Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Reactivity of formal Cu (Ⅲ) – alkyl species toward aniline: a DFT investigation

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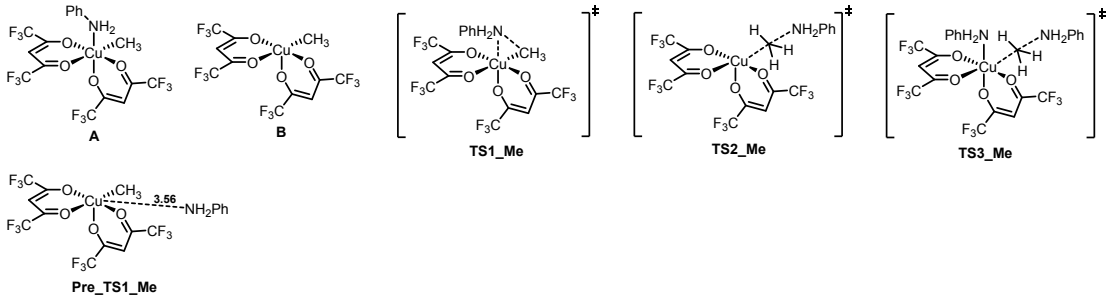
Detailed computational methods

Unless otherwise stated, quantum chemical calculations in this work were carried out using Gaussian 16 program[S1]. Geometry optimization and single point energy calculations were performed at B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP level of theory[S2-S4]. For R=Me, single point energy calculations were also carried out at the M06/def2-TZVP[S5] and PBE0-D3(BJ)/def2-TZVP[S6] level of theory (see SI). Frequency calculations were also carried out to evaluate the nature of optimized structures. For transition states with one imaginary frequency, IRC calculations were also performed to confirm its connectivity between substrates and products. The solvation effects were evaluated by the SMD[S7] model and the wave function analysis were carried out with Multiwfn[S8] program.

Table S1. Relative Gibbs free energy (kcal/mol) for R=Me with single point energy calculated by several different functionals.

	A_Me	B_Me+$PhNH_2$	Pre_TS1_Me	TS1_Me	TS2_Me	TS3_Me
B3LYP-D3(BJ)	0	0.04	3.23	17.36	8.95	7.54
PBE0-D3(BJ)	0	-1.28	2.93	18.13	8.62	8.61
M06	0	-2.69	3.39	18.05	9.18	9.61



In addition to calculate single point energy with different functionals, the binding energy between $Cu(hfac)_2$ and aniline was calculated at B3LYP-D3(BJ)/def2-TZVP-SMD//B3LYP-D3(BJ)/def2-SVP level of theory. Our calculated results (ΔG = -1.8 kcal/mol) fit well with the experimental value demonstrated by Larionov (ΔG = -2.4 kcal/mol)[S9], thus further confirmed the reliability of our computational method:

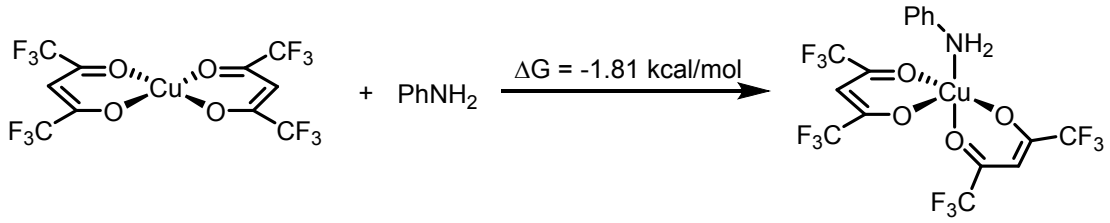


Table S2. Orbital decomposition analysis of complex A_Me and B_Me (LUMO orbital of theses complex were analyzed).

	Cu (complex A)	C* (complex A)	Cu (complex B)	C* (complex B)
Mulliken	33.08%	39.10%	34.28%	42.28%
Stout-Politzer	32.53%	38.47%	32.78%	39.30%

SCPA	29.92%	24.42%	34.88%	30.45%

* C represents the carbon atom on the methyl ligand.

Further discussion on the nature of "reductive elimination" step

Based on IRC calculation, a Pre complex of aniline and complex B_Me (weakly-interacting B_Me and aniline; Pre_TS1_Me) can be located, this indicated that the formation of TS1_Me was also need to dissociate one molcule aniline from complex A_Me at first. This feature is sharp contrast to the classical reductive elimination transition states, in which are directly connect to the substrate. For this and another reasons that we have dissussed in main text, we believe the "reductive elimination" description of this transition state is just formal. Although the reductive elimination transition state initial proposed by Larionov et al.[S9], TS1_Me_2, is directly connect to A_Me that confirmed by IRC calculation*, this structure is much higher in energy than TS1_Me (figure S1). And due to the stucture similarity of TS1_Me and TS1_Me_2, we believe these two transition states have silmilar electronic stuctures.

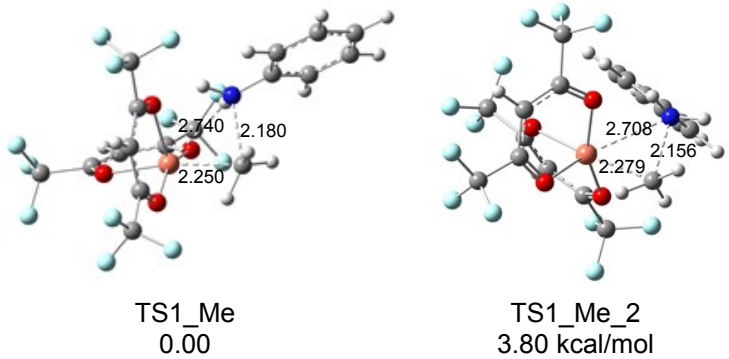


Figure S1. Geometry structure and relative Gibbs free energy of TS1_Me and TS1_Me_2

*A more careful look at the geometry structure of TS1_Me and TS1_Me_2 can explain this difference of connectivity (figure 1). The vacant coordinate site (which was occupied by aniline in A_Me and TS1_Me_2) in TS1_Me is far away from the aniline group, thus the TS1_Me may more properly be viewed as the transition state of the reaction between B_Me and one molecular of external aniline via a weakly-interacting complex Pre_TS1_Me (at least the aniline group should dissociate from copper at first to reach TS1_Me).

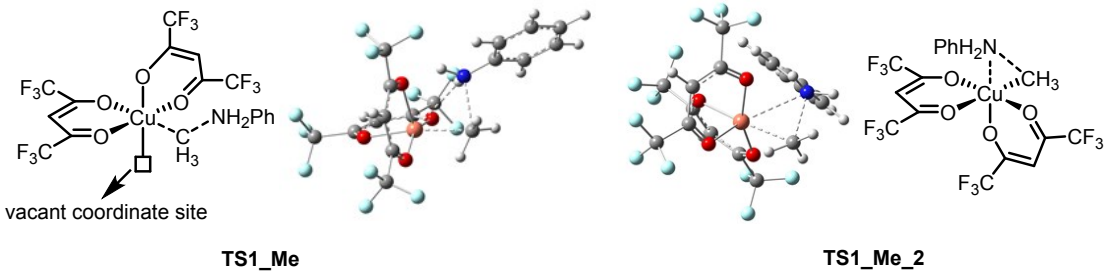


Figure S2. Geometry and molecular structure of TS1_Me and TS1_Me_2.

Discussion on the ground state electronic structure of substrates and transition states

To further probe the electronic nature of both substrates and transition states in this coupling reaction, we tried to compute these structures on different multiplicity. However, all of the efforts to optimize these structures on triplet or another higher spin multiplicity only lead to decomposition to form a Cu (Ⅱ) complex and R• radical. This decomposition process is endothermic, consistent with the results of Larionov et al.[S9], which have demonstrated that the combination of Cu (Ⅱ) complex $Cu(PhNH_2)(hfac)_2$ and methyl radical is highly exothermic. Thus, we believe the ground state multiplicity of these species is singlet.

However, we also compute to check the corresponding close-shell singlet wavefunction stability (key word "stable=opt" was used) and finally find that for several structures, the ground state electronic structure is open-shell singlet rather than close-shell singlet (for these structures, geometry re-optimization and single point energy re-calculation were performed; single point energy reported in table S4 were calculated at B3LYP-D3(BJ)/def2tzvp level of theory):

Table S3. Compute ground state electronic structures of substrates and transition states in this reaction.

	B3LYP-D3(BJ)/def2svp
A_Me	close-shell singlet
B_Me	close-shell singlet
Pre_TS1_Me	open-shell singlet
TS1_Me	close-shell singlet
TS2_Me	close-shell singlet
TS3_Me	close-shell singlet
B_Et	close-shell singlet
TS1_Et	open-shell singlet
TS2_Et	close-shell singlet
B_Cy	close-shell singlet
TS1_Cy	open-shell singlet
TS2_Cy	open-shell singlet
B_i-Pr	close-shell singlet
TS1_i-Pr	open-shell singlet
TS2_i-Pr	open-shell singlet
B_t-Bu	open-shell singlet
TS1_t-Bu	open-shell singlet
TS2_t-Bu	open-shell singlet

In these complexes with open-shell singlet electronic structure, the carbo-ligands were partially oxidized (see table S4 for spin density) and radical components were generated in corresponding coupling reactions. However, for most structures, this change in electronic structure only slightly altered the geometry structure and electronic energy of these species (figure S2 and table S4). Thus, we proposed that the electronic nature of this coupling reaction is mainly ionic but with minor radical character (and this radical character seems more profound in intramolecular than intermolecular coupling).

Table S4. Comparison of electronic energy between close-shell singlet and open-shell singlet; Mulliken spin density of R group.

	close-shell singlet (hartree)	open-shell singlet (hartree)	ΔE (kcal/mol)	Mulliken spin density of R group (a.u.)
Pre_TS1_Me	-3850.419465	-3850.419318	0.09	0.132
TS1_Et	-3889.740484	-3889.741561	-0.68	0.213
TS1_Cy	-4045.878676	-4045.879016	-0.21	0.179
TS2_Cy*	-4045.886113	-4045.886119	0.00	0
TS1_i-Pr	-3929.085048	-3929.085857	-0.51	0.253
TS2_i-Pr*	-3929.092701	-3929.092702	0.00	0
B_t-Bu	-3680.685171	-3680.685442	-0.17	0.277
TS1_t-Bu	-3968.423658	-3968.424006	-0.22	0.461
TS2_t-Bu*	-3968.421753	-3968.421806	-0.03	0

*Although the ground state electronic structure of these two transition states were estimated as open-shell singlet at B3LYP-D3(BJ)/def2svp level of theory, subsequent calculation with a larger basis set (def2tzvp) identified the ground state electronic structure of these two species as close-shell singlet.

