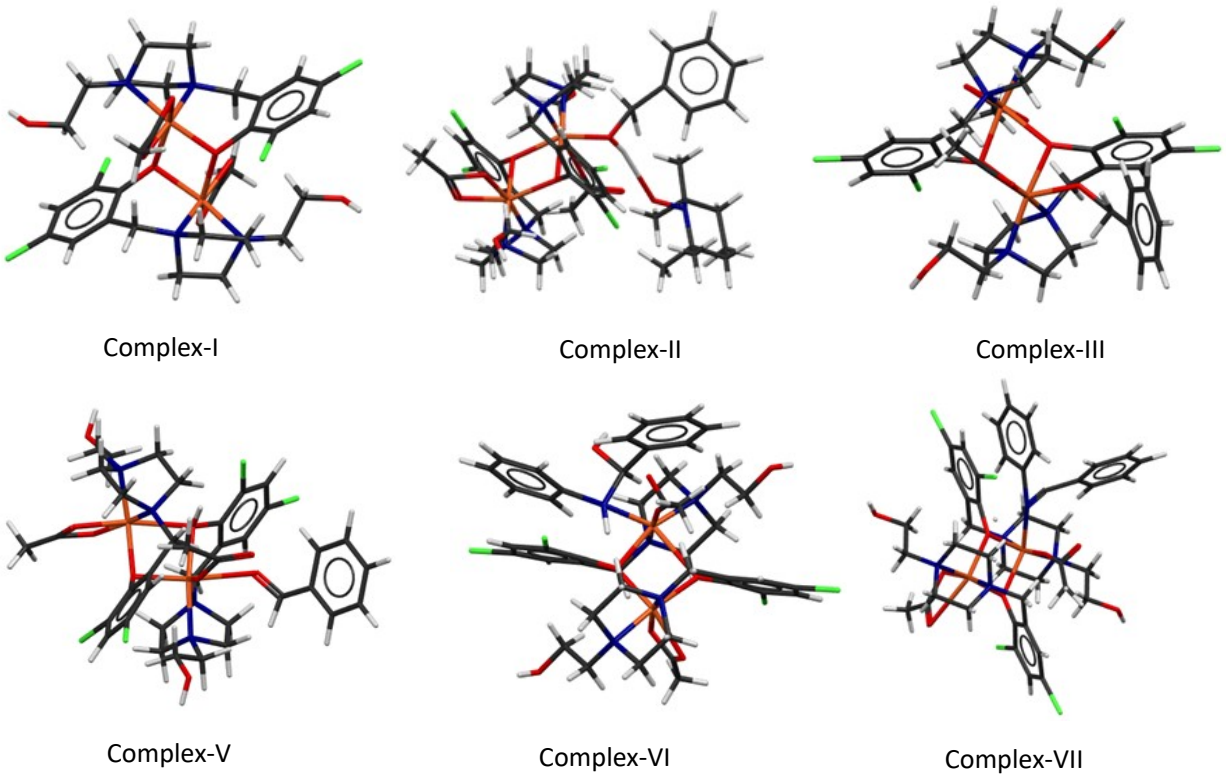

Figure S17. Optimized structures of the complex and intermediates.

Table S1. Crystallographic data and structure refinement parameters.

Complex	1
Empirical formula	$C_{15}H_{20}Cl_2CuN_2O_4$
Formula weight	426.77 g/mol
Crystal system	monoclinic
Space group	P 1 21/n 1
a (Å)	10.4399(4)
b (Å)	14.9215(5)
c (Å)	11.5303(5)
α (°)	90°
β (°)	102.3293(13)°
γ (°)	90°
V (Å^3)	1754.75(12)
λ (Å)	0.71073
ρ_{Calcd} g/cm^3	1.615
Z	2
T (K)	148(2)
F (0 0 0)	876
μ (mm−1)	1.571
Crystal size (mm^3)	0.040 x 0.060 x 0.100
ϑ ranges (°)	2.27 to 28.30
Reflections collected	35789
h/k/l	-13,13/-19,19/-15,15
Independent reflections	4353
Tmax and Tmin	0.9400 and 0.8590
Data/restraints/parameters	4353 / 0 / 219
Goodness-of-fit (GOF) on F2	1.065
Final R indices[I > 2σ(I)]	R1 = 0.0428, wR2 = 0.0828

R indices (all data)	R1 = 0.0888, wR2 = 0.1059
Largest peak and hole(e $Å^{-3}$)	0.560 and -0.512

Table S2. Selected bond lengths (Å) and bond angles (°).

Bond Lengths (Å)		Bond angles (°)	
Cu1-O2	1.947(2)	O1-Cu1-O2	91.90(10)
Cu1-O3	2.374(2)	O1-Cu1-N1	92.52(10)
Cu1-N1	2.020(3)	O2-Cu1-O3	94.13(10)
Cu1-N2	2.066(3)	O2-Cu1-N1	164.74(10)
Cu1-O1	1.943(2)	O1-Cu1-N2	165.28(10)
C1-O1	1.328(4)	O2-Cu1-O1	92.86(9)
C13-O4	1.418(4)	O3-Cu1-O1	84.96(9)
C14-O3	1.242(4)	O2-Cu1-N2	100.06(11)
C14-O2	1.268(4)	N1-Cu1-N2	73.76(11)

Table S3. Cartesian coordinates, multiplicity and energies (in Hartree) for all the species

