Supplementary Information (SI) for Dalton Transactions.
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Supplementary Information

Selective Hydroxylation of Benzene to Phenol via $Cu^{II}(\mu\text{-}O^{\bullet})Cu^{II}$ intermediate by a Nonsymmetric Dicopper Catalyst

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Experimental Section

Materials. Commercially available chemicals and solvents were used as received unless otherwise noted. The synthesis routes of $[Cu_2(TPMAN)(\mu\text{-}OH)(H_2O)](CF_3SO_3)_3$ ($\mathbf{1}(CF_3SO_3)_3$)came from our reported literature.[1,2]

Instrumentation. GC data were obtained on a Shimazu 2010 Plus GC system containing an Rxi®-5ms capillary column. Nitrobenzene was used as a standard. NMR spectra were obtained on NMR spectrometer with 400 MHz for ^1H NMR.

Abbreviations

TPMAN: 1-(7-((bis(pyridin-2-ylmethyl)amino)methyl)-1,8-naphthyridin-2-yl)-N-methyl-N-(pyridin-2-ylmethyl)methanamine.

TON: Turnover number.

BQ: *p*-Benzoquinone

Cov.: Conversion ratio

Supplementary tables and figures:

Table S1. Screening the reaction condition of the catalyst for hydroxylation of benzene.

entry	[cat.**1**](μM)	[H_2O_2]M	base(2 mM)	[benzene](M)	T °C	Yield (%)		Selectivity (%)
						phenol	benzoquinone	
1	20	4	Et_3N	0.78	45	1.36	0.2	87
2	40	4	Et_3N	0.78	45	1.91	0.82	70
3	80	4	Et_3N	0.78	45	2.3	1.15	67
4	40	2	Et_3N	0.78	45	1.15	0.19	86
5	40	1	Et_3N	0.78	45	0.14	0	100
6	40	4	DETA	0.78	45	2.04	0.82	71
7	40	4	DBU	0.78	45	1.94	0.83	70
8	40	4	Et_3N(0.4mM)	0.78	45	2.02	0.81	71
9	40	4	Et_3N	0.78	35	0.93	0.79	54
10	40	4	Et_3N	0.78	55	3.75	0.81	82
11	40	4	Et_3N	0.78	30(rt)	0.39	0.39	50
12	40	4	Et_3N	0.78	30(rt)	0.49	0.55	47

Note: The reaction time is 11 h; The p*K*a of the base is : DETA (18.29 in AN), DBU (23.9 in AN), and Et_3N (17.61 in AN)

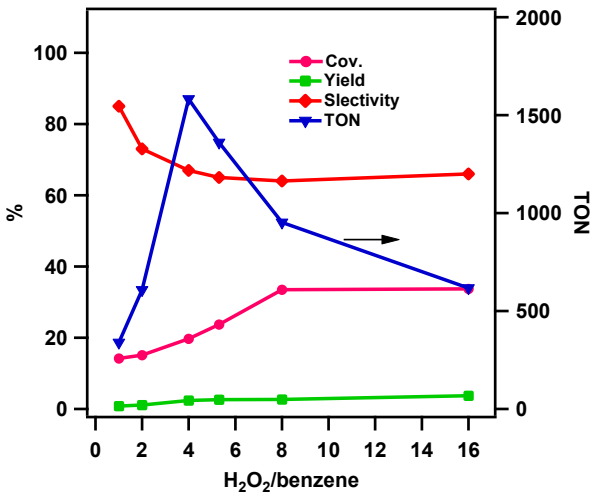


Figure S1. The effect of different ratio of H_2O_2/benzene on the oxidation of benzene to phenol catalyzed by catalyst **1** (0.44 μmol) under 45°C at 12 h.

Table S2. Different amounts of Et_3N for hydroxylation of benzene.

Entry	Et_3N[a]	Conv. (%)	Yield (%)	Selectivity (%)
1	-	36.8	3.1	81.5
2	0.17mol%	41.9	3.2	89.2
3	17mol%	37.8	3.2	100[b]
4[c]	0.17mol%	21	4.7	86.0
5[c]	0.017mol%	30.9	5.2	88.7

Condition: 0.44 μmol catalyst **1**, 11 mmol benzene, 44 mmol H_2O_2 (30%), 6.3 mL CH_3CN, 45°C,24 h. [a] As compared with benzene. [b] The selectivity obtained after 44h reaction. [c] The reaction is done in a sealed tube.

Table S3. Different kinds of base for hydroxylation of benzene.

Entry	additive[a]	additive	pKa(MeCN)	Yield%	Slectivity%
2	0.36mol%	Et_2NH	18.75	4.7	85.9
3	0.29mol%	*i*-$PrNH_2$	17.96	4.2	82.9
4	0.26mol%	NH_3	16.46	4.9	86.2
5	0.017mol%	morpholine	16.61	5.6	88.5
6	0.17mol%	DMAP	17.95	4.3	91.2
7	0.18mol%	L-Ascorbic Acid Sodium	-	3.8	86.5
8	2.5mol%	$BaCO_3$	-	5.05	83.3

Condition: 0.44 μmol catalyst, 11 mmol benzene, 44 mmol H_2O_2 (30%), 6.3mL CH_3CN, 45°C, 21 - 24 h. [a]As compared with benzene.

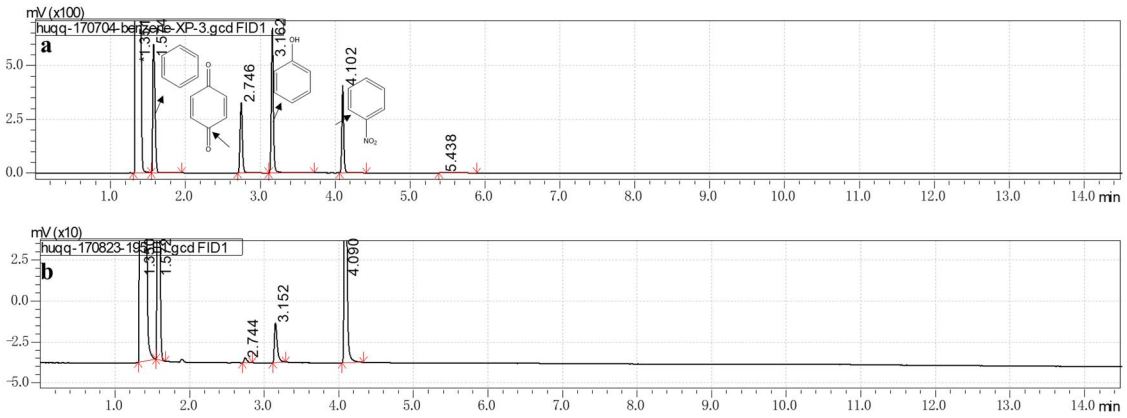
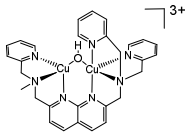
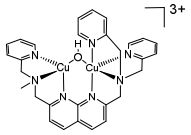
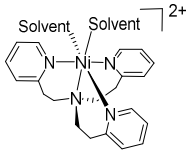
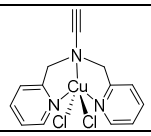
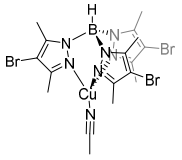
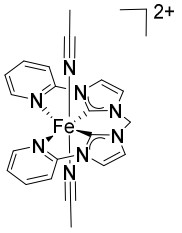
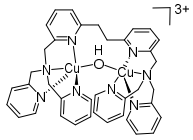
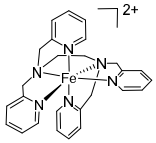
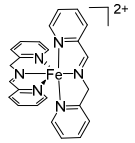
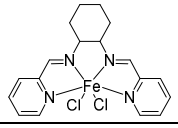
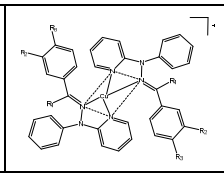
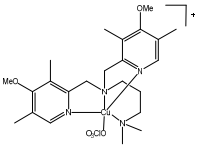
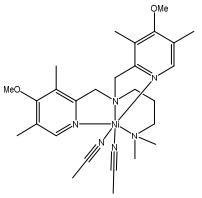
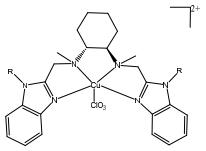


Figure S2. Gas chromatographs of the standard samples (a) and the reaction mixture of benzene oxidation (b). Reaction condition: catalyst **1** (0.48 mg, 0.44 μmol), benzene (860 mg, 11 mmol), base (Et_3N, 0.5 mg, 5 μmol), 30% H_2O_2 (4.5 mL, 44 mmol), 6.3 mL CH_3CN, 45 °C, 23 h.

Table S4. Comparison of catalytic activity of various catalysts for oxidation of benzene with H_2O_2.

Entry	compound	Yield (%)	TON	Selectivity (%)	Time (h)	Temp. (°C)	C/S/O[a]	Ref.
1[a]		6.7	2100	92	24	65	1/25000/100000	This work
2[b]		6.1	14000	97	29	65	1/220000/8800000	This work
3		7.5	749	99	216	60	1/10000/50000	Ref. 3
4		11.7	37	28.1	4	80	1/3333/5000	Ref. 4
5		-	-	92	2	80	1/200/300	Ref. 5
6		5.6	-	94	1	25	1/100/50	Ref. 6
7		20	6250	93.2	40	50	1/30000/120000	Ref. 7
8		0.4	11.8	-	2	20	1/3000/200	Ref. 8
9		26	-	82	1.5	25	1/100/250	Ref. 9
10		64	89	98	3	50	1/100/250	Ref. 10

11		29	586	98	5	60	1/2000/10000	Ref. 11
12		38	760	98	5	60	1/2000/10000	Ref. 12
13		41	820	97	5	60	1/2000/10000	Ref. 13
14		22.4		95	24	25	1/50/500	Ref. 14

[a] Condition: 0.44 μmol catalyst **1**; [b] Condition: 0.05 μmol catalyst **1**.

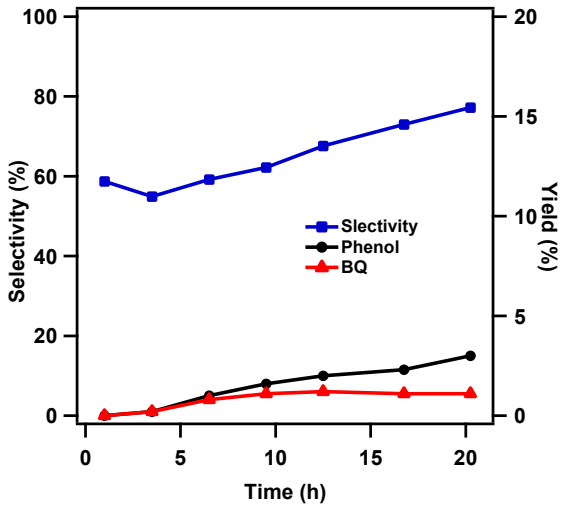


Figure S3. The catalytic selectivity and yield of the hydroxylation of benzene catalyzed by catalyst **1** at 45 °C. Condition: catalyst **1** (0.48 mg, 0.44 μmol), benzene (860 mg, 11 mmol), base (Et_3N, 0.5 mg, 5 μmol), 30% H_2O_2 (4.5 mL, 44 mmol), 6.3 mL CH_3CN, 45 °C, 20 h.

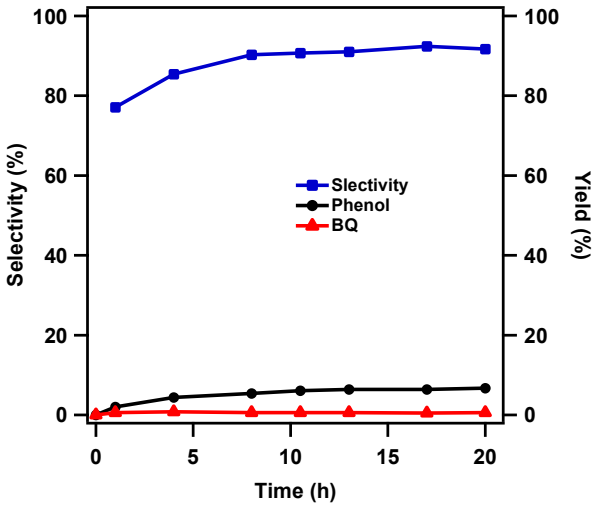


Figure S4. The catalytic selectivity and yield of the hydroxylation of benzene catalyzed by catalyst **1** at 65 °C. Condition: catalyst **1** (0.48 mg, 0.44 μmol), benzene (860 mg, 11 mmol), base (Et_3N, 0.5 mg, 5 μmol), 30% H_2O_2 (4.5 mL, 44 mmol), 6.3 mL CH_3CN, 65 °C, 20 h.

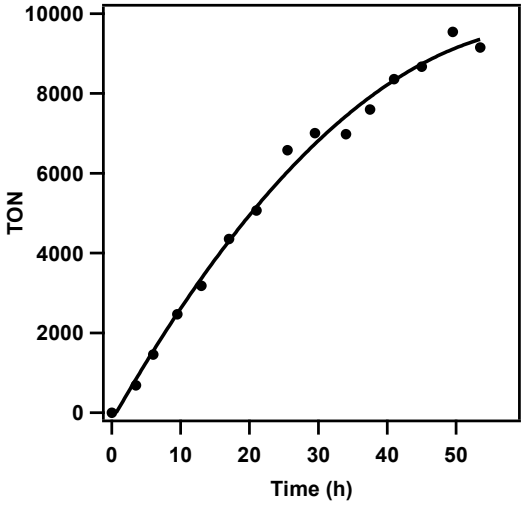


Figure S5. Time profile formation of phenol in the hydroxylation of benzene, catalyzed by catalyst **1** (0.05 μmol) 11 mmol benzene, 44 mmol 30% H_2O_2, 5 μmol Et_3N in 6.3 mL CH_3CN, 45°C.

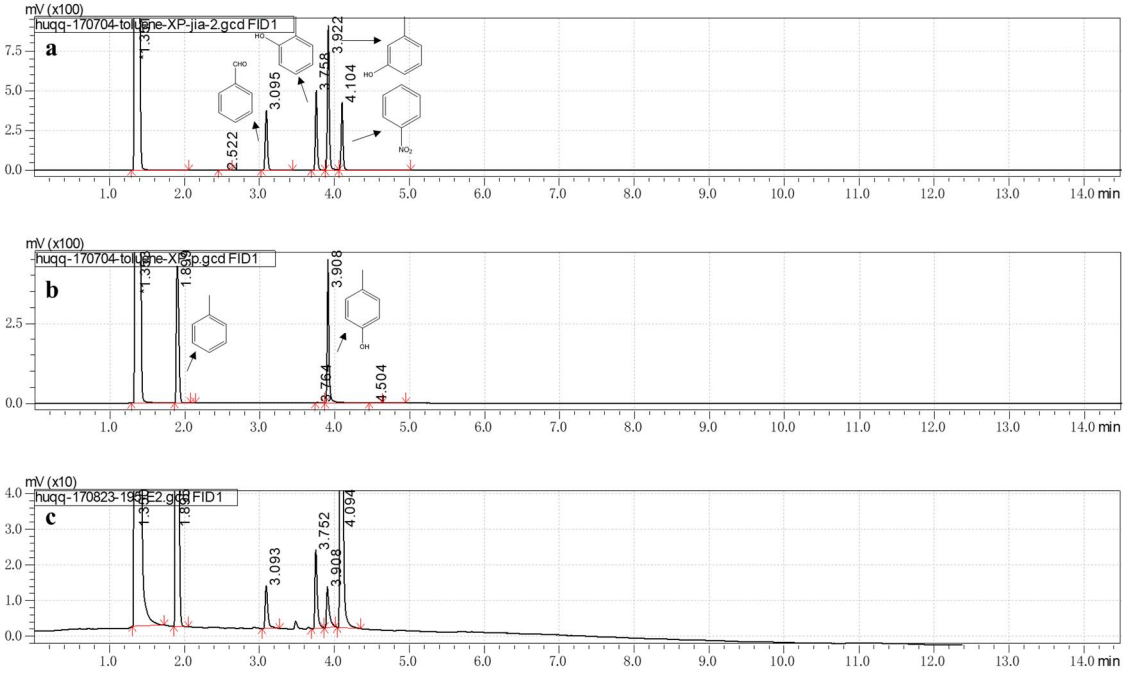


Figure S6. Gas chromatographs of the standard samples (a, b) and the reaction mixture of toluene oxidation (c). Reaction condition: catalyst **1** (0.48 mg, 0.44 μmol), toluene (780 mg, 8.5 mmol), base (Et_3N, 0.5 mg, 5 μmol), 30% H_2O_2 (4.5 mL, 44 mmol), 6.3 mL CH_3CN, 45 °C, 23 h.