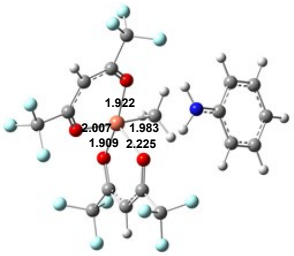
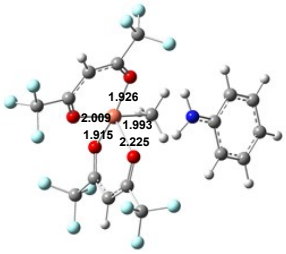
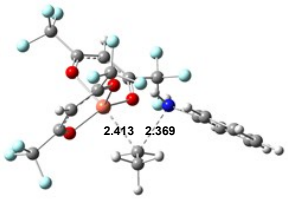
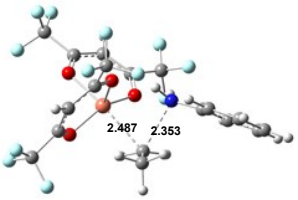
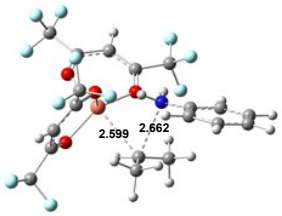
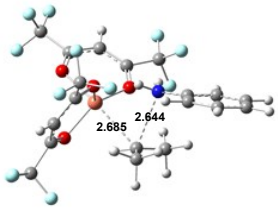
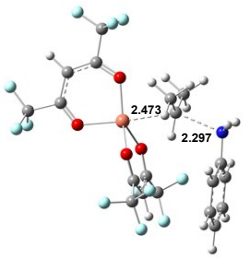
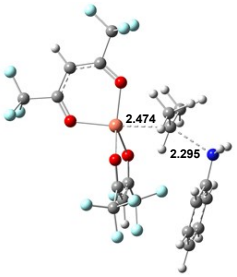
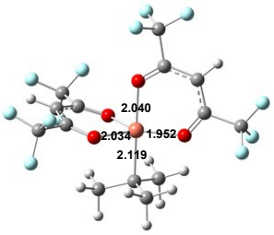
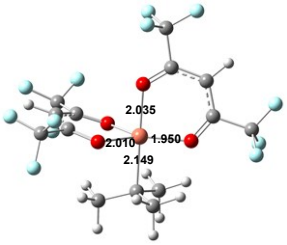
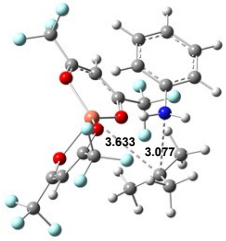
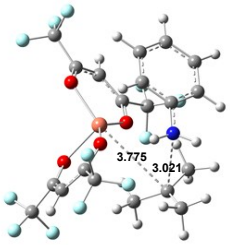
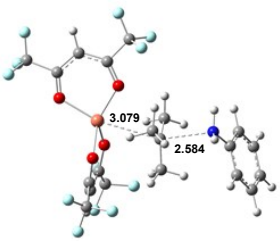
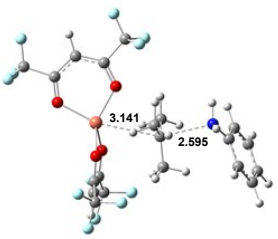
	close-shell singlet	open-shell singlet
Pre_TS1_Me		
TS1_Et		
TS1_i-Pr		
TS2_i-Pr		
B_t-Bu		
TS1_t-Bu		
TS2_t-Bu		

Figure S3. Comparison of geometry structures between close-shell singlet and open-shell singlet. Selected bond length were represented.

Outer-sphere radical capture pathway

To elaborate all of the mechanistic possibility of this C-N coupling reaction, the consideration of the outer-sphere radical capture pathway is essential. After a literature screening, we found although this kind of mechanism has been widely proposed for a variety of copper catalyzed C-X coupling reactions, the geometry structure of this coupling transition state has never been computationally located (to the best of our knowledge)[S10]. The only exception is a very recently report of C-S coupling reaction[S11].

In the current reaction system developed by Larionov, two pathways (pathway a and pathway b) can be imagined for this outer-sphere radical capture mechanism:

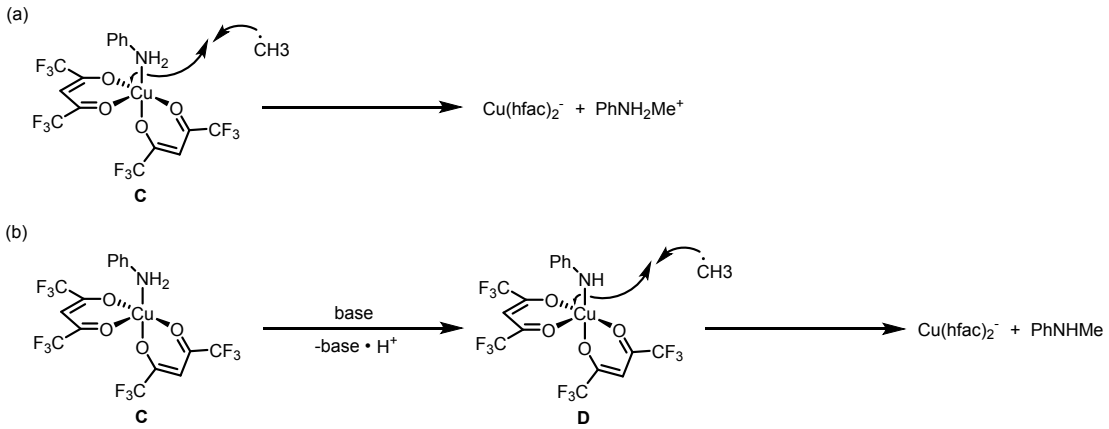


Figure S4. Two possible outer-sphere radical capture pathways.

In addition, as the deprotonation of complex C has been proven to be highly thermodynamically disfavored, we will only discuss pathway a in following sections. For R=Me, a transition state, TS4_Me can be located. In TS4_Me, the aniline group dissociate from the copper center and interact with methyl radical with a C-N distance at 2.49 Å. Through the IRC calculation, a nucleophilic-coupled electron transfer mechanism was indicated. As the reaction progresses, C-N bond formation and electron transfer from methyl radical to $Cu(hfac)_2$ becomes complete (figure 2b). The coordinate environment of copper is slightly deviated from square planar, also indicate an intermediate oxidation state between + Ⅰ and + Ⅱ.

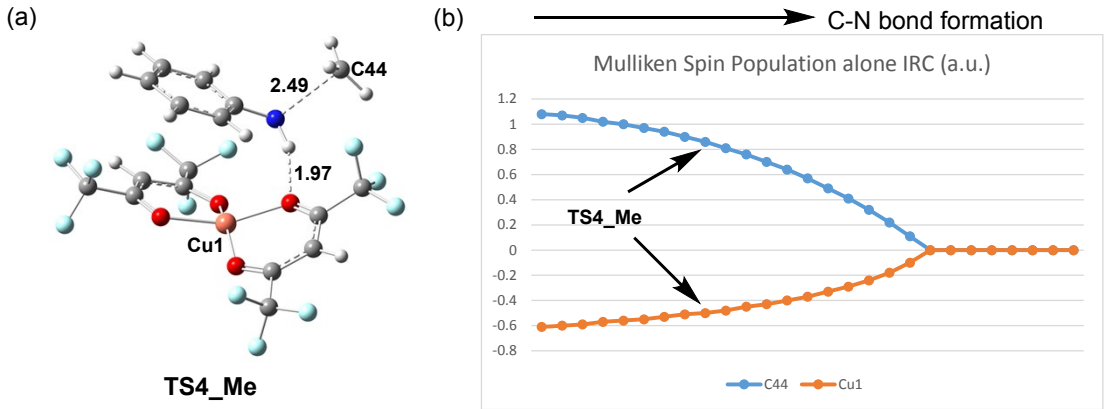


Figure S5. (a) Geometry structure of TS4_Me. (b) Mulliken spin population alone IRC (a.u.; for separate methyl radical and $Cu(hfac)_2$, the Mulliken spin density of C44 and Cu1 is 1.14 a.u. and -0.61 a.u., respectively).

While the energy difference between TS2_Me (S_N2 transition) and TS4_Me is 6.49 kcal/mol in gas phase (table 1), this value was increased to 14.41 kcal/mol in Ethyl Acetate. This solvation effect can be rationalized by the difference between the dipole moment of TS2_Me (12.11 Debye) and TS4_Me (4.04 Debye). Another factor that may also affect the energy difference between TS2 and TS4 is the nature of R group (stability of carbocation/steric effect; table 1).

Table S5. Calculated Gibbs free energy of TS2_R/TS4_R and $\Delta\Delta G$ value ($\Delta G_{TS2\_R} - \Delta G_{TS4\_R}$).

R	TS2_R (hartree)	TS4_R (hartree)	$\Delta\Delta G$ (kcal/mol)
Me	-3850.196243	-3850.185908	-6.49
Et	-3889.507594	-3889.504741	-1.79
i-Pr	-3928.824328	-3928.821727	-1.63
Cy	-4045.554779	-4045.546849	-4.98
t-Bu	-3968.132747	-3968.137012	2.68

In summary, we have evaluated the feasibility of the outer-sphere radical capture mechanism and discovered a nucleophilic-coupled electron transfer transition state, TS4. For a variety of R group (Me, Et, i-Pr and Cy), the free energy of TS4 is higher than TS2 and this energy difference become more profound in polar solvent. The only exception is t-Bu, which the free energy of TS4 is lower than TS2 in gas phase.

Additional supplementary figures

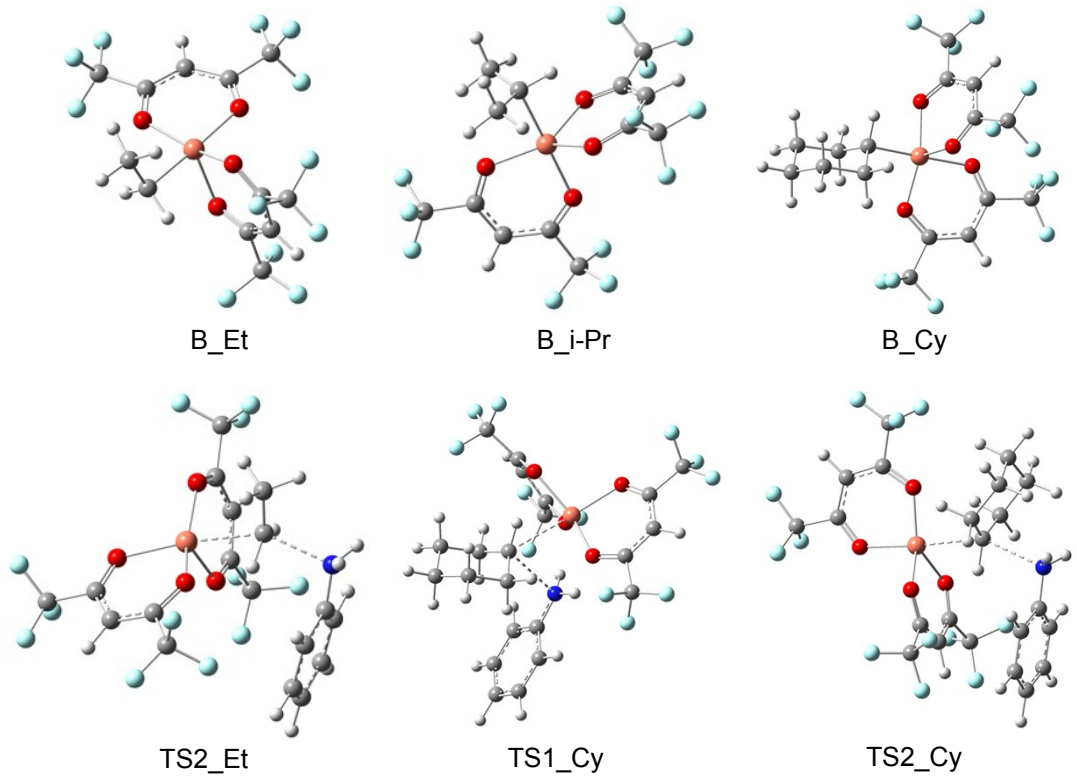


Figure S6. Geometry structures of B_Et, B_i-Pr, B_Cy, TS2_Et, TS1_Cy and TS2_Cy.