H_2O

8 0.000000 0.000000 0.110812

1 0.000000 0.783976 -0.443248

1 0.000000 -0.783976 -0.443248

-76.3861166

$PhCH_2OH$

Multiplicity 1

6 -2.316877 0.119570 -0.180763

6 -1.717197 -1.140425 -0.130471

6 -1.541575 1.268911 -0.014465

1 -2.320383 -2.034616 -0.259851

1 -2.008127 2.249191 -0.053592

6 -0.342212 -1.251079 0.086120

6 -0.166590 1.158257 0.202125

1 0.124340 -2.231359 0.125247

1 0.436596 2.052448 0.331506

6 0.433090 -0.101738 0.252418

1 -3.386617 0.205659 -0.349270

6 1.949548 -0.223778 0.491293

1 2.225368 -1.240560 0.793264

1 2.285155 0.457647 1.281317

8 2.694983 0.092215 -0.699537

1 3.294683 0.825559 -0.509870

-346.6852127

$PhNH_2$

Multiplicity 1

7 2.327472 -0.010181 -0.071739

6 0.927847 -0.004802 -0.039781

6 0.235098 1.205568 -0.021740

6 0.225783 -1.210671 -0.025580

6 -1.159706 1.210829 0.009303

1 0.788074 2.156003 -0.033295

6 -1.168675 -1.205335 0.005934

1 0.772209 -2.164880 -0.039750

6 -1.861508 0.005492 0.022981

1 -1.705699 2.165211 0.023072

1 -1.722272 -2.155535 0.017141

1 -2.960829 0.009455 0.047628

1 2.673184 0.840996 0.323206

1 2.669995 -0.786465 0.457469

-287.5376479

TEMPO

Multiplicity 2

6 -1.270439 -0.080812 0.036157

6 -1.270439 1.209423 -0.798772

6 0.000000 2.038928 -0.554396

6 1.270439 1.209424 -0.798772

6 1.270440 -0.080811 0.036157

7 0.000000 -0.910315 -0.208219

1 -2.162938 1.806510 -0.575585

1 -1.329777 0.947889 -1.865179

1 -0.000001 2.930982 -1.192454

1	0.000000	2.399468	0.484428
1	2.162937	1.806510	-0.575585
1	1.329777	0.947889	-1.865180
8	0.000000	-2.262842	-0.606680
6	-1.353541	0.285466	1.529654
1	-2.242745	-0.150957	1.998652
1	-0.478094	-0.078867	2.079163
1	-1.404382	1.370936	1.672060
6	-2.523630	-0.919203	-0.277228
1	-2.502911	-1.298905	-1.305093
1	-2.603356	-1.783224	0.392264
1	-3.438744	-0.327172	-0.162454
6	1.353541	0.285467	1.529654
1	0.501747	-0.119516	2.087816
1	2.266840	-0.111169	1.987555
1	1.356632	1.371799	1.674505
6	2.523631	-0.919203	-0.277228
1	3.398967	-0.547294	0.267362
1	2.381806	-1.969061	0.003473
1	2.764240	-0.892947	-1.346119

-483.5922355

TEMPOH

Multiplicity 1

6	-1.268916	-0.054644	0.030875
6	-1.260609	1.254555	-0.773949
6	0.015109	2.070020	-0.510557
6	1.280217	1.238275	-0.774205
6	1.271910	-0.070924	0.030620
7	-0.003807	-0.886389	-0.232773
1	-2.149273	1.852019	-0.536905
1	-1.321570	1.018173	-1.846121
1	0.020854	2.976593	-1.127784
1	0.017369	2.406398	0.536339
1	2.176513	1.824301	-0.537340
1	1.337929	1.001132	-1.846389
8	-0.011474	-2.076910	-0.613692
6	-1.349741	0.277473	1.532463
1	-2.241746	-0.163988	1.991318
1	-0.476672	-0.105091	2.073299
1	-1.393632	1.359657	1.699974

6 -2.527439 -0.877506 -0.301716

1 -2.509104 -1.233426 -1.338100

1 -2.612732 -1.756271 0.347595

1 -3.438747 -0.282440 -0.173169

6 1.357286 0.260128 1.532191

1 0.502888 -0.152207 2.080909

1 2.268002 -0.152850 1.980691

1 1.367331 1.342772 1.702160

6 2.519718 -0.909847 -0.302224

1 3.397393 -0.556266 0.250745

1 2.371155 -1.964993 -0.045897

1 2.760541 -0.860385 -1.370244

1 -0.183262 -2.858307 -0.083118

-484.1901072

$PhCH_2NHPh$ (Product)

Multiplicity 1

7 -0.502003 -0.231705 -0.970103

1 -2.397692 1.494300 -1.796932

6 -1.874450 -0.101559 -0.459857

6 -2.737628 0.857086 -1.007438

6	-2.319671	-0.936132	0.574159
6	-4.046026	0.981161	-0.521000
1	-2.397692	1.494300	-1.796932
6	-3.628069	-0.812058	1.060596
1	-1.660615	-1.668079	0.992248
6	-4.491247	0.146590	0.513017
1	-4.705083	1.713107	-0.939091
1	-2.397692	1.494300	-1.796932
1	-3.968005	-1.449271	1.850091
1	-5.490237	0.241325	0.884425
1	-0.183306	0.656941	-1.299862
6	0.379826	-0.698817	0.109287
6	1.864528	-0.290038	0.121881
6	2.263282	0.881152	0.780085
6	2.816853	-1.089238	-0.524863
6	3.614361	1.253140	0.791547
1	1.536160	1.491359	1.273888
6	4.167932	-0.717250	-0.513401
1	2.512396	-1.983467	-1.027416
6	4.566687	0.453938	0.144806

