Supporting Information:

Mechanism of the Visible-Light-Mediated Copper-Catalyzed Coupling Reaction of Phenols and Alkynes

Pin Xiao[1], Chun-Xiang Li[1], Wei-Hai Fang[1], Ganglong Cui[1],* and Walter Thiel[2]*

[1]*Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education, Chemistry College, Beijing Normal University, Beijing 100875, China* and [2]*Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany*

E-mail: ganglong.cui@bnu.edu.cn and thiel@mpg.kofo.de

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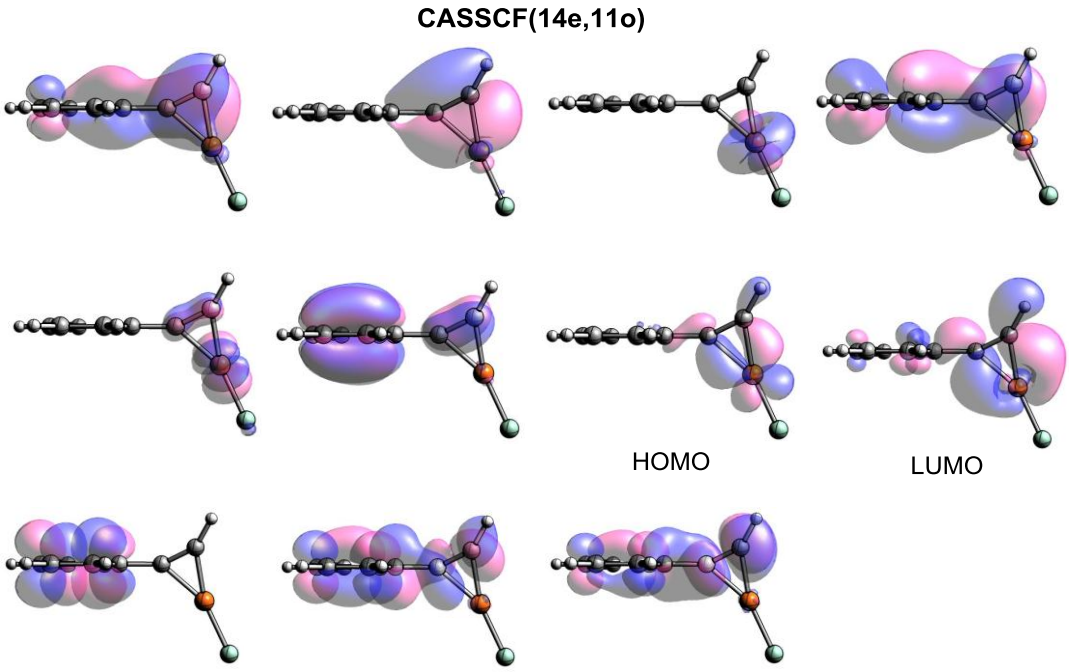


Figure S1: Active spaces used in the CASSCF and MS-CASPT2 calculations of phenylacetylene-CuCl (**9**).

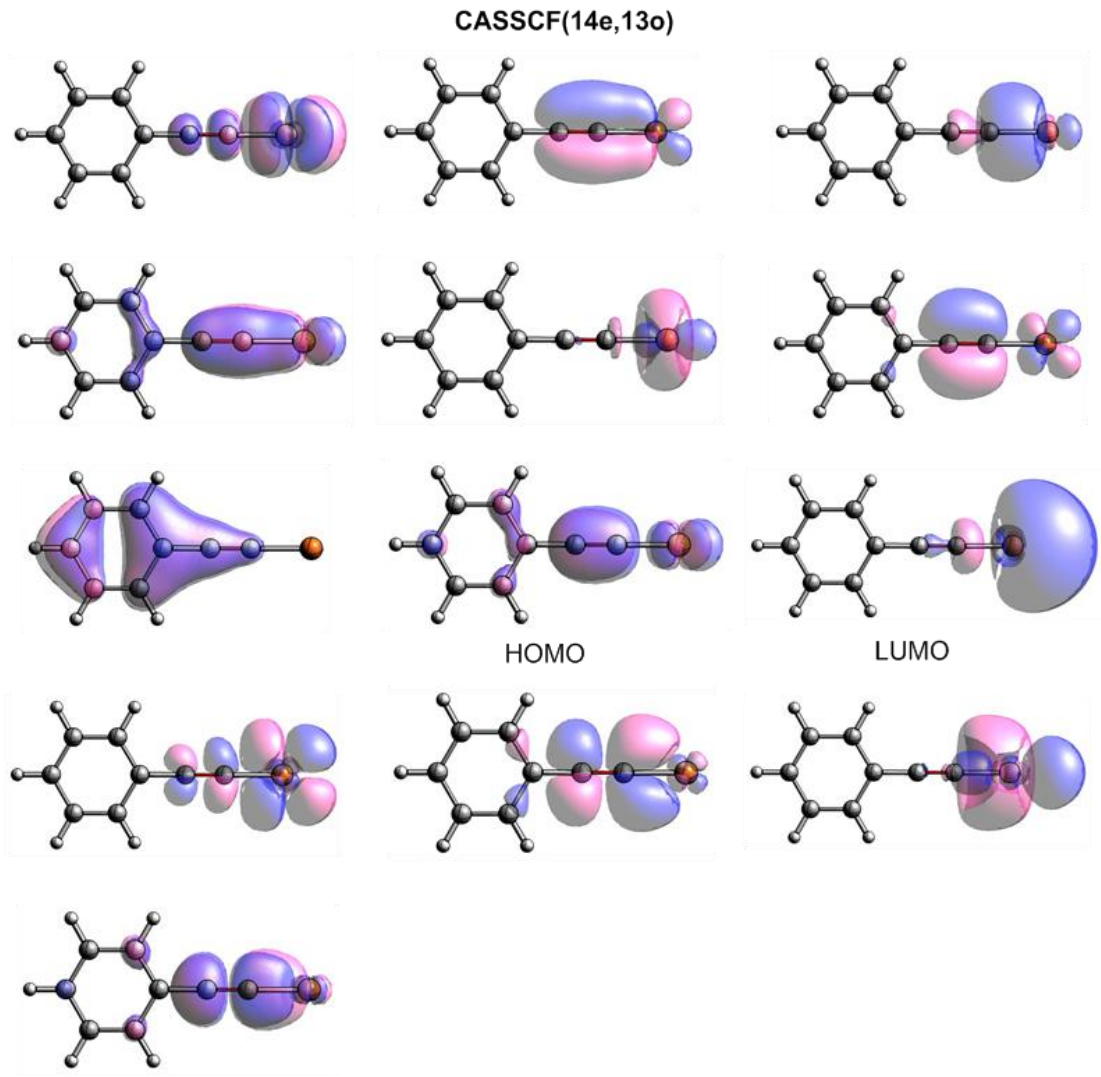


Figure S2: Active spaces used in the CASSCF and MS-CASPT2 calculations of Cu(I)-phenylacetylide (**10**).

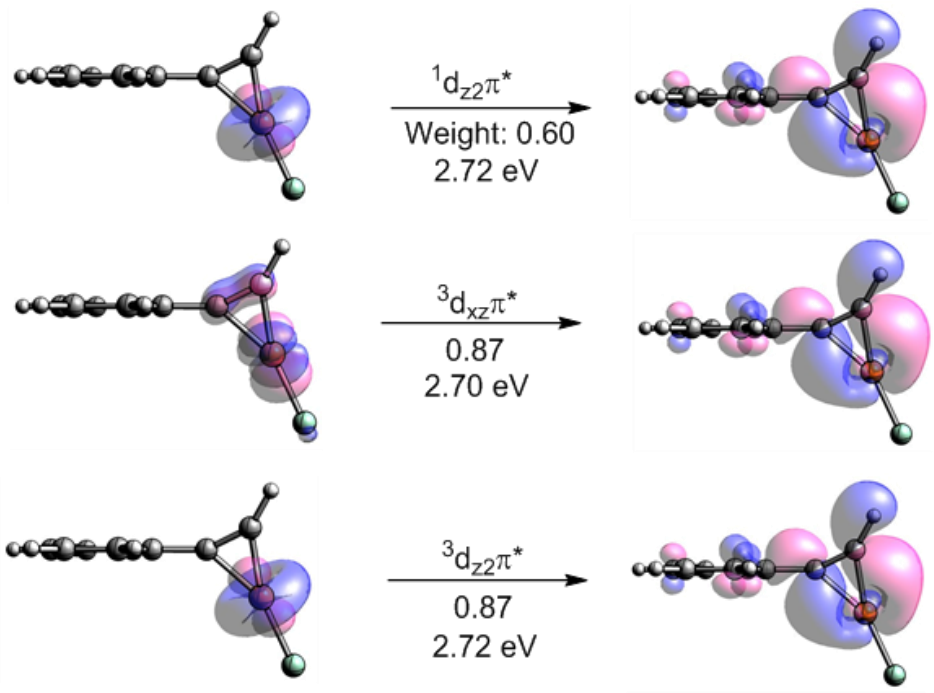


Figure S3: MS-CASPT2/PCM computed primary molecular orbitals involved in the vertical excitation to the relevant S_1, T_1, and T_2 electronic states of phenylacetylene-CuCl (**9**).

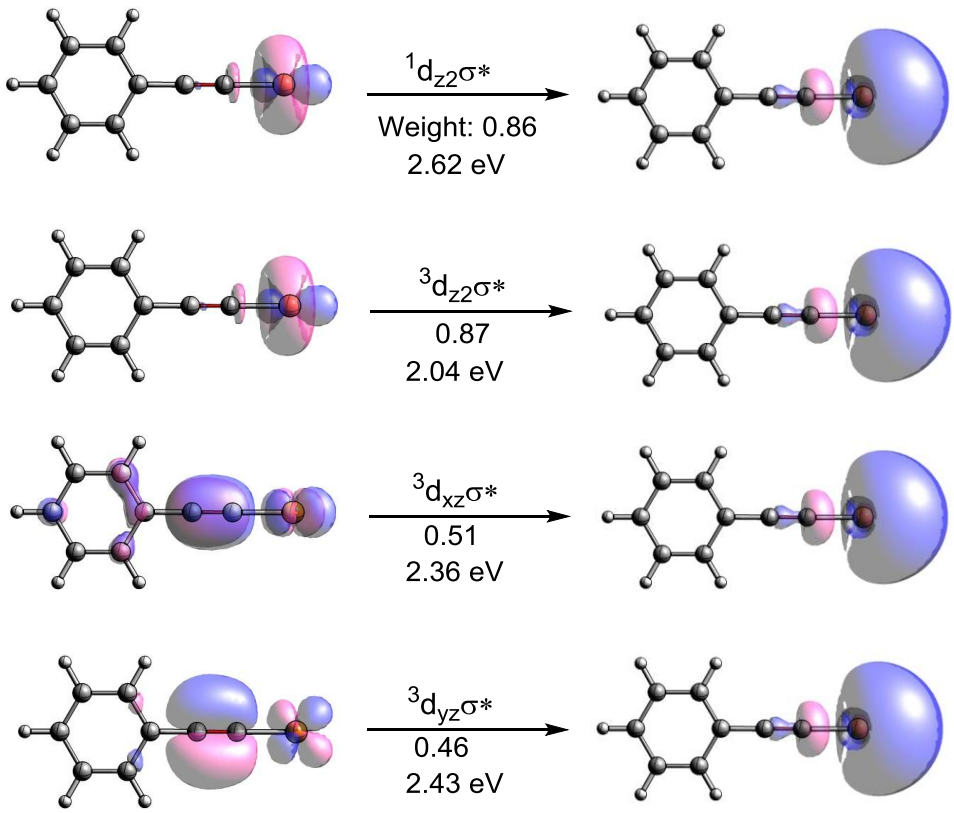


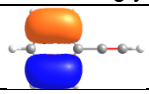
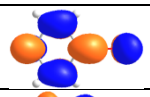
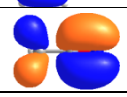
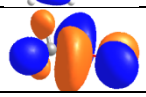
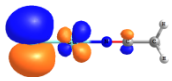
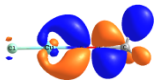
Figure S4: MS-CASPT2/PCM computed primary molecular orbitals involved in the vertical excitation to the relevant S_1, T_1, T_2, and T_3 electronic states of Cu(I)-phenylacetylide (**10**).

II、Tables

Table S1: MS-CASPT2(10,8)/cc-pVDZ-SDD/PCM (Solvent = Acetonitrile) Computed Absolute Energies (A.E., Hartree), Relative Energies (ΔE, kcal/mol/eV), Absorption Wavelengths (nm), Occupations, and Corresponding Weights of Different Substrates and Complexes Optimized at the B3LYP/6-31G**/LANL2DZ level. **2**: Phenylacetylene; **S**: Acetonitrile; **10**: Cu(I)-phenylacetylene.

		A.E. (hartree)	ΔE (kcal/mol)	eV	nm	Occupation	Weight
2	Root 1	-307.4294				22222000	0.85
	Root 2	-307.2674	101.6	4.4	281.6	222u2d00	0.39
	Root 3	-307.2202	131.2	5.7	218.0	2222ud00	0.76
	Root 4	-307.1993	144.3	6.3	198.1	22u22d00	0.85
S	Root 1	-132.3606				22222000	0.92
	Root 2	-132.0533	192.8	8.4	148.3	222u20d0	0.51
	Root 3	-132.0408	200.6	8.7	142.6	2222u00d	0.5
	Root 4	-132.0407	200.7	8.7	142.5	2222u0d0	0.5
CuCl + **S**	Root 1	-788.6298				22222000	0.66
	Root 2	-788.4414	118.2	5.1	241.9	u2222d00	0.56
	Root 3	-788.4385	120.1	5.2	238.2	u22220d0	0.63
	Root 4	-788.4383	120.2	5.2	237.9	2u2220d0	0.55
10 + **S**	Root 1	-634.4342				22222000	0.92
	Root 2	-634.2435	119.7	5.2	239.0	2222u00d	0.94
	Root 3	-634.2305	127.8	5.5	223.7	22u22d00	0.87
	Root 4	-634.2171	136.2	5.9	209.9	22u2200d	0.83

Table S2: TD-CAM-B3LYP/6-311++G**/SDD/SMD Computed Vertical Excitation Energies ($E_{\perp}$, kcal/mol), Absorption Wavelengths (nm), Oscillator Strengths (f), and Corresponding Orbitals to the Lowest Singlet Excited States of Different Substrates and Complexes. The Coulomb-attenuated hybrid exchange-correlation functional (CAM-B3LYP) was employed because it performs well in dealing with the charge transfer excited states, as verified in previous work. [1-3]

	S_n	$E_{\perp}$	nm	f	singly occupied orbitals	
2	1	118.7	241.0	0.0007		
S	1	176.3	162.2	0.0000		
CuCl + **S**	1	118.2	241.9	0.0000		

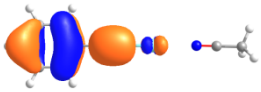
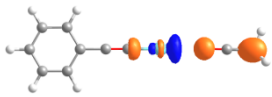
10 + S	1	100.6	284.2	0.0056		

Table S3: MS-CASPT2/PCM (Solvent = Acetonitrile) Computed Vertical and Adiabatic Excitation Energies (in kcal/mol [eV]) to the relevant S_1, T_1, and T_2 Electronic States of Phenylacetylene-CuCl (**9**). See Fig. S3 for Relevant Molecular Orbitals.