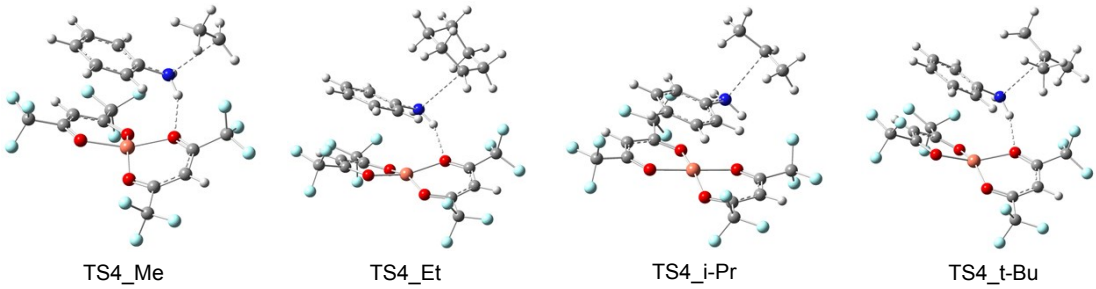


Figure S7. Geometry structures of TS4_Et, TS4_Cy, TS4_i-Pr and TS4_t-Bu.

Reference

S1. Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

S2. (a) Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, 98, 5648-5652 (b) Lee, C.; Yang, W.; Parr, R. G. Development ofthe Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1988**, 37, 785-789.

S3. (a) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010**, 132, 154104-154119. (b) Grimme, S.; Ehrlich, S.; Goerigk, L. Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem.* **2011**, 32, 1456-1465.

S4. Weigend, F.; Anlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **2005**, 7, 3297-3305

S5. Zhao Y.; Truhlar D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* **2008**, 120, 215-241.

S6. Adamo C..; Barone V. Toward reliable density functional methods without adjustable parameters: The PBE0 model. *J. Chem. Phys.* **1999**, 110, 6158-6170.

S7. (a) Marenich A. V.; Cramer C. J.; Truhlar D. G. Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *J. Phys. Chem. B* **2009**, 113, 6378-6396. (b) For ethyl acetate, eps=6.02 was used.

S8. (a) Lu T.; Chen F. Multiwfn: a multifunctional wavefunction analyzer. *J. Comput. Chem.* **2012**, 33, 580-592. (b) Wave function analysis were carried out at the same level of single point energy calculations.

S9. Nguyen V. T.; Nguyen V. D.; Haug G. C., et al. Visible Light-Enabled Direct Decarboxylative N-Alkylation. *Angew. Chem. Int. Ed.* 2020. doi: 10.1002/anie.201916710

S10. (a) Jang E. S., McMullin C. L., Käß M., et al. Copper (II) anilides in sp3 CH amination. *J. Am. Chem. Soc.*, **2014**, 136, 10930-10940. (b) Johnson M. W., Hannoun K. I., Tan Y., et al. A mechanistic investigation of the photoinduced, copper-mediated cross-coupling of an aryl thiol with an aryl halide. *Chem. Sci.*, **2016**, 7, 4091-4100. (c) Matier C. D., Schwaben J., Peters J. C., et al. Copper-catalyzed alkylation of aliphatic amines induced by visible light. *J. Am. Chem. Soc.*,

2017, 139, 17707-17710.
S11. Zhu F., Zhang S. Q., Chen Z., et al. Catalytic and Photochemical Strategies to Stabilized Radicals Based on Anomeric Nucleophiles. *J. Am. Chem. Soc.*, 2020. doi: 10.1021/jacs.0c03298

Cartesian coordinate of optimized structures

A_Me

0 1

C	1.63827900	0.04182100	-1.43538300
C	2.53769700	0.98420400	-0.94773000
C	2.12261700	2.10531500	-0.18793100
H	3.59032700	0.87349200	-1.18961400
C	-1.44185900	-2.22401000	0.28207000
C	0.72123800	-1.69358300	1.36892300
C	-0.18250600	-2.59360900	0.82180600
H	0.10628600	-3.63994100	0.78460000
Cu	-0.49466500	0.65072400	0.39893900
O	-1.93318700	-1.08864300	0.20576800
O	0.64502800	-0.43079100	1.51139200
O	0.97019800	2.38724500	0.18657400
O	0.38595000	-0.03077200	-1.25060700
C	2.17427900	-1.10784700	-2.30647900
C	3.19760200	3.13764400	0.22170000
C	-2.34881500	-3.35953200	-0.24795600
C	2.07946500	-2.22836300	1.86068700
F	1.96329000	-2.27835300	-1.68527200
F	1.52826800	-1.14142000	-3.47881500
F	3.48478400	-1.00748800	-2.55910100
F	2.91323500	4.32810500	-0.32693900
F	3.20579500	3.28528600	1.55087400
F	4.43444100	2.79352900	-0.16396300
F	-2.97385300	-2.97029300	-1.36478500
F	-3.28502600	-3.65158000	0.66908400
F	-1.67523400	-4.48515400	-0.51897300
F	2.30628200	-1.84497400	3.12091900
F	2.16218100	-3.56336300	1.81258300
F	3.05775500	-1.72719700	1.09095000
N	-1.66729100	1.76709000	-0.80204400
H	-1.58333100	1.15076700	-1.61499700
C	-3.01728800	2.11764500	-0.50544900
C	-4.01765200	1.14037200	-0.59340800
C	-3.32202500	3.41391000	-0.07609600
C	-5.33080200	1.48067500	-0.27110200
H	-3.75048100	0.12005900	-0.87394700
C	-4.64066300	3.74089800	0.24781900
H	-2.53102900	4.16514300	-0.00488300
C	-5.64773800	2.77803100	0.14783700
H	-6.11288300	0.72156400	-0.34098900

H	-4.87909600	4.75472300	0.57640900
H	-6.67843900	3.03571700	0.40004300
C	-1.39194500	1.33372500	1.98225600
H	-1.27045700	2.41588400	1.86808200
H	-2.41080600	0.95561800	1.85666500
H	-0.83010200	0.89876000	2.81225300
H	-1.05413900	2.57360700	-0.94200100

B_Me
0 1

Cu	-0.11693600	-0.31884000	1.11509300
C	-1.69504800	1.45283600	-0.48857800
C	-2.84359000	0.64945000	-0.33966500
C	-2.85868200	-0.44843200	0.51461300
H	-3.75154600	0.91624200	-0.87167300
O	-0.57917900	1.28798500	0.04892700
O	-1.91835100	-0.93069200	1.21667000
C	-1.77750500	2.70593600	-1.38615500
C	-4.17477400	-1.22681400	0.70714800
F	-1.58489000	3.80241300	-0.64781100
F	-0.83060000	2.65362100	-2.32466700
F	-2.96547100	2.81544700	-1.99490900
F	-3.98613000	-2.51773200	0.42363500
F	-5.15579900	-0.76484300	-0.07588600
F	-4.57471500	-1.12819800	1.97917900
C	1.79799100	-1.10071700	-1.05074800
C	2.80391200	-0.35960400	-0.36924300
C	2.61616400	0.28854300	0.84208200
H	3.78874200	-0.29880500	-0.82269300
O	0.62520400	-1.29323800	-0.70059000
O	1.58005600	0.37892700	1.57889000
C	2.19029200	-1.78005800	-2.38560100
C	3.81545100	1.01538600	1.48272800
F	1.34249000	-1.41460800	-3.34974300
F	3.43254900	-1.46919500	-2.78333900
F	2.12315800	-3.11016800	-2.24665300
F	3.50480200	2.28815800	1.73498500
F	4.90175500	0.99776300	0.70149700
F	4.13000600	0.42157300	2.64179800
C	0.36455300	-1.85648700	2.23285900
H	0.19159200	-1.45160400	3.23651100
H	-0.37389000	-2.58276400	1.88304900
H	1.40743900	-2.08887800	2.00652600

$PhNH_2$

0 1

C	0.22170700	1.20943900	-0.00450100
C	0.94480300	0.00000000	-0.00931700
C	0.22171200	-1.20944100	-0.00450200
C	-1.17252600	-1.20356200	0.00315300
C	-1.88442500	0.00000000	0.00721000
C	-1.17252800	1.20355800	0.00315500
H	0.76549500	2.15842700	-0.01063600
H	0.76550200	-2.15842800	-0.01060600
H	-1.70917300	-2.15595900	0.00794700
H	-2.97617700	0.00001000	0.01423000
H	-1.70917700	2.15595400	0.00792400
N	2.33183100	0.00001100	-0.06819400
H	2.79413800	0.84421600	0.24872200
H	2.79411800	-0.84425800	0.24859000

Pre_TS1_Me

0 1

C	-2.63724200	-1.39314500	0.04356000
C	-3.32966400	-0.16274700	0.10059900
C	-2.76257300	1.01277800	-0.37631600
H	-4.33356400	-0.13612400	0.51349800
C	1.59410200	-0.96480400	1.28970500
C	1.89972000	-2.02055900	-0.93440400
C	2.22550200	-1.87624100	0.41235000
H	3.02457400	-2.49719800	0.80616800
Cu	-0.23863200	-0.14002900	-0.99694900
O	0.66527600	-0.17597200	1.03589700
O	1.03468600	-1.41900600	-1.63752400
O	-1.61283400	1.20482300	-0.87848700
O	-1.48905700	-1.59393000	-0.39815000
C	-3.34326600	-2.66309200	0.56596100
C	-3.58250700	2.31429000	-0.31875900
C	2.08782100	-0.91465200	2.75386500
C	2.69608400	-3.04167300	-1.77387800
F	-3.47823300	-3.54682400	-0.42622200
F	-2.61268000	-3.22020100	1.53453500
F	-4.56139100	-2.40082600	1.05956000
F	-2.88442600	3.25604000	0.34639800
F	-3.81224400	2.77057000	-1.55164300
F	-4.75468200	2.16172900	0.30037400
F	1.12413700	-1.34372800	3.57408700
F	2.37905400	0.35494000	3.08769400

F	3.18067800	-1.65576600	2.96841500
F	3.34825600	-2.40480900	-2.75444500
F	3.59749700	-3.71395200	-1.04699600
F	1.86597200	-3.92764700	-2.32852000
N	0.24851600	2.70655600	1.08242000
H	0.41461400	1.78514000	1.47758100
C	1.28828500	3.37996100	0.50719700
C	2.62907500	3.01549400	0.78333700
C	1.05467300	4.45344600	-0.38567900
C	3.68253400	3.71713200	0.20359800
H	2.82196900	2.19188000	1.47332100
C	2.12169300	5.14551000	-0.95424000
H	0.02397800	4.73940600	-0.61223500
C	3.44330800	4.78807100	-0.66658200
H	4.70928600	3.42434500	0.43750800
H	1.91659100	5.97565300	-1.63492200
H	4.27533500	5.33440200	-1.11473900
C	0.98537100	1.23427500	-1.76086600
H	0.35152300	2.12195000	-1.72965300
H	1.81246600	1.22570800	-1.04632800
H	1.22217900	0.83687700	-2.75293500
H	-0.68773700	2.87557900	0.73760500