1 3.918818 2.147369 1.294100

1 4.895054 -1.327457 -1.007203

1 5.598266 0.737957 0.153561

-557.7545981

Complex I

Multiplicity 1

29	-0.04180000	1.40880000	-0.03470000
6	-2.53440000	0.09970000	0.30310000
6	-3.52510000	0.01170000	1.30760000
6	-4.90430550	0.12631147	1.03786608
1	-5.56420550	0.02251147	1.75586608
6	-5.28510000	0.38620000	-0.25670000
6	-4.35740000	0.58840000	-1.26020000
1	-4.65680000	0.82890000	-2.16220000
6	-2.99730000	0.45100000	-0.99520000
6	-1.98220000	0.63670000	-2.08720000
1	-1.55410000	-0.25390000	-2.29930000
1	-2.44680000	0.96920000	-2.92430000
6	0.14870000	1.62040000	-2.75750000
1	-0.16510000	1.97590000	-3.65250000

1	0.50010000	0.68140000	-2.88780000
6	1.25290000	2.52870000	-2.18190000
1	2.12070000	2.01530000	-2.11020000
1	1.40030000	3.32490000	-2.78970000
6	-0.36760000	3.86400000	-1.04240000
1	-0.13240000	4.62680000	-1.66560000
1	-0.66940000	4.25240000	-0.15820000
6	-1.49240000	3.00200000	-1.65500000
1	-2.30810000	3.01620000	-1.05750000
1	-1.75330000	3.36380000	-2.56490000
6	1.89050000	3.72350000	-0.12170000
1	1.49030000	4.17550000	0.69090000
1	2.25320000	4.44830000	-0.73090000
6	3.04470000	2.83430000	0.32910000
1	2.70540000	2.14120000	0.98210000
1	3.43840000	2.35190000	-0.46950000
6	0.16810000	1.85210000	1.86310000
6	0.40310000	1.99100000	3.35470000
1	0.84640000	2.87280000	3.54210000
1	0.99390000	1.24440000	3.67240000

1	-0.47810000	1.95090000	3.83520000
17	-3.08506495	-0.19698945	2.81066948
17	-6.84153128	0.50292102	-0.56001153
7	-0.92940000	1.60430000	-1.69490000
7	0.82180000	2.99010000	-0.83310000
8	-1.15530000	-0.14190000	0.59410000
8	1.07190000	1.01630000	1.38930000
8	-0.86800000	2.58000000	1.24280000
8	4.04600000	3.63080000	0.95430000
1	4.54080000	4.01970000	0.34730000
29	0.20470000	-1.60720000	0.07980000
6	2.66530000	-0.37380000	-0.20960000
6	3.65590000	-0.28580000	-1.21400000
6	5.01110000	-0.39850000	-0.94910000
1	5.67090000	-0.29460000	-1.66710000
6	5.41600000	-0.66040000	0.35020000
6	4.48820000	-0.86260000	1.35380000
1	4.78760000	-1.10310000	2.25580000
6	3.12830000	-0.72520000	1.08880000
6	2.11300000	-0.91080000	2.18090000

1	1.68500000	-0.02020000	2.39290000
1	2.57760000	-1.24340000	3.01790000
6	-0.06720000	-1.88510000	2.76110000
1	0.24670000	-2.24060000	3.65610000
1	-0.41860000	-0.94610000	2.89140000
6	-1.17130000	-2.79340000	2.18560000
1	-2.03910000	-2.28000000	2.11380000
1	-1.31890000	-3.58970000	2.79340000
6	0.44910000	-4.12880000	1.04600000
1	0.21390000	-4.89160000	1.66920000
1	0.75100000	-4.51720000	0.16180000
6	1.57390000	-3.26680000	1.65860000
1	2.38960000	-3.28100000	1.06100000
1	1.83480000	-3.62860000	2.56850000
6	-1.77440000	-3.92810000	0.09770000
1	-1.37430000	-4.38010000	-0.71490000
1	-2.13710000	-4.65280000	0.70690000
6	-2.92860000	-3.03890000	-0.35310000
1	-2.58950000	-2.34580000	-1.00620000
1	-3.32230000	-2.55640000	0.44560000

6	-0.00090000	-2.09150000	-1.93670000
6	-0.23600000	-2.23030000	-3.42830000
1	-0.67920000	-3.11220000	-3.61560000
1	-0.82680000	-1.48370000	-3.74600000
1	0.64520000	-2.19030000	-3.90890000
17	3.22702838	-0.08240489	-2.67902545
17	6.89410420	-0.77124706	0.63833350
7	1.06030000	-1.87850000	1.78840000
7	-0.70580000	-3.19470000	0.80900000
8	1.27660000	-0.13050000	-0.50250000
8	-0.78230000	-1.29870000	-1.30630000
8	1.04260000	-2.82440000	-1.31200000
8	-3.93000000	-3.83540000	-0.97840000
1	-4.42480000	-4.22430000	-0.37120000

-4220.6080899

Complex II

Multiplicity 2

29	-0.464313	-0.599140	1.478413
6	0.788783	-2.522845	-0.094414
6	2.062111	-2.652792	-0.687791

6	2.772418	-3.838876	-0.696642
1	3.611923	-3.898018	-1.138274
6	2.237186	-4.938214	-0.050960
6	1.047797	-4.842961	0.637690
1	0.720423	-5.590904	1.122440
6	0.323758	-3.655816	0.624895
6	-0.989083	-3.549829	1.342826
1	-1.719209	-3.469118	0.679548
1	-1.142969	-4.375614	1.867460
6	-2.387759	-2.138695	2.778833
1	-2.663878	-2.884600	3.368132
1	-3.035398	-2.069561	2.034140
6	-2.348352	-0.822620	3.572857
1	-3.022367	-0.191598	3.215429
1	-2.555067	-0.994807	4.524979
6	-0.060928	-1.171406	4.141641
1	-0.344194	-1.291974	5.082206
1	0.858259	-0.802902	4.136241
6	-0.094222	-2.521389	3.399564
1	0.812378	-2.758694	3.082065