	S_1	**T_1**	**T_2**
Vertical excitation	62.6 [2.72]	62.2 [2.70]	62.8 [2.72]
Adiabatic excitation	60.9 [2.64]	51.5 [2.23]	58.3 [2.53]

Table S4: MS-CASPT2/PCM (Solvent = Acetonitrile) Computed Vertical and Adiabatic Excitation Energies (in kcal/mol [eV]) to the relevant S_1, T_1, T_2, and T_3 Electronic States of Cu(I)-phenylacetylide (**10**). See Fig. S4 for Relevant Molecular Orbitals.

	S_1	**T_1**	**T_2**	**T_3**
Vertical excitation	60.5 [2.62]	47.0 [2.04]	54.5 [2.36]	56.1 [2.43]
Adiabatic excitation	60.1 [2.61]	46.9 [2.04]	54.5 [2.36]	56.0 [2.43]

Table S5: MS-CASPT2/PCM (Solvent = Acetonitrile) Computed Absolute Energies (A.E., in Hartree), Relative Energies (ΔE, in kcal/mol) of the S_0, S_1, T_1, and T_2 (T_3) Minima of Phenylacetylene-CuCl (**9**) and Cu(I)-phenylacetylide (**10**).

Structures		MS-CASPT2 (Singlets)			MS-CASPT2 (Triplets)		
			A.E.	**ΔE**		**A.E.**	**ΔE**
9	**S0-MIN**	Root1 (S_0)	-964.04223	**0.0**	Root1	-963.94315	62.2
		Root2	-963.94250	62.6	Root2	-963.94224	62.8
		Root3	-963.93685	66.2	Root3	-963.92330	74.6
	S1/T1/T2-MIN	Root1	-963.96454	48.8	Root1 (T_1)	-963.96039	**51.5**
		Root2 (S_1)	-963.94533	**60.9**	Root2 (T_2)	-963.94939	**58.3**
		Root3	-963.94417	61.6	Root3	-963.94506	61.0
10	**S0-MIN**	Root1 (S_0)	-503.65121	**0.0**	Root1	-503.57638	47.0
		Root2	-503.55483	60.5	Root2	-503.56436	54.5
		Root3	-503.55058	63.1	Root3	-503.56176	56.1
		Root4	-503.54735	65.2	Root4	-503.51971	82.5
	S1/T1/T2/T3-MIN	Root1	-503.64940	1.1	Root1 (T_1)	-503.57635	**46.9**

		Root2 (S_1)	-503.55544	**60.1**	Root2 (T_2)	-503.56413	**54.5**
		Root3	-503.55034	63.3	Root3 (T_3)	-503.56200	**56.0**
		Root4	-503.54765	65.0	Root4	-503.52107	81.7

Table S6: Energy Decomposition Analysis (EDA, in kcal/mol) of Intermediate **11** and of Transition States **TS(11-12)** and **TS(11-12a)** at the M06/QZ4P/ZORA Level. Also Shown are the Corresponding Entropy (S, in kcal/mol/K) Values.

	E_{Pauli}	E_{elstat}	E_{orb}	E_{dist}	E_{tot}	S
11	0.47	-1.31	-3.63	7.34	2.87	0.127
TS(11-12)	123.77	-55.51	-65.81	18.96	21.42	0.129
TS(11-12a)	131.74	-59.66	-68.99	19.36	22.45	0.134
	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{orb}	ΔE_{dist}	ΔE_{tot}	ΔS
TS(11-12) – 11	123.30	-54.2	-62.18	11.62	18.55	0.002
TS(11-12a) – 11	131.27	-58.35	-65.36	12.02	19.58	0.007

The energy decomposition analysis (EDA) was carried out at the M06/QZ4P/ZORA level using ADF2016. Within the Morokuma−Ziegler scheme,[4-6] the total binding energy E_{tot} can be decomposed into four terms

$$E_{tot} = E_{dist} + E_{elstat} + E_{Pauli} + E_{orb}$$

where E_{dist} refers to the distortion energy involving conformational changes of the fragments from their equilibrium structures to their counterparts in intermediates and transition states; E_{elstat} denotes the electrostatic interaction between interacting fragments; E_{Pauli} corresponds to the non-classical Pauli or exchange repulsion interaction between occupied orbitals of interacting fragments; E_{orb} describes orbital interactions involving both mixing of empty/occupied orbitals on the same fragment, and charge transfer between occupied molecular orbitals of one fragment and unoccupied orbitals of another one.

III、Additional Figures

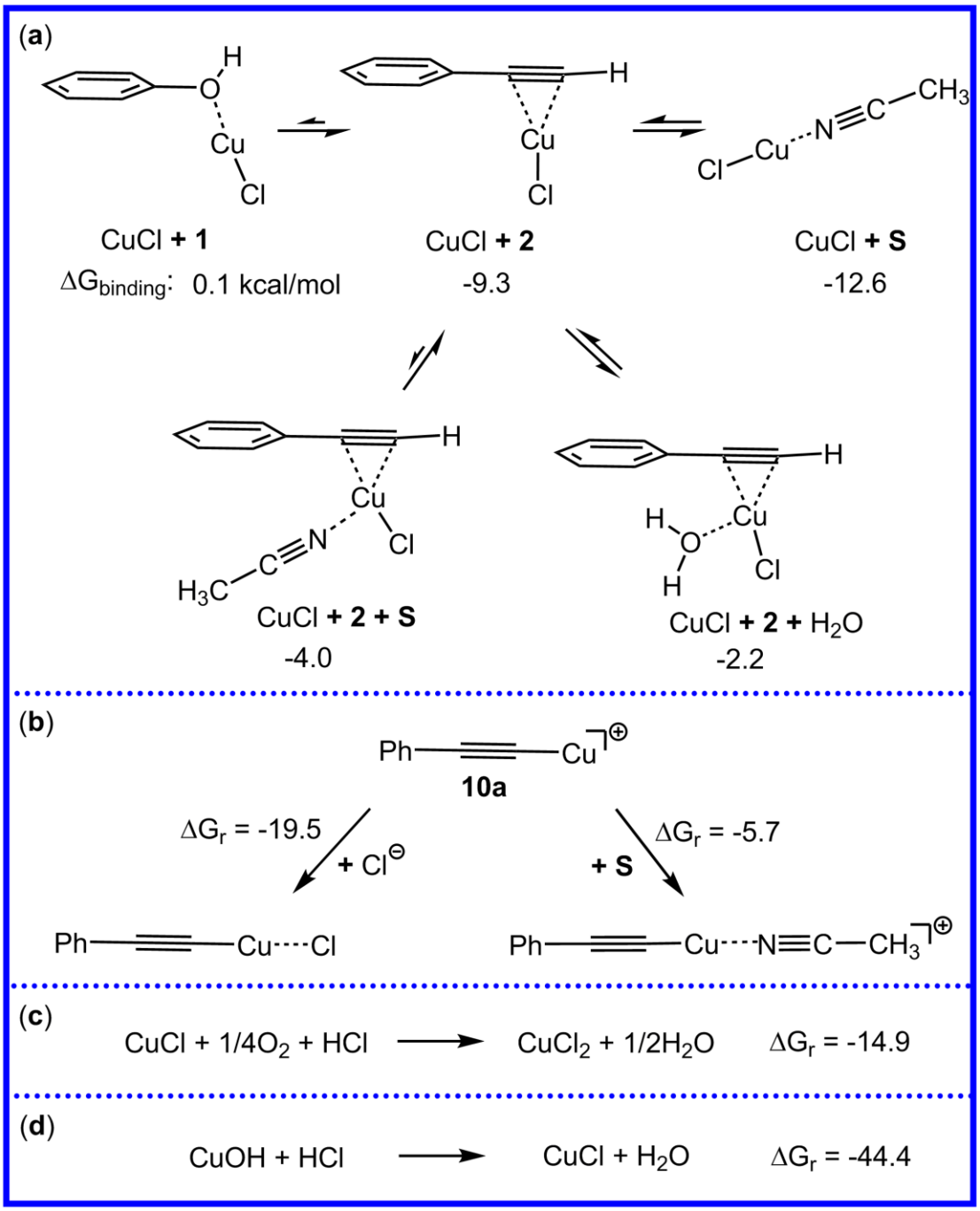


Figure S5: M06/BSII/SMD calculated free energies (in kcal/mol) of (a) the binding of Cu(I)Cl with phenol (**1**), phenylacetylene (**2**), water, and solvent (acetonitrile, **S**); (b) the binding of Cu(II)-phenylacetylide cation (**10a**) with chloride anion and **S**; (c) the oxidation reaction of Cu(I)Cl to Cu(II)Cl_2 by the dioxygen molecule; (d) the neutralization reaction of CuOH and HCl.

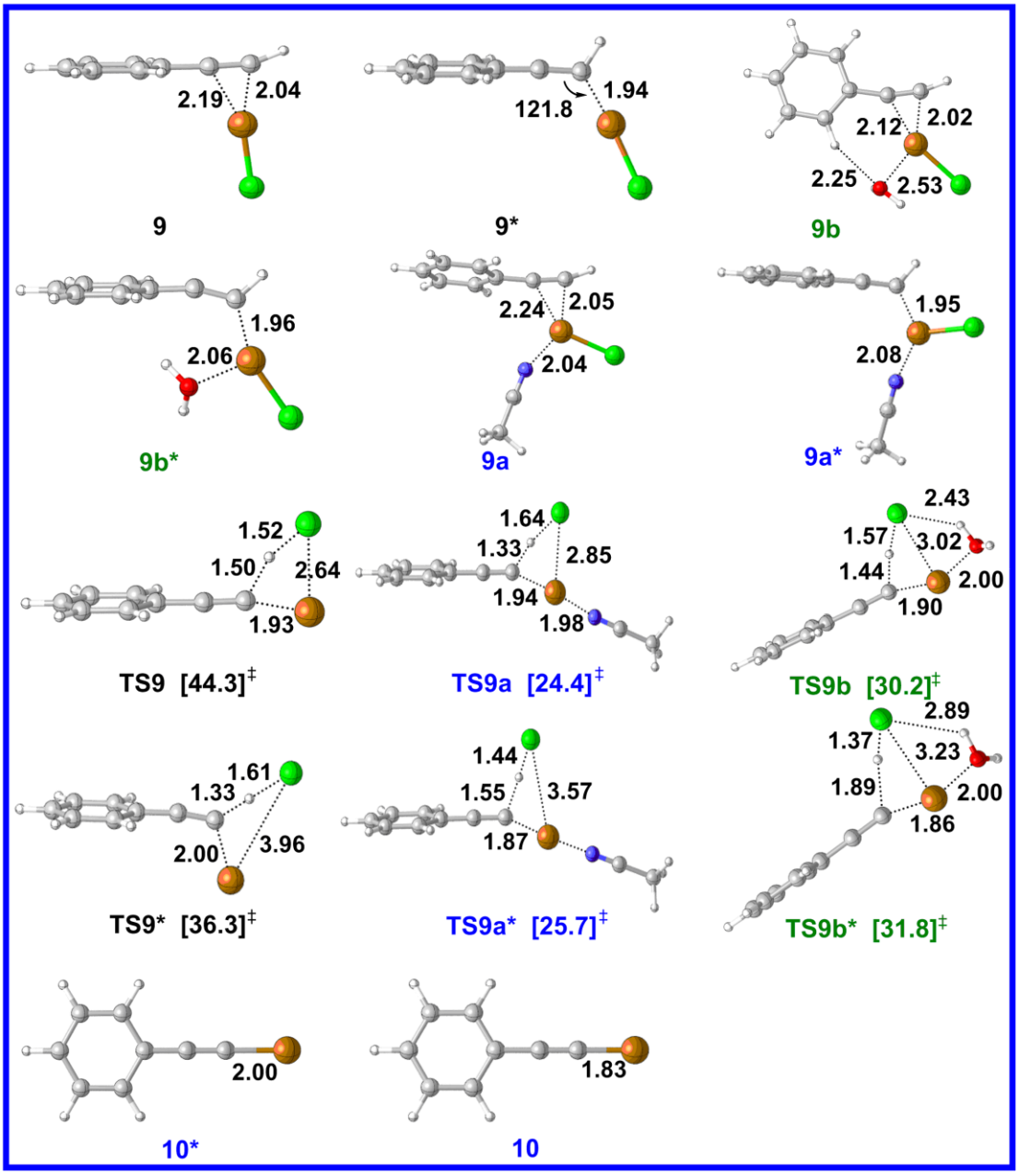


Figure S6: B3LYP/BSI optimized structures of intermediates and transition states for the formation of copper(I)-phenylacetylide (**10**) from CuCl and phenylacetylene (**2**). Selected distances are given in Å.