TS1_Me

0 1

C	-2.94020000	-1.06529600	0.33034700
C	-3.48411200	0.24340800	0.24299400
C	-2.76312400	1.31069800	-0.27494800
H	-4.49104600	0.41960300	0.60990400
C	1.84310900	-1.26032300	1.16429500
C	1.57694800	-2.47647900	-0.96852500
C	2.15236300	-2.32422100	0.30780000
H	2.90632800	-3.04022900	0.62112900
Cu	-0.31298700	-0.21151000	-0.74568400
O	0.98352700	-0.35861500	1.00798300
O	0.72418000	-1.75944200	-1.53592900
O	-1.58660000	1.32092100	-0.75032500
O	-1.81180000	-1.44708200	-0.01911500
C	-3.82605000	-2.17730900	0.93862400
C	-3.40828700	2.70583600	-0.30618200
C	2.66674600	-1.10444500	2.45823300
C	2.07302700	-3.64492500	-1.84902400
F	-3.99637700	-3.16199700	0.05123900
F	-3.23482300	-2.68665000	2.02432300

F	-5.04017800	-1.73294700	1.30012100
F	-2.56363000	3.60210600	0.24284400
F	-3.63419400	3.08705800	-1.56957600
F	-4.56379600	2.77034100	0.36070300
F	1.86886100	-1.06913400	3.52727200
F	3.33814500	0.06881700	2.41144100
F	3.56797100	-2.07548000	2.64026300
F	2.68926800	-3.15713000	-2.93613100
F	2.93993700	-4.44699200	-1.21344500
F	1.04220200	-4.39008500	-2.25407800
N	0.85005900	2.14613700	0.02817800
H	1.03459600	1.39135700	0.70363900
C	1.75974200	3.19491100	-0.02578200
C	3.07221600	3.00593900	0.44565600
C	1.39145600	4.41711600	-0.61688200
C	3.99738400	4.04149800	0.33691800
H	3.34535200	2.05537600	0.90897600
C	2.32806900	5.44384800	-0.71971200
H	0.36683500	4.55586600	-0.97156800
C	3.63205300	5.26064700	-0.24636200
H	5.01253200	3.89734400	0.71309700
H	2.03739500	6.39575500	-1.16939700
H	4.36228700	6.06824700	-0.32886900
C	1.07709000	1.13615600	-1.89234000
H	0.85855100	2.13692400	-2.26488600
H	2.12506400	0.95245000	-1.64925400
H	0.62822800	0.35138100	-2.51932000
H	-0.14543200	2.36697500	-0.06219000

TS2_Me

0 1

Cu	-0.53082000	0.11156000	-0.09123600
C	-3.29447800	-0.28487100	-0.94768500
C	-3.70599500	0.92186200	-0.33204300
C	-2.81652600	1.77132100	0.32060900
H	-4.75370300	1.20268900	-0.37961600
O	-2.14793700	-0.76433800	-1.00123800
O	-1.56992100	1.64234800	0.50008500
C	-4.36787600	-1.13541200	-1.66329600
C	-3.35739000	3.07533000	0.93344400
F	-4.07474600	-1.23877300	-2.96485100
F	-4.40051600	-2.36610100	-1.14258100
F	-5.60006200	-0.61199700	-1.56049200
F	-3.12369000	3.09577700	2.25303500

F	-4.67324900	3.23711300	0.74659400
F	-2.73229900	4.13064000	0.39099300
C	0.60121000	-2.32450200	1.31572000
C	1.48906100	-2.56302900	0.24001500
C	1.56186300	-1.74808900	-0.89316700
H	2.17354700	-3.40343400	0.31250900
O	-0.25374400	-1.42872900	1.42855300
O	0.87450100	-0.73883100	-1.19953500
C	0.75810200	-3.21376900	2.57060100
C	2.70240700	-2.02063200	-1.89469100
F	-0.42771800	-3.59697000	3.03968000
F	1.49608000	-4.31267400	2.35203800
F	1.37556100	-2.49729400	3.53211200
F	2.28251300	-1.91966100	-3.15267100
F	3.26846600	-3.22395300	-1.73561000
F	3.67292200	-1.09359200	-1.70831400
C	1.12616500	1.16161400	0.85923900
H	1.77760500	0.86626200	0.04289100
H	0.59559900	2.11033200	0.81757400
H	0.98087400	0.51135800	1.71999100
N	2.86210200	2.05486000	1.73974300
H	2.55127400	2.79926900	2.36212300
H	3.23378000	1.27855000	2.28540700
C	3.72445500	2.48776900	0.70017600
C	4.44073100	1.53422000	-0.03635300
C	3.77797300	3.83959000	0.33932900
C	5.21505800	1.93833500	-1.12317800
H	4.37382500	0.47503200	0.22128500
C	4.56065300	4.23461800	-0.74710100
H	3.20807200	4.58041600	0.90661100
C	5.28088200	3.28830500	-1.48133500
H	5.75805200	1.18634600	-1.69908500
H	4.60348100	5.29082000	-1.02176200
H	5.88636700	3.60090100	-2.33430200

TS3_Me

0 1

C	-3.40606100	-1.45517600	0.51588400
C	-4.09196900	-0.49063100	-0.25494400
C	-3.44154300	0.42577600	-1.09437200
H	-5.17734600	-0.47931000	-0.22048100
C	1.86705400	-1.21185800	1.34486400
C	1.62648200	-1.95085000	-0.99442100
C	2.39592800	-1.76785100	0.16267500

H	3.44705800	-2.03723000	0.13539700
Cu	-0.75975600	-0.38083500	-0.17475600
O	0.71062300	-0.79323500	1.54393300
O	0.41270000	-1.69785800	-1.18529100
O	-2.21477200	0.57101800	-1.30920900
O	-2.17679700	-1.62489100	0.63484500
C	-4.25213600	-2.41711200	1.37951400
C	-4.31255900	1.45946200	-1.83818900
C	2.81580600	-1.06007500	2.55557200
C	2.33735100	-2.47824100	-2.25764400
F	-3.91751500	-3.68496600	1.13417800
F	-4.02209700	-2.16647500	2.67857700
F	-5.57190500	-2.28884700	1.16973500
F	-4.09092100	2.68465400	-1.31029500
F	-3.99070400	1.51316600	-3.13167000
F	-5.62606100	1.21838300	-1.74487100
F	2.33665500	-1.72238500	3.61133700
F	2.91162600	0.24373100	2.90569700
F	4.06212400	-1.49770100	2.32302500
F	2.29994300	-1.52615800	-3.21454300
F	3.62817600	-2.78790300	-2.05570200
F	1.72455600	-3.56105900	-2.73787800
N	-1.36644400	1.08481000	1.54102500
H	-1.03067300	0.44627500	2.25902100
C	-0.74167900	2.33729800	1.51718600
C	0.51306600	2.51545300	2.12480100
C	-1.29918800	3.38923900	0.76785600
C	1.19060900	3.72835800	1.98605700
H	0.96067100	1.69239300	2.68274000
C	-0.60896000	4.59377600	0.63120100
H	-2.25919700	3.24506000	0.26798700
C	0.64223200	4.77418200	1.23433200
H	2.15711900	3.85829000	2.47983600
H	-1.05635900	5.40125000	0.04649500
H	1.17246500	5.72388300	1.13646700
C	0.54010700	1.05876100	-0.92989400
H	-0.24262600	1.80713300	-1.01777300
H	1.10194400	0.95416200	-0.00907300
H	0.85678300	0.51672400	-1.81691200
H	-2.38219900	1.10722000	1.49141300
N	2.12002700	2.54157900	-1.32957300
H	1.97539400	2.88386000	-2.27639300
H	1.91243800	3.25806300	-0.63321000
C	3.31159900	1.81634200	-1.12469300

C	3.86360500	1.72519600	0.16089900
C	3.86596200	1.07015200	-2.17426800
C	4.97354200	0.90982300	0.38438000
H	3.41161200	2.27816900	0.98511000
C	4.97309300	0.25550900	-1.93957700
H	3.41506700	1.10843100	-3.16871600
C	5.53409400	0.17355000	-0.66194900
H	5.38734400	0.83608600	1.39135500
H	5.38640800	-0.33442800	-2.75986300
H	6.39441000	-0.47327800	-0.47981400

TS4_Me

0 1

Cu	-0.43350200	-0.56429000	0.67149400
C	-3.22288600	-1.28846700	0.32899900
C	-3.66202400	0.03482800	0.12452500
C	-2.77426700	1.11101600	0.14506900
H	-4.71172600	0.21770000	-0.08596200
O	-2.05610600	-1.68703600	0.54328600
O	-1.53933800	1.09308000	0.40743700
C	-4.26515800	-2.42622900	0.27051600
C	-3.29107000	2.50094700	-0.26944200
F	-4.26902300	-3.09742800	1.42520900
F	-5.50647900	-1.96864600	0.05172800
F	-3.95706900	-3.27532900	-0.71289600
F	-2.79653000	3.45014800	0.53352900
F	-4.62312500	2.58860600	-0.25343700
F	-2.87090500	2.76299500	-1.52024200
C	2.23830500	0.15341400	1.39018100
C	2.81104500	-0.90516000	0.68112800
C	2.02919600	-1.87672900	0.03815300
H	3.89051400	-0.94531700	0.57693300
O	1.01498000	0.41015500	1.56281600
O	0.77902400	-1.99261900	0.04669000
C	3.17988500	1.14129200	2.10651800
C	2.74725800	-2.97908100	-0.76749600
F	3.18893500	0.88711600	3.41968400
F	4.43959600	1.06920900	1.66067600
F	2.76285100	2.40981400	1.94177500
F	2.63746900	-4.15165700	-0.13272600
F	4.05311700	-2.72167700	-0.93565700
F	2.19521500	-3.10825800	-1.97879800
N	0.73172100	2.79763400	-0.35241500
H	1.25641900	3.27661500	0.37148000

H	-0.15608900	2.43161000	-0.00782700
C	1.46600400	1.92469200	-1.13540700
C	2.86902800	2.03435000	-1.22555700
C	0.81781500	0.90914700	-1.87023100
C	3.59900400	1.12748100	-1.99061700
H	3.38079200	2.82389800	-0.67160500
C	1.56089300	-0.00169300	-2.61625300
H	-0.27137000	0.84630800	-1.84298800
C	2.95691200	0.09118500	-2.67488600
H	4.68696500	1.21835200	-2.03225300
H	1.04636200	-0.80566700	-3.14617500
H	3.53310100	-0.63631200	-3.24868000
C	-0.26096800	4.74424500	-1.55436600
H	0.68132200	5.28387100	-1.64324000
H	-0.59349700	4.10725500	-2.37237900
H	-0.96205600	4.99855300	-0.76015300

B_Et

0 1

Cu	0.13091800	-0.81218200	-0.21445400
C	1.87183200	1.43985700	-0.66096700
C	3.00275900	0.73364500	-0.19724400
C	2.92950200	-0.60424200	0.17689400
H	3.96289700	1.23893200	-0.15777000
O	0.70496500	1.01337200	-0.77977500
O	1.91903200	-1.36972300	0.21381600
C	2.05119800	2.90691700	-1.10792400
C	4.21730100	-1.33344100	0.60243600
F	1.76926600	3.01926400	-2.40941600
F	1.21962600	3.69558700	-0.42437400
F	3.30122200	3.34916100	-0.91324000
F	4.08321100	-1.81304500	1.84238900
F	5.29016800	-0.53520800	0.57694600
F	4.44433900	-2.36298500	-0.22252000
C	-2.07054500	0.29438300	1.47203500
C	-2.96128100	0.17416300	0.37272900
C	-2.60091100	-0.34246600	-0.86653600
H	-3.98812900	0.50124000	0.50603500
O	-0.87478100	-0.03593800	1.52842800
O	-1.47926300	-0.78089000	-1.26766300
C	-2.63236100	0.87935400	2.79009500
C	-3.67980500	-0.46396000	-1.95987500
F	-1.88347900	1.90889500	3.19066000
F	-3.89832700	1.30595200	2.67278800