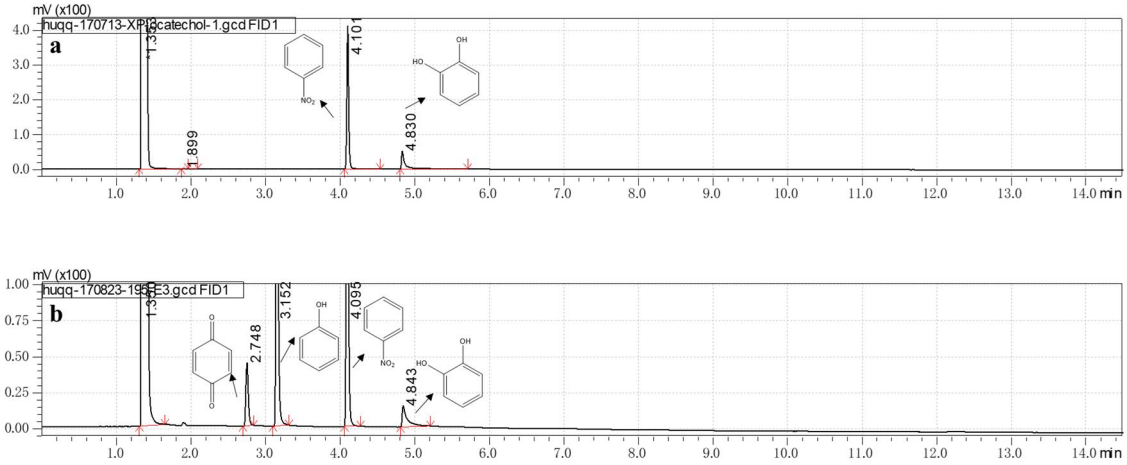


Figure S7. Gas chromatographs of the standard samples (a) and the reaction mixture of phenol oxidation (b). Reaction condition: catalyst **1** (0.48 mg, 0.44 μmol), phenol (770 mg, 8.2 mmol), base (Et_3N, 0.5 mg, 5 μmol), 30% H_2O_2 (4.5 mL, 44 mmol), 6.3 mL CH_3CN, 45 °C, 23 h.

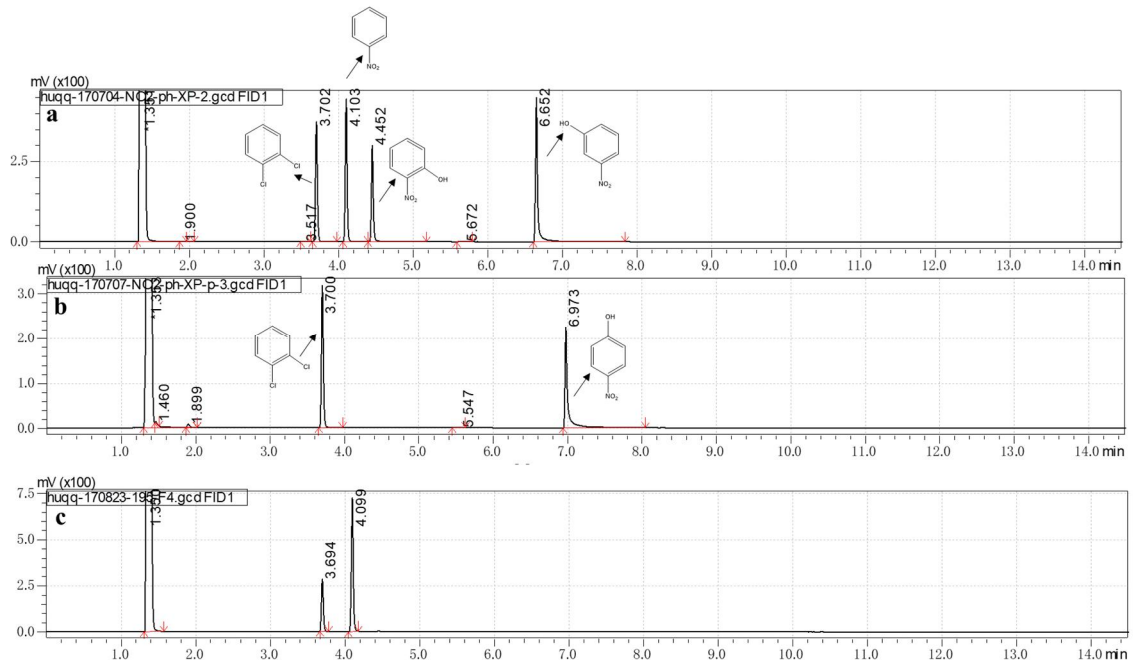


Figure S8. Gas chromatographs of the standard samples (a, b) and the reaction mixture of nitrobenzene oxidation (c). Reaction condition: catalyst **1** (0.48 mg, 0.44 μmol), nitrobenzene (1010 mg, 8.2 mmol), base (Et_3N, 0.5 mg, 5 μmol), 30% H_2O_2 (4.5 mL, 44 mmol), 6.3 mL CH_3CN, 45 °C, 23 h.

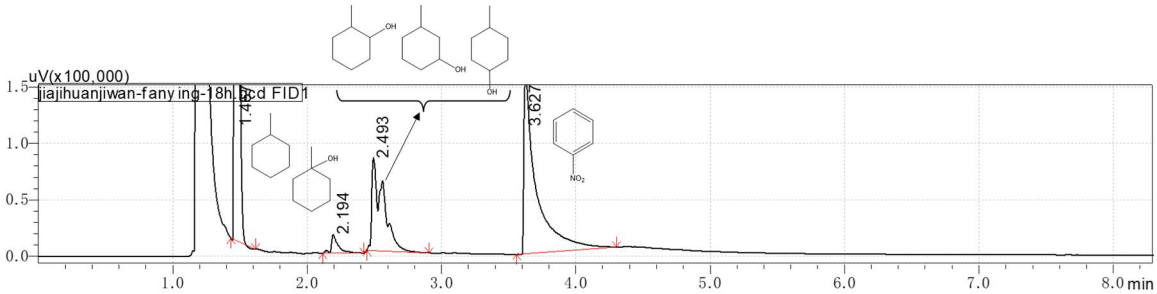


Figure S9. Gas chromatographs of the reaction mixture of methylcyclohexane oxidation. Reaction condition: catalyst **1** (0.48 mg, 0.44 μmol), methylcyclohexane (1142 mg, 10 mmol), base (Et_3N, 0.5 mg, 5 μmol), 30% H_2O_2 (4.5 mL, 44 mmol), 6 mL CH_3CN, 65 °C, 18 h.

Note: $S_{3'\text{-OH}}$ (peak 2.194): $S_{2'\text{-OH}}$ (peak 2.493)= 0.455: 6.624; this result means that the product selectivity of the hydroxylation of methylcyclohexane is about 1 (tertiary alcohol) : 15 (secondary alcohol).

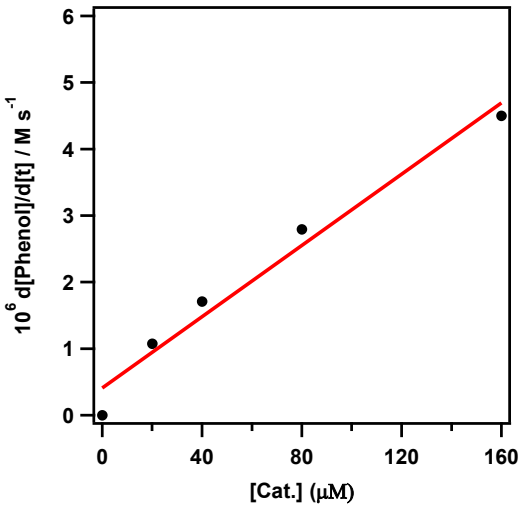


Figure S10. Dependence of the initial rate of phenol production by oxidation of benzene catalyzed by different concentration of catalyst **1** under 45°C.

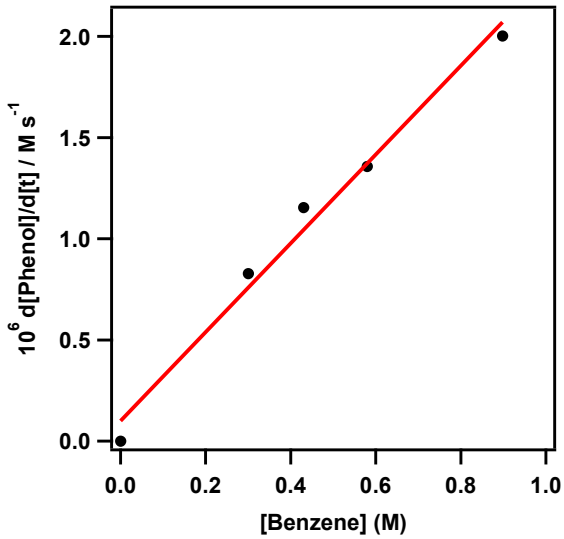


Figure S11. Dependence of the initial rate of phenol production by oxidation of benzene catalyzed by catalyst **1** with different concentration of benzene under 45°C.

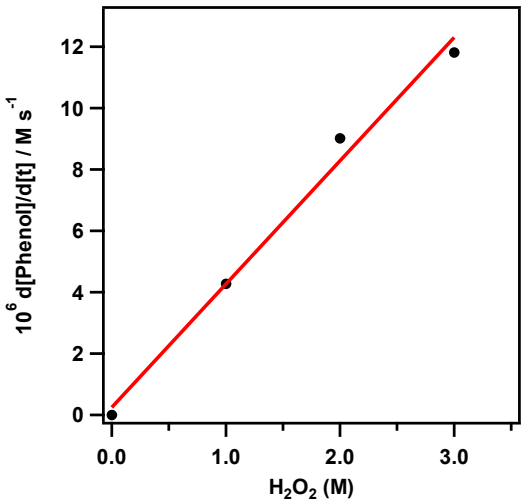


Figure S12. Dependence of the initial rate of phenol production by oxidation of benzene catalyzed by catalyst **1** with different concentration of the oxidant (H_2O_2) under 45°C.

DFT calculations

Computational Details

All density functional calculations in the present study were performed by using the B3LYP[15]-D3 functional (with D3BJ dispersion),[16,17] as implemented in the Gaussian 16 program package.[18] For the geometry optimizations, the SDD pseudopotential[19] and its corresponding basis sets were used for Cu, and the 6-31G(d,p) basis sets[20,21] were used for the C, N, O, and H elements. Analytic frequency calculations were carried out at the same level of theory as the geometry optimization to obtain the Gibbs free energy corrections and to identify all the stationary points as minima (no imaginary frequency) or transition states (one imaginary frequency). To obtain more accurate energies, single-point calculations using these optimized geometries were done employing a larger basis set, where all elements, except Cu (ECP10MDF pseudopotentials),[22] were described by 6-311+G(2df,2pd). Solvation effects from the acetonitrile solvent were calculated using the SMD continuum solvation model[23] with the larger basis set at the B3LYP-D3(BJ) levels. For pK_as calculations, the Gibbs free energy of a proton in acetonitrile is -264.7 kcal/mol, which is composed of the experimental solvation free energy of a proton in acetonitrile (-258.4 kcal/mol)[24,25] and the Gibbs free energy correction (-6.3 kcal/mol)[25] resulting from the translation entropy of a proton in the gas phase.

The concentration correction of +1.9 kcal/mol at room temperature (derived from the free-energy change of 1 mol of an ideal gas from 1 atm (24.5 L/mol, 298.15 K) to 1 M was added for all species. Unless otherwise specified, the B3LYP-D3(BJ) energies are reported, including Gibbs free energy corrections and D3(BJ) dispersion from B3LYP. The 3D images of the computed structures were prepared using CYLView.[26]

Ab initio molecular dynamics (AIMD) calculations in the gas phase were conducted using the Quickstep Module of the CP2K package[27,28] to demonstrate that the metastable intermediate **Int4'** generated via **TS1** can isomerize to the intermediate **Int4** without any applied potential and rapidly. The DFT-optimized structure of **Int4'** was used as the starting configuration for the AIMD simulation. The PBE functional[29] with D3 dispersion corrections[30] was used. The motion of the atoms was generated using molecular dynamics, using a timestep of 0.5 fs. The simulations used a periodic cubic box (L = 16.12 Å). All elements were described with the DZVP-MOLOPT-SR-GTH basis set, using the Goedecker–Teter–Hutter (GTH) pseudopotentials.[31] The plane wave cutoff was 280 Ry for the calculations. To avoid the nonergodic and glassy behavior,[32] the temperature was set slightly above room temperature (T = 300 K) and controlled using a CSVR thermostat.[33] The simulations were carried out for 8.5 ps, in which all the atoms were relaxed, and the length of the O2-Cu2 bond was calculated as the average of the last five ps of the trajectory.

Table S5. Optimized structures of complexes **1** ($[Cu^{II}_2(TPMAN)(\mu\text{-}OH)(H_2O)]^{3+}$) and **Int1**. Distances are shown in Å in black, and Mulliken spin populations on selected atoms are shown in red. For clarity, unimportant hydrogen atoms are not shown.

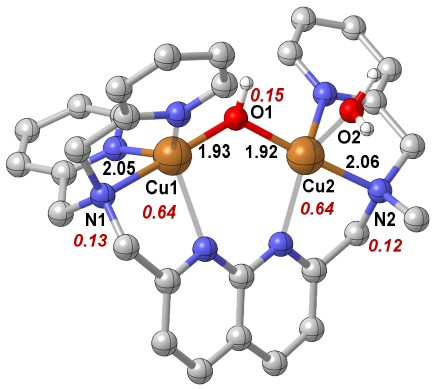
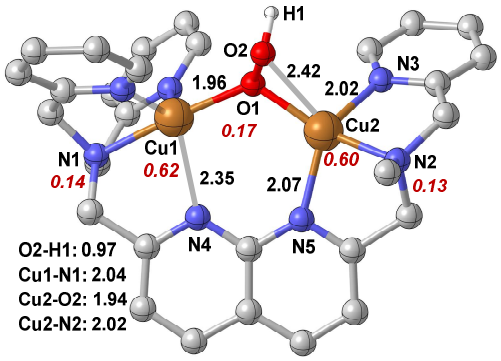
 **^{3}1**	 **^{3}Int1**
BS-singlet: 0.4 Triplet: 0.0	BS-singlet: 0.1 Triplet: 0.0

Table S6. Optimized structures of **Int2**, its possible isomers (complexes **Int2A** and **Int2B**), and **Int3**. Distances are shown in Å in black, and Mulliken spin populations on selected atoms are shown in red. For clarity, unimportant hydrogen atoms are not shown.

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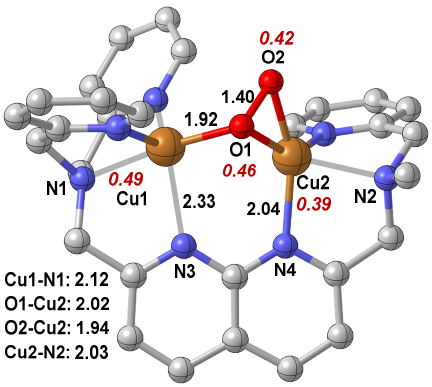
<td> 

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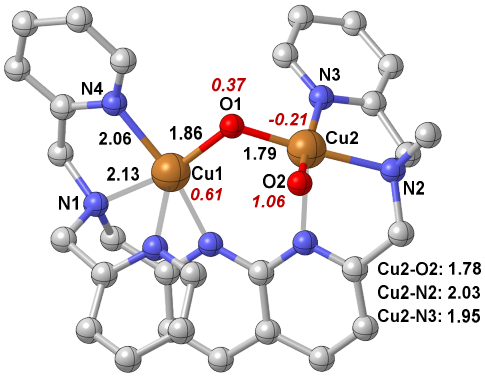
<td> 

^{3}Int2A</td>
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Triplet: +26.8 kcal/mol relative to complex ^{3}Int2</td>
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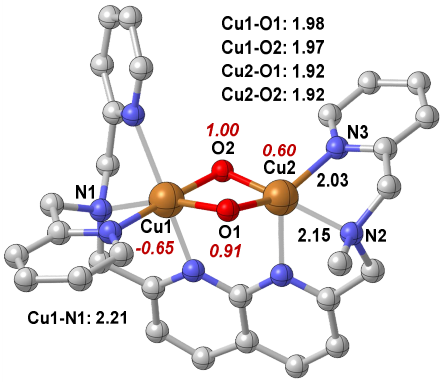
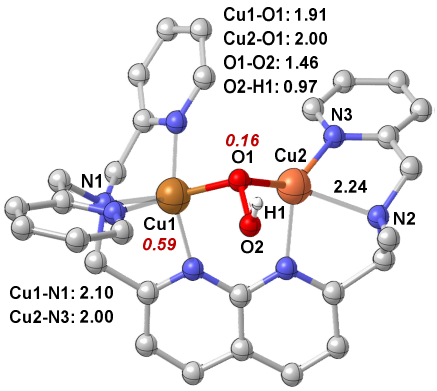
<td> 

^{3}Int2B</td>
<td> 

^{2}Int3</td>
</tr>
<tr>
<td>BS-singlet: +36.0 kcal/mol relative to complex ^{3}Int2
Triplet: +32.7 kcal/mol relative to complex ^{3}Int2</td>
<td>Doublet: 0.0
Quartet: 19.0</td>
</tr>
</table>

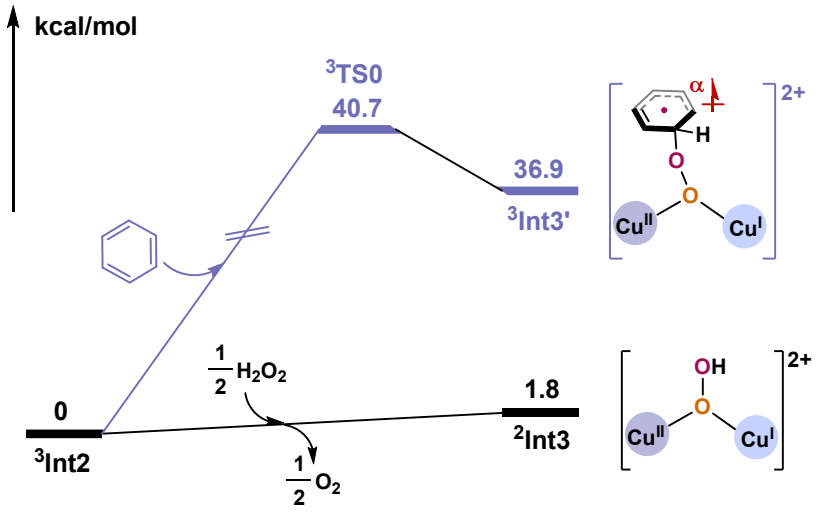


Figure S13. The Gibbs free energy diagram for benzene and H_2O_2 react with **Int2**.

