

Supporting Information

Mechanistic Insights into Copper-Mediated Benzylic C(*sp*³)-H Bond Trifluoromethylation

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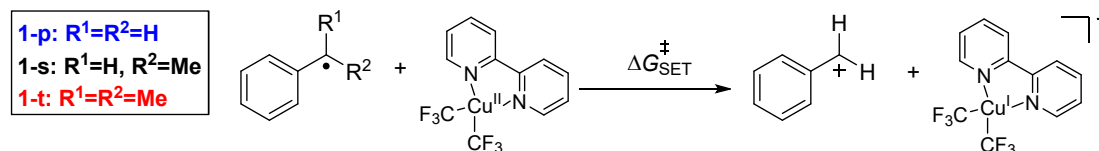
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Marcus theory calculations for the free energy of activation of single-electron transfer

The activation free energies of the single-electron transfer reactions were calculated using modified Marcus theory using (U)M06/def2-TZVP(IEFPCM $\epsilon = 9.2$)/(U)M06/6-31G(d)-SDD level of theory. The SET pathway is shown as Scheme S1:



Scheme S1. The SET pathway of copper-mediated benzylic C(sp^3)-H bond trifluoromethylation

The following equation was used to calculate the activation free energy of activation ($\Delta G_{\text{SET}}^\ddagger$) in the SET pathway:

$$\Delta G_{\text{SET}}^\ddagger = \Delta G_0^\ddagger \left(1 + \frac{\Delta_r G}{4\Delta G_0^\ddagger}\right)^2$$

Here, the reaction energies for **1-p**, **1-s**, and **1-t** obtained from DFT calculations are $\Delta_r G_p = 38.0$ kcal/mol, $\Delta_r G_s = 30.1$ kcal/mol, and $\Delta_r G_t = 24.8$ kcal/mol, respectively. The intrinsic barrier is determined using $\Delta G_0^\ddagger = \lambda_0/4$, where λ_0 is the solvent reorganization energy that can be calculated as follows:

$$\lambda_0 = A * [(2r_D)^{-1} + (2r_A)^{-1} - (r_D + r_A)^{-1}]$$

where r_D and r_A are the hard sphere radii of electron donor and acceptor, respectively. The r_D and r_A values were calculated using the Multiwfn program. A is an empirical constant. Here we use $A = 99$ kcal/mol Å as suggested in the Coote and Matyjaszewski's study.¹ Thus,

$$\text{primary: } \lambda_0 = 99 \times [1/(3.17 \times 2) + 1/(4.14 \times 2) - 1/(3.17 + 4.14)] = 14.0 \text{ kcal/mol}$$

$$\text{secondary: } \lambda_0 = 99 \times [1/(3.34 \times 2) + 1/(4.14 \times 2) - 1/(3.34 + 4.14)] = 13.5 \text{ kcal/mol}$$

$$\text{tertiary: } \lambda_0 = 99 \times [1/(3.48 \times 2) + 1/(4.14 \times 2) - 1/(3.48 + 4.14)] = 13.2 \text{ kcal/mol}$$

¹Lin, C. Y.; Coote, M. L.; Gennaro, A.; Matyjaszewski, K. Ab Initio Evaluation of the Thermodynamic and Electrochemical Properties of Alkyl Halides and Radicals and Their Mechanistic Implications for Atom Transfer Radical Polymerization. *J. Am. Chem. Soc.* **2008**, *130*,

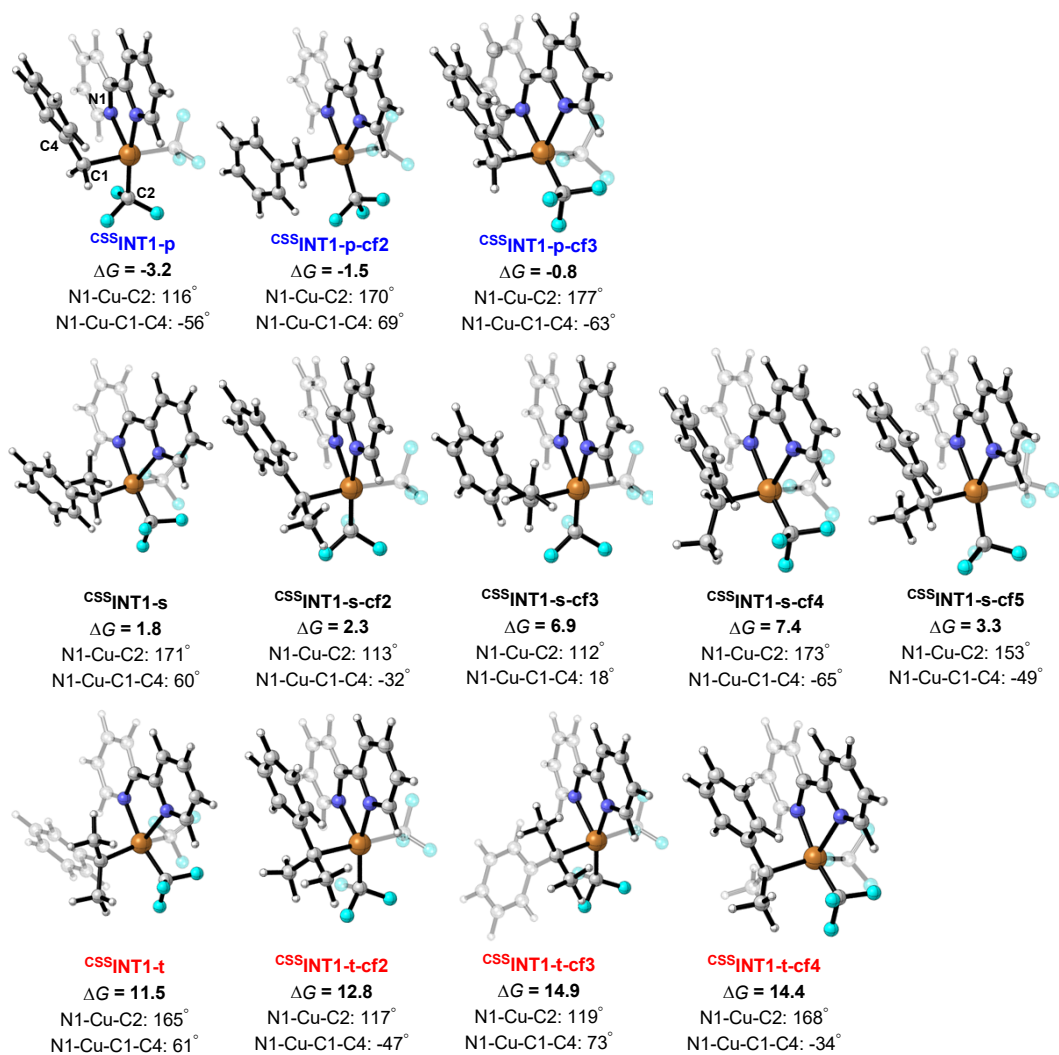


Figure S1. Different conformers for the CSS|INT1-p , CSS|INT1-s and CSS|INT1-t . The energies are shown in kcal/mol.

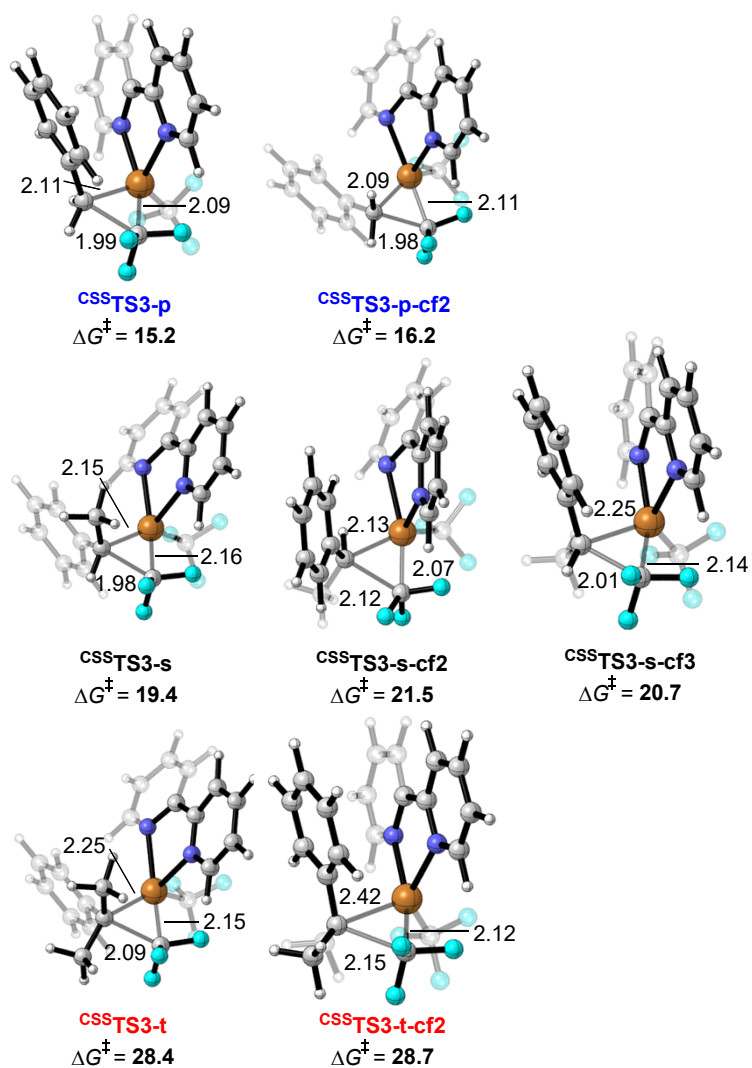


Figure S2. Different conformers for the reductive elimination transition state CSS-TS3-p , CSS-TS3-s and CSS-TS3-t . Distances are in Å, and energies are in kcal/mol.