F	-2.60223000	-0.06016900	3.74462100
F	-3.30896400	0.20191200	-3.05550800
F	-4.86913700	0.00748500	-1.56725500
F	-3.83540300	-1.75557700	-2.28779700
C	-0.40870200	-2.66312800	0.27141400
C	-0.07080600	-3.50420500	-0.90756700
H	1.00330900	-3.46843400	-1.14209800
H	-0.31376100	-4.55812700	-0.65761600
H	-0.67117700	-3.23334200	-1.78857700
H	0.23937600	-2.74577000	1.15106800
H	-1.47048500	-2.54849900	0.51108400

TS1_Et

0 1

C	-3.24229100	-0.36230900	0.38134500
C	-3.43250100	1.03455700	0.21755400
C	-2.44763300	1.86017700	-0.30951100
H	-4.37584400	1.47560600	0.52604500
C	1.45478100	-1.69376700	1.22592300
C	0.89016300	-2.83629300	-0.88883700
C	1.50327300	-2.80960800	0.37673800
H	2.08971700	-3.67088500	0.68309200
Cu	-0.47033400	-0.24734300	-0.63395800
O	0.81732900	-0.62637900	1.06804500
O	0.19356400	-1.95628500	-1.44428300
O	-1.28973500	1.55024600	-0.72450500
O	-2.23504500	-1.03442800	0.10333100
C	-4.40614600	-1.18516600	0.98072400
C	-2.72430200	3.36682600	-0.44063400
C	2.32026900	-1.71163300	2.50230800
C	1.17598600	-4.05177400	-1.79576300
F	-4.79976600	-2.11904900	0.10891200
F	-4.00338400	-1.79661500	2.09910800
F	-5.47265500	-0.42894200	1.28475700
F	-1.70274100	4.06081900	0.09821700
F	-2.80977300	3.71235200	-1.73170600
F	-3.84881800	3.75278100	0.16838300
F	1.57176300	-1.49101600	3.58464000
F	3.23414300	-0.71892800	2.42679100
F	2.98610600	-2.85802700	2.68007600
F	2.03814000	-3.68094800	-2.76010800
F	1.72459200	-5.07995100	-1.13360900
F	0.05950500	-4.48299500	-2.38112500
N	1.27738100	1.91023500	0.12886800

H	1.29782600	1.12770100	0.78999800
C	2.34128800	2.79356200	0.12961100
C	3.56457400	2.43025000	0.72862400
C	2.23060900	4.03342600	-0.53032000
C	4.65216700	3.29925100	0.66562500
H	3.64061000	1.47446500	1.25175700
C	3.32719800	4.89091100	-0.58575100
H	1.27397500	4.31945300	-0.97523800
C	4.54253700	4.52895100	0.00685100
H	5.59423800	3.01475000	1.13978500
H	3.23148000	5.85408200	-1.09220400
H	5.39816200	5.20566900	-0.03868100
C	1.34828200	0.81740200	-1.95383300
H	1.32565900	1.87755900	-2.20907700
H	0.55719000	0.24105600	-2.44805100
H	0.33996700	2.28295500	-0.02828700
C	2.66409100	0.15524500	-1.81964900
H	3.11280700	0.09084800	-2.83251200
H	3.36969800	0.73072900	-1.20297100
H	2.58552900	-0.87327500	-1.44669400

TS2_Et

0 1

Cu	-0.10794200	-0.71202900	-0.82885900
C	-2.28524600	-2.13183400	0.53233800
C	-3.22658300	-1.13329300	0.17559100
C	-2.90970900	-0.07688100	-0.67342800
H	-4.23474500	-1.19935300	0.57337700
O	-1.09443400	-2.22132700	0.18806600
O	-1.81000900	0.18486400	-1.24154600
C	-2.76227400	-3.27297800	1.45951200
C	-4.00442900	0.94739500	-1.01804600
F	-2.00978400	-3.31130200	2.56418300
F	-4.04331000	-3.13573700	1.83992100
F	-2.64653200	-4.44994300	0.83337500
F	-3.60045100	2.18817400	-0.67989100
F	-5.16343600	0.71634200	-0.39180400
F	-4.24037200	0.94994000	-2.33705800
C	1.97842600	-0.00229200	1.27046000
C	2.95444500	-0.71610500	0.52255500
C	2.69092300	-1.38982200	-0.66975500
H	3.96844500	-0.75573800	0.91346700
O	0.78236100	0.17765500	1.00952100
O	1.60615200	-1.50654100	-1.30524500

C	2.51872500	0.69554200	2.54530300
C	3.86531500	-2.07096000	-1.39703300
F	3.30665000	-0.11540300	3.26464400
F	3.26867100	1.76883500	2.19424300
F	1.53453200	1.12810500	3.32682500
F	3.61068500	-3.36396900	-1.60600400
F	5.02549700	-1.97841200	-0.73151700
F	4.04049200	-1.48457600	-2.59757900
C	0.75413600	1.14346300	-1.89120500
H	1.61420300	1.09152200	-1.22781000
H	-0.20284800	1.43312300	-1.47069800
N	1.04457300	3.27763000	-1.89784800
H	2.03570500	3.47776000	-2.02523700
H	0.50742200	3.63381200	-2.68724300
C	0.53128500	3.65489500	-0.62891700
C	-0.84828900	3.83634600	-0.47065200
C	1.37700600	3.67623300	0.48581800
C	-1.37392400	4.05769700	0.80233200
H	-1.51595800	3.77304800	-1.33298300
C	0.84182400	3.89836000	1.75446600
H	2.44690200	3.48778200	0.37001200
C	-0.53220200	4.09259800	1.91700300
H	-2.45211700	4.18091600	0.91901500
H	1.50463700	3.89447500	2.62072900
H	-0.94796700	4.25269600	2.91361300
C	0.87839900	0.69521800	-3.30624500
H	-0.10542600	0.60290200	-3.78676800
H	1.49489700	1.39857600	-3.89361300
H	1.40186100	-0.27327200	-3.34500600

TS4_Et

0 1

Cu	-0.35265900	-0.70557600	0.55532300
C	-3.09871400	-1.59671000	0.24074600
C	-3.63632800	-0.29426200	0.27487500
C	-2.81905000	0.82904300	0.39847600
H	-4.70974300	-0.16049500	0.17661500
O	-1.89592200	-1.93206700	0.31552000
O	-1.56609100	0.86479200	0.55727700
C	-4.06677400	-2.78841400	0.07562400
C	-3.46368000	2.22090200	0.25741300
F	-3.94071900	-3.62178600	1.11136300
F	-5.34769400	-2.39763100	0.00956200
F	-3.77847400	-3.45585600	-1.04430200

F	-2.89060500	3.09897800	1.08522200
F	-4.77687300	2.20685800	0.49870200
F	-3.27824100	2.66288600	-1.00042900
C	2.24282100	0.03827100	1.49853700
C	2.88953100	-0.88642000	0.67160100
C	2.18107300	-1.82086900	-0.09558300
H	3.97325300	-0.87770700	0.61817800
O	1.00660400	0.21251900	1.65966700
O	0.93533400	-1.97079400	-0.17977700
C	3.10881200	0.96979500	2.36932200
C	2.98086800	-2.84683700	-0.92296100
F	2.97578000	0.64730500	3.65911900
F	4.40801900	0.91227500	2.05543900
F	2.71369800	2.24860300	2.22440500
F	2.89983700	-4.05420500	-0.35134300
F	4.27778500	-2.52036700	-1.01907200
F	2.48691700	-2.93756600	-2.16126700
N	0.65222500	2.74581900	-0.06103500
H	1.16400800	3.19965900	0.68649400
H	-0.24357500	2.36747600	0.23846600
C	1.39299200	1.96312700	-0.91386600
C	2.79349600	2.12693800	-1.02119200
C	0.77023700	0.98415100	-1.72251100
C	3.53545700	1.32594400	-1.88300800
H	3.28887600	2.88246000	-0.40753200
C	1.53039500	0.17801800	-2.56907100
H	-0.31587800	0.88173500	-1.69290300
C	2.91723100	0.33172000	-2.65110800
H	4.61798900	1.46401300	-1.93976000
H	1.03221000	-0.59351900	-3.15974000
H	3.50646800	-0.31248300	-3.30543800
C	-0.68248000	4.81102400	-1.38301100
H	-1.51357700	4.73376500	-0.68017700
H	0.12064000	5.51165300	-1.14264400
C	-0.69964000	4.10299100	-2.68280700
H	0.28584100	3.66490000	-2.92318100
H	-1.44840000	3.29762800	-2.70074600
H	-0.93833500	4.79035500	-3.52167500

B_Cy
0 1

Cu	-0.28844800	0.58708900	-0.43370300
C	-0.52368700	-2.26491200	-0.78948100
C	-1.89946900	-2.24266900	-0.46846000

C	-2.59858300	-1.04656900	-0.34131600
H	-2.43320200	-3.18135300	-0.35415500
O	0.22400100	-1.28682200	-0.98624800
O	-2.16209000	0.14244400	-0.39920700
C	0.18595500	-3.62870800	-0.92040900
C	-4.11848100	-1.08718800	-0.10477100
F	0.73003300	-3.75172500	-2.13374100
F	1.16057400	-3.70712900	-0.00885900
F	-0.64735300	-4.66127900	-0.73032200
F	-4.42520900	-0.39844500	1.00386100
F	-4.58630400	-2.33121100	0.03794800
F	-4.75519800	-0.51672100	-1.13452400
C	1.89039000	-0.09934600	1.45238900
C	2.83497300	0.31032600	0.47924700
C	2.49911200	0.99046600	-0.68721200
H	3.88217100	0.07943400	0.64969700
O	0.66312000	0.10216300	1.46273100
O	1.35934100	1.33950100	-1.12308500
C	2.40560100	-0.92346300	2.65401300
C	3.63296100	1.43211500	-1.63249200
F	1.92622900	-2.17135700	2.57067800
F	3.74359100	-0.99752200	2.70634800
F	1.97774100	-0.38706500	3.80213200
F	3.44361500	0.92135800	-2.85260600
F	4.84347500	1.04967800	-1.20603800
F	3.63776300	2.76906200	-1.73687000
C	-0.76310400	2.45224700	0.17228300
C	-1.46281000	3.04597100	-1.00736100
C	-1.55917800	2.33558000	1.43044800
H	0.26458900	2.80408300	0.31570900
C	-1.91981300	4.47971400	-0.60598200
H	-2.35468300	2.45035300	-1.25762200
H	-0.80019300	3.09134000	-1.88418800
C	-1.99882500	3.77758000	1.82078100
H	-2.45980400	1.72765000	1.26403700
H	-0.96774900	1.87740700	2.23470200
C	-2.75557300	4.45096200	0.67473700
H	-2.48566200	4.91182300	-1.44656100
H	-1.02959900	5.11457300	-0.45826700
H	-2.61984500	3.71298900	2.72829900
H	-1.10873400	4.37461000	2.08380800
H	-3.03827500	5.47749700	0.96100500
H	-3.69642200	3.90430700	0.48685600