1	-0.410757	-3.236117	4.007857
6	-0.901590	1.112475	4.024001
1	0.051442	1.375273	4.085993
1	-1.267867	1.091691	4.944038
6	-1.650615	2.164437	3.219555
1	-1.258770	2.232949	2.313121
1	-2.600242	1.899689	3.126916
6	0.391481	2.826567	0.154975
6	-0.378341	3.828149	-0.678993
1	-0.652499	4.580741	-0.114331
1	-1.171993	3.396388	-1.056907
1	0.193071	4.155669	-1.404898
6	2.802236	-1.259973	-1.420123
6	3.131221	-6.434659	-0.077090
7	-1.019736	-2.381774	2.249520
7	-0.987366	-0.240247	3.443966
8	0.086650	-1.401499	-0.203097
8	-0.022567	1.169150	0.795278
8	1.471096	3.429841	0.277168
8	-1.563921	3.417603	3.875684

1	-2.124778	3.446089	4.500645
29	-1.859741	-0.747348	-1.393994
6	-3.112885	1.176445	0.178846
6	-4.386165	1.306305	0.772211
6	-5.096519	2.492476	0.781073
1	-5.935978	2.551531	1.222693
6	-4.561241	3.591726	0.135379
6	-3.371851	3.496474	-0.553271
1	-3.044477	4.244417	-1.038020
6	-2.647860	2.309416	-0.540464
6	-1.334885	2.203390	-1.258421
1	-0.604893	2.122718	-0.595117
1	-1.180999	3.029175	-1.783054
6	0.063705	0.792207	-2.694414
1	0.339777	1.538200	-3.283701
1	0.711343	0.723074	-1.949721
6	0.024337	-0.523732	-3.488439
1	0.698265	-1.154802	-3.130998
1	0.231099	-0.351632	-4.440574
6	-2.263127	-0.175081	-4.057221

1	-1.979908	-0.054426	-4.997774
1	-3.182361	-0.543498	-4.051810
6	-2.229832	1.174902	-3.315145
1	-3.136432	1.412207	-2.997645
1	-1.913212	1.889678	-3.923451
6	-1.422511	-2.458875	-3.939569
1	-2.375497	-2.721760	-4.001574
1	-1.056235	-2.438091	-4.859606
6	-0.673487	-3.510837	-3.135123
1	-1.065285	-3.579436	-2.228702
1	0.276227	-3.246041	-3.042498
6	-3.995307	-2.311932	-1.357474
6	-4.912368	-3.454616	-0.977482
1	-5.087302	-4.008826	-1.766499
1	-4.485857	-3.998374	-0.283556
1	-5.758240	-3.094559	-0.637338
17	-5.126291	-0.086514	1.504542
17	-5.455323	5.088259	0.161522
7	-1.304319	1.035286	-2.165101
7	-1.336689	-1.106241	-3.359547

8	-2.410665	0.055147	0.287515
8	-2.788495	-2.407316	-0.981210
8	-4.440286	-1.349295	-2.005365
8	-0.760133	-4.764090	-3.791265
1	-0.199237	-4.792440	-4.416227
6	5.472673	-0.717848	0.569713
6	4.265992	-1.391571	0.760735
6	3.881539	-1.783992	2.042696
6	4.704494	-1.503758	3.134223
6	5.911095	-0.830612	2.943109
6	6.295054	-0.437269	1.660819
1	5.775386	-0.408152	-0.441027
1	3.617503	-1.611945	-0.099579
1	4.401184	-1.813317	4.144902
1	6.559904	-0.609614	3.803157
1	7.246225	0.093564	1.510421
6	2.531578	-2.461840	1.743153
1	2.786088	-1.617288	1.057608
1	1.863711	-2.314483	2.626466
8	1.646167	-1.741140	0.882026

1	2.196335	-1.018355	0.571388
6	5.665567	2.847073	-2.384954
17	4.355144	2.115429	-2.177509
17	4.211377	3.027331	0.147110
6	5.522165	3.758527	-0.059750
6	5.745279	4.089256	-1.521352
1	6.518256	2.162921	-2.133487
1	5.769668	3.132494	-3.463927
1	5.524075	4.703352	0.543448
1	6.367068	3.120394	0.310919
1	4.971721	4.828210	-1.858845
1	6.749467	4.571003	-1.648325
6	4.075305	2.659558	1.543078
1	4.110017	3.540725	2.149080
1	4.875532	2.005086	1.819130
1	3.139953	2.161470	1.691153
6	3.109396	3.911002	-0.180399
1	2.182890	3.400681	-0.018971
1	3.180679	4.204729	-1.206821
1	3.151431	4.779685	0.442917

6	3.277400	2.928686	-2.648657
1	3.071425	2.690444	-3.671259
1	3.548805	3.960744	-2.570571
1	2.405547	2.743393	-2.056679
6	4.352514	0.910430	-2.947490
1	4.494678	1.147381	-3.981194
1	3.415599	0.409071	-2.822077
1	5.145299	0.273195	-2.615340
7	4.133471	1.783965	-0.715742
8	2.916493	1.196991	-0.560740

-5050.9073010

Complex III

Multiplicity 2

29	-0.16250000	-1.09170000	0.79890000
6	-2.24910000	0.66020000	0.23210000
6	-3.30260000	0.68820000	-0.70580000
6	-4.58910000	1.07860000	-0.38340000
1	-5.26480000	1.11990000	-1.05040000
6	-4.87360000	1.40890000	0.92890000
6	-3.91240000	1.29740000	1.90950000