Table S7. Optimized structures of **TS0** and **Int3'**. Distances are shown in Å in black, Mulliken spin populations on selected atoms are shown in red, and the imaginary frequency (in cm^{-1}) for **TS0** is also shown. For clarity, unimportant hydrogen atoms are not shown.

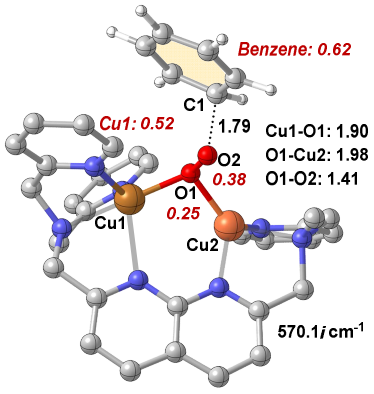
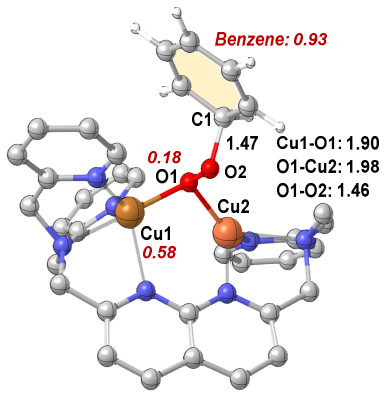
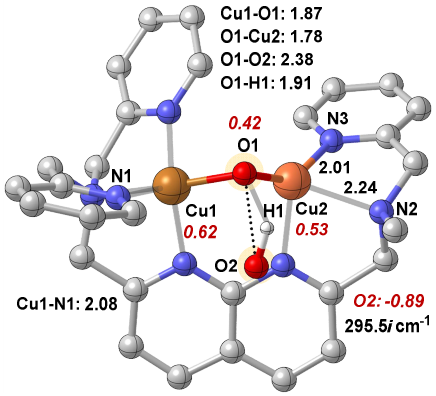
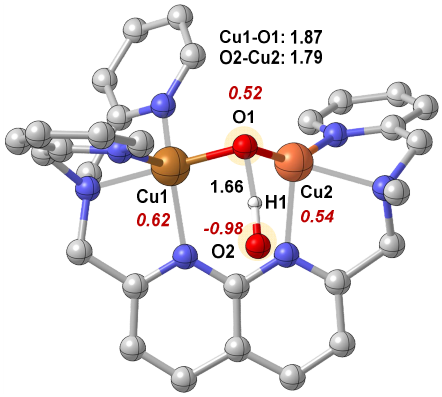
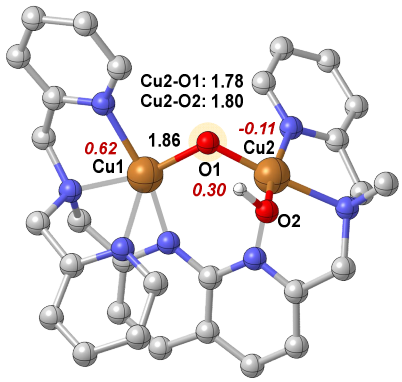
 **3TS0**	 **3Int3'**
BS-singlet: 1.1 Triplet: 0.0	BS-singlet: 0.7 Triplet: 0.0

Table S8. Optimized structures of **TS1**, **Int4'**, and **Int4**. Distances are shown in Å in black, Mulliken spin populations on selected atoms are shown in red, and the imaginary frequency (in cm^{-1}) for **TS1** is also shown. For clarity, unimportant hydrogen atoms are not shown.

 ^{2}TS1	 ^{2}Int4'
Doublet: 0.0	Doublet: 0.0
 ^{2}Int4	
Doublet: 0.0 Quartet: 4.8	

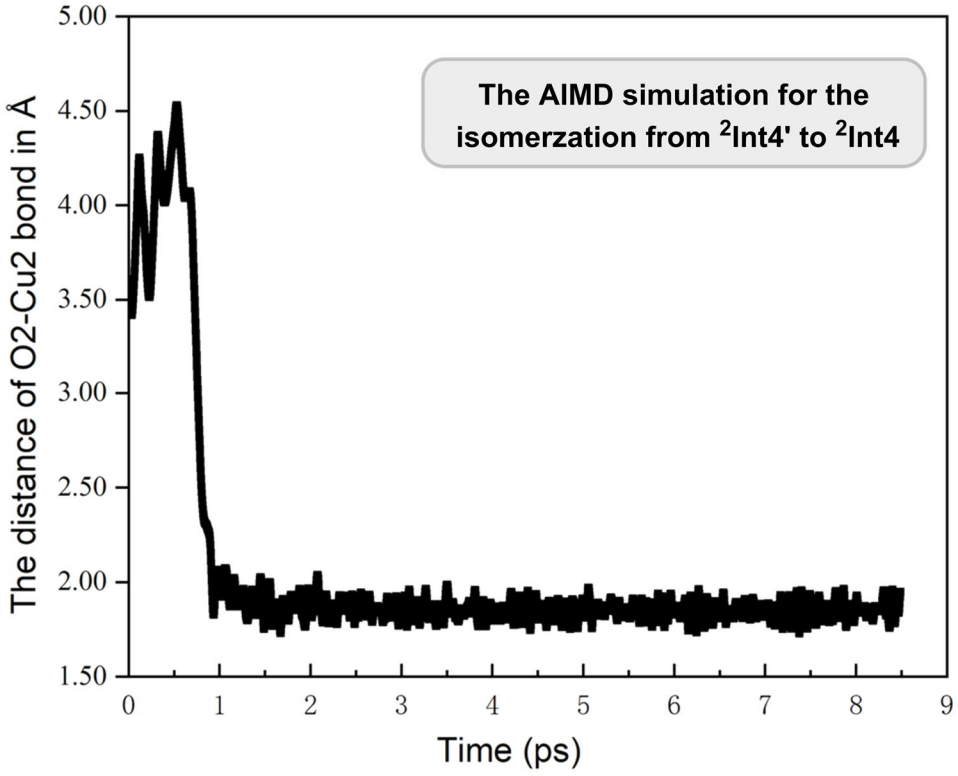


Figure S14. Collective variables of O2-Cu2 distance (in Å) as a function of simulation time (in ps)

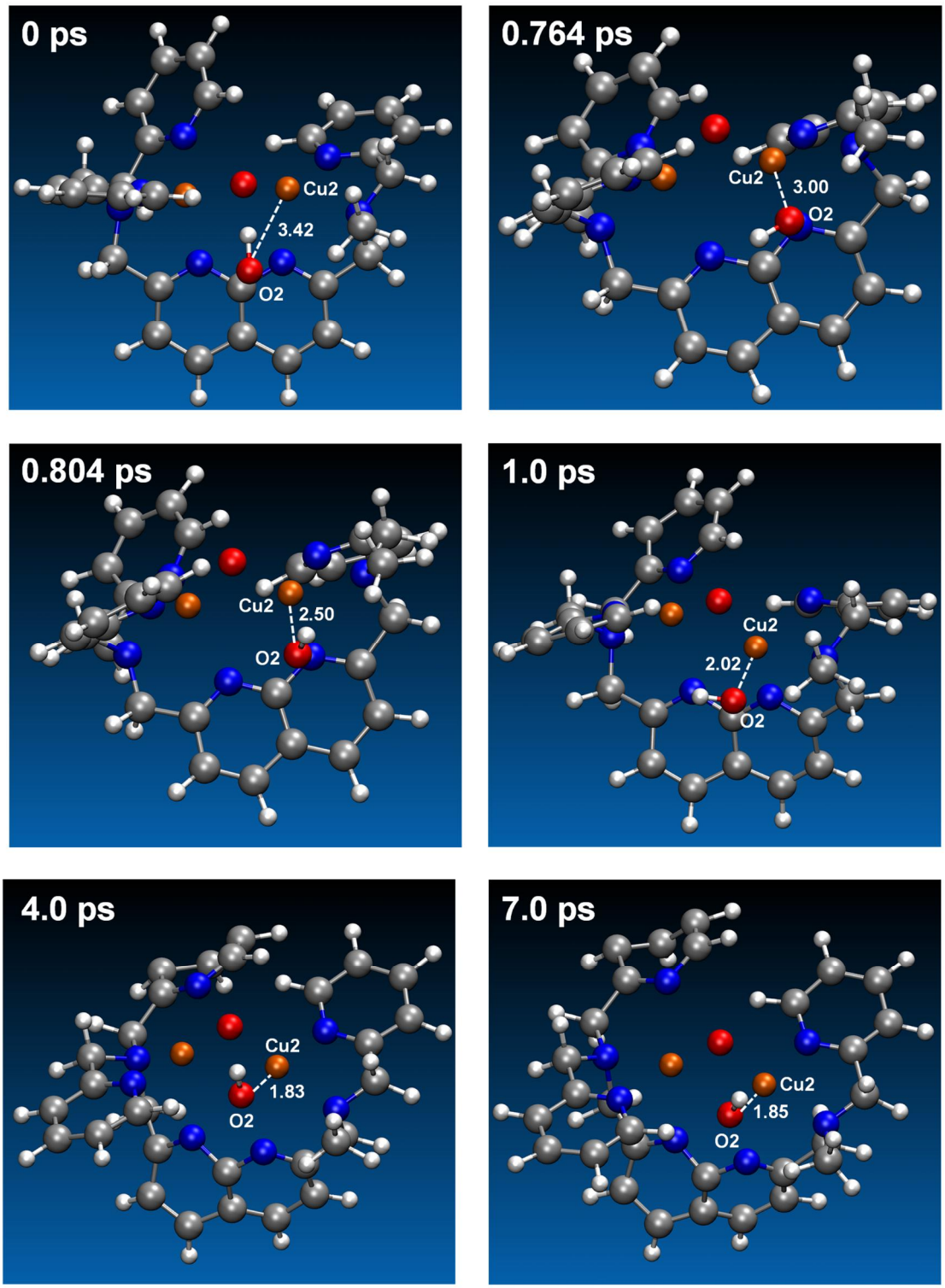


Figure S15. Snapshots for the isomerization process of **Int4'** to **Int4** in the gas phase, the distance of O2-Cu2 is shown in Å. The average distance of the O2-Cu2 bond is 1.85 Å.

Table S9. Optimized structures of **TS1'** and **Int4"**. Distances are shown in Å in black, Mulliken spin populations on selected atoms are shown in red, and the imaginary frequency (in cm^{-1}) for transition state **TS1'** is also shown. For clarity, unimportant hydrogen atoms are not shown.

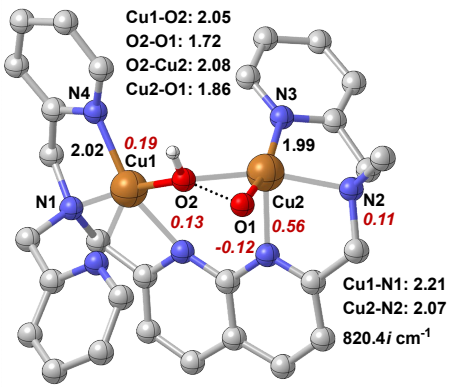
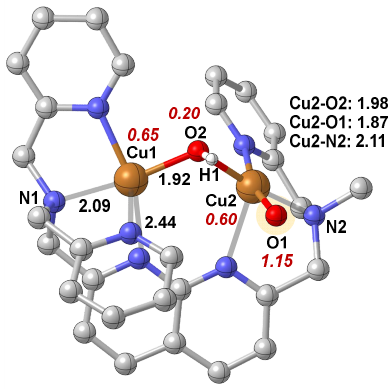
 **^{2}TS1'**	 **^{4}Int4"**
Doublet: 0.0	Doublet: 3.0 Quartet: 0.0

Table S10. Optimized structures of **TS2**, **Int5**, **TS3**, **Int6**, benzene and phenol. Distances are shown in Å in black, Mulliken spin populations on selected atoms are shown in red, and the imaginary frequencies (in cm^{-1}) for transition states are also shown. For clarity, unimportant hydrogen atoms are not shown.

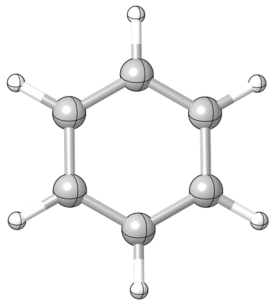
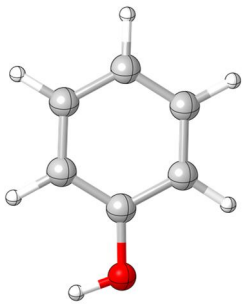
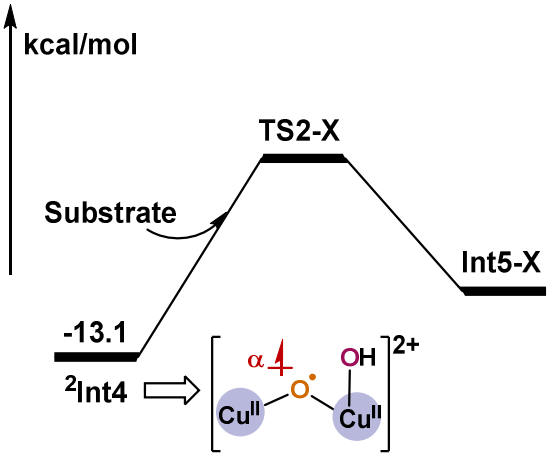
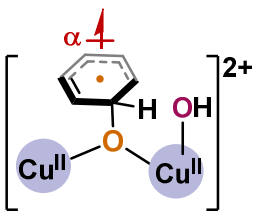
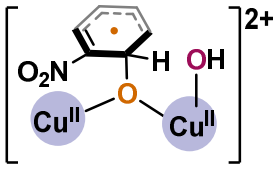
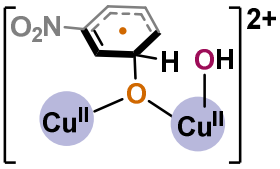
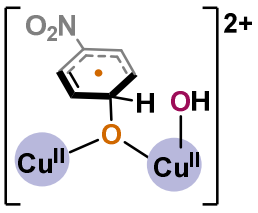
Doublet: 0.1 Quartet: 0.0	Doublet: 0.3 Quartet: 0.0
Doublet: 0.0	Doublet: 0.0 Quartet: 13.9
	
benzene	phenol

Table S11. The calculated barriers for different substrates react with the catalytic active species **Int4**.



Substrate	The calculated barrier (TS2-X) relative to Int4 in kcal/mol	Structure for Int5-X
Benzene	+14.0	
Nitrobenzene	+16.7	
	+16.9	
	+15.4	

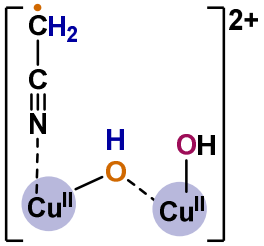
CH_3CN	+15.8	

Table S12. Optimized structures of **TS2-*o*-nitrobenzene**, **TS2-*m*-nitrobenzene**, **TS2-*p*-nitrobenzene**, **TS2-CH_3CN**, nitrobenzene and CH_3CN. Distances are shown in Å in black, Mulliken spin populations on selected atoms are shown in red, and the imaginary frequencies (in cm^{-1}) for transition states are also shown. For clarity, unimportant hydrogen atoms are not shown.