TS1_Cy

0 1

Cu	0.75641000	-0.40654200	-0.20309400
C	3.67292900	-0.26848500	0.28753100
C	3.71499000	1.13009100	0.04162200
C	2.57502800	1.86200000	-0.26404900
H	4.66754400	1.64725300	0.11109100
O	2.68568800	-1.02111100	0.25976400
O	1.38103400	1.45585500	-0.39193800
C	5.00030000	-0.97745700	0.64435800
C	2.68696400	3.37823400	-0.48604000
F	4.90867400	-1.53298200	1.85716200
F	5.25438900	-1.94464900	-0.24280400
F	6.05017000	-0.14038800	0.65297100
F	2.31755000	3.68858400	-1.73932000
F	3.91652500	3.85847800	-0.28619700
F	1.84911200	4.02170200	0.35000600
C	-0.63816800	-2.97068800	-0.73216400
C	-1.19529500	-3.09013800	0.55399400
C	-1.05971600	-2.09381600	1.53338200
H	-1.81998800	-3.95188300	0.77031600
O	0.12188400	-2.08178300	-1.17630500
O	-0.40191300	-1.02887000	1.47300400
C	-1.08600100	-3.98832300	-1.80174500
C	-1.86820000	-2.24691600	2.83781800
F	-0.05773900	-4.39902400	-2.54081000
F	-1.68799800	-5.06677400	-1.28355400
F	-1.97296900	-3.38458500	-2.62293000
F	-1.07461000	-2.13845400	3.90405300
F	-2.52730600	-3.40854900	2.92291500
F	-2.78462500	-1.25587400	2.90544300
C	-1.29474900	0.57554100	-1.45764500
C	-2.61473000	0.00654900	-1.12058300
C	-1.25562200	1.92417500	-2.05451800
H	-0.57020600	-0.13756100	-1.86223800
C	-3.38701900	-0.10974500	-2.47476300
H	-3.18213100	0.67875700	-0.45870300
H	-2.53690400	-0.98233900	-0.65190800
C	-2.01878400	1.80308200	-3.41364800
H	-1.79614800	2.65556500	-1.43530200
H	-0.22579200	2.27140000	-2.20979400
C	-3.42490500	1.23792100	-3.19823800
H	-4.40198200	-0.47941100	-2.25861300
H	-2.89497500	-0.87097300	-3.10164300

H	-2.05237300	2.80169000	-3.87756500
H	-1.45104000	1.14907100	-4.09676700
H	-3.93822300	1.12884600	-4.16772400
H	-4.01853000	1.95509400	-2.60421800
N	-1.05371400	1.64825900	0.93645300
H	-1.00406500	0.77902800	1.46879800
H	-0.14969700	2.04095500	0.68392400
C	-2.11005000	2.50189400	1.14816400
C	-3.31299900	2.02474700	1.71427300
C	-2.03423300	3.85202000	0.73999000
C	-4.40627100	2.87703100	1.85295100
H	-3.36666300	0.98871400	2.05446500
C	-3.13788400	4.69039600	0.88403300
H	-1.09404000	4.23332200	0.33402100
C	-4.33172300	4.21047900	1.43397300
H	-5.32805500	2.49559400	2.29878000
H	-3.06161400	5.73429000	0.57029300
H	-5.19229100	4.87284300	1.54655400

TS2_Cy

0 1

Cu	-0.77155500	-0.14157000	-0.09778400
C	-3.25006000	-1.74524300	-0.07937200
C	-4.06761200	-0.58865300	0.00683900
C	-3.54235600	0.69964500	0.01726100
H	-5.14428400	-0.71335300	0.07387400
O	-2.01166200	-1.80583300	-0.14984200
O	-2.33292700	1.06661600	-0.05538300
C	-3.95152300	-3.12322000	-0.08774300
C	-4.50317100	1.89247500	0.14918500
F	-3.66740700	-3.77364700	-1.22174000
F	-3.52014000	-3.86363100	0.93883800
F	-5.28826200	-3.02926800	0.00697900
F	-4.21383400	2.58936800	1.26141400
F	-5.79045400	1.53703500	0.20931400
F	-4.35404500	2.72586400	-0.89514300
C	1.58437400	-1.27206500	1.25577800
C	2.21349000	-1.59761900	0.04006200
C	1.68282700	-1.28149900	-1.22208000
H	3.17690400	-2.09480400	0.07954200
O	0.49747900	-0.68163600	1.44534900
O	0.61113800	-0.69663700	-1.50313200
C	2.30169200	-1.65519700	2.56793100
C	2.50220500	-1.66605200	-2.47179900

F	1.54432400	-2.48618200	3.28835200
F	3.49219300	-2.24679600	2.37405700
F	2.51846300	-0.55117400	3.30878100
F	1.80820500	-2.50297900	-3.24684300
F	3.67667400	-2.25049000	-2.18298300
F	2.77089400	-0.56281700	-3.19769900
C	0.53511800	1.90452500	-0.06612000
C	0.10772800	2.39980500	-1.40731100
C	-0.00806300	2.50418500	1.18489800
H	1.25691900	1.10025800	-0.00009800
C	-0.17291900	3.91235300	-1.44517800
H	-0.84419500	1.89095700	-1.64414400
H	0.81987400	2.06448600	-2.17551000
C	-0.29339600	4.01309300	1.07526000
H	-0.97991300	2.01256700	1.37005300
H	0.63213800	2.23941400	2.03940200
C	-1.00089100	4.35743100	-0.23760500
H	-0.69142000	4.15590500	-2.38484400
H	0.77934100	4.47243100	-1.46522800
H	-0.90225100	4.32382700	1.93762800
H	0.65127800	4.58260900	1.14298400
H	-1.19471500	5.44060500	-0.28957400
H	-1.98036000	3.85386600	-0.26637000
N	2.64748100	3.02323900	-0.01369300
H	2.69510900	3.58468000	-0.86006200
H	2.61384200	3.62272400	0.80691100
C	3.61568100	2.00045300	0.05636200
C	4.13440600	1.44099900	-1.12009300
C	4.00014500	1.47973700	1.30036800
C	5.05156200	0.39269500	-1.04716400
H	3.81329600	1.82094000	-2.09278200
C	4.91833800	0.43161000	1.36251900
H	3.57429000	1.88977500	2.21922900
C	5.45232400	-0.11245000	0.19197500
H	5.44018200	-0.04213500	-1.96934900
H	5.20214400	0.02730400	2.33533200
H	6.16342700	-0.93889700	0.24484200

TS4_Cy

0 1

Cu	-0.00190300	-1.33093200	0.50603500
C	-2.42619100	-2.81271600	-0.07131100
C	-3.28544200	-1.77988700	0.34581000
C	-2.78877000	-0.53775900	0.74608500

H	-4.35993300	-1.94086400	0.32621800
O	-1.17447200	-2.79856100	-0.11400200
O	-1.58290600	-0.18397800	0.85721700
C	-3.04757200	-4.13884900	-0.55923000
C	-3.81582100	0.57918400	1.02437100
F	-2.59320000	-5.15308000	0.18043900
F	-4.38590700	-4.13177300	-0.47897200
F	-2.70939000	-4.35634100	-1.83263600
F	-3.30191900	1.52268400	1.81458100
F	-4.92632700	0.10380600	1.59615900
F	-4.16833300	1.15882700	-0.13787000
C	2.33355000	-0.13366000	1.62631100
C	3.18322000	-0.72936600	0.68929500
C	2.72128000	-1.68696300	-0.22259100
H	4.22669200	-0.43351400	0.65873700
O	1.09584900	-0.30986600	1.78171100
O	1.55305100	-2.13597000	-0.34858000
C	2.94494500	0.84346900	2.64946900
C	3.73676300	-2.33850700	-1.18219900
F	2.94890200	0.28830500	3.86533900
F	4.20038300	1.19025300	2.34414700
F	2.21721500	1.97262700	2.71759100
F	3.97442400	-3.59978900	-0.80273600
F	4.90692600	-1.68464300	-1.20171900
F	3.25646000	-2.36123900	-2.42858300
N	0.05688600	2.32457600	0.48820300
H	0.46937200	2.74140900	1.31504300
H	-0.71518400	1.70231100	0.71264600
C	0.95507100	1.86144900	-0.44860500
C	2.26921700	2.37569300	-0.50975500
C	0.57864300	0.88470900	-1.39751800
C	3.16758800	1.91810100	-1.46955500
H	2.57630000	3.13520000	0.21259300
C	1.49465100	0.42340600	-2.34353100
H	-0.44908800	0.51525700	-1.40308400
C	2.79807800	0.92665300	-2.38508200
H	4.18042200	2.32802700	-1.48917400
H	1.18864600	-0.35443700	-3.04635100
H	3.51218600	0.55202500	-3.11984800
C	-2.06533500	3.32765700	-1.48977500
C	-1.08408700	3.85350700	-2.47764800
C	-2.74643500	4.24728400	-0.53760900
H	-2.43892000	2.30612300	-1.59741600
C	-0.20644900	4.98613200	-1.91683200

H	-1.64686000	4.25089600	-3.35463000
H	-0.45977600	3.03758500	-2.87551800
C	-1.81547200	5.35042200	-0.00712900
H	-3.59788500	4.73711100	-1.06550600
H	-3.20400400	3.68238600	0.28892100
C	-1.03487300	6.01625000	-1.14387100
H	0.34754700	5.46772100	-2.73866200
H	0.54542500	4.54734200	-1.24203200
H	-2.39999100	6.09579400	0.55623900
H	-1.10127300	4.89374300	0.69797200
H	-0.37912800	6.80726700	-0.74363300
H	-1.74219500	6.51664500	-1.83197500

B_i-Pr

0 1

Cu	0.14653100	-0.59579100	0.00007500
C	1.95057200	1.68490000	0.00133700
C	3.10095200	0.86350900	0.00073900
C	3.00590200	-0.52400300	0.00000800
H	4.08360500	1.32538700	0.00086300
O	0.75787800	1.32306600	0.00135000
O	1.96905900	-1.25169600	-0.00020700
C	2.14223600	3.21745800	0.00187200
C	4.29221600	-1.36811500	-0.00068100
F	1.56927500	3.74682800	-1.08241100
F	1.56758800	3.74641000	1.08541600
F	3.43579700	3.57069900	0.00293600
F	4.31802200	-2.15619700	1.08226500
F	5.40169600	-0.62280600	-0.00037500
F	4.31771300	-2.15484400	-1.08461400
C	-2.43141600	0.02184300	1.23695000
C	-3.07590300	0.18824600	-0.00016000
C	-2.43090700	0.02358200	-1.23724000
H	-4.13125800	0.44375200	-0.00019600
O	-1.23462400	-0.27879500	1.46212700
O	-1.23402100	-0.27673000	-1.46234400
C	-3.26830600	0.17495500	2.52463500
C	-3.26725400	0.17852500	-2.52505800
F	-2.73154800	1.10276900	3.31979000
F	-4.54017000	0.51867200	2.28190500
F	-3.27670400	-0.99144000	3.18809100
F	-2.73029500	1.10763200	-3.31855500
F	-4.53928200	0.52166200	-2.28237600
F	-3.27517300	-0.98686600	-3.19030500