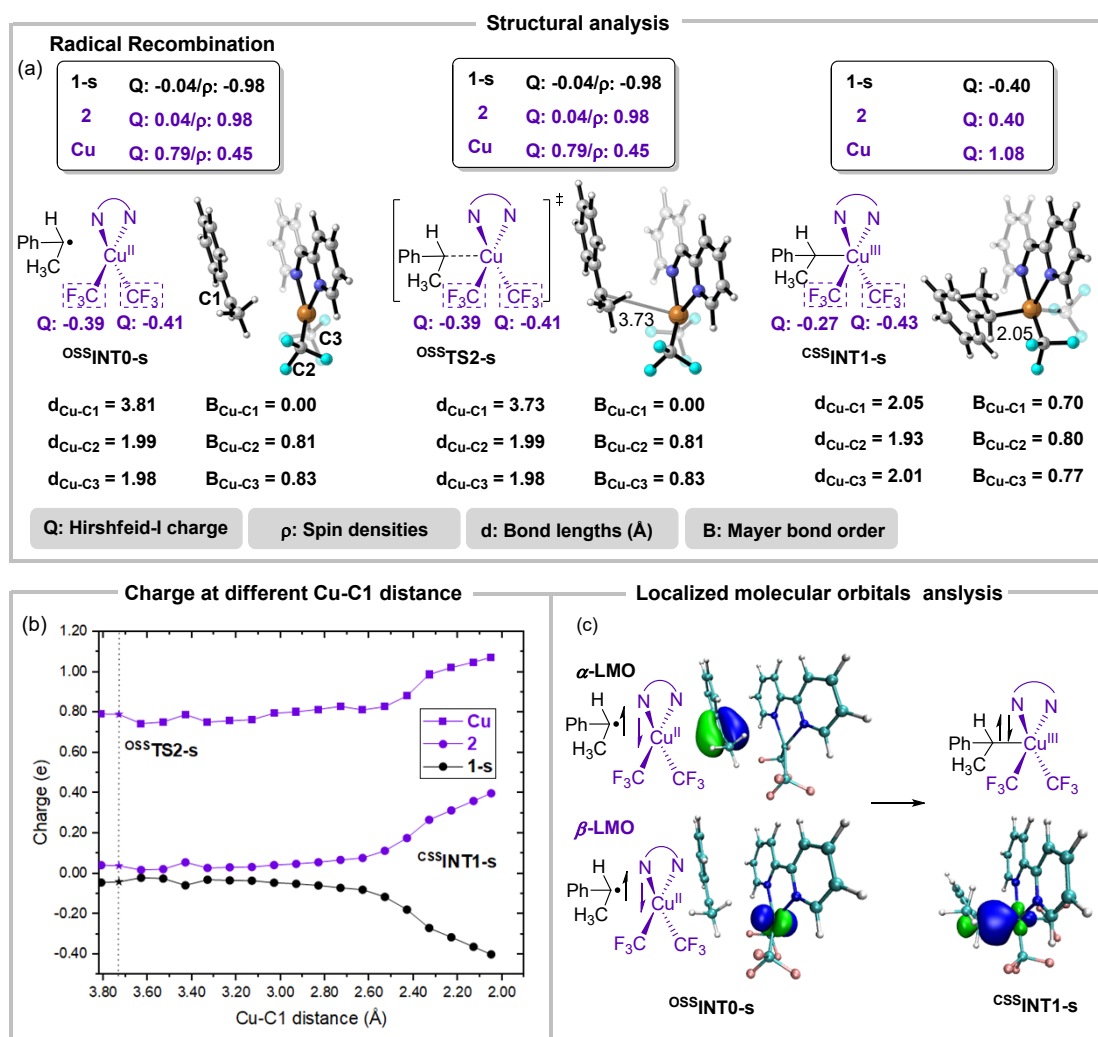


Figure S3. (a) Optimized geometries, Hirshfeld-I charge, spin densities, bond lengths, and Mayer bond orders of computed structures in the radical recombination step (secondary radical); (b) Hirshfeld-I charge changes along the reaction coordinate. (c) Localized molecular orbitals analysis of OSS|INT0-s and CSS|INT1-s.

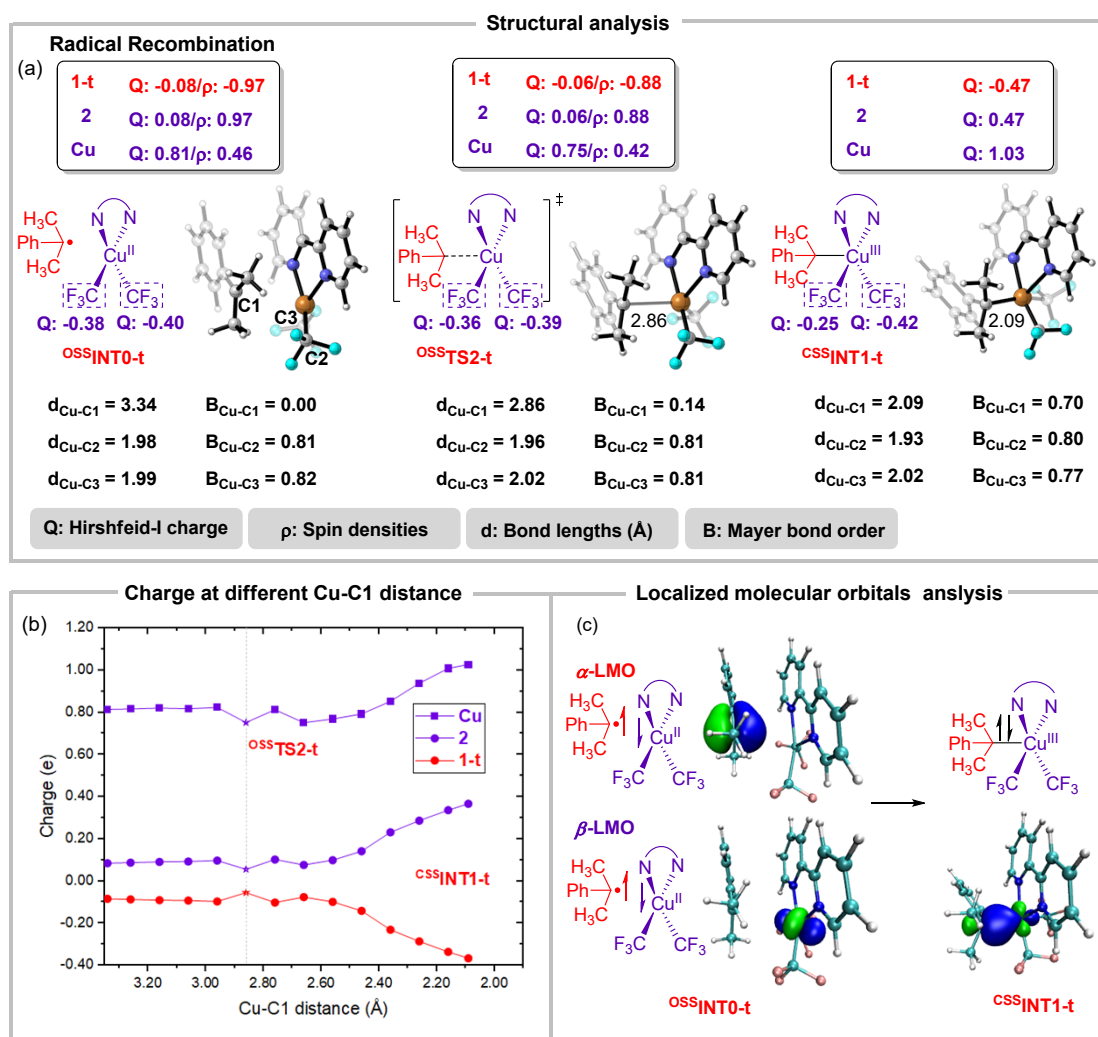


Figure S4. (a) Optimized geometries, Hirshfeld-I charge, spin densities, bond lengths, and Mayer bond orders of computed structures in the radical recombination step (tertiary radical); (b) Hirshfeld-I charge changes along the reaction coordinate. (c) Localized molecular orbitals analysis of OSSINT0-t and CSSINT1-t.

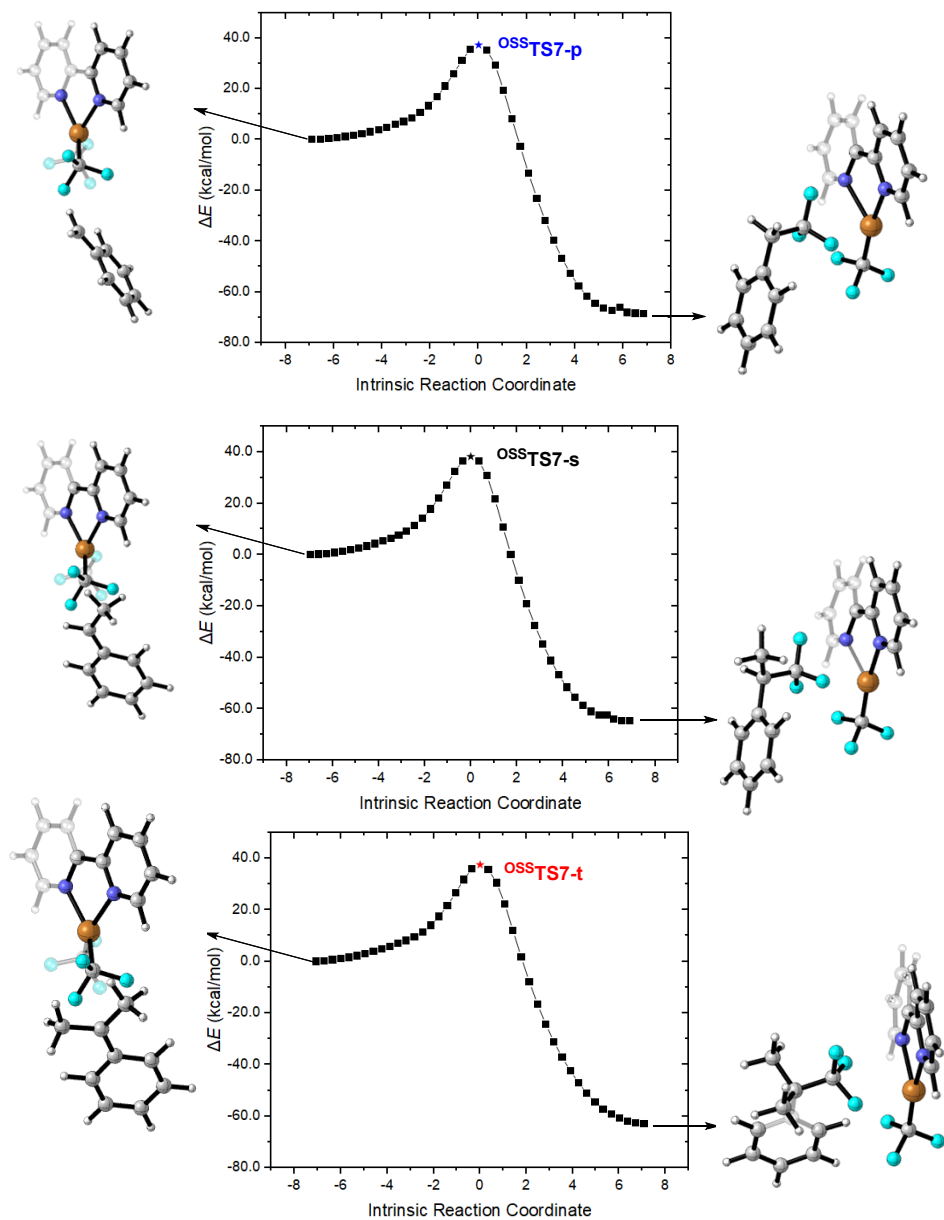


Figure S5. The IRC path for $\text{OSS}^{\text{TS7-p}}$, $\text{OSS}^{\text{TS7-s}}$ and $\text{OSS}^{\text{TS7-t}}$. The displayed intermediates were obtained through structural optimization.