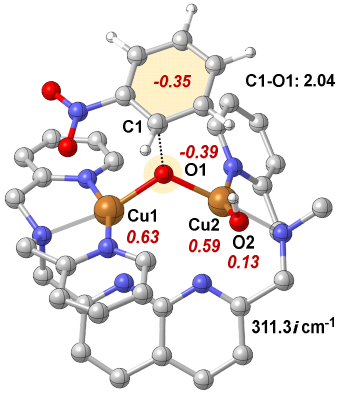
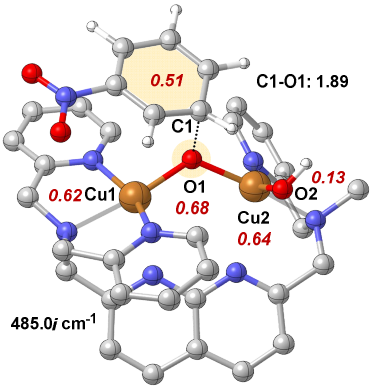
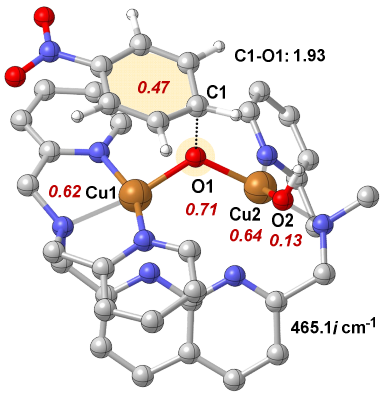
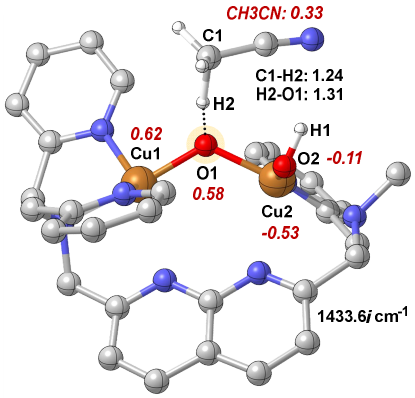
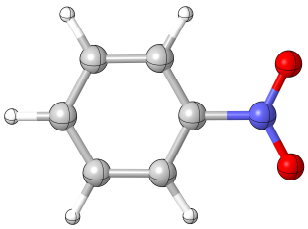
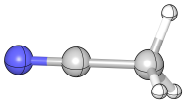
	
^{2}TS2-*o*-nitrobenzene	**^{4}TS2-*m*-nitrobenzene**
Doublet: 0.0 Quartet: 1.0	Doublet: 0.8 Quartet: 0.0
	
^{4}TS2-*p*-nitrobenzene	**^{2}TS2-CH_3CN**
Doublet: 0.2 Quartet: 0.0	Doublet: 0.0 Quartet: 0.8
	
nitrobenzene	CH_3CN

Table S13. Calculated energies in Hartree for all ground-state stationary points

Stationary point	Opt (Hartree)	Gibbs (Hartree)	Large basis set in SMD (Hartree)
H_2O_2	-151.54151	0.00473	-151.62397
H_2O	-76.41873	0.00373	-76.47195
Et_3N	-292.46075	0.17234	-292.55807
Et_3NH^+	-292.20220	0.17198	-292.37820
O_2	-150.31706	-0.01620	-150.38264
Benzene	-232.27201	0.07325	-232.35493
Phenol	-307.49338	0.07596	-307.61340
1	-2052.32114	0.51610	-2053.40028
Int1	-2050.99335	0.49660	-2052.07262
Int2	-2050.76731	0.48292	-2051.61167
Int2A	-2050.71784	0.48379	-2051.56990
Int2B	-2050.72215	0.48175	-2051.55844
Int3	-2051.39018	0.49365	-2052.22815
TS0	-2283.01521	0.57349	-2283.91607
Int3'	-2283.02332	0.57620	-2283.92475
TS1	-2051.36009	0.49069	-2052.21313
Int4'	-2051.36330	0.49115	-2052.21742
Int4	-2051.40569	0.49754	-2052.25591
TS2	-2283.68840	0.58866	-2284.60325
Int5	-2283.70535	0.59123	-2284.62039
TS3	-2283.69539	0.58878	-2284.60740
Int6	-2283.77658	0.58629	-2284.68413
TS1'	-2051.34048	0.49133	-2052.18850
Int4''	-2051.39421	0.49494	-2052.24466
TS2-*o*-nitrobenzene	-2488.20161	0.59035	-2489.18780
TS2-*m*-nitrobenzene	-2488.19338	0.59001	-2489.18723
TS2-*p*-nitrobenzene	-2488.19338	0.59001	-2489.18723
TS2-CH_3CN	-2184.15381	0.53038	-2185.05638
nitrobenzene	-436.77464	0.07179	-436.94061
CH_3CN	-132.76040	0.02143	-132.81994

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Coordinates for the calculated structures

H_2O_2

(charge: 0, multiplicity: singlet, E = -151.54151 Hartree)

O 1.0515765432 0.8791886715 -0.0165543062

H 2.0148978291 0.9948882621 -0.0073816957

O 0.6342705452 2.2733460775 0.0288203249

H 0.1703957199 2.3345097582 -0.8212017821

H_2O

(charge: 0, multiplicity: singlet, E = -76.41873 Hartree)

O 1.0514171441 0.9335360506 0.

H 2.0150788739 0.980156106 0.

H 0.7736862427 1.8574856734 0

Et_3N

(charge: 0, multiplicity: singlet, E = -292.46075 Hartree)

N -0.9122777351 0.3981806274 0.0005787044

C -0.4852068291 -0.9930054792 0.1743926501

H -0.5400149253 -1.4879656259 -0.7995315986

H 0.5752825156 -1.0518101705 0.4882659303

C -0.4860312037 1.2439789481 1.1190363176

H	-0.5431729293	0.648311913	2.0346992904
H	0.5750482906	1.5437942782	1.014825305
C	-0.4839632936	0.9435320925	-1.2905726523
H	-0.5404635878	2.0343900362	-1.2326985716
H	0.5772201611	0.7026306222	-1.496699289
C	-1.3659390489	0.4776735271	-2.4481927016
H	-1.0368680528	0.9322818511	-3.388506295
H	-1.3340078011	-0.6083746434	-2.5794154036
H	-2.405972871	0.7619325618	-2.2649802457
C	-1.3697658398	-1.7622967264	1.1545649983
H	-1.0418370793	-2.8042857101	1.2311521733
H	-1.3393616004	-1.3334365979	2.1609814943
H	-2.4091274347	-1.7445695853	0.8147827881
C	-1.3692559538	2.4786694833	1.2935086246
H	-1.3363886552	3.1358348449	0.4189857536
H	-2.4092912079	2.1768774783	1.4461054101
H	-1.0421664885	3.0655479545	2.1582252972

Et_3NH^+

(charge: +1, multiplicity: singlet, E = -292.20220 Hartree)

N	-0.0001534853	-0.0002318298	0.7124015826
C	1.1103084192	-0.9419576019	0.7001775337
H	2.030876071	-0.3843527024	0.8785863805
H	0.9500046	-1.6331945424	1.5375597055
C	-1.370954037	-0.4909453493	0.6992972598
H	-1.3484020251	-1.5672675987	0.8760191067
H	-1.8893575341	-0.0077378289	1.5374600841
C	0.2602359399	1.4322791071	0.6994660617
H	-0.6831303443	1.9507424606	0.8767317343
H	0.9383647838	1.6396732598	1.5372317302
C	0.9088230914	1.8935576006	-0.6206607156
H	1.0730735942	2.9715365447	-0.5542557477
H	1.8753943789	1.4134176083	-0.7873304092
H	0.2549442218	1.6921865456	-1.471282665
C	1.186938147	-1.7339227911	-0.6200735487

H 2.0382397942 -2.4152366904 -0.5528493299

H 0.2880164541 -2.3308358843 -0.7879564063

H 1.3405468807 -1.0667492211 -1.4703404097

C -2.0952206445 -0.1590415258 -0.6203031895

H -2.1626272169 0.9181904671 -0.786474274

H -1.5945142042 -0.624313355 -1.471462375

H -3.1109408848 -0.5556266728 -0.5534881085

O_2

(charge: 0, multiplicity: triplet, E = -150.31706 Hartree)

O 0. 0. 0.6070803132

O 0. 0. -0.6070803132

Benzene

(charge: 0, multiplicity: singlet, E = -232.27201 Hartree)

C -0.6374300675 0.1424117976 0.000074399

C 0.7586503252 0.142383002 0.0005823832

C 1.4566584626 1.3512093239 -0.0000887348

C 0.7586719689 2.5603037916 -0.0010253548

C -0.637204199 2.5603308209 -0.0014195517

C -1.335317186 1.3513359036 -0.0009830972

H -1.1803024831 -0.797947708 0.0004346786

H 1.3013944682 -0.798061823 0.0013718544

H 2.5424643685 1.351304813 0.0001681936

H 1.301779847 3.5005197716 -0.001450981

H -1.1801659076 3.5006426106 -0.0022427996

H -2.4211305172 1.3515078963 -0.0013319897

Phenol

(charge: 0, multiplicity: singlet, E = -307.49338 Hartree)

C -1.330573969 -0.4200406433 0.0000022291

C -0.3024519663 -1.3683493602 0.0000112152

C 1.0334739729 -0.9540093509 0.000004988

C 1.3360498675 0.4078690946 -0.0000085127

C 0.3167713222 1.3600767613 -0.0000187839

C -1.0146776848 0.9363448712 -0.0000147143

H -2.359285077 -0.7635681954 0.00000912

H 1.8310612033 -1.6939194494 0.0000115914

H 2.375758915 0.7216662808 -0.0000122751

H 0.5558797003 2.4184466518 -0.0000289837

H -1.8171592679 1.6682076537 -0.0000224621

O -0.6638524958 -2.6866183322 0.0000222188

H 0.1339975095 -3.230921402 0.0000382992

1

(charge: +3, multiplicity: triplet, E = -2052.32114 Hartree)

C 2.0890373317 4.0079252828 -0.3564226103

C 0.9308036211 4.6095594727 -0.7874128719

C -0.2692191925 3.8597985421 -0.8147561687

C -0.2379530807 2.5027598849 -0.363954093

C 2.0476128952 2.6468139636 0.0105845891

H -1.5266456079 5.4296486051 -1.6253218289

H 3.0261910734 4.5519056818 -0.321986892

H 0.9233394887 5.6451140371 -1.1137338278

C -1.4934089323 4.4050868077 -1.2671734255

C	-2.5373003506	2.32476008	-0.7057487776
C	-2.6271842348	3.630029513	-1.225631743
H	-3.5863930387	4.0151223697	-1.5522413441
N	0.9296909334	1.9158181779	0.0096358265
N	-1.3923938111	1.7661229646	-0.2918586257
Cu	1.5351737372	-0.2626809664	0.0115935349
Cu	-1.8526258131	-0.1723953414	0.4835290101
C	3.3155859025	1.9271197767	0.4158163334
H	4.2001641427	2.5262007275	0.1738791506
H	3.3086944743	1.7684098758	1.4984550432
C	-3.7804656424	1.4830423897	-0.5495118767
H	-3.8585602593	0.7723952641	-1.3807403972
H	-4.6787735134	2.1105339974	-0.5631840507
N	3.3804742407	0.6009169518	-0.2451708165
N	-3.690892614	0.7174456531	0.7200125851
C	4.334509029	-0.3169832532	0.4310143083
H	4.4820407919	-1.1784519973	-0.2297650299

H	5.310355284	0.1636006553	0.5669291594
C	3.6660039993	0.722986035	-1.7012056332
H	4.7456299457	0.7462040613	-1.8839533361
H	3.2623376184	1.6818728559	-2.0423132152
C	-4.7425777067	-0.3340073667	0.7909084536
H	-4.8740870036	-0.594689758	1.8459333556
H	-5.7040258525	0.05755021	0.4398076603
C	-3.8060956477	1.6332626331	1.8864925426
H	-3.0378072808	2.404553123	1.8308393127
H	-4.7916561288	2.1114653451	1.901845194
C	-4.3354023613	-1.5680935435	0.0295634773
C	-5.2556593938	-2.4821677666	-0.4734800213
C	-4.7848567937	-3.6471717291	-1.0805798091
H	-6.3197302662	-2.2896467242	-0.3858775931
C	-2.548139373	-2.8912022642	-0.6681583424
C	-3.4075662311	-3.8576766905	-1.1747640605
H	-5.482894923	-4.3778609789	-1.4759108417

H	-1.4706302251	-2.9864038065	-0.7254488477
H	-3.0060771413	-4.7516725925	-1.637891378
C	2.9919218974	-0.3842609861	-2.4735265941
C	3.4657328447	-0.849334432	-3.6956354494
C	2.7242698684	-1.8132815214	-4.3812204641
H	4.3940565148	-0.4652758681	-4.1050484782
C	1.1340040981	-1.7823628641	-2.5885460618
C	1.5350216107	-2.2831471512	-3.82162545
H	3.073029003	-2.1936650465	-5.3356717821
H	0.2304188393	-2.1134830463	-2.0912601676
H	0.9355104669	-3.0319884584	-4.3261763444
C	3.7612626635	-0.7806359284	1.7483609738
C	4.5575522157	-1.1587363426	2.8244588191
C	3.9419307841	-1.619391787	3.9889036781
H	5.6382519217	-1.0978590137	2.7520552919
C	1.8187596101	-1.2622174288	2.935157744
C	2.548080776	-1.6694256841	4.0459304842

H 4.5408657979 -1.926403033 4.8399661418

H 0.7335637088 -1.2623177577 2.9360205598

H 2.0363610778 -2.0138424028 4.9373032502

N 2.4122874883 -0.8333111093 1.8064411823

N 1.8481706462 -0.8526116905 -1.9312034903

N -3.0050470967 -1.7724039279 -0.0739057347

O -0.1892039186 -1.1055790572 0.2309272881

H -0.1335052592 -1.7727698147 0.9277123425

H -3.6719401854 1.059875237 2.8022326583

O -1.6854578789 -0.7248859044 2.7941912494

H -1.5247201316 -0.1297372683 3.5400593434

H -2.1792084525 -1.4741728715 3.1577769306

Int1

(charge: +3, multiplicity: triplet, E = -2050.99335 Hartree)

C -2.0440959814 -3.4915258543 -1.877659343

C -0.8651932362 -4.1112033757 -2.2062158914

C 0.353624803 -3.5419209305 -1.7684510455

C	0.3127133703	-2.3308377535	-1.0083538924
C	-1.9996192608	-2.2963061354	-1.1278272793
H	1.6365850813	-5.0612063419	-2.6287092169
H	-2.9992737873	-3.9017838659	-2.1853270519
H	-0.8519760796	-5.0274650297	-2.7884639217
C	1.601908055	-4.1453706869	-2.0463421071
C	2.6438632602	-2.3982685603	-0.7905296719
C	2.749526639	-3.5756032365	-1.55151133
H	3.7225124155	-4.0216254184	-1.7238108271
N	-0.8680398138	-1.7152966018	-0.7163129422
N	1.4787862889	-1.7811574551	-0.5365386506
Cu	-1.4844486173	0.373283707	0.1765080023
Cu	1.9077940946	-0.0364431398	0.4909960271
C	-3.3070784209	-1.6639737812	-0.7105213351
H	-4.1226262909	-2.0041726643	-1.3585266136
H	-3.5392949061	-2.0000943283	0.305304885
C	3.8917804153	-1.7630642022	-0.2204983448

H 4.2914505263 -1.0382141167 -0.9398377977

H 4.6661718713 -2.520052581 -0.0513080023

N -3.2364852146 -0.1887482563 -0.7013720202

N 3.5696160128 -1.0483122608 1.0384168533

C -4.2864588758 0.4012122094 0.1738726127

H -4.3091109359 1.4790236602 -0.0181844113

H -5.2741030337 -0.0002470904 -0.0799377996

C -3.2646927253 0.373611771 -2.0783662926

H -4.2891937361 0.3976090693 -2.4661235916

H -2.6857638106 -0.2961696513 -2.723018853

C 4.6271006355 -0.0653365054 1.4078683749

H 4.522032557 0.1417384276 2.4777725696

H 5.6234058245 -0.496212155 1.25979457

C 3.3188631324 -2.0052095997 2.1524209072

H 2.5545974731 -2.7235903626 1.8550937592

H 4.2388357998 -2.5439510153 2.4047392471

C 4.4562282079 1.2204385051 0.6388532362

C	5.5037780349	2.1008940849	0.3913590742
C	5.2334135632	3.304014449	-0.2625529406
H	6.5113913203	1.8523474364	0.7073730715
C	2.9298043801	2.6562321743	-0.3899957817
C	3.9246347913	3.5865349361	-0.6600941366
H	6.0343333542	4.007867402	-0.4640665417
H	1.9003312107	2.8120663918	-0.6894303351
H	3.6814297418	4.5076594393	-1.1769195784
C	-2.636342709	1.7437307496	-2.0843646347
C	-3.0171787386	2.755191286	-2.9595920137
C	-2.3589514709	3.9847173681	-2.8946583845
H	-3.8174903378	2.5884783803	-3.6726817911
C	-1.0315868779	3.1122241461	-1.0999205654
C	-1.3523793511	4.1681951051	-1.9449838631
H	-2.6400114274	4.7912132641	-3.5639345082
H	-0.2801298968	3.20055053	-0.32429734
H	-0.8375201114	5.1172797346	-1.849403146

C	-3.9380039354	0.1373858426	1.6187539835
C	-4.9038999272	-0.0126122982	2.6060997996
C	-4.4939004121	-0.2299993567	3.9232027761
H	-5.9570867721	0.0401572588	2.3514266279
C	-2.220247537	-0.1522897707	3.1620872581
C	-3.1301059055	-0.3053821471	4.2030268585
H	-5.2285339403	-0.3469142504	4.713107562
H	-1.1520222177	-0.1953183754	3.3270495081
H	-2.7717097552	-0.4825462134	5.21053903
N	-2.6132859797	0.0713562744	1.8941239803
N	-1.6509212853	1.9210878952	-1.1785283691
N	3.1916982424	1.5015245082	0.251954079
O	0.2809049211	0.9973208328	0.7445249123
O	0.4893271504	0.9318514206	2.1927367907
H	0.6481060753	1.867592314	2.4112440142
H	2.9724520651	-1.4556302058	3.0287247921

Int2

(charge: +2, multiplicity: triplet, E = -2050.76731 Hartree)

C	-2.8299389775	3.6906098891	-0.8403831474
C	-1.8023005708	4.2197568202	-1.5808667137
C	-0.5746466621	3.5189379297	-1.6644621704
C	-0.4503486079	2.2819779067	-0.9683925294
C	-2.6488146899	2.443746385	-0.2001466129
H	0.4652618629	4.9195380849	-2.9525737244
H	-3.777469338	4.2082899023	-0.7420896478
H	-1.9126788883	5.1693796126	-2.0954125104
C	0.537866349	3.9846204195	-2.4055799226
C	1.7415547908	2.0391759581	-1.6741178843
C	1.6892314478	3.2378927662	-2.4239309077
H	2.5579936437	3.557899921	-2.9885678387
N	-1.5049421042	1.7640133394	-0.2737444431
N	0.7149935901	1.5728586099	-0.9691589136
Cu	-1.4927943043	0.0135648967	0.7678803172
Cu	1.4582077103	-0.2017102666	0.3482662311

C	-3.8052102774	1.8054613237	0.5452360352
H	-4.4727032069	2.5893934142	0.9280615094
H	-4.3831010823	1.2377580919	-0.1937984814
C	3.0519702094	1.2827666554	-1.6132097249
H	3.684431467	1.7753317178	-0.8659025315
H	3.5772421183	1.3646771572	-2.5745175943
N	-3.363674165	0.8940231923	1.6070636285
N	2.8895456465	-0.121102215	-1.2101064315
C	-4.239377373	-0.27751888	1.7452739192
H	-3.9207827934	-0.817193175	2.6441605044
H	-5.293489084	-0.0011273869	1.8915257737
C	-3.1412957448	1.5951413833	2.882891037
H	-4.0753207602	1.9928773092	3.3036134923
H	-2.4483182463	2.4238148636	2.7189009727
C	4.1254098594	-0.6580700275	-0.5946286858
H	4.0214699128	-1.7474544184	-0.5474645644
H	5.0082336588	-0.4404691649	-1.2088763988