C	-0.44533700	-2.54811100	-0.00138000
C	0.08213300	-3.07483700	-1.29369200
H	-0.31191300	-2.51334300	-2.15215100
H	1.18044700	-3.09512500	-1.31409400
H	-0.27711800	-4.11989000	-1.39292600
C	0.08187000	-3.07659100	1.29031600
H	-0.31221000	-2.51613200	2.14944400
H	-0.27759600	-4.12169600	1.38819100
H	1.18017600	-3.09707100	1.31085000
H	-1.52271800	-2.34556100	-0.00135500

TS1_i-Pr

0 1

C	-3.36995300	-0.61979500	0.48528000
C	-3.59522600	0.76019100	0.23322000
C	-2.60373800	1.59242400	-0.26800500
H	-4.57309000	1.18082400	0.44883300
C	1.61863300	-1.71283700	1.27738900
C	1.11572500	-2.84257700	-0.85577600
C	1.79275200	-2.77420700	0.37325800
H	2.53213400	-3.53677500	0.59995100
Cu	-0.56205000	-0.46055100	-0.42312600
O	0.83110400	-0.74327700	1.19137800
O	0.22312500	-2.08503500	-1.30367900
O	-1.40907800	1.30472800	-0.58430500
O	-2.32502800	-1.26768100	0.31125000
C	-4.54642900	-1.45222600	1.04643600
C	-2.90959400	3.08110000	-0.49424900
C	2.54451200	-1.65149600	2.50990400
C	1.56975500	-3.91370900	-1.86798400
F	-4.85045200	-2.43948500	0.19764200
F	-4.20327400	-1.99532700	2.21829100
F	-5.65420600	-0.71894900	1.23965900
F	-2.02573700	3.83316100	0.18987600
F	-2.77147500	3.38684500	-1.79449100
F	-4.13741500	3.43765300	-0.11222400
F	1.83192100	-1.56250400	3.63358800
F	3.31656200	-0.54642700	2.42364700
F	3.36198300	-2.70586500	2.61469700
F	2.26547200	-3.30695300	-2.84980400
F	2.36351600	-4.84624600	-1.32478500
F	0.52455400	-4.52713200	-2.42091900
N	1.16437600	1.90357800	0.30903700
H	1.27071300	1.08940700	0.91547100

C	2.12280400	2.89280400	0.36639900
C	3.42551900	2.59896700	0.82375900
C	1.83578400	4.19740500	-0.08950900
C	4.41011500	3.58490100	0.81091500
H	3.64412200	1.59827500	1.20187700
C	2.83195500	5.17163400	-0.09812200
H	0.81979500	4.43764400	-0.41226600
C	4.12536100	4.87346100	0.34516000
H	5.41214000	3.34464300	1.17445500
H	2.59282400	6.17901500	-0.44738500
H	4.90117500	5.64160800	0.33864900
C	1.24008900	0.69726200	-2.04254600
H	0.56455700	-0.13347100	-2.26600200
H	0.19501500	2.18210500	0.17557500
C	2.63687600	0.31061600	-1.76546800
H	3.08369500	-0.01097000	-2.73050400
H	3.24452400	1.14063500	-1.37802600
H	2.70449300	-0.55976400	-1.09927900
C	0.87111300	1.99989600	-2.62581100
H	0.94776100	1.89989100	-3.72935300
H	-0.17807600	2.24969800	-2.40922900
H	1.53669200	2.81646500	-2.31464000

TS2_i-Pr

0 1

Cu	-0.81670500	0.17276200	-0.00008900
C	-3.32884200	-1.36379800	-0.00022200
C	-4.10940800	-0.17837600	-0.00031400
C	-3.54421700	1.09263600	-0.00031300
H	-5.19185200	-0.26555800	-0.00038800
O	-2.09134200	-1.46781100	-0.00013100
O	-2.32095900	1.42177100	-0.00023600
C	-4.07682500	-2.71713800	-0.00022800
C	-4.46831500	2.32038300	-0.00041400
F	-3.74102500	-3.42574000	-1.08388000
F	-3.74121400	-3.42564400	1.08354500
F	-5.41274000	-2.57602400	-0.00035100
F	-4.22619600	3.07634300	1.08276900
F	-5.76877800	2.00682200	-0.00049700
F	-4.22604400	3.07627900	-1.08360800
C	1.58365900	-1.01233600	1.23843700
C	2.15510000	-1.35456600	0.00022200
C	1.58386500	-1.01243400	-1.23811500
H	3.10229400	-1.88363600	0.00032100

O	0.52221500	-0.38974500	1.46901500
O	0.52246000	-0.38985800	-1.46891800
C	2.33854400	-1.41586900	2.52263900
C	2.33896100	-1.41607300	-2.52215900
F	1.59208400	-2.23578800	3.26631400
F	3.51059100	-2.02798800	2.28447900
F	2.60228300	-0.31926900	3.26042100
F	1.59262300	-2.23605600	-3.26588800
F	3.51096900	-2.02817000	-2.28375500
F	2.60282000	-0.31953500	-3.25999100
C	0.54714900	2.23645000	-0.00004800
H	1.19100200	1.36632900	0.00002200
N	2.62832500	3.20478000	0.00007700
H	2.63353700	3.78456000	-0.83637000
H	2.63340400	3.78463100	0.83647600
C	3.60807900	2.18692100	0.00019700
C	4.05929200	1.64865100	1.21305200
C	4.05948700	1.64855200	-1.21254100
C	4.97829900	0.59950100	1.20773400
H	3.68164300	2.04112300	2.16004200
C	4.97849300	0.59940300	-1.20699100
H	3.68199000	2.04094700	-2.15962400
C	5.44581400	0.07485600	0.00043000
H	5.31409000	0.17851900	2.15663700
H	5.31443700	0.17834500	-2.15580600
H	6.15741500	-0.75286600	0.00052100
C	0.06015400	2.78228900	1.29451100
H	-1.03680800	2.66295200	1.33833200
H	0.51288100	2.26499600	2.15003500
H	0.24012500	3.86943000	1.35702700
C	0.06033900	2.78221800	-1.29470600
H	0.51318300	2.26487300	-2.15013700
H	-1.03661800	2.66288700	-1.33867400
H	0.24032800	3.86935400	-1.35726000

TS4_i-Pr

0 1

Cu	0.06578400	0.60279100	-0.82708900
C	-2.43540400	2.02440500	-0.43510600
C	-3.23611800	0.91539900	-0.77362300
C	-2.66736500	-0.27692500	-1.22646500
H	-4.31452200	0.98509800	-0.66664800
O	-1.19201400	2.12314200	-0.51024800
O	-1.44792700	-0.54847900	-1.39223800

C	-3.12540900	3.26537300	0.16873300
C	-3.59190400	-1.46989200	-1.53192900
F	-2.68008700	4.38200800	-0.40250100
F	-4.45842400	3.22648200	0.03400700
F	-2.84840400	3.32295800	1.48259300
F	-3.47259800	-1.84842700	-2.80414900
F	-4.87965700	-1.21057800	-1.28777500
F	-3.23093500	-2.51516200	-0.75465400
C	2.55481900	-0.79086100	-1.32468000
C	3.35139100	0.21856500	-0.77302800
C	2.78119100	1.40007400	-0.27394300
H	4.42479000	0.07314700	-0.70012800
O	1.31325800	-0.78740500	-1.51189500
O	1.57003200	1.72297200	-0.24735100
C	3.21841300	-2.12649400	-1.70858600
C	3.71199300	2.45508700	0.35977000
F	2.88901800	-2.49127100	-2.94554700
F	4.55149400	-2.09629600	-1.61695300
F	2.77594900	-3.08755400	-0.86265500
F	3.51210900	3.64744200	-0.20302900
F	5.00798500	2.13955000	0.22018000
F	3.45747300	2.56123600	1.67145600
N	-0.14542000	-2.48753500	0.63054600
H	0.62082000	-2.97145900	0.17396100
H	-0.94323100	-2.37287400	0.01309000
C	0.21312700	-1.37392300	1.36274500
C	1.52873500	-1.22135200	1.85310300
C	-0.73304300	-0.36985500	1.67313100
C	1.87681600	-0.10794100	2.61234400
H	2.27388200	-1.98336900	1.61548500
C	-0.36612100	0.74681900	2.42992400
H	-1.76557500	-0.48569300	1.34136000
C	0.93884900	0.89017800	2.90139200
H	2.90584200	-0.00272900	2.96348700
H	-1.11031100	1.52145800	2.62594800
H	1.23019200	1.77470500	3.46884300
C	-1.40722700	-4.18178000	2.53035100
H	-1.41834800	-4.97778600	1.78086200
C	-2.60567500	-3.31780500	2.67128100
H	-2.33525200	-2.31628200	3.04840100
H	-3.14826100	-3.20253700	1.72040400
H	-3.32869600	-3.73827900	3.40336000
C	-0.27692800	-4.09954400	3.48689100
H	-0.57799600	-4.42354200	4.50585600

H	0.57621700	-4.72336200	3.18200700
H	0.07771700	-3.05718700	3.59673300

B_t-Bu
0 1

Cu	-0.20952400	-0.72806300	-0.08820400
C	-1.74324400	1.77463100	-0.07540600
C	-2.98470100	1.10252300	-0.01299600
C	-3.05811400	-0.28704000	-0.00738800
H	-3.90256900	1.68143500	0.02364600
O	-0.60643200	1.26754600	-0.12493900
O	-2.11697200	-1.13201000	-0.04095100
C	-1.74337400	3.31883900	-0.09299800
C	-4.43655300	-0.96804400	0.04057300
F	-1.03974400	3.78555400	0.94249800
F	-1.17763400	3.76005400	-1.22062400
F	-2.97979400	3.83289200	-0.02037200
F	-4.60178500	-1.73484400	-1.04622200
F	-5.44789600	-0.09547700	0.09183600
F	-4.51472400	-1.76065500	1.11871900
C	2.32915200	0.08025500	-1.18215100
C	2.84729600	0.42474700	0.07359900
C	2.21562000	0.10669600	1.28947400
H	3.82189200	0.90218900	0.11152800
O	1.23611700	-0.47375500	-1.46207100
O	1.10349700	-0.43823700	1.47473000
C	3.22227600	0.29790400	-2.41990200
C	3.00272700	0.34709800	2.59442600
F	2.54683500	0.91529900	-3.38977300
F	4.32130300	1.01503000	-2.15404200
F	3.61772000	-0.90154900	-2.88524100
F	2.23872400	0.94906500	3.50615900
F	4.10292800	1.08959500	2.41478300
F	3.38758500	-0.84293200	3.09143200
C	0.18335200	-2.84091400	-0.05347800
C	1.67194800	-3.02780200	-0.04259200
H	2.15232500	-2.65882700	-0.95573500
H	2.14519300	-2.59083400	0.84462400
H	1.84560900	-4.12141900	0.00349300
C	-0.50072400	-3.18928300	-1.34151400
H	-0.38229500	-4.28216600	-1.48890300
H	-1.57386800	-2.96478900	-1.32269400
H	-0.01806800	-2.69663500	-2.19857100
C	-0.50911400	-3.17000000	1.23538800