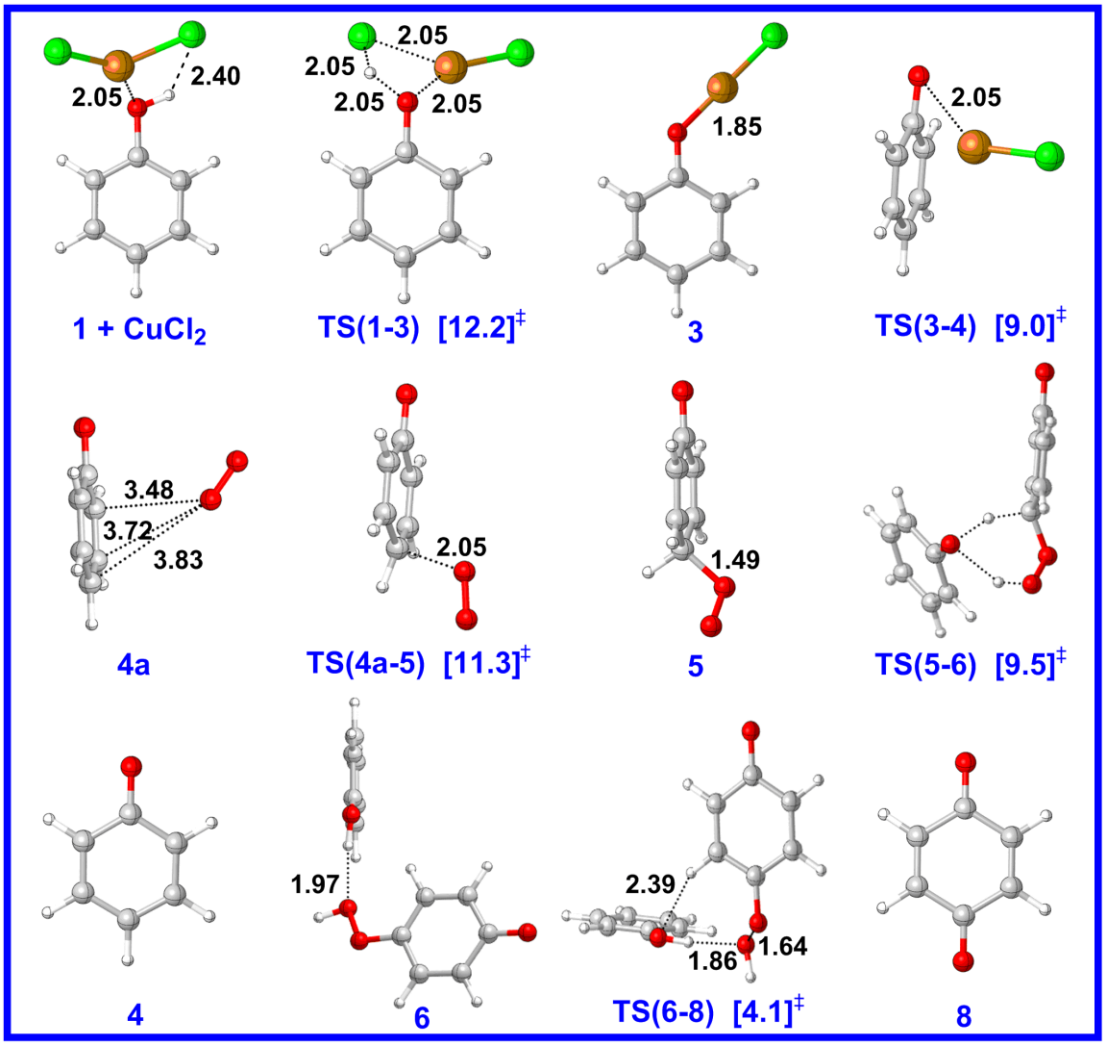


Figure S7: B3LYP/BSI optimized structures of intermediates and transition states for the formation of benzoquinone (**8**) from $CuCl_2$ and phenol (**1**). Selected distances are given in Å.

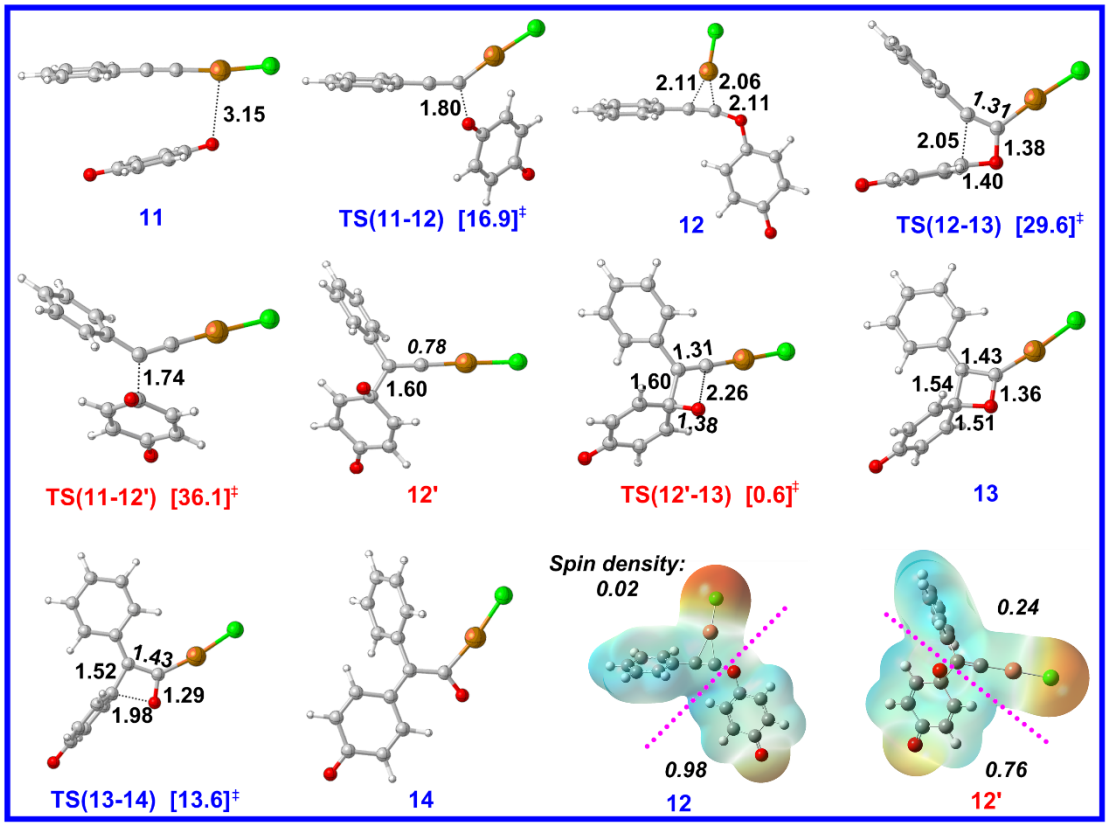


Figure S8: B3LYP/BSI optimized structures of intermediates and transition states for the formation of Cu(II)-coordinated quinone methide (**14**) from complex **11** of PhCCCu(II)Cl with benzoquinone. Selected distances are given in Å. Also shown are electrostatic potential plots of intermediates **12** and **12'** along with fragment spin densities (bottom right).

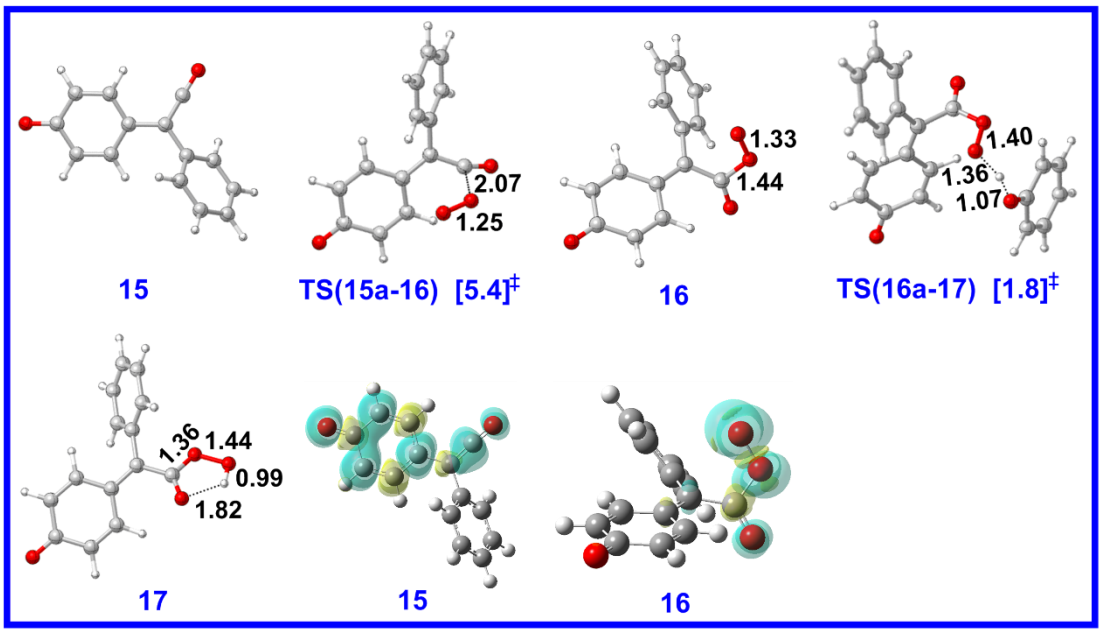


Figure S9: B3LYP/BSI optimized structures of intermediates and transition states for per-acid **17** formation from radical **15**. Selected distances are given in Å. Also shown are the spin densities of radical species **15** and **16** (bottom right).

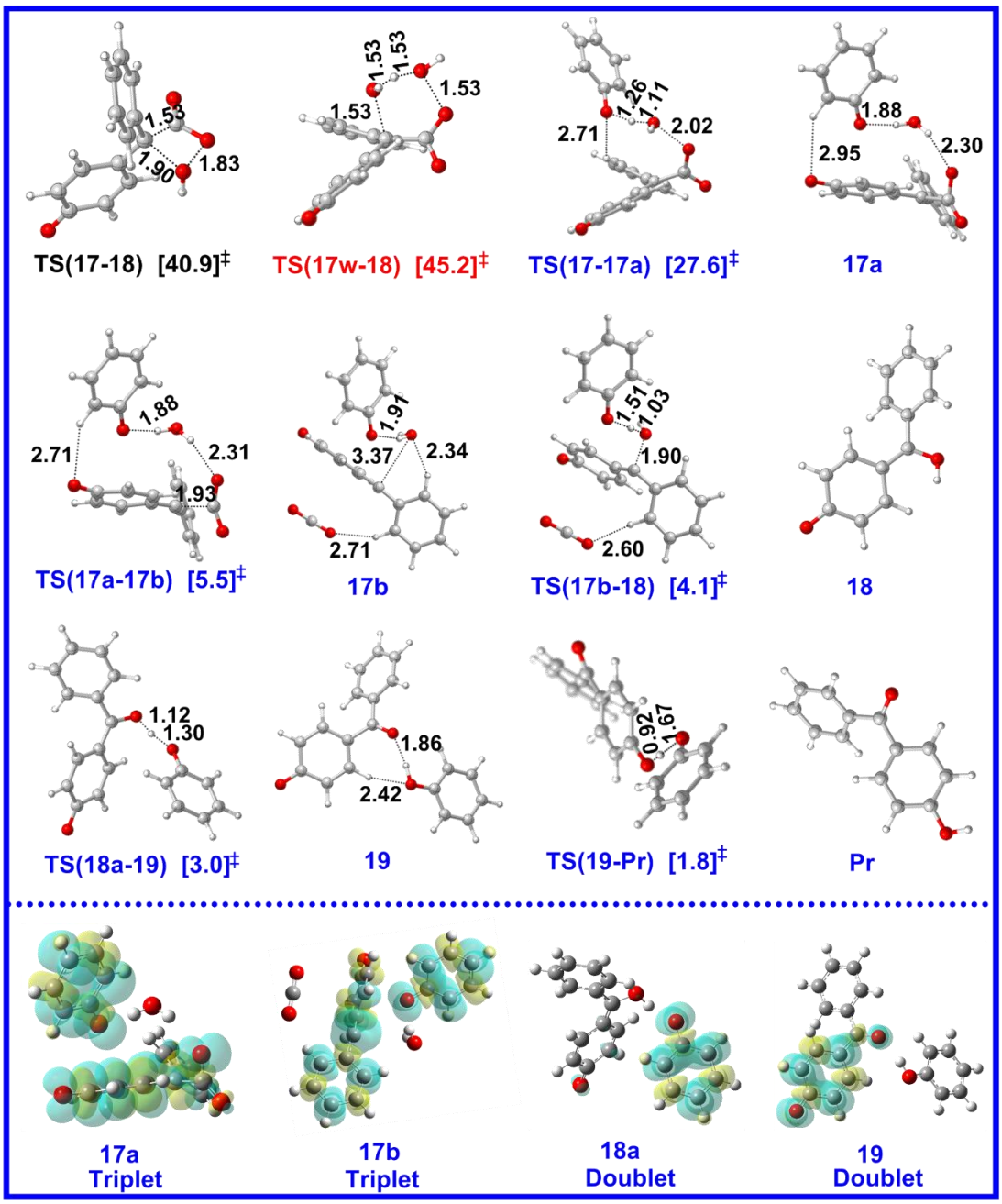


Figure S10: B3LYP/BSI optimized structures of intermediates and transition states for product formation from peracid **17**. Selected distances are given in Å. Also shown are the spin densities of radical species **17a**, **17b**, **18a**, and **19** (bottom panel).