C	2.3712670719	-0.9701250991	-2.3027187409
H	1.635944608	-0.3767162499	-2.8561808813
H	3.1646212262	-1.2481351353	-3.0078822316
C	1.6905949556	-2.2011307605	-1.7450977177
C	1.7013875447	-3.4241800982	-2.4079269149
C	0.4144131431	-3.0818026047	-0.0087939543
C	1.0283703507	-4.5068144409	-1.8376351862
H	2.2331369574	-3.5299193994	-3.3475898674
C	0.3774953437	-4.3337617831	-0.6172825734
H	-0.0632122264	-2.8720096841	0.9429271158
H	1.0273394172	-5.471830241	-2.3338059347
H	-0.1399706099	-5.1535623525	-0.1324154995
C	4.2902640334	-0.1175077685	0.8106389125
C	5.5300774457	0.0554267325	1.4157758872
C	5.5747095811	0.4884728482	2.7428183994
H	6.4415157583	-0.1500946571	0.8645172667
C	3.1788315072	0.555379493	2.745826723

C 4.3820011356 0.7396879081 3.4204963616

H 6.5295990623 0.6279175006 3.2386706292

H 2.2145226258 0.7268195864 3.2125125103

H 4.3792792062 1.0735523516 4.4515717024

C -4.1092191471 -1.2019847505 0.5499350277

C -5.1635854365 -2.0100742045 0.1282782482

C -4.9720655512 -2.8715117869 -0.9504584427

H -6.1183799896 -1.962589382 0.6410515723

C -2.7307190486 -2.0508578153 -1.1199023363

C -3.7319348822 -2.8919785195 -1.5897160816

H -5.7800946172 -3.5102311442 -1.2914545982

H -1.7497419553 -2.0262668857 -1.5817586857

H -3.5448379158 -3.5403357547 -2.4379317766

N -2.9129623062 -1.2280026274 -0.0728684955

N 3.1425390069 0.1409567535 1.4697845964

N 1.0477674327 -2.0370289062 -0.5694395494

O 0.2343858439 0.0130456266 1.8155859613

O -0.572978966 -1.10143681 2.0565479348

H -2.686981996 0.9061700453 3.597205577

Int2A

(charge: +2, multiplicity: triplet, E = -2050.71784 Hartree)

C -1.4329518919 2.9702457042 2.5435635151

C -0.441999172 3.8548856224 2.1854088565

C 0.6231128715 3.4007671524 1.3730636621

C 0.6302532616 2.0287409229 0.9796987651

C -1.3601691852 1.6356170356 2.0844076931

H 1.700234503 5.2763051846 1.1994217255

H -2.2696787615 3.2843144285 3.1572495506

H -0.4734343516 4.8919483739 2.5054278421

C 1.6763674021 4.2301075797 0.9100082331

C 2.5716198128 2.3259575978 -0.24354862

C 2.6481549634 3.699570235 0.0953177445

H 3.4593235042 4.3113207628 -0.2841935812

N -0.3641417821 1.1707811842 1.339201537

N	1.6199158954	1.5257065668	0.2035750965
Cu	-1.2209417245	-0.5653870375	-0.0184972682
Cu	1.7966997986	-0.554214365	-0.9606979148
C	-2.4286748822	0.63194771	2.4507038218
H	-2.0015837553	-0.0522029981	3.1903618854
H	-3.2859642864	1.128576845	2.9197077972
C	3.5665241434	1.7152524357	-1.2118500756
H	4.556236082	2.1753338187	-1.0982974146
H	3.2237345505	1.9188547397	-2.2319851366
N	-2.8593786968	-0.1744344091	1.2833009891
N	3.6645799658	0.2449939728	-1.0627841715
C	-3.8506003396	0.5506275907	0.4378535659
H	-4.3742727356	-0.2034493074	-0.1591031133
H	-4.5993778701	1.045657822	1.067439152
C	-3.4128198636	-1.4895811458	1.7046700644
H	-4.4386855223	-1.3903887059	2.0790358404
H	-2.7983253517	-1.8597291032	2.5315176221

C	4.3552590802	-0.1146637789	0.2114943962
H	5.4414229564	-0.1077141314	0.0697220173
H	4.1119484909	0.6483368835	0.956733142
C	4.3493658432	-0.3648403445	-2.2346397547
H	3.7390800878	-0.1998734664	-3.1228151623
H	5.3434300455	0.0756668921	-2.3701934175
C	3.8654985534	-1.445276046	0.715102377
C	4.6002331367	-2.2938410211	1.5351380191
C	4.0022271081	-3.4711682613	1.9886818515
H	5.6183666568	-2.0409337855	1.8100211255
C	2.0190952138	-2.8824478224	0.776172577
C	2.6931904722	-3.7698289667	1.6069558075
H	4.5570772007	-4.1513794312	2.6263698805
H	1.0088195834	-3.0353345253	0.4104666916
H	2.2063330979	-4.6807326732	1.9350073094
C	-3.3369073671	-2.4772490749	0.5660853844
C	-4.2521089314	-3.5068149947	0.3780008598

C -4.0432432368 -4.4041155049 -0.6719552432

H -5.1076790785 -3.6059626626 1.0374538279

C -2.0665314871 -3.1785701398 -1.2591211203

C -2.9337458334 -4.2402554681 -1.5008707579

H -4.7428844582 -5.2157261531 -0.842231372

H -1.1891174927 -2.9758438291 -1.8637722406

H -2.7451398969 -4.914345556 -2.3283697792

C -3.2022089109 1.5290963969 -0.5125484147

C -3.8063266302 2.7286311792 -0.8737968071

C -3.1854626533 3.5259476003 -1.837985646

H -4.7459915735 3.0280818264 -0.4217106015

C -1.4317272658 1.8923358239 -1.9729180084

C -1.9836003667 3.0994860495 -2.3991484002

H -3.6378359299 4.4633729476 -2.1447167513

H -0.4884928851 1.5083886869 -2.3516211456

H -1.4765386508 3.68809681 -3.1552499168

N -2.0353480939 1.1282625063 -1.0501158215

N -2.2719307211 -2.3246336109 -0.243351567

N 2.6031215789 -1.7513185505 0.3540510806

O 0.1929349896 -1.3433014083 -0.9340747278

O 1.2186972382 0.2599999115 -2.4347258701

H 4.4523885477 -1.4382145208 -2.0667174852

Int2B

(charge: +2, multiplicity: triplet, E = -2050.72215 Hartree)

C -3.1368866112 -3.539047747 0.8319638712

C -2.2006828671 -4.0802539459 1.6860593179

C -0.9458786595 -3.4404937224 1.8523226969

C -0.7087878961 -2.2516520941 1.1110363338

C -2.8344629667 -2.3262149589 0.169181243

H -0.0466000543 -4.7843647463 3.304752053

H -4.0967081215 -4.0190496477 0.6759920919

H -2.4107483856 -4.9971514114 2.2284512295

C 0.0968268461 -3.8916255679 2.7037808687

C 1.4366182893 -2.0424803886 1.9277887747

C	1.2757437516	-3.1869297763	2.7561429546
H	2.0876300073	-3.5052783344	3.4014677386
N	-1.6723633082	-1.715485008	0.3224689209
N	0.4786610949	-1.5988908542	1.1409706039
Cu	-1.5617761861	0.2381706912	-0.557195861
Cu	1.2819083742	0.2148842133	-0.3903109638
C	-3.8404139509	-1.6048546311	-0.7031991005
H	-4.4608868458	-2.3230458989	-1.2538431689
H	-4.510589477	-1.0425810447	-0.0436000573
C	2.7887475156	-1.3615112601	1.8575967767
H	3.4418157628	-2.0365018155	1.2928724254
H	3.220178521	-1.2904535587	2.8655043701
N	-3.1901144338	-0.6508230091	-1.6380426745
N	2.8142434019	-0.0470455077	1.1860565458
C	-4.0913996763	0.4819046615	-1.9466674552
H	-3.6568056483	1.025498057	-2.7927088281
H	-5.0860862252	0.1380464595	-2.2580162072

C	-2.7237515236	-1.3413351102	-2.8594368329
H	-3.5688105271	-1.7361355206	-3.4367121238
H	-2.0687870807	-2.1646748098	-2.5705560601
C	4.094686886	0.1166983932	0.4546462357
H	4.2718498551	1.1836946089	0.3045284346
H	4.9418280365	-0.2737330008	1.0310373422
C	2.5469207983	1.0685516583	2.117062759
H	1.5989398324	0.8476878467	2.6187277217
H	3.3290567714	1.1399364335	2.8856937279
C	2.4228676034	2.3890047947	1.3801095163
C	2.6698825855	3.601546903	2.0207825251
C	1.8967485031	3.4687000473	-0.6005465387
C	2.5029771348	4.7864705437	1.3040285715
H	2.9889586285	3.6176187035	3.0578553244
C	2.1087495677	4.7221367365	-0.0324951431
H	1.5987924098	3.3629729196	-1.6394926046
H	2.6880594265	5.7440536657	1.7794796605

H	1.978458969	5.619518847	-0.626444128
C	4.0074386284	-0.5445124308	-0.8989332633
C	5.1099927521	-1.0839345814	-1.5532915797
C	4.9461456538	-1.6082803165	-2.8360814817
H	6.0798841943	-1.0884204959	-1.0675974207
C	2.6215281505	-1.040721332	-2.7108570895
C	3.682571959	-1.5844579945	-3.4260294128
H	5.7936165768	-2.0314915395	-3.3651257515
H	1.6123651341	-0.9875587209	-3.1033441695
H	3.5171823252	-1.9808620843	-4.4210026503
C	-4.1849084695	1.4039889142	-0.7518586033
C	-5.3014217528	2.1843870039	-0.4713071562
C	-5.2672573322	3.0355242392	0.6345422933
H	-6.1788671832	2.127971798	-1.1064947956
C	-3.0477370173	2.2595853894	1.0981584915
C	-4.1235981655	3.074378093	1.432876484
H	-6.125523422	3.6553847596	0.871890647

H -2.1280708729 2.2337599753 1.6723837632

H -4.0650391606 3.7198039003 2.3015318285

N -3.0851854858 1.4474396393 0.0286586264

N 2.7878955787 -0.5353638659 -1.4762453653

N 2.051129212 2.3294161614 0.0895242499

O -0.1018519872 -0.0308916512 -1.7809321521

O -0.2392115546 0.9016457743 0.6639327646

H -2.147905889 -0.6453164488 -3.4688591447

TS0

(charge: +2, multiplicity: triplet, E = -2283.01521 Hartree)

C 0.936273 -4.485853 -1.195048

C -0.137119 -4.628718 -2.037782

C -1.070731 -3.570285 -2.151173

C -0.857622 -2.397946 -1.368307

C 1.098017 -3.267427 -0.491472

H -2.381547 -4.494181 -3.610656

H 1.666277 -5.278918 -1.074423

H	-0.28409	-5.538607	-2.611594
C	-2.205164	-3.616275	-2.99685
C	-2.803436	-1.429983	-2.195564
C	-3.059689	-2.541362	-3.03059
H	-3.930778	-2.536031	-3.676271
N	0.240575	-2.258555	-0.56921
N	-1.746263	-1.366833	-1.387898
Cu	1.183238	-0.322189	0.453876
Cu	-1.70193	0.360954	-0.244574
C	2.354714	-3.078145	0.33193
H	2.620551	-4.017986	0.834481
H	3.172031	-2.854812	-0.361861
C	-3.790003	-0.279002	-2.136484
H	-4.505198	-0.509334	-1.337395
H	-4.36439	-0.232149	-3.073265
N	2.258311	-1.970007	1.293914
N	-3.13891	0.997744	-1.823365

C	3.581684	-1.357418	1.550694
H	3.46692	-0.660474	2.388142
H	4.326721	-2.107419	1.845586
C	1.548251	-2.365099	2.526644
H	2.203495	-2.925292	3.206167
H	0.735161	-3.036783	2.231023
C	-4.025919	1.923001	-1.109444
H	-3.519265	2.894451	-1.076293
H	-4.981137	2.080683	-1.632424
C	-2.526083	1.602207	-3.01445
H	-1.854624	0.875421	-3.476629
H	-3.277131	1.913784	-3.755377
C	-4.291246	1.466264	0.312927
C	-5.502775	1.737803	0.945585
C	-5.688695	1.340163	2.268524
H	-6.288707	2.253848	0.404236
C	-3.479225	0.4212	2.220239

C	-4.655511	0.6667	2.919173
H	-6.624629	1.54479	2.777574
H	-2.651318	-0.104601	2.683095
H	-4.758848	0.329814	3.944378
C	0.945604	-1.166511	3.225153
C	0.745428	-1.120491	4.602612
C	0.126549	0.001082	5.155784
H	1.069951	-1.944724	5.22885
C	-0.021019	0.933532	2.953157
C	-0.265818	1.046065	4.317798
H	-0.037851	0.061177	6.226607
H	-0.290355	1.708203	2.243441
H	-0.740932	1.936973	4.712205
C	4.02779	-0.606786	0.314209
C	5.35526	-0.526881	-0.087338
C	5.66518	0.186628	-1.248575
H	6.130945	-1.017083	0.491205

C	3.33072	0.674967	-1.500622
C	4.637779	0.791651	-1.967539
H	6.694011	0.259061	-1.5856
H	2.487979	1.147367	-1.991549
H	4.835527	1.351538	-2.873809
N	3.037422	-0.011471	-0.387135
N	0.565705	-0.153344	2.424796
N	-3.291075	0.814125	0.947074
O	0.101543	1.164592	-0.04981
O	0.496721	1.807368	-1.231015
H	-1.92839	2.46404	-2.714081
C	0.972948	3.486875	-0.792305
C	2.02594	3.37435	0.192528
C	1.333983	4.036069	-2.080316
C	3.335487	3.646255	-0.138585
H	1.767177	3.044856	1.192708
C	2.652674	4.287129	-2.393899

H	0.549732	4.221143	-2.806822
C	3.665952	4.092761	-1.433254
H	4.118069	3.538537	0.606204
H	2.911045	4.675907	-3.373808
H	4.698106	4.315046	-1.682775
H	-0.019958	3.721178	-0.415808

Int3'

(charge: +2, multiplicity: triplet, E = -2283.02332 Hartree)

C	5.0090205824	-2.4948613214	-2.2322572894
C	4.7814644732	-1.2564604467	-2.779182451
C	3.5365040525	-0.6197086927	-2.5563937432
C	2.5625725544	-1.2995151445	-1.7680935184
C	4.0056056849	-3.0785619157	-1.4228369679
H	3.9301802166	1.1955485298	-3.6762074977
H	5.9441754241	-3.0194295386	-2.3957372433
H	5.5348834787	-0.7645433555	-3.3868038197
C	3.2008055665	0.6500793272	-3.0853977766

C	1.0254450591	0.4097523928	-2.0879603179
C	1.9531518613	1.1687621325	-2.8392666234
H	1.6636130129	2.1406374459	-3.2231922076
N	2.831772656	-2.5067961068	-1.1887645917
N	1.3210912343	-0.7806341674	-1.5722707999
Cu	1.7791680728	-3.5802608813	0.5728861759
Cu	-0.3026240014	-1.6624451895	-0.5486201697
C	4.3048285517	-4.3916688278	-0.7307942055
H	4.8392591854	-5.0662186041	-1.4128145575
H	4.9858343429	-4.1835004942	0.100549857
C	-0.398579806	0.9044164934	-1.9230269687
H	-0.9752618497	0.4916079685	-2.7598435036
H	-0.4278122419	1.9988433531	-2.0283023064
N	3.1000361875	-5.0394769522	-0.182572163
N	-1.0153002201	0.4568495237	-0.6695079775
C	3.4132012675	-5.8442374906	1.0220126961
H	2.5208073754	-6.4283492377	1.2712283451

H	4.2285794348	-6.5533602228	0.8316586139
C	2.3568536759	-5.7990697368	-1.211073837
H	2.8303551334	-6.7684091396	-1.4116825785
H	2.39751986	-5.2158071732	-2.1370540991
C	-2.4694347976	0.2935694174	-0.7900601877
H	-2.862172621	0.1349835023	0.2208713345
H	-2.9647675025	1.1924965321	-1.186570457
C	-0.6312183971	1.3179780075	0.4568575455
H	0.4566875286	1.3213579923	0.5492043715
H	-0.9853228383	2.3517659709	0.3290667812
C	-2.8309707613	-0.9077132211	-1.6427146818
C	-3.9845536011	-0.9208725336	-2.4238145826
C	-4.30354618	-2.0633204138	-3.1559579714
H	-4.622377635	-0.0438353358	-2.4554814101
C	-2.3080102109	-3.07218687	-2.301724861
C	-3.4462672021	-3.1613296893	-3.0943710512
H	-5.1989243196	-2.0919606705	-3.7678316849