H	-1.58278500	-2.95180200	1.20704000
H	-0.38427300	-4.25939200	1.40083600
H	-0.03559500	-2.65824200	2.08590600

TS1_t-Bu

0 1

Cu	-1.14939400	0.36709800	0.03957800
C	-3.98743000	-0.32730200	0.37520100
C	-3.75523700	-1.70214800	0.12352300
C	-2.48564600	-2.21129000	-0.15419100
H	-4.59849000	-2.38612800	0.14832700
O	-3.16617900	0.60741400	0.39390100
O	-1.38759000	-1.60101200	-0.23080900
C	-5.44015200	0.11042000	0.67092500
C	-2.33043200	-3.71967900	-0.41273000
F	-5.51330900	0.67519900	1.88244500
F	-5.84247800	1.01218000	-0.23287100
F	-6.31352300	-0.91099100	0.64415000
F	-1.80280600	-3.92704600	-1.63514400
F	-3.47520100	-4.40558400	-0.34122900
F	-1.47404400	-4.25529600	0.47916300
C	0.21234800	2.70627800	-1.17977000
C	0.67007400	3.18572800	0.06063600
C	0.58805100	2.42783300	1.24185700
H	1.19984700	4.13373800	0.08814100
O	-0.43303200	1.66278700	-1.42382000
O	0.03207300	1.32089100	1.42476300
C	0.64608400	3.47683800	-2.44343900
C	1.39076200	2.92626600	2.46053800
F	-0.35684900	3.59800000	-3.31095300
F	1.12680700	4.70030200	-2.18515500
F	1.63411300	2.77785700	-3.05449500
F	0.70304100	2.78214600	3.59151100
F	1.76951600	4.20772800	2.36118000
F	2.51690900	2.18095600	2.56593500
C	1.67433600	-0.83697800	-0.62718200
N	3.34011200	-2.74245200	-1.19878100
H	2.76572200	-3.54743000	-0.96426500
H	3.47366500	-2.66103800	-2.20273500
C	4.48688400	-2.57061900	-0.42362500
C	5.53524700	-1.75098400	-0.88414900
C	4.56975100	-3.12809000	0.86594100
C	6.63709800	-1.49595500	-0.06733100
H	5.48746900	-1.32660300	-1.89068800

C	5.67486000	-2.86163700	1.67425900
H	3.77147000	-3.78244200	1.22493100
C	6.71185400	-2.04332400	1.21653900
H	7.44524600	-0.86313300	-0.44096900
H	5.72652800	-3.30406400	2.67162100
H	7.57484300	-1.83961700	1.85303400
C	0.97413200	-1.13177600	-1.89639000
H	0.29849500	-0.27755700	-2.09854800
H	1.68640500	-1.12163000	-2.73702900
H	0.37770400	-2.04843200	-1.86643700
C	1.40629400	-1.51515000	0.65742600
H	2.36418500	-1.76316800	1.14809300
H	0.93172800	-0.77904700	1.33309000
H	0.74976500	-2.38541300	0.56450700
C	2.63000700	0.29110600	-0.60073600
H	2.54600500	0.85853000	0.33623900
H	3.65598900	-0.12794800	-0.59268200
H	2.52999300	0.95579800	-1.46785000

TS2_t-Bu

0 1

C	-2.47890000	1.69958200	-0.73666000
C	-3.03723100	1.06000300	0.39724000
C	-2.36008300	0.09250500	1.13698200
H	-4.05430300	1.31044900	0.68393300
C	2.91682500	0.12083700	-1.12834000
C	2.42915500	1.79804300	0.60860600
C	3.32955600	1.12699000	-0.25702000
H	4.38668400	1.37145000	-0.20306300
Cu	0.08975400	0.24219300	-0.40962500
O	1.75025600	-0.30695600	-1.35297700
O	1.19987400	1.65214700	0.69852800
O	-1.18746900	-0.34704000	0.98315600
O	-1.34214500	1.56930800	-1.22144100
C	-3.41055400	2.62587500	-1.55092400
C	-3.09259500	-0.58709500	2.30816800
C	3.98567400	-0.64857600	-1.92262000
C	3.04371200	2.74341100	1.66504100
F	-2.78473300	3.74953700	-1.90000600
F	-3.78276000	1.98930800	-2.67958700
F	-4.53050000	2.96118500	-0.89177400
F	-3.25787300	-1.89866200	2.05384600
F	-2.35921600	-0.49056900	3.42900000
F	-4.29874700	-0.06656100	2.55784900

F	3.78006300	-0.53647200	-3.23624700
F	3.89732600	-1.96705800	-1.61204700
F	5.23554200	-0.25933000	-1.65764800
F	3.13120200	2.07874500	2.83481000
F	4.27927500	3.15371100	1.34072200
F	2.28387300	3.81819900	1.85474200
N	0.70226900	-3.01096800	-0.96824900
H	0.93116500	-3.98041600	-0.78977900
C	-0.61281900	-2.70442000	-1.25108200
C	-1.66099200	-3.47198400	-0.69798500
C	-0.94272300	-1.57765600	-2.04196000
C	-2.98640800	-3.10564200	-0.90203700
H	-1.42210700	-4.35472800	-0.10086400
C	-2.28260000	-1.23016600	-2.24424000
H	-0.15195700	-1.03927400	-2.56571500
C	-3.30823300	-1.97485200	-1.66512000
H	-3.78146600	-3.70334600	-0.45071900
H	-2.51622500	-0.35693900	-2.85462500
H	-4.35000200	-1.68481100	-1.81256100
C	1.39795200	-2.42988300	1.91399100
H	1.42144400	-2.46770500	-1.43621000
C	2.52944900	-3.29993200	1.50542300
H	3.22512200	-3.41145400	2.36349000
H	2.21151600	-4.30587400	1.20096700
H	3.12362600	-2.83917600	0.69927200
C	0.05253900	-2.95686000	2.18947700
H	-0.25990600	-2.70787500	3.22142300
H	-0.68734200	-2.42056800	1.55987400
H	-0.03445400	-4.03864800	2.02556900
C	1.70932400	-1.04322300	2.33295600
H	2.56110600	-0.61934800	1.78497100
H	0.83747900	-0.38008100	2.26739600
H	2.00935900	-1.06817000	3.40308900

TS4_t-Bu

0 1

Cu	-0.32050800	-1.04603400	0.52284800
C	-3.05445900	-1.92454600	0.06257300
C	-3.62789700	-0.67343700	0.36437200
C	-2.83868800	0.44373100	0.64476400
H	-4.70916400	-0.56906600	0.35036800
O	-1.84107200	-2.22747500	0.03286200
O	-1.58194800	0.50321900	0.72796700
C	-3.99486700	-3.09529400	-0.29708000

C	-3.55062600	1.80166700	0.81220400
F	-3.79295700	-4.11603800	0.53984700
F	-5.28929100	-2.75036000	-0.22629200
F	-3.74570600	-3.51181800	-1.54172100
F	-2.87889600	2.59794400	1.64559400
F	-4.79983200	1.66927700	1.26674600
F	-3.61546600	2.42220500	-0.38424700
C	2.24714400	-0.36987300	1.58807200
C	2.93318500	-1.15788500	0.65893200
C	2.26293500	-1.98879400	-0.24982800
H	4.01576200	-1.09796000	0.61600500
O	1.00306700	-0.25918000	1.75348600
O	1.02582100	-2.17673100	-0.36257500
C	3.07644800	0.45366100	2.59314000
C	3.10641500	-2.82783700	-1.23139500
F	3.02966700	-0.12219100	3.80028200
F	4.36159300	0.56371100	2.23571200
F	2.58182300	1.69778900	2.71738800
F	3.06197700	-4.11895500	-0.88042000
F	4.39350100	-2.45073600	-1.25238200
F	2.62724200	-2.71911000	-2.47517800
N	0.60465900	2.52763400	0.45877400
H	1.06590800	2.83171200	1.30967100
H	-0.25439400	2.02101100	0.66640600
C	1.44206400	1.90506200	-0.45018800
C	2.82896900	2.16504400	-0.45800100
C	0.92994500	1.01328100	-1.41590700
C	3.66510800	1.54598200	-1.38532800
H	3.24487800	2.85248400	0.28180300
C	1.77736400	0.39022700	-2.33066100
H	-0.14326300	0.81739100	-1.44436700
C	3.15294900	0.64355700	-2.32236500
H	4.73702800	1.75735900	-1.35978700
H	1.35910500	-0.32270600	-3.04411500
H	3.81256300	0.13890500	-3.02999400
C	-0.67085100	4.38353600	-1.76925800
C	0.73058600	4.82903200	-1.97669800
C	-1.49176600	5.01995000	-0.70508300
H	0.77279800	5.66882300	-2.70392100
H	1.36402000	4.02376100	-2.37808300
H	-1.29624100	6.10412800	-0.62935000
H	-2.56960100	4.85441700	-0.84747700
C	-1.28011700	3.34371200	-2.63683400
H	-1.77875700	2.56734200	-2.02882100

H	-2.08478900	3.77559600	-3.26731700
H	-0.54600400	2.85944700	-3.29468500
H	1.18014300	5.19698300	-1.04103700
H	-1.22076700	4.58312800	0.27622900

TS1_Me_2

0 1

C	-0.99686900	-0.95308800	1.58183500
C	-2.20956200	-1.30731000	0.95287400
C	-2.41948100	-1.17919000	-0.42215400
H	-3.02439100	-1.67619200	1.56847000
C	2.66447500	1.22036600	-0.11494100
C	2.93414800	-1.13531700	-0.76144100
C	3.39192800	0.03849000	-0.10426300
H	4.33454200	0.00763400	0.43427100
Cu	0.14458500	0.00264900	-0.94107400
O	1.55082200	1.44729100	-0.67925000
O	1.87984800	-1.28861800	-1.39877400
O	-1.62459500	-0.77437400	-1.31256700
O	0.04326400	-0.50331000	1.06263300
C	-0.93402800	-1.05593800	3.12140100
C	-3.78878100	-1.59933800	-0.99054600
C	3.20605200	2.44550100	0.63490200
C	3.83071600	-2.39357900	-0.69174400
F	0.19100800	-1.65216700	3.51338500
F	-0.95075500	0.18563800	3.64738000
F	-1.96868600	-1.72827800	3.64683200
F	-4.25233800	-0.66424800	-1.83484000
F	-3.67089100	-2.74376300	-1.67608800
F	-4.71475900	-1.78246400	-0.03888700
F	2.34715100	2.80010000	1.60656100
F	3.31284800	3.48844700	-0.20589600
F	4.40199000	2.24314800	1.19559000
F	4.16763700	-2.78280100	-1.92843500
F	4.96571100	-2.19220000	-0.00318700
F	3.16755200	-3.39611700	-0.10569300
N	-0.59682500	2.42887800	-1.88958800
H	-0.78941400	3.02851600	-2.68911600
C	-1.65425600	2.36800800	-0.95232300
C	-2.98029100	2.31873000	-1.40239500
C	-1.36625600	2.28264700	0.41985900
C	-4.01745000	2.18965100	-0.48125600
H	-3.19510300	2.35467500	-2.47309200
C	-2.41267700	2.14701600	1.33034000

H	-0.33143100	2.30900800	0.76334200
C	-3.73746400	2.09928700	0.88589000
H	-5.04866000	2.13805100	-0.83536000
H	-2.18339500	2.05767100	2.39320300
H	-4.55143500	1.98099900	1.60383200
C	-0.05471600	0.72491200	-3.09349000
H	-1.08157100	0.42444000	-3.30271500
H	0.37109200	1.49937100	-3.73376200
H	0.66165300	-0.09462500	-2.94165900
H	0.32707000	2.60081100	-1.47130800