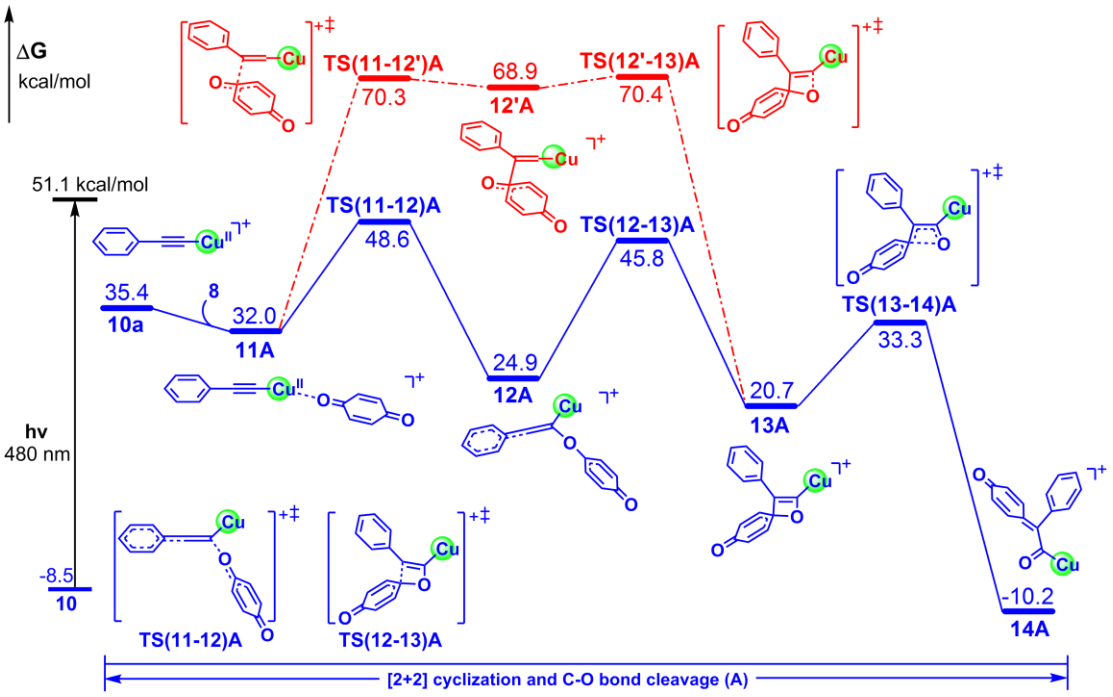


Figure S11: M06/BSII/SMD calculated energy profiles (in kcal/mol) for the [2+2] cycloaddition and the C-O bond cleavage reaction between the PhCCCu(II) cation and benzoquinone.

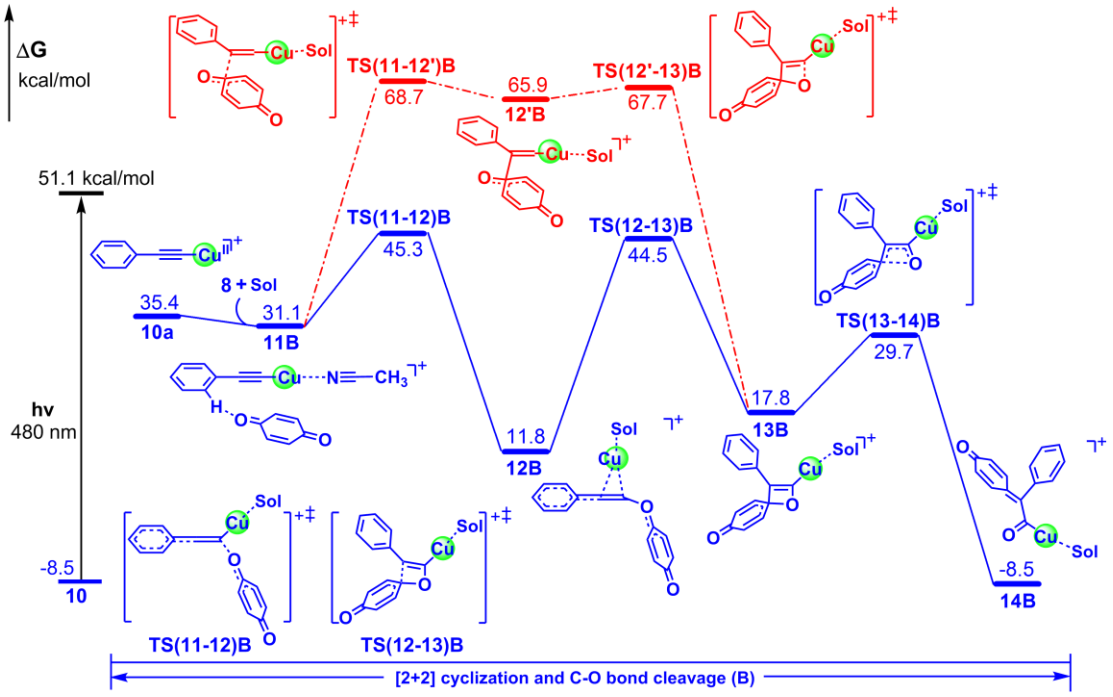


Figure S12: M06/BSII/SMD calculated energy profiles (in kcal/mol) for the [2+2] cycloaddition and the C-O bond cleavage reaction between the PhCCCu(II) cation and benzoquinone with a solvent molecule (acetonitrile) coordinated to Cu.

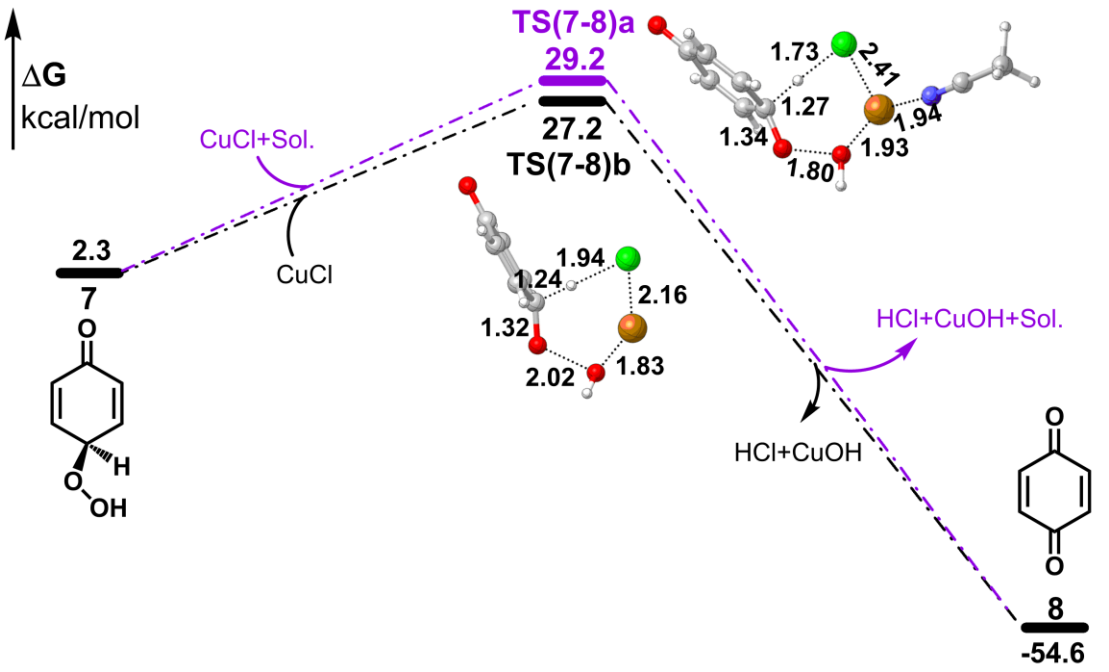


Figure S13: M06/BSII/SMD calculated energy profiles (in kcal/mol) for the formation of benzoquinone (**8**) from species **7** by CuCl with and without a solvent (acetonitrile) molecule coordinated. Selected distances are given in Å.

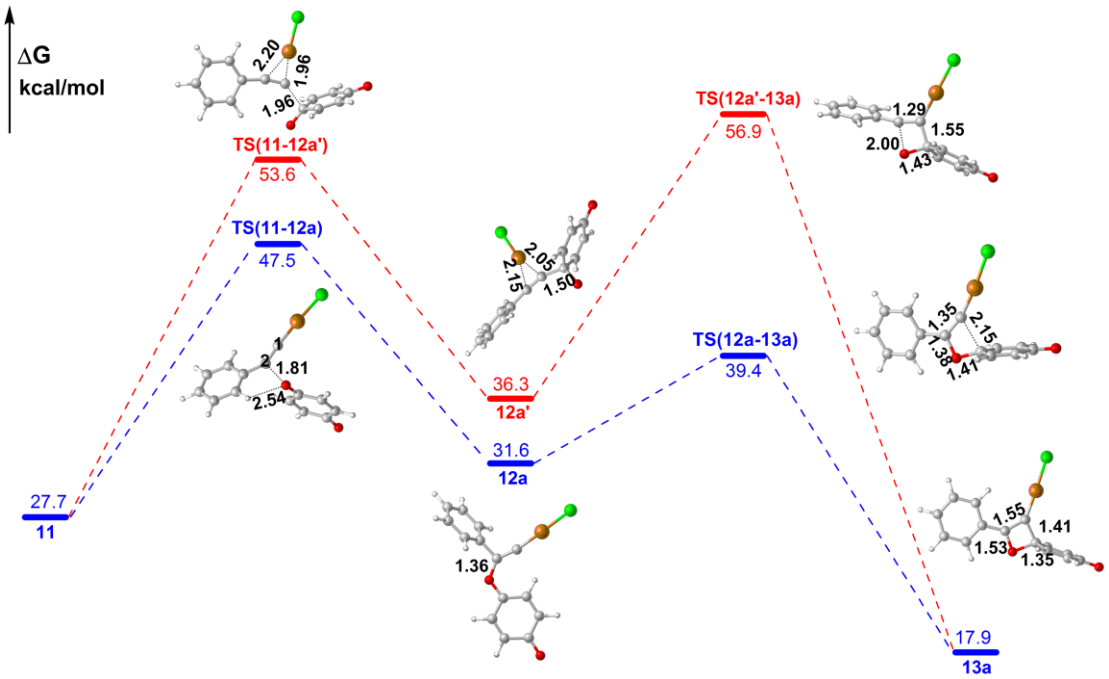


Figure S14: M06/BSII/SMD calculated energy profiles (in kcal/mol) for the [2+2] cyclization from the complex **11** of PhCCCu(II)Cl with benzoquinone. Selected distances are given in Å.

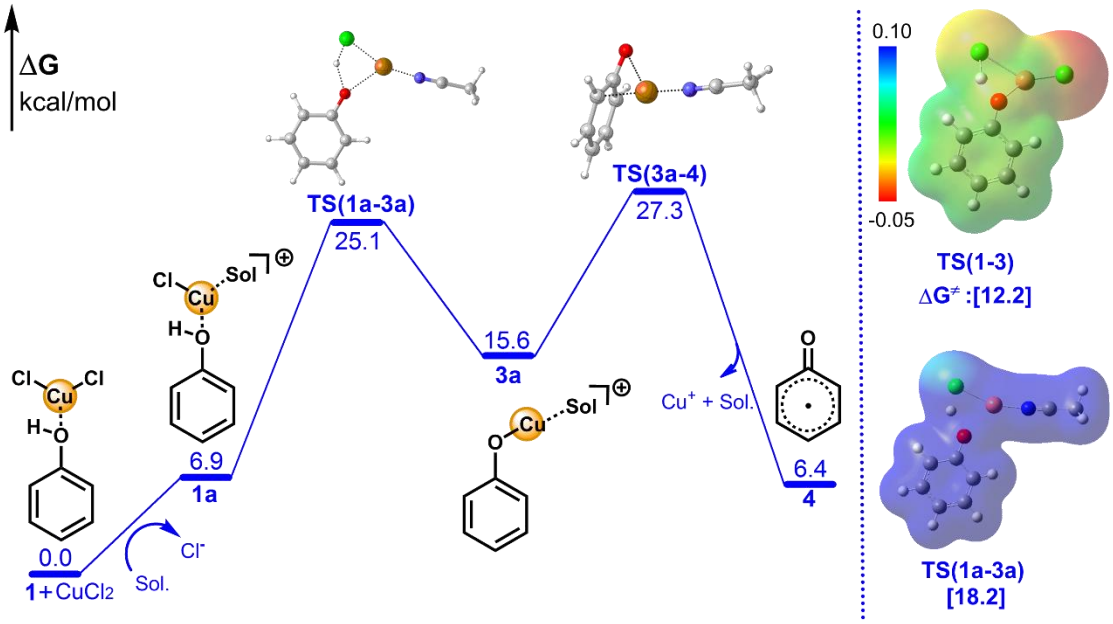


Figure S15: M06/BSII/SMD calculated energy profiles (in kcal/mol) for the formation of the phenol radical PhO· (**4**) from phenol and Cu(II)Cl_2 with a solvent molecule (acetonitrile) replacing one chloride anion coordinated to Cu(II). Also shown are the electrostatic potentials for selected transition states.

IV、References

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(2) Hiyama, M.; Akiyama, H.; Wang, Y.; Koga, N. Theoretical Study for Absorption Spectra of Oxyluciferin in Aqueous Solutions. *Chem. Phys. Lett.* **2013**, *577*, 121–126.
(3) Cheng, Y.-Y.; Zhu, J.; Liu, Y.-J. Theoretical Tuning of the Firefly Bioluminescence Spectra by the Modification of Oxyluciferin. *Chem. Phys. Lett.* **2014**, *591*, 156–160.
(4) Morokuma, K. *J. Chem. Phys.* **1971**, *55,* 1236–1244.
(5) Kitaura, K.; Morokuma, K. *Int. J. Quantum Chem.* **1976**, *10,* 325–340.
(6) Ziegler, T.; Rauk, A. *Theor. Chem. Acc.* **1977**, *46*, 1–10.