H -1.6105951388 -3.8990730527 -2.2267410022

H -3.648915193 -4.0676013508 -3.6536664803

C 0.9082864312 -5.9740913224 -0.8131642671

C 0.1323407795 -7.0537027463 -1.2265480681

C -1.209844623 -7.1004469742 -0.8462187239

H 0.5700578073 -7.8427067778 -1.8287711392

C -0.8940625889 -5.0322927776 0.3234045943

C -1.7333302906 -6.0738862866 -0.0585290541

H -1.8344421874 -7.9331679191 -1.1524583412

H -1.2301949007 -4.2043129906 0.9379408809

H -2.7679203004 -6.0828232803 0.2644996059

C 3.7578174272 -4.9139989131 2.1649782179

C 4.6608625677 -5.2511533079 3.1654177465

C 4.9133880267 -4.3269019914 4.1826455949

H 5.1594896515 -6.2143884082 3.1488401988

C 3.3776383393 -2.8247347425 3.1170244552

C 4.2677753279 -3.0935917303 4.1534525249

H	5.6130838688	-4.5671271608	4.9763570269
H	2.8411742718	-1.8880777653	3.0425142207
H	4.4396575364	-2.3451082936	4.9176921308
N	3.1246346434	-3.7198210765	2.1499555608
N	0.3936928413	-4.9875892318	-0.0558737245
N	-2.0021196701	-1.9750233479	-1.5841865396
O	0.3859759687	-2.4248363114	1.1462267894
O	0.9397975829	-1.3583860481	1.9680352396
H	-1.0475663309	0.9113076991	1.3799786385
C	0.1532769686	-1.3131558221	3.2147299103
C	0.206973271	-2.6050181829	3.9690616903
C	0.7258116133	-0.1504125087	3.9600522973
C	0.7704878429	-2.692925449	5.2111565594
H	-0.2279672306	-3.4749910828	3.4909311059
C	1.2908828592	-0.2961195888	5.1970404239
H	0.684590788	0.8194495848	3.4754730368
C	1.3309504374	-1.5559945243	5.8457702213

H 0.7861437424 -3.6479262261 5.7284511045

H 1.6968397737 0.5737643844 5.7046918239

H 1.7687825763 -1.6439503786 6.8338344004

H -0.8796761071 -1.1073567938 2.8866267712

Int3

(charge: +2, multiplicity: doublet, E = -2051.39018 Hartree)

C 1.9589565726 3.4989402918 -1.7987640386

C 0.8018291844 4.239048086 -1.8089817072

C -0.3865259822 3.6749912158 -1.2850885464

C -0.3294751705 2.3539830296 -0.7538538746

C 1.9395196261 2.2121889658 -1.2130350626

H -1.7059255604 5.3554379221 -1.6610948135

H 2.8811292106 3.8894701689 -2.2151718942

H 0.7814001968 5.2405609867 -2.227779094

C -1.6366034906 4.3409074889 -1.2810090617

C -2.6117642025 2.3509680553 -0.3438888225

C -2.7430865706 3.6839544226 -0.8008836866

H	-3.715731215	4.1629230098	-0.7829862905
N	0.848628523	1.6644749891	-0.6916770404
N	-1.4441992029	1.7148354725	-0.3150121766
Cu	1.4153017568	-0.1022947278	0.5935904275
Cu	-1.5931502502	-0.2751568662	0.4158671651
C	3.2296233881	1.42562043	-1.1195266461
H	3.7973501802	1.5147884315	-2.0551862529
H	3.845657248	1.8746519656	-0.333765028
C	-3.8454199284	1.5568813387	0.0399508373
H	-4.1848798469	1.0474723345	-0.8704050384
H	-4.65274992	2.2415202521	0.3378568409
N	3.0046863668	0.0108397503	-0.7683324418
N	-3.5783443582	0.5442106766	1.0674949629
C	4.1559242387	-0.5582105361	-0.0286524732
H	4.0174867128	-1.6434825884	0.016484597
H	5.1012326121	-0.3691467425	-0.5521123025
C	2.6079862867	-0.8101196085	-1.9347056508

H 3.4730814784 -1.0521801268 -2.5644802599

H 1.919249252 -0.208251636 -2.536542813

C -4.4507223252 -0.6300410279 0.9337247669

H -4.3120045237 -1.2405268802 1.833361373

H -5.5170010252 -0.3625304757 0.89171691

C -3.6160942742 1.1284123894 2.4157628905

H -2.8843980909 1.9363164246 2.4748568119

H -4.6111313526 1.5234802071 2.668508975

C -4.0846858556 -1.4650091493 -0.2782604837

C -5.0523013653 -2.1624906242 -0.9979841493

C -4.6662179856 -2.9513402771 -2.0804650659

H -6.0954972508 -2.0847553402 -0.7105466576

C -2.4070015757 -2.2794205229 -1.6633966872

C -3.3153650975 -3.0087279632 -2.4212524145

H -5.4063917259 -3.5026771337 -2.6506129986

H -1.3478868502 -2.2906569027 -1.8943352747

H -2.9699167003 -3.6008105158 -3.2610550322

C	1.8968575807	-2.0670739912	-1.4817328738
C	1.9300515044	-3.2603092305	-2.1981759716
C	1.2169436902	-4.3567106276	-1.7092271584
H	2.5076196686	-3.3329820325	-3.1135739542
C	0.5185565799	-3.0073538399	0.1444200601
C	0.501099723	-4.2309317285	-0.5178253328
H	1.231521468	-5.2995156344	-2.2461085092
H	-0.0144664054	-2.8417817889	1.0744387334
H	-0.052507656	-5.0647078248	-0.1018943389
C	4.1863992651	0.0077630769	1.3738414071
C	5.364732539	0.1750213794	2.0927320761
C	5.2937644326	0.6769935376	3.3934588033
H	6.3185810675	-0.0819788134	1.6444988411
C	2.9145812593	0.8242932295	3.1419491748
C	4.0492190959	1.0105722843	3.9257417227
H	6.1984986167	0.8141563305	3.9763194383
H	1.9190119881	1.0766331275	3.4863218003

H 3.9545677427 1.4143886618 4.927079091

N 2.9831904285 0.327400501 1.8964523046

N 1.1961681469 -1.9527450469 -0.337387519

N -2.774064316 -1.5263310968 -0.6093957964

O -0.0889841831 -0.3993558261 1.7251804554

O -0.2224309138 0.7222219547 2.6563404162

H -0.319579138 0.2357369187 3.491890263

H -3.3419893219 0.3664278191 3.1477200883

TS1

(charge: +2, multiplicity: doublet, E = -2051.36009 Hartree)

C -1.915055 -2.625757 -2.851704

C -0.866152 -3.511292 -2.848115

C 0.274568 -3.232478 -2.056018

C 0.290884 -2.025350 -1.301128

C -1.841480 -1.478696 -2.027546

H 1.400616 -5.024968 -2.524746

H -2.801374 -2.804493 -3.450592

H	-0.897160	-4.419530	-3.442005
C	1.396378	-4.091504	-1.970501
C	2.415267	-2.499621	-0.487808
C	2.455975	-3.734951	-1.172750
H	3.321084	-4.379384	-1.064705
N	-0.782232	-1.185119	-1.282753
N	1.381598	-1.670568	-0.570759
Cu	-1.366320	0.268493	0.311775
Cu	1.486446	-0.017389	0.733620
C	-3.050083	-0.573903	-1.917145
H	-3.482378	-0.390402	-2.909955
H	-3.809602	-1.107491	-1.336264
C	3.604774	-2.045866	0.333008
H	4.245857	-1.450867	-0.327664
H	4.194355	-2.918173	0.643917
N	-2.749899	0.689901	-1.221214
N	3.217691	-1.221232	1.489136

C	-3.938753	1.227120	-0.515863
H	-3.704848	2.252974	-0.212661
H	-4.810923	1.272397	-1.179938
C	-2.120518	1.687587	-2.115118
H	-2.863787	2.166034	-2.765140
H	-1.417279	1.150252	-2.759892
C	4.227541	-0.193811	1.783162
H	3.969911	0.258523	2.747579
H	5.238822	-0.612159	1.886440
C	2.881754	-2.053224	2.659740
H	2.053882	-2.713036	2.394852
H	3.741369	-2.648559	2.996240
C	4.215431	0.880517	0.715515
C	5.347771	1.622904	0.389408
C	5.253211	2.619465	-0.580650
H	6.288315	1.419202	0.889874
C	2.941549	2.058426	-0.842093

C	4.027482	2.841129	-1.210651
H	6.124660	3.208433	-0.846796
H	1.966806	2.186555	-1.300226
H	3.915682	3.600136	-1.976145
C	-1.362174	2.717099	-1.306457
C	-1.192119	4.036945	-1.715878
C	-0.455060	4.900816	-0.903048
H	-1.633565	4.384223	-2.644054
C	-0.140358	3.092793	0.638440
C	0.076948	4.424330	0.296051
H	-0.313097	5.935959	-1.195870
H	0.233382	2.656297	1.559084
H	0.635420	5.072725	0.961435
C	-4.228766	0.389574	0.710378
C	-5.506089	0.246218	1.240195
C	-5.669902	-0.521553	2.394927
H	-6.354217	0.724104	0.761426

C	-3.311949	-0.958204	2.370536
C	-4.557380	-1.137686	2.965731
H	-6.654942	-0.646101	2.832327
H	-2.415587	-1.443143	2.735358
H	-4.648484	-1.755476	3.851550
N	-3.155147	-0.201274	1.273562
N	-0.834066	2.262322	-0.155220
N	3.032667	1.102214	0.101123
O	-0.064130	-0.013404	1.617711
O	-0.389848	-2.358728	1.864263
H	-0.226035	-1.673021	2.543601
H	2.554849	-1.405826	3.475903

Int4'

(charge: +2, multiplicity: doublet, E = -2051.36330 Hartree)

C	-1.868135	-2.752650	-2.813201
C	-0.774032	-3.581818	-2.827261
C	0.361577	-3.244936	-2.051420

C	0.330439	-2.035583	-1.300406
C	-1.840874	-1.602440	-1.992272
H	1.560030	-4.989157	-2.520862
H	-2.755331	-2.980244	-3.393731
H	-0.768265	-4.492463	-3.418172
C	1.518271	-4.056256	-1.967312
C	2.467636	-2.429910	-0.476214
C	2.559179	-3.660656	-1.163745
H	3.445893	-4.273698	-1.048629
N	-0.782176	-1.248118	-1.271565
N	1.407419	-1.634819	-0.571386
Cu	-1.365388	0.221903	0.259193
Cu	1.501484	0.065166	0.705915
C	-3.096017	-0.771044	-1.842710
H	-3.600831	-0.657651	-2.811382
H	-3.780478	-1.325304	-1.190655
C	3.626688	-1.948443	0.372080

H	4.274115	-1.342511	-0.272312
H	4.223300	-2.809404	0.700978
N	-2.834367	0.535538	-1.214428
N	3.192452	-1.130647	1.515770
C	-4.027189	1.046169	-0.495132
H	-3.856665	2.108784	-0.292712
H	-4.928725	0.971889	-1.115374
C	-2.284112	1.522564	-2.172309
H	-3.072231	1.939453	-2.811480
H	-1.581339	0.990672	-2.822011
C	4.186411	-0.099835	1.850484
H	3.889269	0.349719	2.804712
H	5.193932	-0.515580	1.992806
C	2.811242	-1.966812	2.671594
H	2.003724	-2.637732	2.372403
H	3.663107	-2.550116	3.046154
C	4.212754	0.974969	0.783307

C	5.353696	1.722707	0.503546
C	5.294720	2.717866	-0.470813
H	6.273551	1.524170	1.042982
C	2.998801	2.145261	-0.828504
C	4.095446	2.932722	-1.152078
H	6.173570	3.310996	-0.700951
H	2.043562	2.268480	-1.327291
H	4.012099	3.690191	-1.922687
C	-1.544955	2.618626	-1.435223
C	-1.492294	3.935887	-1.882830
C	-0.766414	4.868482	-1.138625
H	-2.013776	4.228747	-2.787959
C	-0.236946	3.126297	0.419107
C	-0.130358	4.460138	0.034354
H	-0.713854	5.902647	-1.462812
H	0.214997	2.746264	1.330125
H	0.422084	5.161582	0.649110

C	-4.199943	0.317371	0.819606
C	-5.437247	0.122743	1.423063
C	-5.481461	-0.493206	2.675846
H	-6.345910	0.449306	0.928568
C	-3.092794	-0.679231	2.608725
C	-4.291879	-0.896547	3.281065
H	-6.433610	-0.656353	3.169704
H	-2.133747	-0.969691	3.021145
H	-4.288552	-1.375853	4.253055
N	-3.056323	-0.089380	1.405127
N	-0.917336	2.228924	-0.309867
N	3.054849	1.190497	0.119550
O	-0.061008	-0.071486	1.561042
O	-0.338853	-2.688958	1.569291
H	-0.270228	-1.705088	1.778670
H	2.437510	-1.322088	3.469067

Int4

(charge: +2, multiplicity: doublet, E = -2051.40569 Hartree)

C	-1.251670	3.049739	2.539830
C	-0.180012	3.847888	2.212340
C	0.854143	3.313294	1.409292
C	0.752639	1.948960	1.002565
C	-1.286886	1.719753	2.063655
H	2.081420	5.096104	1.257570
H	-2.071628	3.429720	3.138701
H	-0.127888	4.880487	2.543948
C	1.973893	4.057847	0.958642
C	2.717630	2.096412	-0.209330
C	2.902215	3.456900	0.142295
H	3.762464	4.003525	-0.228245
N	-0.316608	1.175085	1.339382
N	1.699380	1.373439	0.225710
Cu	-1.246348	-0.488570	-0.038901
Cu	1.752289	-0.711209	-0.955745
C	-2.459173	0.818515	2.371627
H	-2.135747	0.091753	3.123161
H	-3.288352	1.390795	2.803746
C	3.666905	1.409278	-1.168473
H	4.681490	1.816926	-1.078782
H	3.313432	1.592470	-2.188109
N	-2.905135	0.063586	1.175190
N	3.682609	-0.057716	-0.974173
C	-3.766444	0.886942	0.277866
H	-4.309436	0.190440	-0.369591
H	-4.511730	1.436427	0.865143
C	-3.619225	-1.182762	1.559630
H	-4.651571	-0.973989	1.864752
H	-3.103906	-1.608665	2.426403
C	4.299680	-0.425403	0.332696
H	5.385064	-0.528392	0.228000
H	4.112258	0.385691	1.042223
C	4.372010	-0.732269	-2.104717
H	3.801923	-0.548220	-3.015207
H	5.394176	-0.352173	-2.212579
C	3.669931	-1.681145	0.869353
C	4.287720	-2.545406	1.766541
C	3.571008	-3.644596	2.242065
H	5.309040	-2.363311	2.082668
C	1.708359	-2.956036	0.898369
C	2.261968	-3.852786	1.804440
H	4.033945	-4.334969	2.939415

H	0.708653	-3.040311	0.484188
H	1.683412	-4.702759	2.146894
C	-3.571375	-2.184549	0.432816
C	-4.565879	-3.129053	0.203681
C	-4.380726	-4.061331	-0.819376
H	-5.463192	-3.137359	0.813170
C	-2.267817	-3.034072	-1.301644
C	-3.212962	-4.016639	-1.580702
H	-5.141285	-4.808574	-1.020283
H	-1.339360	-2.926755	-1.851643
H	-3.037698	-4.722806	-2.384042
C	-2.968623	1.822223	-0.600052
C	-3.416976	3.097401	-0.928810
C	-2.653474	3.869778	-1.806797
H	-4.345388	3.476193	-0.514650
C	-1.077285	2.063663	-1.925079
C	-1.466409	3.344752	-2.313125
H	-2.982666	4.865248	-2.086310
H	-0.148746	1.610577	-2.263824
H	-0.846335	3.913751	-2.996573
N	-1.821304	1.319458	-1.092448
N	-2.452086	-2.143023	-0.313941
N	2.405478	-1.899455	0.456077
O	0.107489	-1.391519	-0.934941
O	1.406332	0.124779	-2.517612
H	0.641716	-0.362004	-2.863154
H	4.407741	-1.805747	-1.910005

TS2

(charge: +2, multiplicity: quartet, E = -2283.68840 Hartree)

C	-2.372009	-2.473573	-2.902788
C	-1.488174	-3.527906	-2.870529
C	-0.282732	-3.398557	-2.144537
C	-0.010760	-2.157243	-1.491322
C	-2.031724	-1.285826	-2.220486
H	0.486668	-5.397266	-2.500946
H	-3.315900	-2.547104	-3.431195
H	-1.712165	-4.462323	-3.376250
C	0.661310	-4.446530	-2.006517
C	1.959641	-2.975954	-0.610747
C	1.778133	-4.236208	-1.241423
H	2.520917	-5.014587	-1.106136
N	-0.888973	-1.122231	-1.566245

N	1.110582	-1.966557	-0.740391
Cu	-1.212207	0.519926	0.046003
Cu	1.902359	-0.243895	0.988499
C	-2.976020	-0.101524	-2.227213
H	-2.567128	0.650785	-2.908116
H	-3.958672	-0.394910	-2.614488
C	3.144473	-2.808310	0.310371
H	3.971161	-3.451860	-0.020953
H	2.826952	-3.136988	1.306142
N	-3.124230	0.538078	-0.892571
N	3.591431	-1.417853	0.463372
C	-4.044477	-0.200367	0.001178
H	-4.420545	0.509601	0.744939
H	-4.911113	-0.588216	-0.546836
C	-3.484247	1.968605	-1.037467
H	-3.778183	2.338248	-0.050350
H	-4.334751	2.110879	-1.715619
C	4.141179	-0.851762	-0.786050
H	5.150742	-1.231204	-0.989289
H	3.495444	-1.155879	-1.615590
C	4.576409	-1.330055	1.566245
H	4.085684	-1.647212	2.485817
H	5.447766	-1.966049	1.365416
C	4.139416	0.654035	-0.686093
C	5.112839	1.467383	-1.260786
C	5.022854	2.848738	-1.090642
H	5.931842	1.024711	-1.817357
C	3.032775	2.497587	0.194054
C	3.967684	3.375304	-0.343280
H	5.774549	3.502662	-1.520336
H	2.185614	2.838686	0.778039
H	3.878213	4.441415	-0.168184
C	-2.273341	2.736153	-1.508242
C	-2.342246	3.893066	-2.277946
C	-1.153685	4.530715	-2.637322
H	-3.304181	4.283645	-2.592393
C	0.049046	2.822115	-1.463903
C	0.063110	3.982178	-2.230557
H	-1.179053	5.434440	-3.237184
H	0.950397	2.340781	-1.111879
H	1.006928	4.438746	-2.505730
C	-3.325443	-1.305423	0.734807
C	-3.969410	-2.470424	1.133571
C	-3.258839	-3.409450	1.883549