1	-4.13720000	1.47440000	2.81490000
6	-2.61330000	0.92770000	1.57860000
6	-1.54970000	0.83550000	2.63240000
1	-0.89050000	1.56120000	2.49650000
1	-1.96110000	0.95980000	3.52470000
6	0.34470000	-0.47690000	3.46830000
1	0.07530000	-0.39820000	4.41760000
1	0.93580000	0.28420000	3.24470000
6	1.07950000	-1.80710000	3.23450000
1	2.01590000	-1.63330000	2.96410000
1	1.08840000	-2.34050000	4.06770000
6	-0.96720000	-2.90710000	2.70670000
1	-0.86580000	-3.43130000	3.54000000
1	-1.46610000	-3.45590000	2.05040000
6	-1.73030000	-1.59910000	2.99150000
1	-2.57440000	-1.57730000	2.47580000
1	-1.94960000	-1.53630000	3.95530000
6	1.09210000	-3.73430000	1.71790000
1	0.49830000	-4.28770000	1.15010000
1	1.32120000	-4.26670000	2.52110000

6	2.36840000	-3.43220000	0.94700000
1	2.14770000	-2.94600000	0.11350000
1	2.95980000	-2.85630000	1.49380000
6	1.18510000	-2.20440000	-2.12510000
6	2.34480000	-2.04070000	-3.08410000
1	2.93440000	-2.82090000	-3.01940000
1	2.84630000	-1.23150000	-2.85440000
1	2.00270000	-1.96500000	-3.99950000
17	-2.99550000	0.18250000	-2.34100000
17	-6.49420000	1.91340000	1.32670000
7	-0.85610000	-0.47010000	2.59150000
7	0.36050000	-2.52520000	2.13780000
8	-0.81550000	0.42580000	-0.17810000
8	0.60760000	-1.72750000	-0.87190000
8	0.30370000	-3.00350000	-2.48440000
8	3.03440000	-4.64330000	0.63380000
1	3.46230000	-4.90980000	1.30610000
29	0.96490000	1.71360000	-0.41410000
6	2.85460000	-0.22510000	0.21380000
6	3.89190000	-0.24810000	1.15580000

6	5.19460000	-0.64350000	0.82930000
1	5.87030000	-0.68470000	1.49640000
6	5.47900000	-0.97370000	-0.48290000
6	4.51780000	-0.86220000	-1.46350000
1	4.74270000	-1.03920000	-2.36890000
6	3.21890000	-0.49250000	-1.13270000
6	2.15510000	-0.40030000	-2.18650000
1	1.49610000	-1.12600000	-2.05050000
1	2.56650000	-0.52460000	-3.07870000
6	0.26080000	0.91210000	-3.02230000
1	0.53030000	0.83330000	-3.97160000
1	-0.33040000	0.15100000	-2.79870000
6	-0.47390000	2.24220000	-2.78860000
1	-1.41040000	2.06850000	-2.51820000
1	-0.48290000	2.77570000	-3.62180000
6	1.57270000	3.34230000	-2.26070000
1	1.47130000	3.86640000	-3.09400000
1	2.07160000	3.89100000	-1.60440000
6	2.33570000	2.03430000	-2.54550000
1	3.17990000	2.01250000	-2.02980000

1	2.55510000	1.97140000	-3.50940000
1	-0.49560000	4.19450000	-1.29530000
1	0.09800000	4.74790000	-0.72750000
1	-0.72470000	4.72690000	-2.09850000
6	-1.77200000	3.89240000	-0.52430000
1	-1.55130000	3.40620000	0.30920000
1	-2.36340000	3.31640000	-1.07120000
6	1.27070000	2.92630000	1.23760000
6	1.27440000	3.62300000	2.58130000
6	1.11300000	4.58100000	2.45260000
1	0.56940000	3.24540000	3.14660000
1	2.14470000	3.49360000	3.01330000
17	3.58480000	0.25760000	2.79110000
17	7.09980000	-1.47820000	-0.88070000
7	1.46160000	0.90530000	-2.14550000
7	0.23590000	2.98540000	-1.71520000
8	1.50990000	0.04610000	0.62710000
8	0.11760000	2.15820000	0.92650000
8	2.24460000	3.04590000	0.47480000
8	-2.43800000	5.10350000	-0.21120000

1	-2.86580000	5.36990000	-0.88350000
6	-4.27380000	-2.67860000	-2.41170000
6	-3.74470000	-1.99000000	-1.31980000
6	-3.74750000	-2.57930000	-0.05570000
6	-4.28050000	-3.85730000	0.11710000
6	-4.80990000	-4.54540000	-0.97460000
6	-4.80620000	-3.95620000	-2.23920000
1	-4.27120000	-2.21400000	-3.40840000
1	-3.32440000	-0.98310000	-1.45630000
1	-4.28260000	-4.32170000	1.11390000
1	-5.23000000	-5.55260000	-0.83870000
1	-5.22340000	-4.49900000	-3.09970000
6	-3.08290000	-1.46970000	0.78030000
1	-2.73110000	-1.52310000	-0.27870000
1	-2.51100000	-1.95280000	1.60940000
8	-1.89900000	-0.89090000	0.22490000