V、Cartesian Coordinates

1) CASSCF Optimized Ground- and Excited-state Structures of PhCCH-CuCl (9) and Cu(I)-phenylacetylide (10)

S0-MIN of **9**

Symbol		X	Y	Z
1	C	3.146955276	-0.685346001	1.172137126
2	C	1.882940221	-0.123275719	1.195171212
3	C	1.305526640	0.369320835	0.017126319
4	C	2.016607351	0.273414322	-1.184997113
5	C	3.288230885	-0.299474296	-1.201279521
6	C	3.854463443	-0.779002940	-0.021030081
7	H	3.583287747	-1.054472475	2.090757742
8	H	1.337854168	-0.053987668	2.126955884
9	H	1.576362525	0.646345553	-2.099421087
10	H	3.832708855	-0.369684210	-2.133025795
11	H	4.840220416	-1.223843083	-0.033066413
12	C	-0.031631729	0.965264663	0.040048007
13	C	-0.833061428	1.965824888	-0.029366390
14	H	-0.897982358	3.037404944	-0.102834443
15	Cu	-1.911652235	0.378748064	0.120893114
16	Cl	-3.547967393	-1.033471589	0.229626476

S1/T1/T2-MIN of **9**

Symbol		X	Y	Z
1	C	3.094506799	-0.672792197	1.177793798
2	C	2.051352103	0.221713657	1.242361524
3	C	1.509719270	0.783838344	0.064986999
4	C	2.079170892	0.428328369	-1.173528905
5	C	3.138410625	-0.476481779	-1.228519063
6	C	3.648975672	-1.031481205	-0.054681928
7	H	3.488799948	-1.102087098	2.089552408
8	H	1.633923690	0.502323626	2.200161460
9	H	1.687668709	0.864491699	-2.082556082
10	H	3.563038081	-0.747879565	-2.185835415
11	H	4.470200120	-1.733891098	-0.096455815
12	C	0.440036664	1.745333773	0.136748731
13	C	-0.886360139	1.837645659	0.121508537
14	H	-1.336704366	2.824260820	0.203737411
15	Cu	-1.969192270	0.181591724	-0.020604315

16	Cl	-3.170683415	-1.611149441	-0.206974309

S0-MIN of **10**

	Symbol	X	Y	Z
1	Cu	2.900209127	-0.302011055	1.462606323
2	C	-2.659906304	2.310692834	-1.285107404
3	C	-1.607222893	1.557230365	-0.807794447
4	C	-0.547032123	2.174373959	-0.098885643
5	C	-0.589131031	3.537177184	0.102878862
6	C	-1.662759384	4.301543181	-0.384765011
7	C	-2.687834940	3.702567358	-1.070470688
8	C	0.553493081	1.379144297	0.398859424
9	C	1.491229589	0.703437630	0.823263796
10	H	-3.465751760	1.831609467	-1.825527040
11	H	-1.579148558	0.488708504	-0.968834853
12	H	0.214012609	4.019627880	0.642344836
13	H	-1.673132496	5.370183466	-0.213651568
14	H	-3.514421128	4.291503588	-1.445664587

S1/T1/T2/T3-MIN of **10**

	Symbol	X	Y	Z
1	Cu	2.934387151	-0.326400512	1.478115037
2	C	-2.659906299	2.310692834	-1.285107404
3	C	-1.607222898	1.557230365	-0.807794447
4	C	-0.547032129	2.174373954	-0.098885649
5	C	-0.589131031	3.537177184	0.102878868
6	C	-1.662759378	4.301543181	-0.384765005
7	C	-2.687834935	3.702567358	-1.070470688
8	C	0.553493081	1.379144297	0.398859430
9	C	1.491229589	0.703437630	0.823263801
10	H	-3.465751760	1.831609461	-1.825527040
11	H	-1.579148553	0.488708504	-0.968834848
12	H	0.214012604	4.019627880	0.642344836
13	H	-1.673132491	5.370183466	-0.213651568
14	H	-3.514421123	4.291503588	-1.445664587

2) Formation of Benzoquinone (8)

1 + $CuCl_2$

	Symbol	X	Y	Z
1	C	-3.2300940	-1.3751310	0.1791850
2	C	-1.9863450	-1.0348450	0.7085870
3	C	-1.5039220	0.2564750	0.5004370
4	C	-2.2248530	1.2097220	-0.2181150
5	C	-3.4712200	0.8537000	-0.7326840
6	C	-3.9748450	-0.4351010	-0.5385660
7	H	-3.6188430	-2.3766150	0.3336380
8	H	-1.3973720	-1.7459910	1.2784210
9	H	-1.8171800	2.2039570	-0.3781230
10	H	-4.0447400	1.5862120	-1.2916270
11	H	-4.9430360	-0.7061950	-0.9466520
12	O	-0.2504580	0.5626740	1.0417470
13	H	-0.0577130	1.5208690	0.9759990
14	Cu	1.4312460	-0.1168080	0.0970280
15	Cl	2.4125720	-1.9508560	-0.4404820
16	Cl	1.9829630	2.0423200	-0.1779010

TS(1-3)

	Symbol	X	Y	Z
1	C	-3.0323850	-1.5730450	0.1166140
2	C	-1.7835300	-1.1602650	0.5536040
3	C	-1.4075170	0.2029270	0.4262530
4	C	-2.3171760	1.1339670	-0.1377130
5	C	-3.5644110	0.7034960	-0.5604230
6	C	-3.9282660	-0.6476610	-0.4396840
7	H	-3.3185760	-2.6157920	0.2106550
8	H	-1.0785130	-1.8563150	0.9974620
9	H	-2.0200680	2.1743090	-0.2240710
10	H	-4.2629510	1.4152160	-0.9892270
11	H	-4.9063150	-0.9760860	-0.7766790
12	O	-0.2139920	0.6000020	0.8591320
13	H	0.4105860	1.8064190	0.4100020

14	Cu	1.4136010	-0.1867660	0.1302550
15	Cl	2.6714750	-1.8441130	-0.4066540
16	Cl	1.5692930	2.3565780	-0.1833750

3

	Symbol	X	Y	Z
1	C	2.7213060	1.5574090	-0.0003850
2	C	1.4481500	1.0220470	-0.0018200
3	C	1.2670670	-0.3994020	-0.0012950
4	C	2.4256850	-1.2429160	-0.0003760
5	C	3.6898940	-0.6860460	0.0011480
6	C	3.8469770	0.7119590	0.0014170
7	H	2.8564180	2.6345120	-0.0003090
8	H	0.5655650	1.6554050	-0.0029200
9	H	2.2669340	-2.3160530	-0.0005780
10	H	4.5661050	-1.3268570	0.0023120
11	H	4.8433990	1.1426190	0.0032500
12	O	0.0979240	-0.9517350	-0.0010380
13	Cu	-1.6235920	-0.2827830	0.0001660
14	Cl	-3.5995370	0.4850970	0.0005640

TS(3-4)

	Symbol	X	Y	Z
1	C	-1.3359930	-1.1827660	1.0893850
2	C	-0.9503910	0.1579060	1.1768730
3	C	-1.2695450	1.0850540	0.0924840
4	C	-2.0177330	0.5633780	-1.0353830
5	C	-2.3911400	-0.7630440	-1.0792300
6	C	-2.0408910	-1.6458200	-0.0341590
7	H	-1.1090480	-1.8643910	1.9034600
8	H	-0.5504230	0.5756770	2.0998650
9	H	-2.2546430	1.2578230	-1.8346960
10	H	-2.9447730	-1.1432500	-1.9323330
11	H	-2.3267010	-2.6909280	-0.0938030
12	O	-0.8628960	2.2847620	0.1295950
13	Cu	0.9302060	0.1172270	0.1955770

14	Cl	2.8909960	-0.4176970	-0.4771050

4

	Symbol	X	Y	Z
1	C	-1.0880020	1.2252350	0.0000590
2	C	0.2900750	1.2395370	0.0002930
3	C	1.0473210	0.0001340	0.0000970
4	C	0.2903330	-1.2392810	0.0003460
5	C	-1.0878060	-1.2254060	-0.0000230
6	C	-1.7851390	-0.0001730	-0.0003260
7	H	-1.6459580	2.1571770	0.0001540
8	H	0.8577000	2.1645260	0.0005830
9	H	0.8583090	-2.1640400	0.0008360
10	H	-1.6454510	-2.1575250	-0.0000010
11	H	-2.8710270	-0.0002840	-0.0007450
12	O	2.3057170	-0.0000160	-0.0004380

TS(4a-5)

	Symbol	X	Y	Z
1	C	-0.5007070	-0.3400800	1.2472030
2	C	-0.5007070	1.0128230	1.2558930
3	C	-0.4866240	1.7885000	0.0000000
4	C	-0.5007070	1.0128230	-1.2558930
5	C	-0.5007070	-0.3400800	-1.2472030
6	C	-0.4189820	-1.0753390	0.0000000
7	H	-0.5230910	-0.9055950	2.1742200
8	H	-0.5276330	1.5866760	2.1767670
9	H	-0.5276330	1.5866760	-2.1767670
10	H	-0.5230910	-0.9055950	-2.1742200
11	H	-0.7417270	-2.1110560	0.0000000
12	O	-0.4747450	3.0210510	0.0000000
13	O	1.5797170	-2.8575900	0.0000000
14	O	1.4317500	-1.6138340	0.0000000

5

	Symbol	X	Y	Z
1	C	-0.3287840	-1.1365420	0.2419480

2	C	0.9868240	-1.2793790	0.0381010
3	C	1.8925360	-0.1093090	-0.0650990
4	C	1.2548960	1.2301210	0.0049970
5	C	-0.0609840	1.3779330	0.2039320
6	C	-0.9637190	0.2064100	0.4308630
7	H	-1.0009810	-1.9879520	0.3034250
8	H	1.4517690	-2.2542710	-0.0719600
9	H	1.9178440	2.0804790	-0.1210730
10	H	-0.5249170	2.3601610	0.2393220
11	H	-1.4226160	0.2658530	1.4271300
12	O	3.1001430	-0.2378500	-0.2234720
13	O	-3.1294590	-0.3910460	-0.1305140
14	O	-2.1088990	0.3539370	-0.5091770

TS(4a-5)'

	Symbol	X	Y	Z
1	C	1.9929000	0.5334210	-0.5957570
2	C	0.9321930	1.3559770	-0.3925060
3	C	-0.2161020	0.9016590	0.3949550
4	C	-0.2277510	-0.5340710	0.7881880
5	C	0.9628850	-1.3256640	0.6217440
6	C	2.0171210	-0.8160360	-0.0735260
7	H	2.8577830	0.8857850	-1.1511340
8	H	0.9094030	2.3786180	-0.7540280
9	H	-0.9299140	-0.7845110	1.5766800
10	H	0.9940110	-2.3322890	1.0263950
11	H	2.9095020	-1.4151730	-0.2282390
12	O	-1.1847590	1.6140950	0.6622400
13	O	-2.4017760	-0.4337330	-0.6837720
14	O	-1.3519970	-1.1083810	-0.5945010

5'

	Symbol	X	Y	Z
1	C	-2.1768570	-0.0135130	0.2816840
2	C	-1.4579960	1.1264230	0.1731150
3	C	-0.0274630	1.0911840	-0.1629610

4	C	0.5117420	-0.2714190	-0.6704450
5	C	-0.3198960	-1.4723260	-0.3374810
6	C	-1.5958240	-1.3337790	0.0544440
7	H	-3.2183710	0.0353140	0.5891440
8	H	-1.8725390	2.0991340	0.4167470
9	H	0.5695390	-0.1757380	-1.7664460
10	H	0.1391200	-2.4458150	-0.4819890
11	H	-2.2144210	-2.2072040	0.2358770
12	O	0.7014730	2.0635930	-0.1000950
13	O	2.0186440	-0.6152820	1.0171420
14	O	1.9041880	-0.4564490	-0.2949800

TS(4a-5)"

	Symbol	X	Y	Z
1	C	0.3282910	1.8001500	0.1451700
2	C	1.4260910	0.9766020	0.4236020
3	C	1.4852060	-0.4231450	-0.0203880
4	C	0.3163130	-0.9031490	-0.7457740
5	C	-0.8923380	-0.0928680	-0.9065150
6	C	-0.7840430	1.3328360	-0.5242080
7	H	0.3573680	2.8402710	0.4593750
8	H	2.2861220	1.3495720	0.9698970
9	H	0.3289040	-1.9273210	-1.1041620
10	H	-1.3990680	-0.2546700	-1.8617890
11	H	-1.6315440	1.9789960	-0.7254240
12	O	2.4678580	-1.1445730	0.1907800
13	O	-1.8243570	-0.6152320	1.2893010
14	O	-2.0458630	-0.7563710	0.0237670

5"

	Symbol	X	Y	Z
1	C	0.5859800	1.8089610	0.1133390
2	C	1.6501940	0.9021030	0.2600500
3	C	1.5986220	-0.5398390	-0.0061680
4	C	0.2444080	-0.9809200	-0.2353260
5	C	-0.8331660	-0.0389200	-0.5547180

6	C	-0.6754720	1.3889140	-0.2277320
7	H	0.7683940	2.8639350	0.2988100
8	H	2.6088570	1.2712670	0.6167610
9	H	0.0246750	-2.0436450	-0.2661520
10	H	-0.7371970	0.0103780	-1.6702750
11	H	-1.5155830	2.0555220	-0.3797470
12	O	2.5764930	-1.2928430	0.1016680
13	O	-2.4749630	-0.5724950	0.9280000
14	O	-2.1730980	-0.5595670	-0.3666770

TS(5-7)

	Symbol	X	Y	Z
1	C	2.6881630	1.2884630	-0.2120000
2	C	3.8739140	0.6713020	-0.1332710
3	C	3.9850560	-0.8067600	-0.1134660
4	C	2.7087380	-1.5659270	-0.1116490
5	C	1.5199220	-0.9542650	-0.1836000
6	C	1.3966390	0.5320430	-0.3428190
7	H	2.5970430	2.3707810	-0.2067700
8	H	4.8081420	1.2207130	-0.0665910
9	H	2.7984930	-2.6457220	-0.0410450
10	H	0.5867440	-1.5111400	-0.1638470
11	H	0.9502160	0.7566130	-1.3241390
12	O	5.0696160	-1.3761850	-0.0761560
13	O	-0.0184230	2.2506420	0.2700200
14	O	0.4332530	0.9874990	0.6448130
15	C	-4.0982670	-1.0502120	-0.9689600
16	C	-3.6240600	0.2489690	-0.9915110
17	C	-2.7351850	0.7070890	0.0225650
18	C	-2.3375670	-0.1998460	1.0491530
19	C	-2.8105520	-1.5049380	1.0425670
20	C	-3.6907630	-1.9373940	0.0423980
21	H	-4.7837380	-1.3897670	-1.7397230
22	H	-3.9148420	0.9532950	-1.7636580
23	H	-1.6715630	0.1526200	1.8276800

24	H	-2.5070070	-2.1906050	1.8281150
25	H	-4.0628420	-2.9571450	0.0505730
26	O	-2.3376330	1.9553190	-0.0010030
27	H	-1.2313800	2.1310020	0.3015560

7

	Symbol	X	Y	Z
1	C	-0.2888920	-1.1237650	0.1950120
2	C	1.0294570	-1.2813790	0.0190760
3	C	1.9508450	-0.1232940	-0.0519260
4	C	1.3255900	1.2222720	0.0050070
5	C	0.0075670	1.3854010	0.1741460
6	C	-0.9231340	0.2259170	0.3884790
7	H	-0.9665090	-1.9718480	0.2293080
8	H	1.4852960	-2.2603670	-0.0950790
9	H	2.0007130	2.0654300	-0.1058790
10	H	-0.4465460	2.3726870	0.1964720
11	H	-1.3147780	0.2811230	1.4197800
12	O	3.1625770	-0.2620680	-0.1744960
13	O	-3.0828190	-0.4837370	-0.0970880
14	O	-2.0312130	0.4369620	-0.5059970
15	H	-3.7551410	0.1528140	0.1972800