H	-5.007688	-2.636225	0.866339
C	-1.339382	-1.964839	1.761295
C	-1.928553	-3.148497	2.201522
H	-3.739528	-4.326358	2.208880
H	-0.294938	-1.730793	1.988013
H	-1.338851	-3.848956	2.781948
N	-2.034942	-1.062949	1.046071
N	-1.094979	2.225405	-1.106256
N	3.112888	1.169516	0.015513
O	0.402207	0.973710	0.956349
O	1.535516	-1.446663	2.397304
H	4.910934	-0.296930	1.674629
C	0.003027	1.866642	2.612161
C	-0.785254	0.914297	3.334548
C	-0.650720	3.052358	2.131822
C	-2.159629	1.059753	3.421345
H	-0.294021	0.054449	3.771829
C	-2.021374	3.181252	2.221981
H	-0.055567	3.831448	1.667809
C	-2.787700	2.182323	2.860407
H	-2.750204	0.315889	3.945974
H	-2.509068	4.073367	1.841030
H	-3.861214	2.309995	2.963488
H	1.631607	-0.996992	3.246761
H	1.061671	1.924621	2.839502

Int5

(charge: +2, multiplicity: quartet, E = -2283.70535 Hartree)

C	3.338387	1.902429	-2.503779
C	2.801906	3.167686	-2.423894
C	1.556440	3.351676	-1.782723
C	0.880521	2.204168	-1.264838
C	2.614704	0.826476	-1.948224
H	1.435966	5.509385	-1.993826
H	4.300850	1.727947	-2.971445
H	3.329224	4.026272	-2.828645
C	0.949337	4.620125	-1.604934
C	-0.844889	3.502942	-0.452045
C	-0.245950	4.695533	-0.939704
H	-0.741214	5.647040	-0.780765
N	1.425216	0.963679	-1.374686
N	-0.312849	2.299956	-0.615195
Cu	1.162914	-0.783593	0.131967

Cu	-1.748561	0.776969	0.870842
C	3.171451	-0.580448	-1.984713
H	2.589493	-1.160986	-2.706212
H	4.213600	-0.577937	-2.324206
C	-2.123952	3.620673	0.340674
H	-2.695153	4.496701	0.004075
H	-1.845272	3.766762	1.389997
N	3.064509	-1.265558	-0.668671
N	-2.954889	2.409291	0.302792
C	4.086491	-0.803664	0.301167
H	4.283094	-1.626161	0.996685
H	5.034754	-0.577936	-0.199608
C	3.049571	-2.738144	-0.843250
H	3.177194	-3.191972	0.144547
H	3.875971	-3.082870	-1.476900
C	-3.471043	2.112578	-1.050061
H	-4.307137	2.772670	-1.313422
H	-2.667341	2.285639	-1.771770
C	-4.058979	2.529545	1.283515
H	-3.621717	2.629804	2.276454
H	-4.688427	3.399773	1.059266
C	-3.887427	0.664450	-1.112204
C	-4.955933	0.210013	-1.880308
C	-5.278758	-1.146252	-1.852934
H	-5.532497	0.910249	-2.475032
C	-3.477190	-1.476149	-0.307248
C	-4.531736	-2.003658	-1.044318
H	-6.112404	-1.522497	-2.436712
H	-2.871510	-2.089593	0.350259
H	-4.769642	-3.058790	-0.970381
C	1.714554	-3.160556	-1.406003
C	1.534057	-4.300440	-2.181745
C	0.246974	-4.617681	-2.619274
H	2.382453	-4.925399	-2.439256
C	-0.551171	-2.652821	-1.505508
C	-0.812904	-3.776771	-2.280580
H	0.079018	-5.502375	-3.224432
H	-1.321925	-1.958057	-1.208190
H	-1.823923	-3.981010	-2.613549
C	3.602706	0.384005	1.100179
C	4.479710	1.316110	1.640157
C	3.967147	2.335644	2.445411
H	5.543566	1.241434	1.441146
C	1.766819	1.432843	2.089988

C	2.594893	2.389290	2.674475
H	4.632876	3.073209	2.881746
H	0.679905	1.464674	2.220960
H	2.154975	3.163456	3.292697
N	2.272337	0.449213	1.323378
N	0.682284	-2.361073	-1.075557
N	-3.151218	-0.172741	-0.354497
O	-0.553423	-0.784753	1.043711
O	-1.200468	1.746973	2.395157
H	-4.675275	1.629539	1.249998
C	-0.467688	-1.450309	2.348667
C	0.733461	-2.355441	2.372922
C	-1.751523	-2.195861	2.567382
C	0.614444	-3.713696	2.252351
H	1.706072	-1.892811	2.513192
C	-1.826821	-3.554648	2.440614
H	-2.641491	-1.607378	2.774931
C	-0.659493	-4.333578	2.226214
H	1.503285	-4.339086	2.233769
H	-2.784346	-4.057804	2.541788
H	-0.737096	-5.410796	2.128591
H	-1.448967	1.278771	3.203002
H	-0.348457	-0.661332	3.103300

TS3

(charge: +2, multiplicity: doublet, E = -2283.69539 Hartree)

C	-0.788623	3.765994	-2.181658
C	-2.107561	3.840580	-1.800610
C	-2.679674	2.754164	-1.099966
C	-1.865164	1.605158	-0.856050
C	-0.045743	2.607617	-1.852143
H	-4.654138	3.601711	-0.798727
H	-0.309335	4.584025	-2.707638
H	-2.707697	4.719339	-2.016669
C	-4.016865	2.738636	-0.630768
C	-3.624660	0.513677	0.185421
C	-4.492170	1.620883	0.009738
H	-5.516223	1.566988	0.362638
N	-0.562763	1.552504	-1.237686
N	-2.361756	0.514232	-0.212956
Cu	1.429664	0.626245	0.182645
Cu	-1.344517	-1.464695	0.637871
C	1.442587	2.556641	-2.106145

H	1.683939	1.676500	-2.710028
H	1.768204	3.449070	-2.658277
C	-4.130038	-0.750945	0.847160
H	-5.212760	-0.852623	0.693048
H	-3.936612	-0.683458	1.922720
N	2.183242	2.438701	-0.828507
N	-3.404633	-1.939983	0.354082
C	1.924508	3.561505	0.096681
H	2.806649	3.680888	0.733527
H	1.793166	4.509555	-0.440051
C	3.611456	2.179036	-1.077488
H	4.166908	2.449886	-0.173601
H	4.009544	2.796391	-1.893718
C	-3.619451	-2.165845	-1.096410
H	-4.463327	-2.844507	-1.265811
H	-3.877697	-1.212824	-1.566151
C	-3.776689	-3.148575	1.120162
H	-3.552615	-2.996222	2.175814
H	-4.845567	-3.372858	1.014350
C	-2.370315	-2.683036	-1.768215
C	-2.408264	-3.394803	-2.965441
C	-1.208035	-3.751528	-3.577430
H	-3.361853	-3.661730	-3.408466
C	-0.044879	-2.693432	-1.771654
C	-0.003003	-3.387548	-2.973934
H	-1.213647	-4.307302	-4.509256
H	0.844105	-2.382832	-1.239463
H	0.950651	-3.644853	-3.420274
C	3.873233	0.712609	-1.348270
C	4.934861	0.291865	-2.145664
C	5.207045	-1.071355	-2.249724
H	5.543012	1.023662	-2.666832
C	3.354805	-1.481339	-0.787763
C	4.408577	-1.974459	-1.547503
H	6.031750	-1.420745	-2.862030
H	2.706924	-2.132169	-0.215656
H	4.597609	-3.041253	-1.584305
C	0.732834	3.307136	1.002924
C	-0.080998	4.346613	1.440124
C	-1.126316	4.065396	2.321703
H	0.101872	5.359329	1.096659
C	-0.478142	1.757682	2.247516
C	-1.324408	2.750348	2.734981
H	-1.772153	4.862372	2.675776

H	-0.630514	0.716734	2.516694
H	-2.121999	2.484652	3.419120
N	0.530461	2.033814	1.400978
N	3.083810	-0.166314	-0.698055
N	-1.203841	-2.353493	-1.184335
O	0.597560	-1.121487	0.812625
O	-1.533673	-1.166467	2.519403
H	-3.198622	-3.998943	0.752523
C	1.120040	-1.659302	2.020611
C	2.063121	-0.788350	2.744803
C	1.528043	-3.073806	1.926384
C	3.160873	-1.303337	3.398265
H	1.813835	0.263321	2.825920
C	2.631099	-3.556448	2.580982
H	0.891488	-3.732502	1.341498
C	3.455273	-2.676634	3.321780
H	3.810166	-0.648431	3.970459
H	2.887092	-4.609951	2.528735
H	4.326476	-3.067518	3.837278
H	-1.912947	-1.913917	2.999075
H	0.178164	-1.646133	2.690883

Int6

(charge: +2, multiplicity: doublet, E = -2283.77658 Hartree)

C	0.850144	4.054073	-1.578814
C	-0.212277	4.677736	-0.969301
C	-1.234141	3.882020	-0.397645
C	-1.077997	2.464676	-0.455020
C	0.896983	2.637428	-1.615427
H	-2.558621	5.478418	0.236972
H	1.643442	4.629181	-2.043258
H	-0.288211	5.760304	-0.936852
C	-2.415294	4.403108	0.186237
C	-3.148448	2.147755	0.564304
C	-3.383461	3.540322	0.645621
H	-4.315543	3.909139	1.059726
N	-0.024972	1.865245	-1.058202
N	-2.027859	1.638179	0.069968
Cu	1.553822	-0.223143	-0.082162
Cu	-1.912095	-0.540375	0.339860
C	2.003633	1.928158	-2.369664
H	1.529047	1.347065	-3.165552
H	2.661818	2.668407	-2.847785

C	-4.185227	1.153202	1.054800
H	-5.195422	1.544519	0.873095
H	-4.083378	1.023960	2.136709
N	2.769876	0.992413	-1.532427
N	-3.998388	-0.169904	0.429259
C	3.684656	1.694263	-0.610514
H	4.427393	0.966231	-0.267312
H	4.231641	2.499029	-1.122054
C	3.489451	-0.003299	-2.346431
H	4.371282	0.426484	-2.843065
H	2.806422	-0.333826	-3.136391
C	-4.440416	-0.175627	-0.986205
H	-5.524468	-0.325481	-1.058602
H	-4.215692	0.805535	-1.417077
C	-4.679422	-1.236540	1.198389
H	-4.254971	-1.282181	2.201465
H	-5.758715	-1.050211	1.264463
C	-3.692398	-1.217207	-1.786769
C	-4.224335	-1.834194	-2.915194
C	-3.418945	-2.707270	-3.647256
H	-5.247303	-1.633217	-3.214759
C	-1.646741	-2.296034	-2.087675
C	-2.105870	-2.935967	-3.233366
H	-3.812608	-3.202471	-4.528741
H	-0.642729	-2.427414	-1.699594
H	-1.451507	-3.604274	-3.781016
C	3.895284	-1.214088	-1.531919
C	5.063434	-1.917866	-1.814601
C	5.352158	-3.073436	-1.088964
H	5.733115	-1.566353	-2.592602
C	3.327157	-2.715570	0.139825
C	4.464489	-3.482401	-0.095470
H	6.255121	-3.639099	-1.293362
H	2.616648	-2.986288	0.912934
H	4.648698	-4.372585	0.495073
C	2.971503	2.236278	0.608863
C	3.271245	3.487284	1.145015
C	2.614596	3.907207	2.301045
H	4.010070	4.119562	0.663925
C	1.434668	1.827720	2.284728
C	1.674138	3.059570	2.885757
H	2.834281	4.875895	2.737558
H	0.720830	1.125934	2.706433
H	1.145001	3.341362	3.789265

N	2.062592	1.418340	1.174157
N	3.043815	-1.604180	-0.562104
N	-2.431764	-1.464877	-1.383656
O	-0.108469	-1.251264	0.422872
O	-1.868530	-0.280891	2.510104
H	-1.237589	-0.949422	2.842819
H	-4.517314	-2.193786	0.699257
C	0.004749	-2.220862	1.369907
C	0.773531	-1.997889	2.530963
C	-0.666775	-3.448830	1.225876
C	0.880863	-2.991365	3.509594
H	1.326936	-1.067706	2.622103
C	-0.561114	-4.426873	2.213533
H	-1.259368	-3.627459	0.335146
C	0.210928	-4.206158	3.358539
H	1.491586	-2.812019	4.389026
H	-1.080695	-5.371381	2.086072
H	0.291208	-4.973820	4.120092
H	-1.472090	0.574766	2.723311

TS1'

(charge: +2, multiplicity: doublet, E = -2051.34048 Hartree)

C	1.595341	-2.857569	2.417795
C	0.621507	-3.782348	2.126413
C	-0.512671	-3.371633	1.389120
C	-0.582046	-2.010245	0.963964
C	1.445809	-1.528922	1.957060
H	-1.555027	-5.273433	1.375068
H	2.474517	-3.131674	2.989895
H	0.706675	-4.813319	2.456103
C	-1.587261	-4.234828	1.060111
C	-2.650445	-2.377828	-0.024994
C	-2.659529	-3.740387	0.359725
H	-3.502781	-4.371247	0.100648
N	0.405337	-1.114257	1.240680
N	-1.657032	-1.551442	0.266587
Cu	1.351673	0.488398	-0.346979
Cu	-1.956163	0.329708	-0.984065
C	2.482024	-0.487562	2.338018
H	2.015029	0.167080	3.079914
H	3.334090	-0.974272	2.830110
C	-3.800062	-1.831597	-0.852091
H	-4.743288	-2.304373	-0.546983

H	-3.622484	-2.101655	-1.898734
N	2.920591	0.343307	1.204863
N	-3.901303	-0.360752	-0.788374
C	4.007003	-0.291914	0.424195
H	4.428909	0.476499	-0.233521
H	4.815697	-0.640645	1.080637
C	3.238261	1.731501	1.576003
H	4.282942	1.849845	1.892356
H	2.618024	1.998975	2.437644
C	-4.346958	0.115055	0.544118
H	-5.440066	0.178883	0.591478
H	-4.029384	-0.616283	1.293777
C	-4.758467	0.174055	-1.872696
H	-4.312440	-0.073556	-2.837005
H	-5.771519	-0.242368	-1.815817
C	-3.713448	1.441804	0.897942
C	-4.311083	2.347589	1.769715
C	-3.622937	3.509215	2.117493
H	-5.299456	2.144570	2.167615
C	-1.822081	2.793452	0.711465
C	-2.352831	3.734192	1.584128
H	-4.073244	4.229883	2.791982
H	-0.841392	2.917957	0.265926
H	-1.787951	4.625676	1.830400
C	2.923261	2.718829	0.468141
C	3.643983	3.904982	0.341205
C	3.267441	4.837879	-0.622988
H	4.489896	4.091937	0.994274
C	1.514262	3.345749	-1.269386
C	2.173578	4.555631	-1.441419
H	3.819360	5.764975	-0.736210
H	0.666124	3.083607	-1.892734
H	1.843709	5.249556	-2.205941
C	3.494021	-1.426690	-0.438641
C	4.188354	-2.619239	-0.612033
C	3.656671	-3.587555	-1.467166
H	5.126738	-2.786505	-0.093886
C	1.806405	-2.119554	-1.883703
C	2.447026	-3.335803	-2.112441
H	4.180722	-4.524805	-1.623181
H	0.855237	-1.866048	-2.343174
H	2.003977	-4.064335	-2.781867
N	2.327721	-1.190709	-1.069226
N	1.873757	2.439613	-0.337730

N	-2.490784	1.675329	0.374576
O	-0.061237	0.398590	-1.827894
O	-1.370022	-0.439475	-2.567264
H	0.054279	1.021646	-2.562251
H	-4.815405	1.260277	-1.778938

Int4"

(charge: +2, multiplicity: quartet, E = -2051.39421 Hartree)

C	1.276494	-3.134249	2.442191
C	0.155412	-3.898792	2.218886
C	-0.927211	-3.335088	1.508735
C	-0.808797	-1.989216	1.043205
C	1.307036	-1.810746	1.952549
H	-2.242168	-5.059021	1.581616
H	2.127002	-3.529710	2.985788
H	0.091600	-4.921670	2.577414
C	-2.127878	-4.037376	1.232343
C	-2.924096	-2.076565	0.096861
C	-3.127021	-3.410291	0.533315
H	-4.059680	-3.915347	0.307365
N	0.312518	-1.247802	1.273882
N	-1.815070	-1.396136	0.350744
Cu	1.372910	0.411860	-0.164075
Cu	-1.825696	0.496377	-0.995267
C	2.490883	-0.927900	2.266899
H	2.176847	-0.237494	3.055215
H	3.321451	-1.520869	2.665771
C	-3.983856	-1.404530	-0.749541
H	-4.984895	-1.732974	-0.437936
H	-3.824761	-1.728494	-1.783147
N	2.947682	-0.112923	1.112064
N	-3.871564	0.061276	-0.735922
C	3.849512	-0.887678	0.205689
H	4.373025	-0.159382	-0.423445
H	4.606721	-1.422287	0.790551
C	3.629640	1.127454	1.578729
H	4.675805	0.928143	1.837219
H	3.128892	1.459165	2.493170
C	-4.266605	0.640572	0.567639
H	-5.351758	0.790157	0.622159
H	-3.994541	-0.068548	1.355947
C	-4.636225	0.664598	-1.851678
H	-4.220128	0.307945	-2.794622