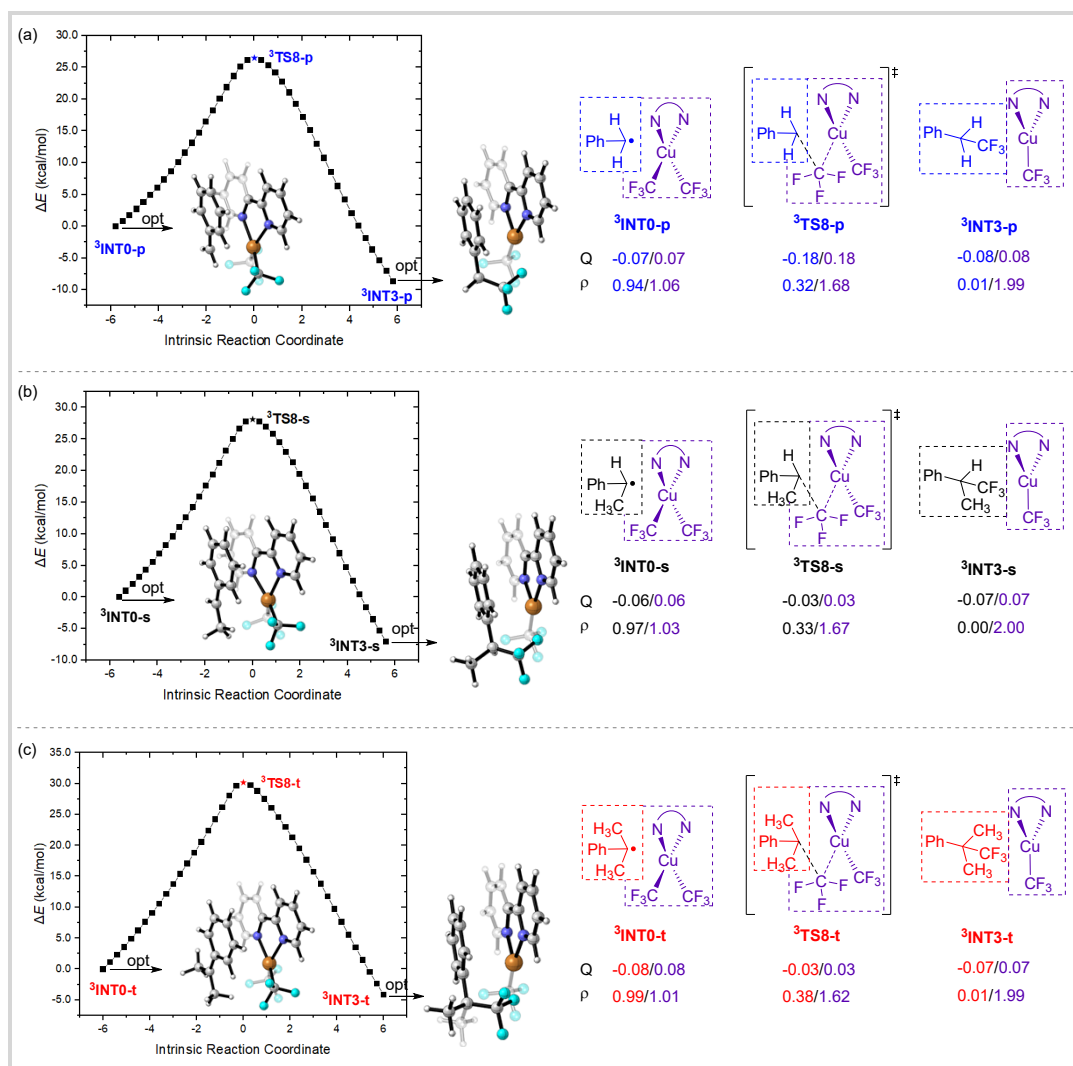


Figure S6. Analysis of the IRC paths for (a) ${}^3\text{TS8-p}$, (b) ${}^3\text{TS8-s}$, and (c) ${}^3\text{TS8-t}$, along with the corresponding changes in Hirshfeld-I charge and spin densities. The displayed intermediates were obtained through structural optimization.

Table S1. Electronic Energies and Free Energies (in Hartree) of the Structures Calculated at the (U)M06/def2-TZVP(IEFPCM $_{\epsilon=9.2}$)/(U)M06/6-31G(d)-SDD Level

Structures	ZPVE	TCE	TCH	TCG	Esol	$G_{\text{sol}}(E_{\text{sol}}+\text{TCG})$
1-p	0.114193	0.119909	0.120853	0.084506	-270.788986	-270.704480
1-s	0.142553	0.149913	0.150858	0.110408	-310.088981	-309.978573
1-t	0.170646	0.179619	0.180563	0.136071	-349.387556	-349.251485
2	0.187111	0.206683	0.207627	0.136377	-2811.027601	-2810.891224
2	0.187004	0.206661	0.207605	0.135472	-2811.013076	-2810.877604

4-p	0.134490	0.143519	0.144463	0.099083	-608.524433	-608.425350
4-s	0.162570	0.173069	0.174013	0.125324	-647.819416	-647.694092
4-t	0.190837	0.202499	0.203443	0.152853	-687.113083	-686.960230
¹5	0.172663	0.187909	0.188853	0.127138	-2473.393676	-2473.266538
²TS1	0.185889	0.205251	0.206196	0.134112	-2811.005566	-2810.871454
^{OSS}TS2-p	0.302312	0.328388	0.329332	0.244562	-3081.830422	-3081.585860
^{OSS}TS2-s	0.330685	0.358388	0.359332	0.270822	-3121.128192	-3120.857370
^{OSS}TS2-t	0.359653	0.388587	0.389531	0.298566	-3160.422286	-3160.123720
^{CSS}TS3-p	0.305702	0.330785	0.331729	0.249461	-3081.820919	-3081.571458
^{CSS}TS3-s	0.333889	0.360581	0.361525	0.275953	-3121.114768	-3120.838815
^{CSS}TS3-t	0.361503	0.389553	0.390497	0.302635	-3160.400155	-3160.097520
^{CSS}TS4-p	0.305551	0.330815	0.331760	0.248941	-3081.818454	-3081.569513
^{OSS}TS5-p	0.302347	0.328506	0.329450	0.243911	-3081.811719	-3081.567808
^{CSS}TS6-p	0.305869	0.331219	0.332163	0.248684	-3081.819974	-3081.571290
^{OSS}TS7-p	0.301441	0.328726	0.329670	0.238810	-3081.752242	-3081.513432
^{OSS}TS7-s	0.330319	0.358950	0.359894	0.266704	-3121.051827	-3120.785123
^{OSS}TS7-t	0.358011	0.388345	0.389289	0.292601	-3160.350979	-3160.058378
³TS8-p	0.303635	0.328959	0.329903	0.247318	-3081.764727	-3081.517409
³TS8-s	0.330943	0.357970	0.358914	0.271989	-3121.055861	-3120.783872
³TS8-t	0.358269	0.386842	0.387786	0.298702	-3160.353403	-3160.054701
^{CSS}INT1-p	0.306626	0.331892	0.332836	0.250574	-3081.851455	-3081.600881
^{CSS}INT1-s	0.335100	0.361978	0.362922	0.276304	-3121.143153	-3120.866849
^{CSS}INT1-t	0.362816	0.391067	0.392011	0.303094	-3160.427413	-3160.124319
^{CSS}INT2-p	0.306719	0.332481	0.333425	0.247886	-3081.852954	-3081.605068

ZPVE = zero-point vibrational energy; **TCE** = thermal correction to energy; **TCH** = thermal correction to enthalpy; **TCG** = thermal correction to Gibbs free energy.

Cartesian coordinates of the structures

1-p

C	1.83280900	0.00000000	-0.00000500
C	1.12959600	1.20885200	-0.00000300
C	-0.25196700	1.21483300	0.00000100
C	-0.99068300	0.00000000	0.00000300
C	-0.25196700	-1.21483300	0.00000000
C	1.12959600	-1.20885200	-0.00000300
H	2.92142200	0.00000000	-0.00000800
H	1.67376700	2.15238600	-0.00000400
H	-0.79913400	2.15800400	0.00000300
H	-0.79913400	-2.15800400	0.00000200
H	1.67376700	-2.15238600	-0.00000500
C	-2.39119600	0.00000000	0.00000700
H	-2.95390900	0.93141200	0.00000900
H	-2.95390900	-0.93141200	0.00000800

1-s

C	-2.29040300	0.35117300	0.00002900
C	-1.32731400	1.36291400	0.00004200
C	0.02123900	1.05282700	0.00002300
C	0.46012900	-0.29736700	-0.00001100
C	-0.53886000	-1.30630400	-0.00001800
C	-1.88274000	-0.98631000	0.00000000
H	-3.34974300	0.60226800	0.00004300
H	-1.63873000	2.40695600	0.00007100
H	0.75974400	1.85410900	0.00004500
H	-0.22348700	-2.35059500	-0.00004100
H	-2.62770300	-1.78110300	-0.00000900
C	1.82568300	-0.64894900	-0.00003000
H	2.06818700	-1.71303700	0.00001200
C	2.94360900	0.33265900	-0.00003700
H	2.91355300	0.99313800	0.88192400
H	3.91694900	-0.16915000	-0.00035900
H	2.91317400	0.99355500	-0.88166700

1-t

C	-2.64835100	0.00000000	-0.00000100
C	-1.94148000	-1.20345000	0.00002600
C	-0.55766000	-1.20839000	0.00002500
C	0.18676100	0.00000000	0.00000000
C	-0.55766000	1.20839000	-0.00002500

C	-1.94148000	1.20345000	-0.00002700
H	-3.73706100	0.00000000	-0.00000100
H	-2.48082300	-2.15014500	0.00004900
H	-0.03171500	-2.16188000	0.00005200
H	-0.03171500	2.16188000	-0.00005200
H	-2.48082300	2.15014500	-0.00005000
C	1.61108200	0.00000000	0.00000000
C	2.36806200	-1.28923800	-0.00003800
H	2.13424200	-1.90891400	-0.88099900
H	3.45037300	-1.11742700	-0.00016500
H	2.13444400	-1.90885000	0.88102400
C	2.36806100	1.28923800	0.00003900
H	2.13424200	1.90891400	0.88100100
H	3.45037300	1.11742800	0.00016600
H	2.13444300	1.90885000	-0.88102300