TS(5-6)"

	Symbol	X	Y	Z
1	C	-0.2299770	-1.2639200	-0.1306070
2	C	1.1142190	-1.2614480	-0.0337350
3	C	1.8843030	-0.0000080	0.0551290
4	C	1.1142390	1.2614490	-0.0337250
5	C	-0.2299580	1.2639420	-0.1305770
6	C	-0.9840030	0.0000180	-0.0592500
7	H	-0.8118730	-2.1754370	-0.2253570
8	H	1.6947680	-2.1783930	-0.0513270
9	H	1.6947960	2.1783880	-0.0513100
10	H	-0.8118460	2.1754690	-0.2253080
11	H	-1.5222090	-0.0000020	1.0718370

12	O	3.1081400	-0.0000200	0.1712930
13	O	-2.8896390	-0.0000390	0.6767030
14	O	-2.2505730	0.0000320	-0.6632390

TS(5-6)'

	Symbol	X	Y	Z
1	C	-0.0223640	-0.9557710	-0.6012080
2	C	1.2969300	-1.1949440	-0.4298640
3	C	2.2253300	-0.1514410	0.0451680
4	C	1.6435640	1.1897270	0.2487580
5	C	0.3232620	1.4301290	0.0720790
6	C	-0.5905480	0.3346290	-0.2070590
7	H	-0.7129320	-1.7073150	-0.9703090
8	H	1.7346840	-2.1578150	-0.6732600
9	H	2.3338760	1.9780300	0.5310700
10	H	-0.0998730	2.4238210	0.1936330
11	H	-1.1477480	-0.1031050	0.9831930
12	O	3.4235260	-0.3753810	0.2309840
13	O	-2.7866690	-0.1947300	-0.7207730
14	O	-1.7890350	0.7480720	-0.8068900
15	O	-2.1219410	-0.6460220	1.5910090
16	H	-2.6262280	-0.6157030	0.6495110
17	H	-2.5458740	0.0126000	2.1642760

TS(5-6)

Symbol		X	Y	Z
1	C	2.4032880	1.0507790	-0.5080060
2	C	3.3381090	0.0891240	-0.6555530
3	C	3.2502710	-1.1956150	0.0656410
4	C	2.1210180	-1.3463420	1.0070790
5	C	1.1848600	-0.3830330	1.1537240
6	C	1.1901520	0.8009270	0.2895820
7	H	2.4660020	2.0086610	-1.0128210
8	H	4.2135010	0.2310570	-1.2815920
9	H	2.0963840	-2.2631690	1.5875380
10	H	0.3652070	-0.4773670	1.8602410

11	H	0.3320930	0.5126990	-0.5911470
12	O	4.0847130	-2.0895950	-0.0864500
13	O	0.2960900	2.9130410	-0.0668860
14	O	0.5780780	1.8955810	0.9297520
15	O	-0.8188160	0.6823960	-1.2925940
16	H	-0.3365720	2.4193330	-0.6400830
17	C	-1.8458160	0.0839530	-0.7103050
18	C	-2.1171610	-1.2842410	-0.9765810
19	C	-2.6987770	0.7981080	0.1727020
20	C	-3.2196270	-1.8991390	-0.4030810
21	H	-1.4514180	-1.8177740	-1.6471920
22	C	-3.7975180	0.1683470	0.7390640
23	H	-2.4697690	1.8369640	0.3879920
24	C	-4.0636230	-1.1784070	0.4548790
25	H	-3.4309060	-2.9423070	-0.6179900
26	H	-4.4517000	0.7197040	1.4075730
27	H	-4.9243940	-1.6659490	0.9020270

6

	Symbol	X	Y	Z
1	C	3.6657990	1.1413300	0.1107090
2	C	4.4661690	0.0357220	0.2453640
3	C	3.9117320	-1.3085210	0.2133150
4	C	2.4756430	-1.4135910	0.0199180
5	C	1.6755230	-0.3031460	-0.1294050
6	C	2.2739440	0.9711250	-0.0827040
7	H	4.0677480	2.1485660	0.1496620
8	H	5.5363460	0.1284600	0.3971470
9	H	2.0543550	-2.4127080	-0.0149150
10	H	0.6112330	-0.4045530	-0.2977770
11	H	-0.1004720	2.8934790	-0.1674920
12	O	4.6367060	-2.3242570	0.3459430
13	O	0.1752480	1.9730400	-0.0182410
14	O	1.6046660	2.1476510	-0.2665830
15	C	-3.9671320	0.2568550	1.4601600

16	C	-2.8299210	0.4968680	0.6874900
17	C	-2.7240230	-0.0720360	-0.5873770
18	C	-3.7525190	-0.8848780	-1.0772800
19	C	-4.8799120	-1.1191470	-0.2939820
20	C	-4.9973890	-0.5497920	0.9769760
21	H	-4.0408060	0.7014320	2.4486810
22	H	-2.0199330	1.1088360	1.0768870
23	H	-3.6499330	-1.3173100	-2.0670880
24	H	-5.6743700	-1.7506790	-0.6813730
25	H	-5.8789620	-0.7349260	1.5823220
26	O	-1.6375550	0.1224740	-1.3964750
27	H	-1.0452090	0.7834080	-1.0022980

TS(6-8)

	Symbol	X	Y	Z
1	C	3.5362800	0.9447620	0.4526390
2	C	4.1946470	-0.2472750	0.5281280
3	C	3.5651360	-1.4895320	0.0686990
4	C	2.2084470	-1.3835970	-0.4827930
5	C	1.5694450	-0.1850010	-0.5830490
6	C	2.2315990	1.0042880	-0.1336580
7	H	3.9754270	1.8733560	0.8023010
8	H	5.1912410	-0.3290760	0.9492960
9	H	1.7480150	-2.3058130	-0.8217780
10	H	0.5706090	-0.1000100	-0.9991540
11	H	0.0768960	3.2061620	0.1787290
12	O	4.1516830	-2.5810900	0.1467070
13	O	0.2195160	2.2669280	0.3923470
14	O	1.7080310	2.2028270	-0.2909370
15	C	-3.6901130	-0.2861760	1.5839200
16	C	-2.6610480	0.3521850	0.8906090
17	C	-2.5907360	0.2416980	-0.5040920
18	C	-3.5487240	-0.5115220	-1.1934060
19	C	-4.5690390	-1.1450230	-0.4880970
20	C	-4.6485390	-1.0374520	0.9030310

21	H	-3.7373560	-0.1949710	2.6655680
22	H	-1.9104090	0.9299360	1.4236110
23	H	-3.4771730	-0.5845370	-2.2737770
24	H	-5.3089370	-1.7266950	-1.0308530
25	H	-5.4464490	-1.5323950	1.4475500
26	O	-1.6084360	0.8421540	-1.2402910
27	H	-1.0323430	1.3733600	-0.6556940

TS(7-8)'

	Symbol	X	Y	Z
1	C	-0.2120960	1.2731950	-0.3619400
2	C	-1.5312600	1.2563780	-0.0807790
3	C	-2.2835550	-0.0061670	0.0823880
4	C	-1.5213800	-1.2505090	-0.1504970
5	C	-0.2010810	-1.2431950	-0.4258890
6	C	0.5686220	0.0205470	-0.4367380
7	H	0.3347080	2.2001950	-0.5170210
8	H	-2.1084270	2.1724380	0.0024630
9	H	-2.0888200	-2.1754450	-0.1137860
10	H	0.3548960	-2.1583850	-0.6126840
11	H	0.9950760	-0.0606150	0.8117480
12	O	-3.4800060	-0.0178890	0.3726570
13	O	3.1422470	0.1193980	-0.2464020
14	O	1.6866230	0.0436990	-1.1863030
15	H	3.5306430	-0.6631130	-0.6682210
16	O	1.8532850	-0.1681300	1.8020020
17	H	1.8328420	0.6612310	2.3047570
18	H	2.6163930	-0.0944300	1.0978440

TS(7-8)"

	Symbol	X	Y	Z
1	C	0.1557400	-1.2566580	0.2175710
2	C	-1.1799550	-1.2583720	0.0387950
3	C	-1.9547640	-0.0053080	-0.1005260
4	C	-1.1909790	1.2543170	0.0282750
5	C	0.1450090	1.2652820	0.2089000

6	C	0.9133600	0.0085860	0.2106040
7	H	0.7229540	-2.1749340	0.3472980
8	H	-1.7516800	-2.1809740	0.0150410
9	H	-1.7699290	2.1719820	-0.0063970
10	H	0.7080190	2.1871100	0.3261270
11	H	1.5986160	0.0056580	-0.9158300
12	O	-3.1699780	-0.0132780	-0.2914440
13	O	2.9886180	0.0907350	-0.7855100
14	O	2.1489580	0.0135680	0.7604680
15	H	3.4207690	-0.7841280	-0.8560650

TS(7-8)

	Symbol	X	Y	Z
1	C	-1.3598550	0.0584040	1.3299560
2	C	-2.0050940	-1.1226100	1.2656900
3	C	-2.9065950	-1.4672340	0.1449850
4	C	-3.1195320	-0.4133740	-0.8712270
5	C	-2.4791040	0.7701030	-0.8210320
6	C	-1.4663720	1.0499220	0.2305590
7	H	-0.7153390	0.3235300	2.1636070
8	H	-1.9155260	-1.8643970	2.0535490
9	H	-3.8453420	-0.6356650	-1.6476530
10	H	-2.6479520	1.5525050	-1.5562860
11	H	-0.4298950	0.7210160	-0.4490030
12	O	-3.4657710	-2.5607030	0.0727050
13	O	0.2967950	2.9746590	0.0202820
14	O	-1.2826640	2.3367610	0.5562570
15	H	-0.1066420	3.6955420	-0.4880710
16	C	2.9672710	-1.9733410	-0.5299830
17	C	1.9233330	-1.1883590	-1.0159590
18	C	1.8091980	0.1338790	-0.5845300
19	C	2.7193010	0.6802020	0.3242700
20	C	3.7617470	-0.1173440	0.7969050
21	C	3.8892770	-1.4420080	0.3751450
22	H	3.0605520	-3.0027970	-0.8619720

23	H	1.1997020	-1.5817410	-1.7221770
24	H	2.6087470	1.7100250	0.6483940
25	H	4.4753700	0.3017700	1.4998550
26	H	4.7027380	-2.0562820	0.7479280
27	O	0.7602920	0.8912030	-1.0900990
28	H	0.7429210	1.8917010	-0.7300020

8

	Symbol	X	Y	Z
1	C	0.6715120	1.2693930	0.0009110
2	C	-0.6712680	1.2693840	0.0007520
3	C	-1.4448330	0.0001200	0.0000380
4	C	-0.6715300	-1.2694330	0.0007620
5	C	0.6712390	-1.2693290	0.0009380
6	C	1.4447250	-0.0000500	0.0000390
7	H	1.2592810	2.1825070	0.0012070
8	H	-1.2590600	2.1825160	0.0008620
9	H	-1.2593990	-2.1825130	0.0008060
10	H	1.2590590	-2.1824660	0.0011370
11	O	-2.6696670	0.0000670	-0.0014890
12	O	2.6697980	-0.0001360	-0.0015920

3) Formation of Cu(I)-phenylacetylide (10)

9

	Symbol	X	Y	Z
1	C	-3.1106620	-0.6824280	-1.1820930
2	C	-1.9401150	0.0679260	-1.2299930
3	C	-1.3847070	0.5741740	-0.0383770
4	C	-2.0135560	0.3138630	1.1951020
5	C	-3.1839960	-0.4375500	1.2283710
6	C	-3.7327220	-0.9360980	0.0435330
7	H	-3.5367630	-1.0727670	-2.1008780
8	H	-1.4477260	0.2670330	-2.1760810
9	H	-1.5776240	0.7016840	2.1098260
10	H	-3.6670930	-0.6380950	2.1794480
11	H	-4.6442110	-1.5252490	0.0756800

12	C	-0.1910810	1.3634520	-0.0808910
13	C	0.8005110	2.0970490	-0.1166120
14	H	1.3894500	2.9907440	-0.1698280
15	Cu	1.7054590	0.2753220	-0.0090900
16	Cl	3.0919770	-1.3452950	0.0841880

9*

	Symbol	X	Y	Z
1	C	3.7490170	-0.5460180	-1.1410230
2	C	2.4931180	-0.9556370	-0.7436270
3	C	1.8010800	-0.2665240	0.3206590
4	C	2.4748440	0.8503970	0.9412030
5	C	3.7284730	1.2352660	0.5136960
6	C	4.3845870	0.5488550	-0.5257190
7	H	4.2531260	-1.0789380	-1.9424960
8	H	2.0075630	-1.8014860	-1.2185680
9	H	1.9747750	1.3783720	1.7460030
10	H	4.2163680	2.0806450	0.9908920
11	H	5.3721080	0.8603300	-0.8488580
12	C	0.5624220	-0.6591360	0.7293790
13	C	-0.6460890	-0.9989940	1.0639360
14	H	-0.7874350	-1.7006630	1.8954980
15	Cu	-2.1954510	-0.3663140	0.0789820
16	Cl	-3.8031260	0.9197420	-0.5802330

TS9

	Symbol	X	Y	Z
1	C	-3.8899300	0.1201690	-1.2107590
2	C	-2.5071970	-0.0362910	-1.2158150
3	C	-1.7963540	-0.1174500	-0.0000170
4	C	-2.5072410	-0.0370640	1.2157990
5	C	-3.8899690	0.1193950	1.2107920
6	C	-4.5839550	0.1979910	0.0000310
7	H	-4.4287390	0.1823720	-2.1515830
8	H	-1.9599850	-0.0966760	-2.1508780
9	H	-1.9600660	-0.0980330	2.1508410

10	H	-4.4288150	0.1809960	2.1516320
11	H	-5.6631570	0.3204600	0.0000510
12	C	-0.3825640	-0.2776560	-0.0000450
13	C	0.8477300	-0.3794490	-0.0000570
14	H	1.7236750	0.8334060	0.0001980
15	Cu	2.6935370	-0.9428410	-0.0002150
16	Cl	2.9918480	1.6754120	0.0003780