H	-5.699420	0.400631	-1.790607
C	-3.528368	1.933451	0.822654
C	-4.045201	2.959681	1.608727
C	-3.264091	4.091783	1.838404
H	-5.042008	2.874042	2.027754
C	-1.548156	3.109497	0.486716
C	-1.991665	4.168385	1.269871
H	-3.647393	4.906306	2.444057
H	-0.580998	3.111551	-0.001781
H	-1.361286	5.037596	1.417740
C	3.515171	2.226057	0.553584
C	4.455121	3.241967	0.417411
C	4.211731	4.261571	-0.504614
H	5.356597	3.236773	1.020735
C	2.159085	3.168845	-1.089243
C	3.043862	4.227153	-1.266912
H	4.928713	5.066128	-0.630288
H	1.246666	3.055842	-1.663855
H	2.825785	4.996938	-1.998085
C	3.079943	-1.829924	-0.689109
C	3.553141	-3.084330	-1.053951
C	2.800511	-3.847945	-1.950437
H	4.491615	-3.454356	-0.655196
C	1.181415	-2.075544	-2.019755
C	1.601290	-3.336034	-2.441400
H	3.149575	-4.828329	-2.257683
H	0.242083	-1.635522	-2.356427
H	0.992431	-3.898483	-3.139910
N	1.916261	-1.344446	-1.165474
N	2.391976	2.197613	-0.189389
N	-2.300748	2.017137	0.274781
O	0.030132	1.105645	-1.321679
O	-1.657673	-0.660349	-2.460094
H	0.110073	0.657142	-2.180070
H	-4.538565	1.751015	-1.805752

TS2-*o*-nitrobenzene

(charge: +2, multiplicity: doublet, E = -2488.20161 Hartree)

C	3.930418	1.670747	-2.078348
C	3.594183	2.998952	-1.954362
C	2.317656	3.344939	-1.457487
C	1.408577	2.294027	-1.123266
C	2.976054	0.694606	-1.718916

H	2.566760	5.500876	-1.504668
H	4.908018	1.369337	-2.437398
H	4.299281	3.782688	-2.214417
C	1.900491	4.682897	-1.248070
C	-0.170461	3.809526	-0.388974
C	0.660264	4.914751	-0.715161
H	0.306868	5.923436	-0.531569
N	1.757760	0.990055	-1.282489
N	0.174689	2.548271	-0.601664
Cu	1.061789	-0.832337	0.037289
Cu	-1.543179	1.193680	0.708313
C	3.305999	-0.776386	-1.858423
H	2.766788	-1.155487	-2.731596
H	4.376212	-0.912834	-2.051144
C	-1.479176	4.097585	0.307516
H	-1.892280	5.052201	-0.047102
H	-1.255912	4.196233	1.374990
N	2.892912	-1.599698	-0.690185
N	-2.472383	3.023048	0.188829
C	3.852303	-1.530569	0.437602
H	3.701943	-2.423411	1.050028
H	4.887991	-1.542045	0.078635
C	2.617205	-2.993577	-1.121446
H	2.542049	-3.616170	-0.227492
H	3.423577	-3.387655	-1.751383
C	-2.972040	2.860378	-1.193092
H	-3.692425	3.645470	-1.455423
H	-2.121960	2.941121	-1.877424
C	-3.583430	3.259459	1.139339
H	-3.175316	3.233288	2.149518
H	-4.063631	4.227564	0.949399
C	-3.588727	1.491275	-1.330293
C	-4.688664	1.212305	-2.136619
C	-5.191555	-0.088676	-2.164410
H	-5.150057	2.003051	-2.718135
C	-3.488051	-0.716740	-0.600832
C	-4.586695	-1.069355	-1.376402
H	-6.053176	-0.328041	-2.779002
H	-2.965899	-1.426537	0.028007
H	-4.962892	-2.085847	-1.353763
C	1.295166	-3.025564	-1.843298
C	0.982864	-3.953005	-2.832506
C	-0.279379	-3.908729	-3.423222
H	1.715686	-4.694334	-3.131866

C	-0.798103	-2.030982	-2.030563
C	-1.183267	-2.923978	-3.022269
H	-0.546555	-4.623236	-4.194743
H	-1.442024	-1.239085	-1.680279
H	-2.166122	-2.842395	-3.472002
C	3.591773	-0.318152	1.296320
C	4.604022	0.323722	2.000299
C	4.275787	1.403347	2.821686
H	5.629302	-0.018596	1.908735
C	1.983186	1.134677	2.153688
C	2.947058	1.813623	2.895819
H	5.048604	1.916997	3.384218
H	0.936984	1.448578	2.154106
H	2.648832	2.654510	3.511615
N	2.305144	0.081493	1.383287
N	0.406712	-2.092398	-1.446590
N	-2.996014	0.532128	-0.592613
O	-0.701289	-0.547012	0.778046
O	-0.913882	2.029240	2.271656
H	-4.328540	2.469120	1.031364
C	-0.959945	-1.639937	2.485549
C	-1.007312	-2.923393	1.881882
C	-2.182705	-1.132910	2.998440
C	-2.188670	-3.622629	1.685383
C	-3.370922	-1.826315	2.819501
H	-2.182012	-0.193213	3.537511
C	-3.380493	-3.067712	2.161087
H	-2.165311	-4.587269	1.194092
H	-4.296644	-1.421532	3.214809
H	-4.310705	-3.612189	2.040151
H	-0.970885	1.442107	3.034512
H	-0.012849	-1.250485	2.828920
N	0.235211	-3.502566	1.406446
O	0.202430	-4.549821	0.769060
O	1.283734	-2.874500	1.645527

TS2-*m*-nitrobenzene

(charge: +2, multiplicity: quartet, E = -2488.19338 Hartree)

C	-0.074530	3.817809	2.567147
C	1.194062	4.258676	2.268522
C	2.057780	3.420222	1.529157
C	1.587249	2.126157	1.143340
C	-0.464908	2.534999	2.126667

H	3.747681	4.778248	1.422661
H	-0.771431	4.438957	3.118324
H	1.534603	5.242242	2.577779
C	3.365265	3.802644	1.138329
C	3.579186	1.659675	0.069708
C	4.124737	2.925100	0.409801
H	5.131058	3.178220	0.094858
N	0.334370	1.708765	1.462371
N	2.362682	1.269111	0.421609
Cu	-1.141164	0.362421	0.094004
Cu	1.940057	-0.820761	-0.863264
C	-1.866206	2.029508	2.369580
H	-1.817545	1.151714	3.020289
H	-2.473934	2.790272	2.873514
C	4.406900	0.721210	-0.773674
H	5.475873	0.876996	-0.573949
H	4.206803	0.961742	-1.823242
N	-2.533950	1.609049	1.106674
N	4.037533	-0.691049	-0.594123
C	-2.846705	2.754653	0.216713
H	-3.718762	2.479645	-0.382791
H	-3.113842	3.644215	0.798507
C	-3.733060	0.798487	1.432989
H	-4.387045	0.782153	0.557613
H	-4.300415	1.243800	2.259249
C	4.308970	-1.182575	0.776212
H	5.377900	-1.381253	0.923448
H	4.010821	-0.406797	1.486691
C	4.733909	-1.528153	-1.596629
H	4.452542	-1.190831	-2.593757
H	5.822588	-1.453753	-1.482865
C	3.488925	-2.423350	1.026959
C	3.920188	-3.479759	1.824924
C	3.095245	-4.594475	1.971021
H	4.889782	-3.434471	2.309013
C	1.512390	-3.531002	0.522351
C	1.873361	-4.626997	1.297410
H	3.411492	-5.433086	2.582478
H	0.589581	-3.504176	-0.044697
H	1.220345	-5.490132	1.358684
C	-3.319508	-0.612701	1.763363
C	-4.114379	-1.475598	2.512663
C	-3.679070	-2.783259	2.719000
H	-5.058723	-1.128869	2.917938

C	-1.717436	-2.268657	1.444477
C	-2.455988	-3.185961	2.179716
H	-4.283126	-3.475099	3.296563
H	-0.768240	-2.500804	0.986688
H	-2.080443	-4.191824	2.327990
C	-1.714260	3.055313	-0.735038
C	-1.532234	4.322653	-1.276500
C	-0.530459	4.513727	-2.228912
H	-2.171682	5.141701	-0.964932
C	0.035558	2.189131	-2.012582
C	0.258713	3.429191	-2.604531
H	-0.374341	5.493563	-2.668375
H	0.651501	1.327038	-2.267539
H	1.044721	3.529296	-3.344080
N	-0.935107	2.013302	-1.095900
N	-2.144337	-1.013120	1.239890
N	2.293729	-2.445816	0.407078
O	-0.003578	-0.991492	-0.707952
O	2.042587	0.049181	-2.545395
H	4.436097	-2.570472	-1.472192
C	-0.683854	-1.457898	-2.409489
C	-1.963828	-0.822718	-2.327171
C	-0.657919	-2.895677	-2.347584
C	-3.043364	-1.562172	-1.881352
C	-1.781112	-3.612071	-1.979687
H	0.273116	-3.409896	-2.563954
C	-2.987367	-2.947445	-1.693879
H	-1.744491	-4.694233	-1.912249
H	-3.868153	-3.478034	-1.355215
H	2.315732	-0.567404	-3.237242
H	0.112070	-0.936656	-2.933043
H	-2.072613	0.231170	-2.536206
N	-4.261637	-0.840831	-1.504487
O	-5.184305	-1.477737	-1.011272
O	-4.254443	0.391381	-1.636297

TS2-*p*-nitrobenzene

(charge: +2, multiplicity: quartet, E = -2488.19338 Hartree)

C	-0.711240	3.693387	-2.666664
C	-2.063504	3.833320	-2.452524
C	-2.746609	2.858262	-1.691260
C	-2.009249	1.734950	-1.203410
C	-0.054947	2.567591	-2.124717

H	-4.708785	3.786218	-1.728641
H	-0.150420	4.433407	-3.226369
H	-2.607207	4.689381	-2.840594
C	-4.123160	2.946886	-1.366049
C	-3.881881	0.883610	-0.151963
C	-4.688762	1.964136	-0.596059
H	-5.738394	1.995940	-0.325709
N	-0.678458	1.610753	-1.447683
N	-2.594815	0.764642	-0.447185
Cu	0.936727	0.634598	-0.007561
Cu	-1.782746	-1.187250	0.927023
C	1.441204	2.400405	-2.263097
H	1.642922	1.536392	-2.901741
H	1.891079	3.281145	-2.735921
C	-4.502770	-0.165283	0.738857
H	-5.581521	-0.235143	0.544148
H	-4.352155	0.148539	1.777682
N	2.089479	2.145899	-0.946341
N	-3.858639	-1.481057	0.612074
C	2.091357	3.347592	-0.078860
H	2.973461	3.293052	0.567040
H	2.190528	4.263505	-0.672236
C	3.445980	1.580132	-1.139344
H	3.980708	1.617372	-0.186005
H	4.026884	2.161474	-1.865897
C	-4.016316	-2.067051	-0.736592
H	-5.016323	-2.498115	-0.870501
H	-3.894060	-1.271530	-1.477187
C	-4.375638	-2.399842	1.651672
H	-4.150460	-1.974597	2.628905
H	-5.458801	-2.539939	1.547525
C	-2.946031	-3.106788	-0.954005
C	-3.136820	-4.252763	-1.722043
C	-2.087177	-5.161218	-1.851707
H	-4.094938	-4.434227	-2.196995
C	-0.769821	-3.735717	-0.450077
C	-0.882423	-4.903067	-1.195936
H	-2.214087	-6.064617	-2.438990
H	0.132291	-3.482532	0.092561
H	-0.052588	-5.598609	-1.248891
C	3.336981	0.137904	-1.560032
C	4.354351	-0.535161	-2.228823
C	4.183241	-1.887184	-2.522689
H	5.267984	-0.014811	-2.493550

C	2.019784	-1.776350	-1.498486
C	2.987748	-2.514321	-2.167667
H	4.968546	-2.439367	-3.027515
H	1.078830	-2.196708	-1.176909
H	2.811278	-3.558314	-2.399301
C	0.866003	3.406281	0.801289
C	0.366290	4.611256	1.281180
C	-0.712115	4.589593	2.167154
H	0.819298	5.547808	0.973536
C	-0.712845	2.190688	2.011550
C	-1.251514	3.361225	2.540723
H	-1.117525	5.517497	2.557367
H	-1.126435	1.211836	2.268850
H	-2.084446	3.295355	3.231329
N	0.327048	2.220865	1.156886
N	2.200854	-0.484317	-1.188724
N	-1.773105	-2.850003	-0.344488
O	0.147150	-0.943402	0.778764
O	-2.156595	-0.334101	2.572178
H	-3.883204	-3.369289	1.557200
C	1.052080	-1.346358	2.439386
C	1.803532	-0.145267	2.662968
C	1.771270	-2.518754	2.029343
C	3.107988	-0.044844	2.217278
C	3.072429	-2.423120	1.586501
H	1.263172	-3.476690	2.029111
C	3.703277	-1.169689	1.630136
H	3.620998	-3.275926	1.207915
H	-2.004268	-0.926535	3.319786
H	0.123293	-1.457959	2.982484
H	1.323573	0.693248	3.149787
H	3.683841	0.865171	2.327242
N	5.020972	-1.024455	1.009567
O	5.464150	0.123647	0.890299
O	5.577044	-2.038448	0.601406

TS2-CH_3CN

(charge: +2, multiplicity: doublet, E = -2184.15381 Hartree)

C	-1.730538	-3.462500	-2.163284
C	-0.644229	-4.263843	-1.900887
C	0.517882	-3.682873	-1.349185
C	0.522162	-2.277024	-1.087911
C	-1.644183	-2.084643	-1.872704

H	1.702412	-5.496324	-1.227932
H	-2.642335	-3.870979	-2.583943
H	-0.669379	-5.330063	-2.104539
C	1.681159	-4.428830	-1.030978
C	2.674716	-2.390063	-0.241604
C	2.758310	-3.786242	-0.479537
H	3.663676	-4.323929	-0.220217
N	-0.566447	-1.500105	-1.358611
N	1.608500	-1.665525	-0.548417
Cu	-1.410005	0.392690	-0.089531
Cu	1.861907	0.380852	0.639005
C	-2.803984	-1.178023	-2.208892
H	-2.515984	-0.594043	-3.087831
H	-3.688271	-1.765453	-2.480995
C	3.827100	-1.704212	0.456979
H	4.784277	-2.133474	0.131083
H	3.701894	-1.893487	1.527144
N	-3.135148	-0.218213	-1.124050
N	3.816896	-0.244017	0.278057
C	-3.960450	-0.846043	-0.047446
H	-4.416469	-0.028463	0.521851
H	-4.774332	-1.434709	-0.486488
C	-3.831274	0.977312	-1.672862
H	-4.909550	0.802087	-1.759450
H	-3.454144	1.151519	-2.685017
C	4.139670	0.143066	-1.115464
H	5.224120	0.187956	-1.270156
H	3.741482	-0.623451	-1.787015
C	4.726661	0.420219	1.242450
H	4.389128	0.202049	2.254906
H	5.757277	0.068626	1.111668
C	3.485531	1.455881	-1.455160
C	4.012712	2.352294	-2.379965
C	3.307939	3.520422	-2.666921
H	4.962026	2.139411	-2.859304
C	1.637139	2.825178	-1.096637
C	2.097832	3.760025	-2.015267
H	3.702778	4.236358	-3.380093
H	0.715238	2.951116	-0.546013
H	1.526109	4.661312	-2.203680
C	-3.540261	2.208148	-0.852343
C	-4.414691	3.288666	-0.779833
C	-4.017424	4.430592	-0.083977
H	-5.384546	3.237992	-1.263114

C	-1.950866	3.329302	0.422844
C	-2.760626	4.454490	0.522201
H	-4.680345	5.286600	-0.013982
H	-0.974078	3.271878	0.887419
H	-2.416222	5.323401	1.071141
C	-3.125007	-1.680484	0.894317
C	-3.577053	-2.862588	1.467165
C	-2.744596	-3.524829	2.374052
H	-4.556417	-3.255780	1.216237
C	-1.095464	-1.805712	2.042423
C	-1.491036	-2.990344	2.663632
H	-3.073184	-4.448066	2.840139
H	-0.107725	-1.363486	2.203767
H	-0.816576	-3.481605	3.355807
N	-1.912668	-1.170118	1.186153
N	-2.333843	2.232307	-0.253536
N	2.316140	1.696805	-0.827788
O	0.086533	1.098454	0.798575
O	1.775110	-0.663683	2.204956
H	2.047848	-0.104577	2.945833
H	4.692230	1.499514	1.085853
C	1.126231	2.115270	3.453629
N	2.248350	2.428084	3.484305
C	-0.218289	1.654953	3.252760
H	-0.179447	1.299162	2.061530
H	-0.461049	0.760804	3.827337
H	-0.971651	2.437289	3.352693

nitrobenzene

(charge: 0, multiplicity: singlet, E = -436.77464 Hartree)

C	1.077023	-1.132161	0.000033
C	2.474325	-1.136745	0.000520
C	3.178126	0.065083	0.000067
C	2.456432	1.256470	-0.000880
C	1.063827	1.286071	-0.001397
C	0.374657	0.075786	-0.000925
H	0.534184	-2.072169	0.000392
H	3.016758	-2.076384	0.001266
H	4.259757	0.099440	0.000422
H	0.552952	2.240070	-0.002131
H	-0.710311	0.075966	-0.001310
N	3.192145	2.530473	-0.001373
O	2.533474	3.569697	-0.002060

O	4.421466	2.479437	-0.001157

CH_3CN

(charge: 0, multiplicity: singlet, E = -132.76040 Hartree)

C	0.649397	0.697727	0.028697
H	1.007021	-0.335675	0.016083
H	1.007041	1.203498	-0.872559
H	-0.444113	0.690459	0.016083
C	1.136112	1.386028	1.220880
N	1.522822	1.932904	2.168106