²²

Cu	0.70941300	0.00000000	0.00000200
C	2.00793100	1.34334400	0.65066000
C	2.00792500	-1.34334900	-0.65066100
F	1.47186300	2.11856400	1.63756400
F	3.17132400	0.88566200	1.13106400
F	2.32989900	-2.22243600	0.34471700
F	1.47185400	-2.11855900	-1.63757200
F	3.17132200	-0.88567400	-1.13105900
F	2.32991400	2.22242000	-0.34472300
N	-0.93358800	1.28544000	-0.30242400
C	-0.83217400	2.59668000	-0.52708900
C	-2.14487200	0.73006400	-0.11906900
C	-1.94387200	3.42664400	-0.59096900
H	0.18070700	2.97702000	-0.65142700
C	-3.30429600	1.50175500	-0.14990100
C	-3.19902100	2.86512300	-0.39241100
H	-1.82034300	4.48905600	-0.78285500
H	-4.27814000	1.05184500	0.02640100
H	-4.09340100	3.48433700	-0.41931400
N	-0.93359200	-1.28543800	0.30242200
C	-0.83218300	-2.59667700	0.52709600
C	-2.14487400	-0.73006000	0.11906200
C	-1.94388400	-3.42663700	0.59097700
H	0.18069600	-2.97702000	0.65144200
C	-3.30430100	-1.50174700	0.14989500
C	-3.19903100	-2.86511400	0.39241200
H	-1.82035900	-4.48904700	0.78287300

H	-4.27814300	-1.05183400	-0.02641000
H	-4.09341200	-3.48432500	0.41931800

23

Cu	-0.00004100	-1.19197400	-0.00001000
C	1.00044100	-1.42255200	1.67316400
C	-1.00056700	-1.42244200	-1.67317900
F	1.14302700	-0.29090400	2.41068200
F	0.48407900	-2.34473800	2.52194200
F	-2.27574600	-1.83782800	-1.41426800
F	-1.14305400	-0.29077000	-2.41067900
F	-0.48431100	-2.34466600	-2.52197800
F	2.27558300	-1.83805900	1.41426700
N	1.23292600	0.46100400	-0.55040000
C	2.48630400	0.38050200	-0.98998000
C	0.69929200	1.65473200	-0.24904600
C	3.28504900	1.50157800	-1.17313000
H	2.85738500	-0.62309100	-1.19452000
C	1.44421100	2.82501300	-0.39431900
C	2.74759600	2.74450700	-0.86483200
H	4.30288900	1.39540400	-1.53861900
H	1.02383500	3.79040500	-0.12543600
H	3.34119800	3.64899900	-0.98104400
N	-1.23288000	0.46109700	0.55039700
C	-2.48626000	0.38069100	0.98998800
C	-0.69915200	1.65478500	0.24905300
C	-3.28491400	1.50182900	1.17315600
H	-2.85742100	-0.62287400	1.19452200
C	-1.44397600	2.82512500	0.39434300
C	-2.74736400	2.74471800	0.86486500
H	-4.30275800	1.39573400	1.53865500
H	-1.02352500	3.79048600	0.12546600
H	-3.34089300	3.64925700	0.98109100

4-p

C	-1.87817500	0.00061800	0.09314600
F	-1.73157500	1.05096000	0.90705000
F	-3.13531300	0.01962000	-0.36718700
F	-1.73673100	-1.10608600	0.83030300
C	-0.89162500	0.03796800	-1.04565600
H	-1.11391300	-0.82516400	-1.68696800
H	-1.10974500	0.94365800	-1.62661800
C	0.53347600	0.01887600	-0.57164200
C	1.18393700	-1.19287000	-0.33868900

C	1.21236200	1.21142900	-0.32308600
C	2.49447100	-1.21324200	0.12431400
C	2.52320400	1.19465500	0.13990900
C	3.16723400	-0.01855300	0.36297200
H	0.65153400	-2.12719200	-0.51969000
H	0.70414600	2.16109300	-0.49397600
H	2.99263200	-2.16542500	0.29898100
H	3.04382900	2.13240800	0.32666800
H	4.19478100	-0.03310900	0.72250300

4-s

C	-1.73149600	0.34182600	-0.28510400
F	-1.68110100	-0.43016800	-1.37841500
F	-3.01150500	0.38275000	0.11172900
F	-1.38777500	1.58051900	-0.64859300
C	-0.83611600	-0.17903600	0.82007000
C	0.61690100	-0.10358900	0.41019600
C	1.41426100	0.94071700	0.87856600
C	1.18458500	-1.04850000	-0.44677000
C	2.75217600	1.03717300	0.51266300
C	2.52183600	-0.95450500	-0.81570900
C	3.31023100	0.08662800	-0.33561900
H	0.97611100	1.68955400	1.53981800
H	0.57741700	-1.86387100	-0.83733700
H	3.35958000	1.85741200	0.89181700
H	2.95004800	-1.69966800	-1.48425800
H	4.35791000	0.15710800	-0.62325700
C	-1.28453200	-1.56889000	1.25840000
H	-2.31316700	-1.54793800	1.63487100
H	-1.24753800	-2.28377500	0.42793800
H	-0.62983700	-1.94067000	2.05415400
H	-0.99416800	0.52298800	1.65359600

4-t

C	1.60509900	-0.31639200	-0.52455000
F	1.29389900	0.15776300	-1.73566100
F	2.92335900	-0.13164600	-0.35368900
F	1.40278500	-1.63998000	-0.54938200
C	0.79821700	0.37501800	0.57196100
C	-0.69030100	0.17826500	0.27999700
C	-1.48079000	1.21362900	-0.22394100
C	-1.30227800	-1.06138900	0.49908500
C	-2.83454200	1.02577300	-0.48583800
C	-2.65302800	-1.25341900	0.23679300

C	-3.42822500	-0.20851300	-0.25486300
H	-1.04542200	2.19127900	-0.41749800
H	-0.71852100	-1.90007500	0.87185700
H	-3.42503600	1.85388000	-0.87484100
H	-3.10120100	-2.22907100	0.41838300
H	-4.48741200	-0.35713800	-0.45807700
C	1.20534100	1.85016100	0.57885600
H	0.59677800	2.40252600	1.30528700
H	2.25685200	1.95043800	0.86945200
H	1.08636700	2.32029800	-0.40393400
C	1.18274800	-0.23280200	1.92488500
H	0.99779200	-1.31071000	1.97347200
H	2.24717400	-0.06745200	2.13139900
H	0.59881500	0.24881900	2.71877200

¹⁵

Cu	-0.93807900	-0.70249000	0.00131400
N	0.17718000	1.28780000	-0.28223000
C	-0.34331400	2.51035500	-0.28202900
H	-1.41606000	2.56100700	-0.47198300
C	0.42607000	3.64627300	-0.04382500
H	-0.03065300	4.63279500	-0.05620700
C	1.78006600	3.47981200	0.21841700
H	2.41361700	4.34083800	0.42288800
C	2.32154800	2.19911600	0.23336200
H	3.37310800	2.05214600	0.47044100
C	1.47977400	1.11897200	-0.02904500
N	0.97840000	-1.23398300	0.04563000
C	1.94091800	-0.29049100	-0.02269200
C	3.28781900	-0.64164600	-0.08699800
H	4.05095200	0.12834000	-0.16982100
C	3.64541000	-1.98282200	-0.07238100
H	4.69355300	-2.26996900	-0.12705400
C	2.64935100	-2.94768700	0.00517000
H	2.88287900	-4.00880900	0.01964200
C	1.32865700	-2.52443100	0.06055700
H	0.50671100	-3.23562200	0.12261500
C	-2.83562600	-0.45514500	0.04513800
F	-3.16247700	0.78875700	-0.46335800
F	-3.59620800	-1.31716400	-0.68229400
F	-3.40164000	-0.45815600	1.28493200

²TS1

C	0.51295300	-1.24780700	1.75010200
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C	2.47149700	-0.00118600	-1.17040600
F	0.47252000	-2.59034700	1.62190900
F	1.49930200	-0.95687600	2.61236400
F	-0.64235300	-0.88097700	2.33290600
F	3.13301100	1.09523100	-0.66280600
F	3.44399000	-0.92708600	-1.36015100
F	2.10860200	0.38857500	-2.43037300
N	-1.04402000	-0.94369700	-0.62182800
C	-1.42925300	-2.16400200	-0.99288500
C	-1.95789300	0.02835700	-0.45944800
C	-2.75836100	-2.48598800	-1.23269600
H	-0.63569600	-2.90304600	-1.09671000
C	-3.31268600	-0.22188000	-0.67238300
C	-3.71393200	-1.49200800	-1.06315800
H	-3.03132700	-3.49281200	-1.53692900
H	-4.05246200	0.55929600	-0.51776600
H	-4.76833800	-1.70344800	-1.22877400
N	-0.14850100	1.39799600	0.31051600
C	0.41617500	2.55631600	0.64379000
C	-1.43831700	1.35769400	-0.05530100
C	-0.29463000	3.75063900	0.65874300
H	1.47692100	2.51314300	0.88916400
C	-2.21480000	2.51537500	-0.07816700
C	-1.63390300	3.72158800	0.29174500
H	0.19742000	4.67763700	0.94082200
H	-3.25280800	2.48747200	-0.39996100
H	-2.22391700	4.63580800	0.27911000
Cu	0.91796900	-0.44873800	0.00365400

ossTS2-p

Cu	1.04085300	-0.12325700	0.37875600
N	-0.60604400	1.08727500	0.84206900
C	-0.57521000	2.42092300	0.84339500
H	0.37207400	2.87154300	0.54935600
C	-1.67632600	3.18864900	1.19832000
H	-1.61004300	4.27340000	1.18752100
C	-2.84416100	2.53542000	1.57171200
H	-3.72491500	3.10109800	1.86944700
C	-2.87689800	1.14786300	1.56765000
H	-3.77805000	0.62049900	1.87062700
C	-1.73422600	0.44602800	1.18838900
N	-0.44154200	-1.54806800	0.96102400
C	-1.66765900	-1.03115000	1.14441400
C	-2.78704900	-1.85093800	1.27396300

H	-3.78051800	-1.42271800	1.38402200
C	-2.61936900	-3.22844500	1.23229700
H	-3.48109700	-3.88607300	1.32838100
C	-1.34409000	-3.75426800	1.06231400
H	-1.17090000	-4.82662000	1.02927000
C	-0.28163500	-2.87114400	0.91987100
H	0.73556000	-3.22200100	0.75475900
C	2.22821300	-1.31190700	-0.67520400
C	2.45188100	1.17463200	0.92906400
F	1.57155000	-2.32330500	-1.33856900
F	2.94515700	-0.68376900	-1.63469100
F	3.12229700	-1.95397600	0.10979800
F	2.17955100	1.67993100	2.16719300
F	3.71045600	0.71878200	0.98874700
F	2.49258000	2.26965900	0.10986700
C	0.66821900	1.81768000	-2.49878000
H	0.70228100	2.90552500	-2.45485100
H	1.61048500	1.28384800	-2.60402900
C	-0.54671100	1.12628500	-2.39435600
C	-1.78062800	1.80746800	-2.20512100
C	-0.58039600	-0.29550800	-2.42269400
C	-2.96024200	1.10931100	-2.02630400
C	-1.76664800	-0.98363200	-2.23758200
C	-2.96430000	-0.29158500	-2.03119900
H	-1.77806700	2.89860000	-2.19013200
H	0.34875900	-0.83899500	-2.58149500
H	-3.89249000	1.65378400	-1.87640500
H	-1.75969800	-2.07420000	-2.24797500
H	-3.89591900	-0.83770300	-1.88605000

ossTS2-s

Cu	-1.36000200	-0.44488400	0.32217300
N	0.45304600	0.38522700	0.99536800
C	1.47617800	-0.32843800	1.46401300
H	1.33645500	-1.40870800	1.47665500
C	2.65562900	0.26187600	1.90211200
H	3.47223200	-0.35733900	2.26234600
C	2.76430300	1.64307700	1.83908500
H	3.67623300	2.14113500	2.16237600
C	1.69460400	2.38932300	1.35870500
H	1.76056500	3.47366200	1.31873900
C	0.54437100	1.72699900	0.93978800
N	-1.71458000	1.63748300	0.16647100
C	-0.65469400	2.42432500	0.42286700