-4566.6699028

Complex V

Multiplicity 2

29	-2.07240000	-0.96490000	0.43750000

6	-3.26820000	1.76370000	0.32410000
6	-4.10580000	2.59920000	-0.44230000
6	-4.94140000	3.52960000	0.13650000
1	-5.58700000	4.14250000	-0.46750000
6	-4.93990000	3.65250000	1.52420000
6	-4.10980000	2.87000000	2.29680000
1	-4.11940000	2.99180000	3.36850000
6	-3.23410000	1.94900000	1.70980000
6	-2.25300000	1.21710000	2.58120000
1	-1.24330000	1.56440000	2.35800000
1	-2.47160000	1.46290000	3.62790000
6	-1.07820000	-0.87610000	3.11530000
1	-1.18890000	-0.74220000	4.19820000
1	-0.17140000	-0.36830000	2.79580000
6	-1.03870000	-2.39710000	2.76070000
1	-0.08010000	-2.66130000	2.32790000
1	-1.18880000	-3.00480000	3.66180000
6	-3.42210000	-2.44570000	2.46040000
1	-3.49230000	-3.09190000	3.34420000
1	-4.23250000	-2.69780000	1.78270000

6	-3.47910000	-0.94310000	2.89660000
1	-4.33930000	-0.43730000	2.46480000
1	-3.54600000	-0.86580000	3.98920000
6	-2.52200000	-4.09100000	1.45630000
1	-3.51220000	-4.05990000	1.00900000
1	-2.58910000	-4.66760000	2.39310000
6	-1.57410000	-4.82150000	0.50010000
1	-1.55680000	-4.31900000	-0.45590000
1	-0.55240000	-4.84340000	0.89370000
6	-3.22580000	-2.86470000	-2.52640000
6	-2.08780000	-3.08190000	-3.42810000
1	-1.87870000	-4.14670000	-3.62080000
1	-1.08900000	-2.69960000	-3.07750000
1	-2.20350000	-2.68020000	-4.44030000
17	-4.14140000	2.35970000	-2.24870000
17	-6.02020000	4.88310000	2.31050000
7	-2.24290000	-0.26100000	2.40980000
7	-2.11900000	-2.68910000	1.76520000
8	-2.25170000	0.98490000	-0.32630000
8	-2.43920000	-2.50230000	-1.11370000

8	-4.44460000	-3.18740000	-3.08750000
8	-2.06270000	-6.16640000	0.27630000
1	-1.79390000	-6.74080000	1.02340000
29	0.10590000	1.36460000	-0.22640000
6	0.02900000	-1.60450000	0.32060000
6	0.84440000	-2.61220000	0.87970000
6	0.90160000	-3.89840000	0.36580000
1	1.51440000	-4.64560000	0.83900000
6	0.15890000	-4.19870000	-0.77240000
6	-0.60260000	-3.22530000	-1.40440000
1	-1.13900000	-3.47320000	-2.30460000
6	-0.68010000	-1.93450000	-0.86940000
6	-1.56110000	-0.88510000	-1.51350000
1	-2.39810000	-0.62860000	-0.85620000
1	-1.96000000	-1.25670000	-2.47310000
6	-1.78940000	1.48070000	-2.16870000
1	-2.23430000	1.19260000	-3.12480000
1	-2.60850000	1.90910000	-1.53520000
6	-1.02850000	2.83150000	-2.24970000
1	-1.49990000	3.56650000	-1.60580000

1	-1.01430000	3.23180000	-3.26940000
6	1.02900000	1.66700000	-2.75120000
1	1.02280000	2.14190000	-3.73940000
1	2.05250000	1.51000000	-2.43110000
6	0.27010000	0.31210000	-2.76580000
1	0.92850000	-0.50250000	-2.48240000
1	-0.16770000	0.08810000	-3.74340000
6	1.16140000	3.81060000	-1.53860000
1	2.19140000	3.50830000	-1.37370000
1	1.13130000	4.43150000	-2.44620000
6	0.71310000	4.63690000	-0.32810000
1	0.83370000	4.05100000	0.57750000
1	-0.33770000	4.93310000	-0.41500000
6	2.63700000	1.43330000	0.53310000
6	3.85470000	1.71890000	1.38140000
1	4.46250000	2.48920000	0.90610000
1	3.56330000	2.05940000	2.36970000
1	4.45040000	0.81380000	1.46360000
17	1.87420000	-2.20730000	2.31250000
17	0.21640000	-5.88470000	-1.45550000

7	-0.80290000	0.43200000	-1.74280000
7	0.35940000	2.57560000	-1.75940000
8	-0.05100000	-0.27030000	0.97910000
8	1.37400000	1.96660000	1.00510000
8	2.05400000	0.93160000	-0.46570000
8	1.56080000	5.80360000	-0.19230000
1	1.25570000	6.50130000	-0.80920000
6	-7.86640000	-1.42090000	-1.91360000
6	-6.85140000	-1.05080000	-1.04190000
6	-6.55420000	-1.86750000	0.08160000
6	-7.30720000	-3.02760000	0.32250000
6	-8.32480000	-3.38830000	-0.56110000
6	-8.60670000	-2.59380000	-1.67670000
1	-8.09140000	-0.80490000	-2.77820000
1	-6.24750000	-0.13620000	-1.19900000
1	-7.09240000	-3.65450000	1.18390000
1	-8.89660000	-4.29270000	-0.37900000
1	-9.40150000	-2.88530000	-2.35600000
6	-5.44300000	-1.44870000	0.96480000
1	-5.04000000	-2.13850000	1.73480000

1	-2.54630000	0.98900000	-1.26850000
8	-4.49330000	-0.75730000	0.40790000

-4566.7220646

Complex VI

Multiplicity 2

27	2.42930000	1.43430000	11.30450000
6	1.97730000	0.28250000	8.74570000
6	0.85750000	-0.06370000	7.96050000
6	0.81470000	0.11090000	6.58970000
1	0.05670000	-0.16810000	6.08880000
6	1.89690000	0.69880000	5.96110000
6	2.97390000	1.15540000	6.68880000
1	3.68460000	1.60670000	6.24970000
6	3.02510000	0.95700000	8.06420000
6	4.20770000	1.41950000	8.86280000
1	4.70940000	0.63190000	9.19070000
1	4.81140000	1.94500000	8.27950000
6	4.93260000	2.51180000	10.93430000
1	5.61230000	3.07500000	10.48630000
1	5.35740000	1.65970000	11.20310000