TS9a

	Symbol	X	Y	Z
1	Cu	-1.7115160	-0.2178200	0.0005000
2	Cl	-1.5468120	2.6276290	0.0002010
3	C	4.8892430	-0.4765960	1.2103660
4	C	3.5124970	-0.2740590	1.2155660
5	C	2.8039770	-0.1696770	0.0000200
6	C	3.5122410	-0.2727030	-1.2157920
7	C	4.8889900	-0.4752200	-1.2111100
8	C	5.5801210	-0.5778620	-0.0005020
9	H	5.4262350	-0.5543580	2.1511500
10	H	2.9678510	-0.1913970	2.1504150
11	H	2.9673950	-0.1889980	-2.1504330
12	H	5.4257870	-0.5519070	-2.1520950
13	H	6.6548780	-0.7351280	-0.0007040
14	C	1.3979220	0.0406160	0.0002650
15	C	0.1791530	0.2366110	0.0004290
16	H	-0.4562150	1.3993960	0.0003920
17	C	-4.6209110	-1.1118700	-0.0003770
18	C	-6.0419250	-1.4268530	-0.0012650
19	H	-6.2771930	-2.0862900	-0.8412720
20	H	-6.3128980	-1.9263300	0.9330480
21	H	-6.6225200	-0.5048150	-0.0957200
22	N	-3.4930560	-0.8524860	0.0002420

TS9b

	Symbol	X	Y	Z
1	Cu	2.2984270	-0.9434790	-0.0145080

2	Cl	2.2955540	2.0716220	-0.0186440
3	C	-4.2592550	0.0141380	-1.2015520
4	C	-2.8726270	-0.1015760	-1.2116490
5	C	-2.1539010	-0.1449440	0.0016700
6	C	-2.8611790	-0.0692290	1.2201180
7	C	-4.2478170	0.0465360	1.2201810
8	C	-4.9492960	0.0879890	0.0118220
9	H	-4.8043390	0.0478840	-2.1402040
10	H	-2.3278030	-0.1579700	-2.1483180
11	H	-2.3074910	-0.1007960	2.1527750
12	H	-4.7840110	0.1055240	2.1627130
13	H	-6.0316620	0.1786640	0.0157240
14	C	-0.7368610	-0.2617400	-0.0034780
15	C	0.4974170	-0.3238130	-0.0082340
16	H	1.2486420	0.8990770	-0.0134150
17	O	4.2465870	-0.5123040	-0.0228940
18	H	4.7401980	-0.6755990	0.7925790
19	H	4.1160720	0.4608020	-0.0743060

TS9*

	Symbol	X	Y	Z
1	C	-3.6079880	-0.2483500	1.2144730
2	C	-2.2220920	-0.2999150	1.2246640
3	C	-1.4985400	-0.3275500	0.0003520
4	C	-2.2221140	-0.3043360	-1.2240610
5	C	-3.6080280	-0.2528590	-1.2140150
6	C	-4.3075520	-0.2255690	0.0001980
7	H	-4.1521700	-0.2263080	2.1538370
8	H	-1.6730090	-0.3222020	2.1601370
9	H	-1.6730630	-0.3300910	-2.1594680
10	H	-4.1522420	-0.2344710	-2.1534430
11	H	-5.3925800	-0.1874680	0.0001400
12	C	-0.1013970	-0.3853900	0.0004240
13	C	1.1469830	-0.2391150	0.0001750
14	H	2.2502560	-0.9818730	0.0003130

15	Cu	1.8054740	1.6537270	-0.0010560
16	Cl	3.5857900	-1.8810090	0.0009320

TS9a*

	Symbol	X	Y	Z
1	Cu	-1.8049800	-0.3419560	-0.0003500
2	Cl	-0.6566090	3.0357480	0.0012160
3	C	4.7136780	-0.6406720	1.2311230
4	C	3.3655980	-0.4238110	1.2548770
5	C	2.6044950	-0.2955030	-0.0001270
6	C	3.3661810	-0.4204440	-1.2551110
7	C	4.7142440	-0.6373950	-1.2313080
8	C	5.4222340	-0.7528760	-0.0000800
9	H	5.2596130	-0.7290210	2.1667000
10	H	2.8226030	-0.3343180	2.1896380
11	H	2.8236220	-0.3284530	-2.1898820
12	H	5.2606140	-0.7232630	-2.1668620
13	H	6.4934740	-0.9229870	-0.0000590
14	C	1.2759240	-0.0719820	-0.0001270
15	C	0.0080130	0.1267750	-0.0002230
16	H	-0.3620560	1.6274520	0.0004920
17	C	-4.8011610	-0.9269220	-0.0002230
18	C	-6.2291910	-1.2074920	-0.0004120
19	H	-6.4169550	-2.1880600	-0.4472880
20	H	-6.6072310	-1.2032720	1.0257940
21	H	-6.7568810	-0.4434390	-0.5782850
22	N	-3.6643030	-0.7062400	-0.0001590

TS9b*

	Symbol	X	Y	Z
1	Cu	-2.2123760	-0.9611040	0.0388610
2	Cl	-2.5162210	2.2506750	-0.1342580
3	C	4.2545200	0.2014680	1.2326100
4	C	2.8932530	0.0962650	1.2509820
5	C	2.1417950	-0.1261800	0.0040880
6	C	2.9276250	-0.2402580	-1.2361400

7	C	4.2881860	-0.1282020	-1.2093470
8	C	4.9857930	0.0947960	0.0136660
9	H	4.7936490	0.3680690	2.1613030
10	H	2.3313240	0.1760170	2.1754290
11	H	2.3914460	-0.4113610	-2.1634520
12	H	4.8529710	-0.2117740	-2.1339490
13	H	6.0669440	0.1815780	0.0168700
14	C	0.7937190	-0.2088740	-0.0029480
15	C	-0.4818680	-0.2847040	-0.0071730
16	H	-1.5648090	1.2710840	-0.0934580
17	O	-4.2113600	-0.8847880	0.0212610
18	H	-4.6570340	-1.1731200	0.8304900
19	H	-4.4070790	0.0624920	-0.0823500

10

	Symbol	X	Y	Z
1	C	3.2615110	-1.2075480	0.0000010
2	C	1.8689530	-1.2120090	0.0000000
3	C	1.1485050	-0.0002010	-0.0000020
4	C	1.8685370	1.2118550	0.0000000
5	C	3.2610970	1.2078810	0.0000010
6	C	3.9638060	0.0002890	-0.0000010
7	H	3.8014120	-2.1504150	0.0000000
8	H	1.3210310	-2.1489070	0.0000010
9	H	1.3202910	2.1485650	-0.0000010
10	H	3.8006700	2.1509360	0.0000020
11	H	5.0500180	0.0004760	-0.0000010
12	C	-0.2793640	-0.0004530	0.0000010
13	C	-1.5049970	-0.0003830	0.0000010
14	Cu	-3.3386800	0.0000950	0.0000000

10*

	Symbol	X	Y	Z
1	C	3.3138890	1.2208040	0.0000000
2	C	1.9308470	1.2291960	0.0000000
3	C	1.2040310	-0.0000020	0.0000000

4	C	1.9308510	-1.2291980	0.0000000
5	C	3.3138940	-1.2208010	0.0000000
6	C	4.0079160	0.0000030	0.0000000
7	H	3.8646310	2.1556260	0.0000000
8	H	1.3732140	2.1589370	0.0000000
9	H	1.3732210	-2.1589390	0.0000000
10	H	3.8646390	-2.1556220	0.0000000
11	H	5.0935150	0.0000050	0.0000000
12	C	-0.1879600	-0.0000030	0.0000000
13	C	-1.4481290	-0.0000070	-0.0000010
14	Cu	-3.4469400	0.0000010	0.0000000

4) Cycloaddition of Benzoquinone and PhCCCu(II)

11

	Symbol	X	Y	Z
1	C	-3.7146530	-2.0759150	1.2022830
2	C	-2.3380070	-1.9021420	1.1993240
3	C	-1.6487360	-1.6755100	-0.0226150
4	C	-2.3882460	-1.6369500	-1.2343510
5	C	-3.7646670	-1.8119270	-1.2168140
6	C	-4.4304420	-2.0289490	-0.0017040
7	H	-4.2388210	-2.2450590	2.1385760
8	H	-1.7688270	-1.9334400	2.1222570
9	H	-1.8570900	-1.4662420	-2.1656530
10	H	-4.3271110	-1.7771400	-2.1444340
11	H	-5.5089350	-2.1596640	0.0070510
12	C	-0.2585940	-1.4699530	-0.0316900
13	C	0.9683600	-1.2458870	-0.0386370
14	Cu	2.7984420	-0.8926530	-0.0342030
15	Cl	4.9239110	-0.7025550	-0.0479320
16	C	0.0175820	2.3693820	-1.1686130
17	C	-1.3197330	2.4526930	-1.2618300
18	C	-2.1824690	2.4219800	-0.0526630
19	C	-1.5041040	2.3348120	1.2668880

20	C	-0.1668120	2.2529410	1.3615610
21	C	0.6921050	2.2398880	0.1494510
22	H	0.6698420	2.3817530	-2.0367510
23	H	-1.8383130	2.5390870	-2.2125410
24	H	-2.1554880	2.3345380	2.1358600
25	H	0.3531890	2.1801920	2.3125620
26	O	1.9096340	2.1186260	0.2338230
27	O	-3.4045410	2.4600700	-0.1405390

TS(11-12)

	Symbol	X	Y	Z
1	C	4.5023990	-1.5431300	1.4145250
2	C	3.2281850	-1.0247460	1.2412750
3	C	2.8999380	-0.3192480	0.0502230
4	C	3.8991400	-0.1507200	-0.9488050
5	C	5.1691230	-0.6731470	-0.7577360
6	C	5.4738740	-1.3697820	0.4194340
7	H	4.7485750	-2.0806540	2.3248950
8	H	2.4682450	-1.1445010	2.0061920
9	H	3.6475310	0.3917510	-1.8538460
10	H	5.9286280	-0.5412390	-1.5219530
11	H	6.4707980	-1.7755700	0.5630420
12	C	1.6211410	0.2011710	-0.1385550
13	C	0.4737870	0.7259690	-0.2967960
14	Cu	-0.5102670	2.3248750	-0.0535660
15	Cl	-1.7897410	4.0164200	0.2593630
16	C	-1.5984830	-2.5691520	-1.0032700
17	C	-2.6880470	-3.2436830	-0.5763340
18	C	-3.6871340	-2.6022480	0.3060880
19	C	-3.4361720	-1.1932790	0.6853010
20	C	-2.3510890	-0.5183290	0.2449850
21	C	-1.4009040	-1.1689050	-0.6453660
22	H	-0.8471560	-3.0164910	-1.6461900
23	H	-2.8740680	-4.2780390	-0.8477390
24	H	-4.1738320	-0.7299370	1.3329810

25	H	-2.1728250	0.5157960	0.5216980
26	O	-0.4034280	-0.5795090	-1.1769570
27	O	-4.6724600	-3.2137730	0.7138750

12

	Symbol	X	Y	Z
1	C	3.4148450	2.5893710	-1.1185480
2	C	2.5058190	1.5381530	-1.0450490
3	C	1.7290410	1.3608110	0.1163860
4	C	1.8833330	2.2481750	1.2002450
5	C	2.7931980	3.2973790	1.1131010
6	C	3.5594680	3.4693280	-0.0430040
7	H	4.0134810	2.7199320	-2.0142810
8	H	2.3915760	0.8483700	-1.8750730
9	H	1.2888130	2.1044170	2.0963070
10	H	2.9075420	3.9799640	1.9494550
11	H	4.2715860	4.2866900	-0.1037860
12	C	0.7702400	0.2929270	0.2035380
13	C	-0.1292270	-0.5297260	0.4299580
14	Cu	1.5410760	-1.6671620	0.0268450
15	Cl	2.8417020	-3.3175600	-0.3211080
16	C	-3.6475110	-1.1702510	0.5888440
17	C	-4.8698900	-0.6197140	0.2891800
18	C	-4.9748530	0.6907310	-0.3335120
19	C	-3.7288650	1.3797740	-0.6240070
20	C	-2.5055550	0.8213620	-0.3198790
21	C	-2.4789760	-0.4450720	0.2856390
22	H	-3.5502890	-2.1464890	1.0528690
23	H	-5.7953880	-1.1423380	0.5062300
24	H	-3.8015100	2.3555340	-1.0931870
25	H	-1.5813110	1.3420800	-0.5431790
26	O	-1.2965330	-1.0965550	0.6391380
27	O	-6.0873470	1.2038770	-0.6081850

TS(12-13)

Symbol	X	Y	Z

1	C	1.4515170	3.1795130	-1.2174950
2	C	0.8496400	1.9284560	-1.2229770
3	C	0.5233990	1.2886490	-0.0008210
4	C	0.8406460	1.9327300	1.2215150
5	C	1.4422630	3.1839250	1.2160690
6	C	1.7469220	3.8055910	-0.0007260
7	H	1.6907390	3.6719660	-2.1544700
8	H	0.6092950	1.4307010	-2.1563460
9	H	0.5932400	1.4382920	2.1548440
10	H	1.6743110	3.6798030	2.1530650
11	H	2.2176030	4.7843260	-0.0007050
12	C	-0.0830170	0.0135450	-0.0007920
13	C	-1.0083630	-0.9145820	0.0011370
14	Cu	-2.8543650	-0.3760190	-0.0015460
15	Cl	-4.9585220	0.0550480	-0.0004810
16	C	1.5800280	-1.7656270	1.2462310
17	C	2.9233460	-1.5166340	1.2503230
18	C	3.6714540	-1.3556670	0.0002830
19	C	2.9224000	-1.5223940	-1.2484410
20	C	1.5791380	-1.7712590	-1.2422440
21	C	0.8768520	-1.8015870	0.0023460
22	H	1.0122240	-1.9183360	2.1585540
23	H	3.4917420	-1.4571340	2.1726260
24	H	3.4902270	-1.4672190	-2.1713610
25	H	1.0106590	-1.9280810	-2.1534290
26	O	-0.4679960	-2.1873790	0.0037160
27	O	4.8910030	-1.1093110	-0.0007450

TS(11-12')

	Symbol	X	Y	Z
1	C	3.3832390	-1.8761050	-1.6511910
2	C	2.1943390	-1.2271460	-1.3222980
3	C	1.8866770	-0.9721830	0.0259830
4	C	2.7786130	-1.3659480	1.0375800
5	C	3.9674660	-2.0050090	0.6948490