C	-0.71505800	3.80124100	0.21643400
H	0.14958700	4.43217700	0.40595300
C	-1.89937700	4.36208400	-0.24300100
H	-1.96511100	5.43567300	-0.40823000
C	-2.99254000	3.54097300	-0.48959400
H	-3.93718300	3.94286200	-0.84586100
C	-2.85055900	2.17567700	-0.27921400
H	-3.66179700	1.47618100	-0.47439100
C	-2.70002300	-1.01008100	-1.02879200
C	-1.26448200	-2.16567500	1.30388400
F	-3.96332500	-0.92705800	-0.52809700
F	-2.71614900	-0.20347700	-2.13505700
F	-2.56754900	-2.26312800	-1.50516900
F	-2.37252700	-2.92079900	1.30357900
F	-0.26866900	-2.96428400	0.80910500
F	-0.93697800	-1.98334600	2.61603700
C	1.63514000	-1.55005300	-1.59902400
C	2.87625200	-0.93560600	-1.31923400
C	3.15798100	0.40958700	-1.67327700
C	3.89253000	-1.65445500	-0.63560700
C	4.37326200	0.99129800	-1.35266300
C	5.10626800	-1.06811000	-0.32884400
C	5.35758600	0.26265300	-0.68035200
H	2.40228200	0.99029700	-2.20246100
H	3.69607900	-2.69097700	-0.35671000
H	4.56491000	2.02605400	-1.63596000
H	5.87106600	-1.64738400	0.18748900
H	6.31491100	0.72273200	-0.44109000
C	0.52153400	-0.89746500	-2.33433800
H	-0.34897600	-1.55667900	-2.40576800
H	0.18503400	0.03399500	-1.84143300
H	0.81205300	-0.60959900	-3.35844400
H	1.49580400	-2.57798600	-1.26036200

ossTS2-t

Cu	-0.37497100	-0.63521800	0.36738300
N	0.17082300	1.34234700	0.44497800
C	1.38088400	1.72337400	0.86203000
H	2.10921000	0.92763700	1.00861900
C	1.70320500	3.05065000	1.11332600
H	2.70670200	3.30648000	1.44356600
C	0.72135600	4.01395100	0.93650800
H	0.92784000	5.06367300	1.13581300
C	-0.53960600	3.62108900	0.50723900

H	-1.32672600	4.36014000	0.38345100
C	-0.78905300	2.27271800	0.26289500
N	-2.25119400	0.44230800	-0.19784500
C	-2.10700600	1.77567300	-0.19143600
C	-3.14363200	2.62063000	-0.58903600
H	-3.01258600	3.69960100	-0.60819900
C	-4.35375800	2.06154100	-0.97683500
H	-5.17540300	2.70319800	-1.28918200
C	-4.49968700	0.68031500	-0.96252500
H	-5.43259000	0.20436800	-1.25344600
C	-3.41301500	-0.09234500	-0.57005700
H	-3.46239300	-1.17965900	-0.55046500
C	-1.05489900	-2.42468800	-0.03421700
C	0.21191100	-1.00471300	2.26594600
F	-2.06590600	-2.69788200	0.83111000
F	-1.65590300	-2.52265700	-1.26809700
F	-0.20993800	-3.47088800	0.03784800
F	-0.12438400	-2.17845500	2.82051800
F	1.56734800	-0.90924800	2.41172600
F	-0.29616700	-0.04589800	3.09301500
C	1.02893700	-0.84531500	-2.11224400
C	2.22840300	-0.30390900	-1.50789900
C	2.70955200	0.98355800	-1.83135600
C	2.98462100	-1.06284700	-0.58600000
C	3.89280100	1.46829700	-1.28983000
C	4.14831000	-0.56160800	-0.02413800
C	4.62001300	0.70352800	-0.37991400
H	2.16061000	1.59724000	-2.54492500
H	2.62214300	-2.04284500	-0.27715800
H	4.24995400	2.45601400	-1.58053600
H	4.69260500	-1.16325500	0.70200900
H	5.54414400	1.08712100	0.04917700
C	0.10500000	0.03483200	-2.89174900
H	0.44629000	0.15113100	-3.93758100
H	-0.89645100	-0.41483600	-2.93392600
H	0.00874000	1.04158000	-2.46443200
C	1.03345900	-2.28793200	-2.51422200
H	1.41201200	-2.95891300	-1.73708600
H	0.03306000	-2.63352900	-2.78769800
H	1.68737100	-2.41195600	-3.39604300

^{css}TS3-p

Cu	1.13960700	-0.05699600	-0.03666900
N	0.01647100	1.72918700	-0.17490400

C	0.46268600	2.78955700	-0.84862500
H	1.42180900	2.65620400	-1.35121800
C	-0.23156500	3.99161300	-0.88811100
H	0.15645700	4.83026700	-1.46032700
C	-1.41458900	4.08956200	-0.16474200
H	-1.98338800	5.01740500	-0.15726600
C	-1.85478800	2.99873000	0.57197100
H	-2.75439700	3.07783600	1.17726600
C	-1.11378900	1.81695100	0.54203500
N	-0.56809100	-0.36185200	1.37824500
C	-1.49945900	0.60260800	1.29858800
C	-2.74980600	0.46063600	1.90075100
H	-3.50800600	1.23312800	1.79786800
C	-3.02862100	-0.69764600	2.61252900
H	-4.00008000	-0.82809400	3.08549700
C	-2.05485300	-1.68314100	2.70723400
H	-2.22842700	-2.60334400	3.25937500
C	-0.84092400	-1.47002700	2.06543000
H	-0.04817400	-2.21748300	2.09310100
C	1.58460800	-2.07163800	-0.37099100
C	2.90474000	0.75504600	0.37695700
F	0.88496000	-3.22873500	-0.50250800
F	2.69852900	-2.19726200	-1.08311700
F	1.94309700	-2.12453700	0.94168100
F	2.85025000	1.74415000	1.32503400
F	3.95974300	-0.01113900	0.74419100
F	3.35727800	1.42871200	-0.75563300
C	0.44344500	-1.14516700	-1.70774600
H	0.91076500	-0.24023600	-2.13435700
H	0.79393800	-1.97853700	-2.31706000
C	-1.03786000	-1.07508400	-1.63251200
C	-1.69424400	0.06498200	-2.11641800
C	-1.82131600	-2.12544600	-1.13588400
C	-3.08053700	0.16127500	-2.09478600
C	-3.20614400	-2.02183000	-1.09917000
C	-3.84436100	-0.87959200	-1.57625800
H	-1.10363100	0.88772700	-2.52110900
H	-1.33787100	-3.02509300	-0.76353400
H	-3.56299900	1.05690900	-2.48427400
H	-3.79325700	-2.84768200	-0.69938500
H	-4.93045100	-0.80651400	-1.55289600
cssTS3-s			
Cu	0.23639900	-0.42606400	0.26909600

N	-0.35637100	1.59938000	-0.30565200
C	0.51022500	2.59058400	-0.08284100
H	1.56447000	2.32294800	-0.13896700
C	0.11764200	3.88906900	0.21223100
H	0.86563600	4.65773600	0.38834400
C	-1.24061100	4.16240400	0.30136600
H	-1.59252200	5.16052500	0.55493600
C	-2.14831900	3.13663800	0.07979600
H	-3.21549400	3.31831000	0.18153800
C	-1.67206900	1.86233000	-0.22800100
N	-2.05983200	-0.50438800	-0.31195900
C	-2.58785900	0.72053800	-0.45073900
C	-3.93162300	0.90767600	-0.78444100
H	-4.33096600	1.90830700	-0.93215200
C	-4.74673800	-0.20165500	-0.95365200
H	-5.79512900	-0.07651000	-1.21791700
C	-4.20205100	-1.46832800	-0.78482900
H	-4.80322500	-2.36683400	-0.89973400
C	-2.85275900	-1.56374100	-0.46690400
H	-2.38293500	-2.53686500	-0.32515900
C	0.42981100	-2.57203300	0.17491600
C	0.44876100	0.02666600	2.18404200
F	-0.52483900	-2.59197100	1.13422600
F	0.02898000	-3.58394000	-0.63607800
F	1.56522600	-2.96708200	0.75505700
F	0.93771200	-0.92350600	3.02896000
F	1.26676800	1.11426100	2.39889500
F	-0.74474600	0.40622200	2.75204200
C	1.10064200	-1.52828200	-1.36679300
C	2.10291500	-0.41457100	-1.22904800
C	2.15478700	0.62206100	-2.17120100
C	3.08935200	-0.45350000	-0.22804500
C	3.16955600	1.57148400	-2.13129900
C	4.08052300	0.51822500	-0.17116400
C	4.13380200	1.52759200	-1.12869500
H	1.39931200	0.68558200	-2.95170400
H	3.07094000	-1.24988400	0.51313200
H	3.20103100	2.35398100	-2.88814200
H	4.82207700	0.47699100	0.62425200
H	4.92381900	2.27577600	-1.09335300
C	0.10098900	-1.43386800	-2.49590000
H	-0.62225700	-2.25225000	-2.44194100
H	-0.45313500	-0.48883700	-2.49496100
H	0.62580900	-1.52826200	-3.45892000