6	4.37170000	3.23840000	12.16780000
1	4.60100000	2.73610000	12.98960000
1	4.76400000	4.14420000	12.23520000
6	2.63960000	4.22770000	10.86450000
1	3.07160000	5.10590000	11.01140000
1	1.66590000	4.37200000	10.75580000
6	3.21870000	3.55480000	9.60510000
1	2.50570000	3.41810000	8.93280000
1	3.92090000	4.12790000	9.20570000
6	2.24770000	3.85470000	13.24020000
1	1.30500000	4.07620000	13.03180000
1	2.70050000	4.69310000	13.51060000
6	2.27740000	2.88030000	14.40830000
1	1.78130000	2.05770000	14.16940000
1	3.21390000	2.62940000	14.60950000
6	-0.09850000	-0.29360000	14.20010000
1	-0.24190000	-0.22320000	15.25810000
1	0.54240000	-1.08450000	14.59000000
1	-0.77410000	-1.06120000	14.51510000
17	-0.55550000	-0.71310000	8.73880000

17	1.84270000	0.90400000	4.23070000
7	3.79430000	2.25090000	10.01400000
7	2.88430000	3.27340000	12.00530000
8	2.14680000	-0.15600000	10.17220000
8	1.09800000	1.02290000	12.25560000
8	-0.92370000	0.88220000	13.08380000
8	1.68710000	3.48290000	15.54710000
1	2.24400000	3.99390000	15.91410000
29	3.20050000	-1.53390000	11.34330000
6	4.69050000	0.04180000	14.59750000
6	4.73330000	-0.13280000	15.96840000
1	5.49130000	0.14620000	16.46920000
6	3.65110000	-0.72070000	16.59690000
6	2.57410000	-1.17730000	15.86920000
1	1.86340000	-1.62860000	16.30830000
6	2.52290000	-0.97890000	14.49390000
6	1.34020000	-1.44140000	13.69520000
1	0.83860000	-0.65380000	13.36740000
1	0.73650000	-1.96690000	14.27850000
6	0.61540000	-2.53370000	11.62370000

1	-0.06430000	-3.09690000	12.07180000
1	0.19060000	-1.68160000	11.35490000
6	1.17620000	-3.26030000	10.39030000
1	0.94700000	-2.75800000	9.56850000
1	0.78390000	-4.16610000	10.32280000
6	2.90840000	-4.24960000	11.69350000
1	2.47640000	-5.12780000	11.54670000
1	3.88210000	-4.39390000	11.80230000
6	2.32930000	-3.57670000	12.95290000
1	3.04230000	-3.44000000	13.62520000
1	1.62700000	-4.14980000	13.35230000
6	3.30030000	-3.87660000	9.31790000
1	4.24300000	-4.09810000	9.52620000
1	2.84750000	-4.71500000	9.04750000
6	3.27060000	-2.90220000	8.14980000
1	3.76670000	-2.07960000	8.38860000
1	2.33400000	-2.65130000	7.94860000
6	5.80810000	-1.81300000	10.97940000
6	7.20510000	-1.55330000	10.45780000
1	7.51600000	-2.33460000	9.95460000

1	7.19380000	-0.76930000	9.87100000
1	7.80940000	-1.38900000	11.21190000
17	6.10350000	0.69120000	13.81920000
17	3.70530000	-0.92590000	18.32740000
7	1.75370000	-2.27280000	12.54400000
7	2.65230000	-3.35350000	10.53440000
8	3.52110000	-0.02870000	12.56110000
8	4.65870000	-1.09300000	10.25000000
8	5.63940000	-2.57440000	11.94700000
8	3.86090000	-3.50480000	7.01090000
1	3.30390000	-4.01580000	6.64400000
1	1.11800000	-0.36910000	9.99410000
6	-1.91520000	3.36850000	9.79310000
6	-0.52510000	3.44160000	9.88640000
6	0.08790000	4.64260000	10.24280000
6	-0.68920000	5.77150000	10.50500000
6	-2.07900000	5.69850000	10.41120000
6	-2.69210000	4.49680000	10.05560000
1	-2.39830000	2.42140000	9.51250000
1	1.18360000	4.70010000	10.31700000

1	-0.20570000	6.71840000	10.78590000
1	-2.69170000	6.58810000	10.61780000
1	-3.78770000	4.43940000	9.98200000
6	0.33220000	2.19530000	9.59750000
1	1.39830000	2.25100000	9.66890000
7	0.54920000	1.03470000	9.86720000
6	-0.32840000	1.01600000	8.47550000
6	0.60410000	1.41360000	7.51760000
6	-1.65400000	0.78610000	8.10530000
6	0.21200000	1.58020000	6.18910000
1	1.64890000	1.59450000	7.80900000
6	-2.04610000	0.95320000	6.77720000
1	-2.38910000	0.47270000	8.86080000
6	-1.11290000	1.34990000	5.81890000
1	0.94740000	1.89320000	5.43390000
1	-3.09070000	0.77200000	6.48510000
1	-1.42220000	1.48130000	4.77190000
6	3.56450000	-0.33080000	13.90700000
6	0.18620000	0.52040000	13.16140000