H	1.67664900	-2.45136700	-1.47046900
cssTS3-t			
Cu	0.27003800	-0.24896800	0.31827600
N	-0.73923200	1.55726500	-0.45968400
C	-0.09635300	2.71930500	-0.31964400
H	0.99074700	2.66814800	-0.35179700
C	-0.74622900	3.93161700	-0.13202700
H	-0.17060700	4.84695200	-0.02123700
C	-2.13244600	3.93102500	-0.06157500
H	-2.68267700	4.85400700	0.11097400
C	-2.80994000	2.72785000	-0.19683600
H	-3.89299400	2.69694600	-0.10698000
C	-2.08233400	1.55557600	-0.40291000
N	-1.99863100	-0.84142200	-0.30104500
C	-2.75188600	0.24186800	-0.53657900
C	-4.10088900	0.13836800	-0.88710300
H	-4.68346100	1.02747300	-1.11632300
C	-4.68393200	-1.11738200	-0.96686200
H	-5.73233500	-1.21909200	-1.24111200
C	-3.90735900	-2.23653800	-0.69623200
H	-4.32117700	-3.24103000	-0.73865000
C	-2.56999300	-2.04301200	-0.37216100
H	-1.92386900	-2.89361100	-0.15741500
C	0.75882600	-2.33638900	0.50474300
C	0.29605600	0.41500200	2.18483200
F	-0.21145800	-2.34657900	1.45782300
F	0.45252300	-3.46227900	-0.19133700
F	1.90009000	-2.56627300	1.15932900
F	1.02103100	-0.28593100	3.10272600
F	0.76264500	1.70417600	2.31157500
F	-0.96727900	0.47356000	2.71752300
C	1.45514300	-1.38462900	-1.22126400
C	2.13269500	-0.04637000	-1.07398400
C	2.08040000	0.90009500	-2.10801000
C	2.97474200	0.21342400	0.02307700
C	2.85837600	2.05144200	-2.05930800
C	3.71979500	1.38496500	0.08502300
C	3.67766100	2.30125700	-0.96156300
H	1.43343700	0.73097000	-2.96690800
H	3.03737900	-0.50690500	0.83679900
H	2.81837100	2.76000000	-2.88548900
H	4.34361000	1.57418100	0.95631900
H	4.27963900	3.20747300	-0.92143000

C	0.40775200	-1.49295400	-2.30932700
H	0.90590500	-1.53651400	-3.29201000
H	-0.15633100	-2.42487300	-2.19910600
H	-0.30194700	-0.65941700	-2.31508100
C	2.55756100	-2.41589500	-1.46419200
H	3.31009700	-2.43884500	-0.67276600
H	2.17096400	-3.42563800	-1.62348000
H	3.06536000	-2.09286100	-2.38656200

cssTS4-p

Cu	0.09810900	-0.22270600	-0.66317000
N	-0.97999000	-1.26339600	0.89116200
C	-0.80139400	-2.52831100	1.28720700
H	-0.00725400	-3.07764900	0.79216300
C	-1.57033800	-3.13301700	2.27043500
H	-1.37487000	-4.16444300	2.55171800
C	-2.57223500	-2.38898800	2.87955200
H	-3.18903300	-2.81949100	3.66586600
C	-2.76771000	-1.07858000	2.47453400
H	-3.52685200	-0.46436200	2.95208800
C	-1.96013200	-0.54289600	1.46995600
N	-1.08832000	1.38073700	0.34008300
C	-2.13337400	0.83931200	0.99164800
C	-3.33271000	1.53074500	1.16355900
H	-4.17982900	1.05057900	1.64661600
C	-3.45281500	2.81648400	0.66195500
H	-4.38623500	3.36465000	0.77089400
C	-2.36575200	3.38394400	0.00825400
H	-2.40772900	4.38904900	-0.40286200
C	-1.21532100	2.62408700	-0.12993500
H	-0.35229200	3.03578700	-0.65514200
C	1.47534200	-1.59509300	-0.91590400
C	-1.29358100	-0.03358300	-2.19044200
F	2.40052300	-1.53805800	-1.88110100
F	2.11888200	-1.91472600	0.22073400
F	0.69559200	-2.65375000	-1.22986300
F	-2.61695700	0.02645600	-1.80178100
F	-1.12666800	1.13269800	-2.91294500
F	-1.27323700	-1.01311600	-3.13757600
C	1.67224000	0.93914000	-1.06094600
H	2.08089200	0.63853300	-2.02475100
H	0.98108800	1.77881500	-1.17844800
C	2.63621200	1.07489900	0.02929400
C	3.94685900	0.59354200	-0.10894900

C	2.27789600	1.70476500	1.23194400
C	4.87107200	0.75036000	0.91352100
C	3.20137200	1.85703000	2.25550700
C	4.50192400	1.38142500	2.09926400
H	4.23033900	0.08964500	-1.03210000
H	1.25473100	2.06041700	1.35642400
H	5.88599900	0.37722800	0.78716700
H	2.90828900	2.34959900	3.18132400
H	5.22721400	1.50161500	2.90233100

^{oss}TS5-p

Cu	-0.23895300	0.23937900	0.13777500
N	1.19069000	-1.34869200	0.36690600
C	0.88910500	-2.59824900	0.70791700
H	-0.14751000	-2.77155300	1.00237500
C	1.82593100	-3.62349900	0.68550200
H	1.54318400	-4.63226400	0.97460400
C	3.11718100	-3.31884100	0.27457100
H	3.88125800	-4.09243000	0.23045400
C	3.42667600	-2.01587000	-0.09140700
H	4.42807400	-1.77361600	-0.43744300
C	2.43325200	-1.03861000	-0.03162000
N	1.60067100	1.16980900	-0.50306300
C	2.67798300	0.37695400	-0.40864000
C	3.95643500	0.88180200	-0.64455500
H	4.83395600	0.24827600	-0.54512600
C	4.10368800	2.21932900	-0.98666400
H	5.09530100	2.62768800	-1.17135100
C	2.97821400	3.02720900	-1.07873100
H	3.05203400	4.08020400	-1.33721400
C	1.74014000	2.45339700	-0.81808800
H	0.82103100	3.03804800	-0.85378300
C	-0.69201800	-0.46955700	-1.65126600
C	0.04530900	1.07251600	1.91799300
F	-1.29456600	-1.69184400	-1.59366600
F	-1.50305100	0.30566500	-2.40871000
F	0.41399300	-0.67633600	-2.42351300
F	-0.23885800	2.41049500	1.85566800
F	-0.68348900	0.61320000	2.97903000
F	1.33332900	1.01335900	2.35005800
C	-2.63922700	-1.64276100	1.58596700
H	-2.78057000	-2.71053700	1.42158000
H	-2.06313100	-1.32288600	2.45254200
C	-3.21970800	-0.70540900	0.71993900

C	-3.98105800	-1.11236300	-0.40957000
C	-3.05433100	0.69534600	0.93046700
C	-4.54427400	-0.18404900	-1.26068600
C	-3.61456400	1.61617500	0.05800800
C	-4.36326300	1.18693800	-1.03839200
H	-4.10333700	-2.17904300	-0.59748800
H	-2.52873500	1.03208100	1.82012200
H	-5.12285000	-0.52061200	-2.11953100
H	-3.47561500	2.68041700	0.24417300
H	-4.80203200	1.91281700	-1.72057300

cssTS6-p

Cu	-0.11004200	-0.79306400	-0.08238500
N	-2.16233000	-0.29261500	0.25176000
C	-3.11938200	-1.21714400	0.30176100
H	-2.77921100	-2.24909000	0.38299100
C	-4.47106100	-0.90488000	0.25037100
H	-5.21834900	-1.69264500	0.29771300
C	-4.82837700	0.43143500	0.12444100
H	-5.87520300	0.72329200	0.06688400
C	-3.83265300	1.39560800	0.05751900
H	-4.09972500	2.44117300	-0.07185600
C	-2.49551600	1.00137400	0.12904700
N	-0.14751800	1.44065200	-0.12688300
C	-1.37253000	1.96637100	0.03261500
C	-1.57050900	3.34703100	0.08071500
H	-2.56131200	3.76435600	0.24124500
C	-0.47918900	4.19233400	-0.06457200
H	-0.61511300	5.27153400	-0.02645300
C	0.77916900	3.64108400	-0.26166700
H	1.66081100	4.26348400	-0.39177500
C	0.89379100	2.25550500	-0.28157900
H	1.85966400	1.77420300	-0.43562800
C	0.30743200	-1.21101300	1.99873700
C	-0.23193300	-1.36767500	-1.99481000
F	-0.62028800	-2.17495800	2.12035500
F	1.20350100	-1.44257800	2.98299500
F	-0.24528700	-0.03955900	2.37765500
F	0.01562300	-0.36767400	-2.89591600
F	0.64589700	-2.36993700	-2.37704400
F	-1.45512700	-1.85366200	-2.36685300
C	1.61818900	-1.78972000	0.55998500
H	1.91744600	-2.45894000	1.36584400
H	1.34859800	-2.41272200	-0.29911300

C	2.64079600	-0.75919100	0.24345500
C	3.29228000	-0.03628200	1.25113900
C	2.99164400	-0.51844000	-1.09233600
C	4.26924000	0.89970600	0.93179500
C	3.97704400	0.41036000	-1.40711400
C	4.61725300	1.12574200	-0.39765700
H	3.03068700	-0.21355900	2.29249700
H	2.48050700	-1.06751800	-1.88167900
H	4.76746600	1.45048700	1.72830800
H	4.24264400	0.57702000	-2.44977000
H	5.38824700	1.85359100	-0.64597500

^{oss}TS7-p

Cu	-0.95921700	-0.70594100	-1.01935800
N	-2.45930400	-0.79016300	0.68677200
C	-2.81303000	-1.84824900	1.40874800
H	-2.15343300	-2.71286400	1.32692700
C	-3.95137700	-1.85588200	2.21022000
H	-4.20885300	-2.73733900	2.79209900
C	-4.74463700	-0.71557000	2.23462900
H	-5.65018600	-0.68481300	2.83757300
C	-4.38057600	0.38725100	1.47074200
H	-5.00901400	1.27509800	1.45761300
C	-3.21645400	0.31352500	0.70689900
N	-1.79421600	1.10592300	-1.06280600
C	-2.73840900	1.42235600	-0.15305600
C	-3.22054700	2.72478300	-0.04136600
H	-3.96253400	2.97260900	0.71367700
C	-2.72396900	3.71037800	-0.88318800
H	-3.08810100	4.73261000	-0.80264700
C	-1.75545900	3.37496300	-1.82102200
H	-1.33958900	4.11392700	-2.50057900
C	-1.31913600	2.05848200	-1.87185800
H	-0.56182500	1.73757600	-2.58558700
C	0.97685900	0.39468400	0.51306700
C	-0.05440600	-2.35820900	-1.37016400
F	1.54349100	0.89100600	-0.55739800
F	0.13865500	1.14713600	1.19619300
F	1.36535600	-0.74574500	1.00995700
F	1.26862100	-2.28863000	-1.68015300
F	-0.09984400	-3.18741100	-0.26818800
F	-0.60478000	-3.10788700	-2.36759100
C	3.92301000	0.97733400	1.25197500
C	4.51900500	1.64988500	0.15605700

C	4.49664600	-0.25370100	1.65694200
C	5.62608600	1.12603200	-0.48599500
C	5.60329800	-0.77078200	1.00853800
C	6.17820800	-0.08616700	-0.06509700
H	4.08408900	2.59370700	-0.17540300
H	4.04207700	-0.79281200	2.48867600
H	6.06790200	1.66088600	-1.32570600
H	6.02576600	-1.71976400	1.33550400
H	7.04845100	-0.49739600	-0.57339900
C	2.76574600	1.48810800	1.87507700
H	2.37190200	1.02759200	2.78000000
H	2.39662900	2.48142100	1.62258300

ossTS7-s

Cu	-1.09619500	-0.82076800	-0.97879100
N	-2.58396000	-0.71081300	0.72901200
C	-2.98110800	-1.70450200	1.51645400
H	-2.35184300	-2.59522800	1.49603500
C	-4.12502600	-1.61547500	2.30462700
H	-4.41995100	-2.44473200	2.94275900
C	-4.87584600	-0.44789200	2.24261600
H	-5.78409200	-0.34303700	2.83309200
C	-4.46691200	0.58606500	1.40780600
H	-5.06363100	1.49211400	1.32717200
C	-3.30026000	0.41758200	0.66286200
N	-1.83263400	1.02570300	-1.14356000
C	-2.77221200	1.44267200	-0.26953300
C	-3.20329500	2.76751700	-0.25645700
H	-3.94238000	3.09683900	0.46976200
C	-2.65928800	3.67088300	-1.15905100
H	-2.98339100	4.70963000	-1.15544100
C	-1.69419200	3.23288700	-2.05722900
H	-1.24129000	3.90556300	-2.78056400
C	-1.31064100	1.89998300	-2.01021700
H	-0.55593600	1.50048700	-2.68601400
C	0.98039300	0.29200300	0.40533000
C	-0.33328800	-2.56793400	-1.16519900
F	1.47325000	0.73001800	-0.72720900
F	0.16931300	1.07067900	1.09110600
F	1.40000900	-0.82147700	0.93356200
F	0.97274400	-2.66377800	-1.52862700
F	-0.40028900	-3.24536100	0.03807800
F	-0.99606600	-3.38326000	-2.03496700
C	3.96105900	0.80776300	1.01219500

C	4.66567600	1.31508800	-0.10570700
C	4.36240200	-0.45256400	1.51821400
C	5.70681400	0.60172600	-0.67612800
C	5.40241300	-1.15905300	0.94240900
C	6.08413600	-0.63831300	-0.15953400
H	4.38561500	2.28294200	-0.52059000
H	3.83074900	-0.86337500	2.37709300
H	6.23389800	1.01399600	-1.53577000
H	5.68833900	-2.12714400	1.35106100
H	6.90193500	-1.19579800	-0.61263000
C	2.86539800	1.49906100	1.59566800
C	2.49326400	2.89619000	1.23541300
H	3.28697700	3.61704300	1.49368600
H	2.31214400	3.00624100	0.15441200
H	1.58186300	3.21132600	1.75556800
H	2.45923600	1.08765800	2.52244200

ossTS7-t

Cu	1.21050600	0.97741200	-1.03909800
N	2.41481300	0.74955100	0.89069200
C	2.60822900	1.65692300	1.84250000
H	1.91170000	2.49648300	1.83522300
C	3.63570200	1.54714600	2.77581100
H	3.76313500	2.30459900	3.54524600
C	4.49110800	0.45590300	2.68677100
H	5.31535300	0.34130500	3.38823200
C	4.29640400	-0.48587000	1.68293800
H	4.97832800	-1.32744900	1.58130800
C	3.23329800	-0.30549300	0.79928400
N	2.12569100	-0.77086000	-1.28511100
C	2.93674300	-1.23853100	-0.31378300
C	3.44679900	-2.53406500	-0.36506100
H	4.07780200	-2.90610700	0.43849100
C	3.11471900	-3.35628500	-1.43281600
H	3.50033500	-4.37266400	-1.48098100
C	2.27948800	-2.86709600	-2.42945300
H	1.99239700	-3.47598000	-3.28244700
C	1.80805500	-1.56727000	-2.31144800
H	1.15112400	-1.13036600	-3.06216800
C	-0.83989200	-0.46538100	0.12041900
C	0.28722100	2.65459900	-1.11513600
F	-1.38342000	-0.64450300	-1.05529000
F	-0.05217500	-1.40230300	0.60709600
F	-1.16259700	0.55304400	0.86650500

F	-1.02826400	2.62691600	-1.45987400
F	0.29323400	3.25317200	0.13158300
F	0.84015500	3.59480900	-1.93159300
C	-3.81871000	-0.90013900	0.71234700
C	-4.46684500	-1.08742800	-0.53262300
C	-4.21157800	0.22902000	1.47065600
C	-5.43152200	-0.20350100	-0.98641700
C	-5.17542800	1.11010100	1.01009900
C	-5.79432000	0.90457200	-0.22216800
H	-4.20992200	-1.94712700	-1.14881900
H	-3.74873900	0.41481700	2.43787500
H	-5.90862400	-0.37984900	-1.94973400
H	-5.44855900	1.97080700	1.61908300
H	-6.55009900	1.59990900	-0.58282000
C	-2.79695600	-1.79828700	1.17236000
C	-2.29445400	-1.71091400	2.58070500
H	-1.42856700	-2.36798600	2.72887700
H	-1.98434300	-0.69445400	2.85971100
H	-3.06397500	-2.01568400	3.31055200
C	-2.53908500	-3.07847900	0.43879700
H	-3.38198100	-3.78436700	0.53452400
H	-2.38146900	-2.92551500	-0.63814200
H	-1.64834200	-3.58353100	0.83222900

³TS8-p

Cu	-0.99309400	0.19193700	-0.40830300
N	0.09728500	1.90676100	-0.43663200
C	-0.26588800	3.11022400	0.03914400
H	-1.32963300	3.25470500	0.20401900
C	0.63669600	4.11926800	0.29959300
H	0.28705600	5.07712900	0.67425000
C	2.00058200	3.87239300	0.06117500
H	2.74508300	4.64054300	0.26079100
C	2.38556500	2.64580600	-0.42741000
H	3.43796500	2.43281000	-0.60098400
C	1.42039500	1.65100700	-0.67266300
N	0.67678700	-0.53385400	-1.26883200
C	1.72966600	0.33606500	-1.17966000
C	3.01590800	-0.06469500	-1.57525700
H	3.84843100	0.63079300	-1.50148500
C	3.21969900	-1.33423500	-2.06982900
H	4.21474500	-1.64812800	-2.37896000
C	2.12800500	-2.20690000	-2.18138200
H	2.23731700	-3.21112700	-2.58116400

C	0.88738700	-1.75800600	-1.77484500
H	0.01473800	-2.40043200	-1.84892000
C	-1.88240900	-1.97369900	-0.00448600
C	-2.72617100	1.03531300	0.02676200
F	-1.18251400	-3.12607800	-0.00627300
F	-3.02706200	-2.21083100	0.63058300
F	-2.21585300	-1.77381400	-1.31834200
F	-2.97284800	2.08235600	-0.80010800
F	-3.81164500	0.25055500	-0.04330000
F	-2.72845400	1.56224300	1.28587400
C	-0.86362800	-1.11167000	1.68104800
C	0.57753700	-1.07002900	1.75062900
C	1.26277300	0.13644200	2.00333300
C	1.34070800	-2.25207500	1.61368000
C	2.64451800	0.15788300	2.12023300
H	0.69009200	1.05778900	2.12998100
C	2.71986600	-2.21768900	1.70800200
H	0.82459200	-3.19150200	1.42188300
C	3.38338300	-1.01268300	1.95748000
H	3.14868900	1.10099900	2.32926200
H	3.29070700	-3.13797500	1.59219100
H	4.46880300	-0.99190900	2.03767300
H	-1.41389500	-0.21407700	1.97079000
H	-1.32562500	-2.01234600	2.08052600

³TS8-s

Cu	-0.89228700	0.44555200	-0.56383300
N	0.34046100	2.02012400	-0.23465400
C	0.04271500	3.15980600	0.41089100
H	-1.01501800	3.35827000	0.56023300
C	1.00292900	4.04376900	0.85581500
H	0.70757700	4.95622800	1.36586800
C	2.35484700	3.73143200	0.62122900
H	3.14324400	4.40117000	0.95912000
C	2.67274000	2.56728500	-0.03823500
H	3.71414900	2.30451300	-0.21051500
C	1.65126600	1.69534000	-0.46260000
N	0.77812600	-0.33242800	-1.36119300
C	1.88548200	0.44000400	-1.13035400
C	3.15520300	-0.00555000	-1.53371500
H	4.03016500	0.61537000	-1.35602100
C	3.29051300	-1.22507000	-2.15909800
H	4.27326100	-1.57368000	-2.47065200
C	2.14697500	-2.00088400	-2.40065400

H	2.20404500	-2.96357800	-2.90070400
C	0.92460000	-1.50802700	-1.99090800
H	0.01216700	-2.07109900	-2.16406500
C	-1.96359700	-1.69210400	-0.34915200
C	-2.58465500	1.36046900	-0.13642300
F	-1.39689700	-2.91690900	-0.40581600
F	-3.22214900	-1.86875100	0.05160400
F	-2.07357700	-1.32456500	-1.68272000
F	-2.65546300	2.56128300	-0.76678200
F	-3.70896700	0.70940700	-0.46866600
F	-2.69697500	1.64797700	1.19318900
C	-0.96301200	-1.08897500	1.60886100
C	-1.81791800	-2.05960500	2.36782700
H	-1.69345200	-3.09774800	2.04293200
H	-1.49698000	-2.00695900	3.42022000
H	-2.87754800	-1.79920100	2.32753500
C	0.47203500	-1.29100300	1.59803700
C	1.32684700	-0.21487200	1.91340000
C	1.05615200	-2.55612100	1.37021000
C	2.69898200	-0.39559800	2.00519400
H	0.89483200	0.76639600	2.11877100
C	2.42881100	-2.72008300	1.42989800
H	0.42065600	-3.40119300	1.11504000
C	3.26127900	-1.64308100	1.74671200
H	3.33312000	0.45172600	2.26536300
H	2.86145200	-3.69950100	1.23072900
H	4.33961600	-1.78190600	1.80086100
H	-1.27197900	-0.05244300	1.76850400

³TS8-t

Cu	-0.96065300	0.45493000	-0.64143800
N	0.15672100	2.06373000	-0.10493100
C	-0.23998900	3.13520800	0.59726600
H	-1.30948500	3.21812000	0.77253600
C	0.64022800	4.08184400	1.08165000
H	0.26787900	4.93524900	1.64103300
C	2.01055900	3.90778000	0.82275500
H	2.73795200	4.62922600	1.18985200
C	2.42785100	2.81349200	0.10011600
H	3.48670400	2.65794900	-0.09427500
C	1.48633800	1.87561400	-0.36328800
N	0.78778800	-0.14830400	-1.40901100
C	1.82455800	0.69802100	-1.12583600
C	3.11991800	0.40079300	-1.57617800