-4854.1930025

Complex VII

Multiplicity 2

29	2.42930000	1.43430000	11.30450000
6	1.97730000	0.28250000	8.74570000
6	0.85750000	-0.06370000	7.96050000
6	0.81470000	0.11090000	6.58970000
1	0.05670000	-0.16810000	6.08880000
6	1.89690000	0.69880000	5.96110000
6	2.97390000	1.15540000	6.68880000
1	3.68460000	1.60670000	6.24970000
6	3.02510000	0.95700000	8.06420000
6	4.20770000	1.41950000	8.86280000
1	4.70940000	0.63190000	9.19070000
1	4.81140000	1.94500000	8.27950000
6	4.93260000	2.51180000	10.93430000
1	5.61230000	3.07500000	10.48630000
1	5.35740000	1.65970000	11.20310000
6	4.37170000	3.23840000	12.16780000
1	4.60100000	2.73610000	12.98960000
1	4.76400000	4.14420000	12.23520000

1	2.63960000	4.22770000	10.86450000
1	3.07160000	5.10590000	11.01140000
1	1.66590000	4.37200000	10.75580000
6	3.21870000	3.55480000	9.60510000
1	2.50570000	3.41810000	8.93280000
1	3.92090000	4.12790000	9.20570000
6	2.24770000	3.85470000	13.24020000
1	1.30500000	4.07620000	13.03180000
1	2.70050000	4.69310000	13.51060000
6	2.27740000	2.88030000	14.40830000
1	1.78130000	2.05770000	14.16940000
1	3.21390000	2.62940000	14.60950000
6	-0.09850000	-0.29360000	14.20010000
1	-0.24190000	-0.22320000	15.25810000
1	0.54240000	-1.08450000	14.59000000
1	-0.77410000	-1.06120000	14.51510000
17	-0.55550000	-0.71310000	8.73880000
17	1.84270000	0.90400000	4.23070000
7	3.79430000	2.25090000	10.01400000
7	2.88430000	3.27340000	12.00530000

8	2.14680000	-0.15600000	10.17220000
8	1.09800000	1.02290000	12.25560000
8	-0.92370000	0.88220000	13.08380000
8	1.68710000	3.48290000	15.54710000
1	2.24400000	3.99390000	15.91410000
29	3.20050000	-1.53390000	11.34330000
6	4.69050000	0.04180000	14.59750000
6	4.73330000	-0.13280000	15.96840000
1	5.49130000	0.14620000	16.46920000
6	3.65110000	-0.72070000	16.59690000
6	2.57410000	-1.17730000	15.86920000
1	1.86340000	-1.62860000	16.30830000
6	2.52290000	-0.97890000	14.49390000
6	1.34020000	-1.44140000	13.69520000
1	0.83860000	-0.65380000	13.36740000
1	0.73650000	-1.96690000	14.27850000
6	0.61540000	-2.53370000	11.62370000
1	-0.06430000	-3.09690000	12.07180000
1	0.19060000	-1.68160000	11.35490000
6	1.17620000	-3.26030000	10.39030000

1	0.94700000	-2.75800000	9.56850000
1	0.78390000	-4.16610000	10.32280000
6	2.90840000	-4.24960000	11.69350000
1	2.47640000	-5.12780000	11.54670000
1	3.88210000	-4.39390000	11.80230000
6	2.32930000	-3.57670000	12.95290000
1	3.04230000	-3.44000000	13.62520000
1	1.62700000	-4.14980000	13.35230000
6	3.30030000	-3.87660000	9.31790000
1	4.24300000	-4.09810000	9.52620000
1	2.84750000	-4.71500000	9.04750000
6	3.27060000	-2.90220000	8.14980000
1	3.76670000	-2.07960000	8.38860000
1	2.33400000	-2.65130000	7.94860000
6	5.80810000	-1.81300000	10.97940000
6	7.20510000	-1.55330000	10.45780000
1	7.51600000	-2.33460000	9.95460000
1	7.19380000	-0.76930000	9.87100000
1	7.80940000	-1.38900000	11.21190000
17	6.10350000	0.69120000	13.81920000

17	3.70530000	-0.92590000	18.32740000
7	1.75370000	-2.27280000	12.54400000
7	2.65230000	-3.35350000	10.53440000
8	3.52110000	-0.02870000	12.56110000
8	4.65870000	-1.09300000	10.25000000
8	5.63940000	-2.57440000	11.94700000
8	3.86090000	-3.50480000	7.01090000
1	3.30390000	-4.01580000	6.64400000
1	1.11800000	-0.36910000	9.99410000
6	-1.91520000	3.36850000	9.79310000
6	-0.52510000	3.44160000	9.88640000
6	0.08790000	4.64260000	10.24280000
6	-0.68920000	5.77150000	10.50500000
6	-2.07900000	5.69850000	10.41120000
6	-2.69210000	4.49680000	10.05560000
1	-2.39830000	2.42140000	9.51250000
1	1.18360000	4.70010000	10.31700000
1	-0.20570000	6.71840000	10.78590000
1	-2.69170000	6.58810000	10.61780000
1	-3.78770000	4.43940000	9.98200000

6	0.33220000	2.19530000	9.59750000
1	1.39830000	2.25100000	9.66890000
7	0.54920000	1.03470000	9.86720000
6	-0.32840000	1.01600000	8.47550000
6	0.60410000	1.41360000	7.51760000
6	-1.65400000	0.78610000	8.10530000
6	0.21200000	1.58020000	6.18910000
1	1.64890000	1.59450000	7.80900000
6	-2.04610000	0.95320000	6.77720000
1	-2.38910000	0.47270000	8.86080000
6	-1.11290000	1.34990000	5.81890000
1	0.94740000	1.89320000	5.43390000
1	-3.09070000	0.77200000	6.48510000
1	-1.42220000	1.48130000	4.77190000
6	3.56450000	-0.33080000	13.90700000
6	0.18620000	0.52040000	13.16140000

-4777.7267896

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