H	3.94052300	1.08204500	-1.36370100
C	3.34845600	-0.75200600	-2.29825100
H	4.35148100	-0.98453500	-2.65105900
C	2.27885200	-1.61308100	-2.57214800
H	2.41350400	-2.53136000	-3.13676500
C	1.02253800	-1.26247700	-2.11176600
H	0.15834600	-1.89338300	-2.30246400
C	-1.73310100	-1.90769000	-0.34558600
C	-2.73663700	1.25159200	-0.32799400
F	-1.15572800	-3.10155300	-0.63252700
F	-2.97729900	-2.18919700	0.07245900
F	-1.93416200	-1.36540900	-1.64064100
F	-2.84884200	2.28982500	-1.19822500
F	-3.79112700	0.45668400	-0.55284600
F	-2.94789400	1.79752500	0.90236200
C	-0.63478800	-1.56947900	1.73383300
C	-1.12037200	-2.92067300	2.17567500
H	-0.66842500	-3.75753000	1.63993100
H	-0.84536100	-3.02559600	3.23908000
H	-2.20857000	-3.00667200	2.10608500
C	0.79305600	-1.42024900	1.53909700
C	1.48792100	-0.26947900	1.97567600
C	1.56760200	-2.47087500	0.98689900
C	2.87248800	-0.19975500	1.91441200
H	0.94045500	0.56549400	2.41214600
C	2.94361400	-2.38110500	0.90354400
H	1.06637200	-3.34973200	0.58690400
C	3.61342100	-1.24838800	1.37570100
H	3.37479000	0.69351200	2.28569200
H	3.50736500	-3.20074600	0.45945500
H	4.69926900	-1.18899800	1.32489600
C	-1.43720500	-0.46232900	2.34182600
H	-1.15387700	0.54042900	2.00918000
H	-2.50200600	-0.59868700	2.12098100
H	-1.32592600	-0.49715300	3.44011300

cssINT1-p

Cu	-1.08296100	-0.35113500	0.33186400
N	-0.08970200	1.49334800	-0.49819600
C	-0.43221500	2.76471000	-0.31505800
H	-1.37966200	2.92872900	0.19950500
C	0.36435300	3.82011800	-0.74449500
H	0.05457300	4.84826200	-0.57548900
C	1.55820700	3.51832700	-1.39081400

H	2.21383000	4.31364500	-1.74021500
C	1.91215300	2.19095400	-1.58673100
H	2.85052000	1.94511600	-2.07762300
C	1.05632500	1.19256700	-1.11931600
N	0.46554700	-1.09804100	-0.69591500
C	1.34482500	-0.25414400	-1.26244000
C	2.45260100	-0.74822900	-1.94913700
H	3.16723000	-0.06934400	-2.40622200
C	2.63480300	-2.11946600	-2.05261400
H	3.49646900	-2.51541200	-2.58608400
C	1.70508000	-2.97651000	-1.47691200
H	1.80546800	-4.05633600	-1.54376300
C	0.62976300	-2.41572200	-0.80419000
H	-0.13321100	-3.03170100	-0.32763900
C	-2.68534400	-0.04659300	1.39080300
C	-2.19557300	-0.51479600	-1.32277200
F	-2.63750800	-0.33514500	2.70214100
F	-2.93363300	1.28421300	1.31194100
F	-3.77497100	-0.67836800	0.93763500
F	-1.46596600	-0.31976800	-2.45367900
F	-2.70822100	-1.76095400	-1.44608300
F	-3.22310600	0.34657200	-1.42264300
C	-0.04220900	-0.24674100	2.07455400
H	-0.43350900	0.66678300	2.53554500
H	-0.40209500	-1.12452300	2.62114800
C	1.41757200	-0.22107200	1.92343800
C	2.11939400	0.98586400	1.77584000
C	2.16875400	-1.40935800	1.90658000
C	3.49730200	1.00450700	1.59238000
C	3.54411800	-1.39499200	1.72390200
C	4.21831200	-0.18567200	1.55595700
H	1.56280600	1.92496800	1.80479100
H	1.64637600	-2.35899000	2.04130200
H	4.01163100	1.95897400	1.47962400
H	4.09783100	-2.33356800	1.71670000
H	5.29802500	-0.17230900	1.41546800

cssINT1-s

Cu	-0.08734900	-0.71490000	0.08415700
N	0.24870100	1.24052200	0.42148700
C	1.42571500	1.65296800	0.90102100
H	2.17829900	0.88283000	1.05257900
C	1.68822300	2.98058200	1.20661700
H	2.66669600	3.26220500	1.58615200

C	0.67827400	3.91080700	1.01518000
H	0.83776100	4.96262900	1.24404200
C	-0.55080500	3.48202100	0.53350700
H	-1.35504400	4.19866100	0.39454400
C	-0.74943900	2.13328800	0.24315900
N	-2.12382300	0.28976300	-0.41732400
C	-2.04662800	1.61597700	-0.25561600
C	-3.13358100	2.44600800	-0.53863200
H	-3.07047600	3.52432300	-0.41885200
C	-4.31603100	1.87329900	-0.98674900
H	-5.17451200	2.50318000	-1.21187600
C	-4.38883400	0.49510600	-1.14184900
H	-5.29817600	0.00888100	-1.48585600
C	-3.25776600	-0.25680700	-0.84383700
H	-3.25379800	-1.34228700	-0.94509200
C	-0.67392200	-2.50559100	-0.32955900
C	-0.31479300	-0.96439400	2.06892100
F	-1.75733700	-2.81026400	0.41005600
F	-1.09758600	-2.67429200	-1.60665000
F	0.24812700	-3.45363100	-0.10708700
F	-0.47790400	-2.19548800	2.58094900
F	0.81452200	-0.48513700	2.67893200
F	-1.33152700	-0.21768400	2.57267100
C	0.88431600	-0.73671100	-1.72479700
C	2.24021700	-0.32785000	-1.31485800
C	2.82114400	0.89428800	-1.68744600
C	2.99043600	-1.18085600	-0.48207400
C	4.09655400	1.24522300	-1.25442800
C	4.25499500	-0.82228800	-0.03672700
C	4.81774400	0.39523700	-0.42174800
H	2.26843100	1.57755600	-2.33222000
H	2.55334400	-2.13542800	-0.18349700
H	4.52899700	2.19420200	-1.57057800
H	4.80926700	-1.49939300	0.61153100
H	5.81344500	0.67289100	-0.08002200
C	0.16239400	0.09910800	-2.74805900
H	-0.82211900	-0.33057100	-2.96821600
H	0.00520600	1.13699800	-2.41902600
H	0.72266900	0.14399200	-3.69799300
H	0.89504200	-1.78860400	-2.01731200

CSSINT1-t

Cu	-0.03147100	-0.65442500	0.17813800
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N	0.16492800	1.38251300	0.31372800
C	1.31081500	1.91621600	0.74892200
H	2.13548700	1.22459200	0.89904100
C	1.46232400	3.26876300	1.01616200
H	2.42251900	3.64491500	1.35881800
C	0.36434700	4.09876400	0.85057700
H	0.43038400	5.16333200	1.06641500
C	-0.83238200	3.54813500	0.41585900
H	-1.71110500	4.17776000	0.30995600
C	-0.90974600	2.18258000	0.14367900
N	-2.20273600	0.21914500	-0.30818700
C	-2.16655300	1.55632400	-0.32906900
C	-3.25262200	2.31148400	-0.77858700
H	-3.20309600	3.39601900	-0.83100300
C	-4.40445900	1.65328800	-1.18611900
H	-5.26161400	2.22243900	-1.54092400
C	-4.44339700	0.26619400	-1.13958800
H	-5.32678400	-0.28841200	-1.44607400
C	-3.30932300	-0.40713700	-0.69838100
H	-3.27956600	-1.49527100	-0.65942500
C	-0.69428200	-2.46455200	0.09417200
C	-0.09058600	-0.71422100	2.19961000
F	-1.65565900	-2.62138200	1.02478400
F	-1.32773100	-2.75984800	-1.06817300
F	0.21327400	-3.42634100	0.30370100
F	0.14786400	-1.91110400	2.77326100
F	0.85449000	0.11027200	2.74370900
F	-1.26894900	-0.27919900	2.70275500
C	0.86461400	-0.84196600	-1.69912100
C	2.17068100	-0.28040500	-1.24819800
C	2.71855900	0.89375000	-1.78726800
C	2.91433500	-0.94625600	-0.25448200
C	3.95287900	1.37605600	-1.36255700
C	4.13750300	-0.45270500	0.18428100
C	4.66730600	0.71095000	-0.37077900
H	2.17506300	1.43516900	-2.56052200
H	2.51519700	-1.86071200	0.18761000
H	4.35865800	2.28189300	-1.81218600
H	4.68141000	-0.98443900	0.96353400
H	5.63034100	1.09171300	-0.03482900
C	0.07565400	0.00567500	-2.67104200
H	0.57667000	0.04634900	-3.65662500
H	-0.91490500	-0.43990100	-2.83598200
H	-0.07254700	1.03966400	-2.33308800

C	1.10104100	-2.21661900	-2.31323400
H	1.53445300	-2.94207100	-1.61801100
H	0.18332700	-2.64679000	-2.72247600
H	1.81358600	-2.09702400	-3.14838500

cssINT2-p

Cu	-0.11677300	-0.92690400	0.03872300
N	-2.04990300	-0.22213200	0.01957800
C	-3.05638500	-1.09623900	0.05280200
H	-2.77489700	-2.14530400	0.11069500
C	-4.38568800	-0.70328700	0.01558300
H	-5.17621200	-1.44801900	0.04468100
C	-4.66322800	0.65479800	-0.06250600
H	-5.69118200	1.00994900	-0.09903500
C	-3.61426700	1.56140400	-0.09410200
H	-3.82354700	2.62525100	-0.15875400
C	-2.30001700	1.09579900	-0.04766500
N	0.07718700	1.41112800	-0.06656400
C	-1.12623700	2.00180700	-0.06584200
C	-1.25969600	3.39062200	-0.07367200
H	-2.23784300	3.86399100	-0.06437100
C	-0.11583000	4.17703100	-0.08565700
H	-0.19953100	5.26216100	-0.09055700
C	1.12625300	3.56002500	-0.08867500
H	2.04891400	4.13468400	-0.09706900
C	1.17014000	2.16929700	-0.07759000
H	2.12256000	1.64031800	-0.07742900
C	-0.26392900	-1.04183400	2.01563300
C	-0.30065200	-1.24948300	-1.91313900
F	-1.24693300	-1.95414200	2.27146800
F	0.76860100	-1.42600500	2.80096600
F	-0.70144000	0.11956500	2.55914400
F	-0.74944700	-0.15305500	-2.56961200
F	0.71939400	-1.71550500	-2.67134500
F	-1.28579700	-2.18440900	-2.05542200
C	1.56963100	-1.95448400	0.07548700
H	1.54326100	-2.52236900	1.00580000
H	1.52487200	-2.60991900	-0.79459900
C	2.67443100	-0.97615200	0.01838700
C	3.24867100	-0.46754700	1.19443300
C	3.19522300	-0.54284800	-1.21176300
C	4.30833000	0.42975200	1.14210700
C	4.25476700	0.35450800	-1.26219400
C	4.81772600	0.84611000	-0.08610000

H	2.84915300	-0.78600200	2.15456600
H	2.75272600	-0.91866900	-2.13155800
H	4.74285500	0.80346200	2.06837900
H	4.64700600	0.66956900	-2.22828300
H	5.65245300	1.54441200	-0.12649900