6	C	4.2706570	-2.2641210	-0.6456490
7	H	3.6152240	-2.0755540	-2.6927490
8	H	1.5024460	-0.9163350	-2.0981290
9	H	2.5355010	-1.1546440	2.0722830
10	H	4.6588890	-2.3037380	1.4767600
11	H	5.1982710	-2.7656820	-0.9043600
12	C	0.6057550	-0.3189120	0.3494090
13	C	-0.6099320	-0.7323910	0.1940550
14	Cu	-2.3545540	-1.2445730	-0.0455530
15	Cl	-4.3946240	-1.7827110	-0.2738740
16	C	-0.7847430	1.8501130	1.0202340
17	C	-1.1169160	2.8887230	0.2396690
18	C	-0.1260090	3.5474460	-0.6436940
19	C	1.2745040	3.0619270	-0.5416500
20	C	1.6214430	2.0249350	0.2351860
21	C	0.6091940	1.2708840	1.0490430
22	H	-1.4907730	1.3985310	1.7115460
23	H	-2.1181660	3.3087430	0.2378850
24	H	2.0105240	3.6111180	-1.1217670
25	H	2.6476580	1.6842820	0.3250540
26	O	1.0190080	0.8269670	2.2373280
27	O	-0.4308360	4.4628700	-1.3971780

12'

	Symbol	X	Y	Z
1	C	-1.6260050	3.2758630	-1.6076240
2	C	-1.0412330	2.0513650	-1.2838110
3	C	-1.0641130	1.5963360	0.0453990
4	C	-1.6618940	2.3785640	1.0485090
5	C	-2.2530810	3.5926110	0.7099600
6	C	-2.2322960	4.0451940	-0.6140950
7	H	-1.6066420	3.6249770	-2.6352650
8	H	-0.5768210	1.4416150	-2.0516260
9	H	-1.6702610	2.0189910	2.0711030
10	H	-2.7267230	4.1911690	1.4820650

11	H	-2.6886830	4.9971740	-0.8679390
12	C	-0.4205470	0.2891620	0.3788650
13	C	0.8738960	0.2182680	0.2433170
14	Cu	2.6842710	0.1367850	0.0009620
15	Cl	4.7838680	-0.0139640	-0.2568380
16	C	-0.3826850	-2.2061400	0.8877970
17	C	-0.6980050	-3.2749850	0.1455160
18	C	-1.9322640	-3.3176500	-0.6750980
19	C	-2.8374620	-2.1444270	-0.5673110
20	C	-2.5336410	-1.0673560	0.1689380
21	C	-1.2388160	-0.9583400	0.9387240
22	H	0.4993570	-2.1897680	1.5238390
23	H	-0.0766030	-4.1651660	0.1252930
24	H	-3.7720000	-2.2141890	-1.1165500
25	H	-3.2049390	-0.2190100	0.2574890
26	O	-1.4250520	-0.4867660	2.2170420
27	O	-2.2071250	-4.2739800	-1.3876140

TS(12'-13)

	Symbol	X	Y	Z
1	C	-1.9761920	3.0578210	-1.1857850
2	C	-1.5518940	1.7545390	-0.9444300
3	C	-0.6050660	1.5068800	0.0652580
4	C	-0.0807960	2.5733030	0.8153650
5	C	-0.5123480	3.8750990	0.5632970
6	C	-1.4580560	4.1180510	-0.4340990
7	H	-2.7088320	3.2482170	-1.9638740
8	H	-1.9420770	0.9325050	-1.5349450
9	H	0.6454200	2.3716200	1.5955790
10	H	-0.1079410	4.6971380	1.1454710
11	H	-1.7917370	5.1326430	-0.6293530
12	C	-0.1321420	0.1176820	0.3158620
13	C	1.1411680	-0.1316130	0.1690950
14	Cu	2.9225810	-0.4308440	-0.1042640
15	Cl	4.9907910	-0.7559180	-0.4440550

16	C	-1.1073380	-2.1611880	-0.2177040
17	C	-2.2396140	-2.5753160	-0.8009310
18	C	-3.5581470	-1.9982500	-0.4444900
19	C	-3.5663800	-0.9790000	0.6360680
20	C	-2.4375500	-0.5424130	1.2099190
21	C	-1.0767110	-1.0710630	0.8293370
22	H	-0.1416870	-2.5982450	-0.4590330
23	H	-2.2471690	-3.3637840	-1.5474530
24	H	-4.5432530	-0.6134190	0.9388200
25	H	-2.4441590	0.1910470	2.0108910
26	O	-0.3271260	-1.3887060	1.9427570
27	O	-4.5916810	-2.3512710	-0.9982670

13

	Symbol	X	Y	Z
1	C	-0.9749980	3.6285800	-0.0021820
2	C	-0.9914540	2.2435800	-0.0028570
3	C	0.2304510	1.5120500	-0.0008280
4	C	1.4580720	2.2293200	0.0018190
5	C	1.4585800	3.6147420	0.0025840
6	C	0.2455990	4.3195200	0.0005890
7	H	-1.9107500	4.1783440	-0.0037930
8	H	-1.9341900	1.7051840	-0.0049690
9	H	2.3951040	1.6826040	0.0034500
10	H	2.3997390	4.1555050	0.0047800
11	H	0.2522130	5.4052500	0.0012100
12	C	0.2112310	0.0978430	-0.0012540
13	C	-0.7961890	-0.9131080	-0.0020850
14	Cu	-2.6866960	-1.0097960	-0.0009360
15	Cl	-4.8219280	-0.9248690	0.0028720
16	C	2.0690390	-1.1452360	1.2636270
17	C	3.4069230	-1.2268030	1.2630970
18	C	4.1891350	-1.2390750	0.0006150
19	C	3.4080020	-1.2264650	-1.2625190
20	C	2.0701010	-1.1451410	-1.2639520

21	C	1.2831300	-1.0024920	-0.0004420
22	H	1.4936300	-1.1507570	2.1855350
23	H	3.9802620	-1.3002950	2.1821190
24	H	3.9821190	-1.2996310	-2.1810730
25	H	1.4953430	-1.1507640	-2.1862590
26	O	0.1035340	-1.9373510	-0.0011780
27	O	5.4124370	-1.2754600	0.0011850

TS(13-14)

	Symbol	X	Y	Z
1	C	-1.7358250	3.3726160	0.0038540
2	C	-1.4375280	2.0197860	-0.0212970
3	C	-0.0837960	1.5801300	0.0204360
4	C	0.9453150	2.5602240	0.0860120
5	C	0.6321680	3.9102720	0.1064650
6	C	-0.7071070	4.3231950	0.0657690
7	H	-2.7721270	3.6936990	-0.0271930
8	H	-2.2372070	1.2873660	-0.0748880
9	H	1.9835510	2.2452320	0.1274880
10	H	1.4264290	4.6484390	0.1583690
11	H	-0.9476760	5.3817800	0.0834750
12	C	0.2340170	0.1957650	0.0024090
13	C	-0.5733320	-0.9828560	-0.0734820
14	Cu	-2.4492660	-1.3536000	-0.0328930
15	Cl	-4.5896860	-1.4461310	0.0429640
16	C	2.2758660	-0.7795030	1.2172650
17	C	3.5897110	-1.1045370	1.2509300
18	C	4.4161420	-1.0787360	0.0305100
19	C	3.7425060	-0.6653500	-1.2175160
20	C	2.4311270	-0.3234280	-1.2308390
21	C	1.6233740	-0.4214090	-0.0310100
22	H	1.6693390	-0.7942520	2.1176300
23	H	4.0888340	-1.3929730	2.1704170
24	H	4.3562320	-0.6365600	-2.1124290
25	H	1.9439510	-0.0004640	-2.1460040

26	O	0.3165920	-1.9028170	-0.2130170
27	O	5.6116830	-1.3760160	0.0467180

14

	Symbol	X	Y	Z
1	C	-1.9384840	2.6721370	-0.7647710
2	C	-1.2681110	1.4498470	-0.7583020
3	C	-0.1800130	1.2356440	0.1077050
4	C	0.2141740	2.2757500	0.9698080
5	C	-0.4591700	3.4961910	0.9602510
6	C	-1.5365700	3.6969330	0.0944590
7	H	-2.7754320	2.8182310	-1.4398910
8	H	-1.5727310	0.6727610	-1.4535860
9	H	1.0320130	2.1118280	1.6649810
10	H	-0.1501650	4.2850290	1.6393090
11	H	-2.0651740	4.6452450	0.0941080
12	C	0.5086750	-0.0776160	0.1677740
13	C	-0.3890470	-1.2245910	0.3899520
14	Cu	-2.3377680	-1.2960050	0.0954110
15	Cl	-4.4146630	-1.1501750	-0.4285640
16	C	2.7027160	0.8773540	-0.4359550
17	C	4.0417330	0.7692990	-0.5669880
18	C	4.7491070	-0.4941700	-0.2800070
19	C	3.8969010	-1.6345040	0.1128970
20	C	2.5566040	-1.5193440	0.2299350
21	C	1.8775480	-0.2467720	0.0057900
22	H	2.2040480	1.8094930	-0.6739750
23	H	4.6518790	1.6003930	-0.9066280
24	H	4.4059140	-2.5740450	0.3037060
25	H	1.9649740	-2.3770680	0.5250660
26	O	-0.1579190	-2.3419800	0.8028430
27	O	5.9695250	-0.5969810	-0.3815590

5) Formation of Aryl Ketone from Cu(II)-coordinated Quinone Methide 14

15

	Symbol	X	Y	Z
1	C	3.8353830	-0.3606860	-0.9004670
2	C	2.6471440	0.3704170	-0.9088970
3	C	1.6386680	0.0993240	0.0273010
4	C	1.8410660	-0.9207280	0.9717640
5	C	3.0216710	-1.6603360	0.9651230
6	C	4.0236780	-1.3800450	0.0326910
7	H	4.6077830	-0.1390470	-1.6306560
8	H	2.4926530	1.1478490	-1.6515060
9	H	1.0719200	-1.1271780	1.7092500
10	H	3.1641570	-2.4497850	1.6969770
11	H	4.9451350	-1.9542650	0.0345490
12	C	0.3723850	0.9007220	0.0465780
13	C	0.5471130	2.2264770	0.1247130
14	C	-1.1769870	-1.0222060	-0.3561900
15	C	-2.4390350	-1.5569220	-0.4174370
16	C	-3.6222500	-0.7633760	-0.1241510
17	C	-3.3832480	0.6286370	0.2335260
18	C	-2.1170780	1.1432980	0.2932870
19	C	-0.9733720	0.3397740	0.0026790
20	H	-0.3157160	-1.6367790	-0.5952520
21	H	-2.5992040	-2.5930610	-0.6984470
22	H	-4.2534800	1.2360330	0.4608330
23	H	-1.9745120	2.1832800	0.5798590
24	O	0.7224180	3.3784330	0.1954050
25	O	-4.7761120	-1.2450770	-0.1764960

15a

	Symbol	X	Y	Z
1	C	3.5692060	-1.1652720	-0.7475510
2	C	2.5072610	-0.2966790	-0.4934410
3	C	1.4023550	-0.7267310	0.2556890
4	C	1.3787480	-2.0435490	0.7443710
5	C	2.4334210	-2.9123970	0.4732470
6	C	3.5332240	-2.4749520	-0.2692310

7	H	4.4186040	-0.8194520	-1.3288430
8	H	2.5243460	0.7149170	-0.8873590
9	H	0.5336230	-2.3787700	1.3372810
10	H	2.4015270	-3.9296110	0.8519020
11	H	4.3563260	-3.1529050	-0.4735340
12	C	0.2689010	0.2057880	0.5609800
13	C	0.6260140	1.3465590	1.1664020
14	C	-1.4988010	-1.1325420	-0.5960970
15	C	-2.8141330	-1.3859490	-0.8916800
16	C	-3.8920350	-0.5771570	-0.3432640
17	C	-3.4872140	0.5153980	0.5321900
18	C	-2.1706010	0.7507960	0.8182080
19	C	-1.1334290	-0.0619120	0.2678060
20	H	-0.7168810	-1.7453360	-1.0316650
21	H	-3.0967150	-2.1964430	-1.5560890
22	H	-4.2776440	1.1273140	0.9548720
23	H	-1.9052060	1.5659760	1.4883310
24	O	0.9574130	2.3294550	1.7019490
25	O	-5.0938570	-0.8037180	-0.6068900
26	O	1.3845820	3.1783470	-1.4184820
27	O	1.6799260	4.1166530	-0.7041600

TS(15a-16)

	Symbol	X	Y	Z
1	C	-3.0950970	-1.4976810	1.2367450
2	C	-1.8955160	-0.8245090	1.0127620
3	C	-1.6565660	-0.2049930	-0.2248720
4	C	-2.6484630	-0.2398430	-1.2165630
5	C	-3.8476050	-0.9118730	-0.9856880
6	C	-4.0709990	-1.5443590	0.2388050
7	H	-3.2722530	-1.9753450	2.1954920
8	H	-1.1454020	-0.7593180	1.7941800
9	H	-2.4720410	0.2502640	-2.1694970
10	H	-4.6059740	-0.9419990	-1.7618710
11	H	-5.0062670	-2.0659210	0.4179960

12	C	-0.3732310	0.5236150	-0.4720430
13	C	-0.5646250	1.9046090	-0.6067190
14	C	1.1227800	-1.4118760	-0.0778820
15	C	2.3694970	-1.9385570	-0.0214140
16	C	3.5751600	-1.1088800	-0.1852380
17	C	3.3405680	0.3243860	-0.4157080
18	C	2.0901240	0.8385520	-0.4648950
19	C	0.9131610	0.0048340	-0.2974330
20	H	0.2539020	-2.0528910	0.0203280
21	H	2.5313090	-3.0007180	0.1327910
22	H	4.2195110	0.9497710	-0.5324480
23	H	1.9497200	1.9041720	-0.6267130
24	O	-0.9213230	2.8687920	-1.1597330
25	O	4.7101680	-1.5913480	-0.1368590
26	O	-0.0213590	2.5121080	1.2939550
27	O	0.7315590	1.7368760	1.9289610

16

	Symbol	X	Y	Z
1	C	-2.7459100	-2.1431490	0.8253190
2	C	-1.6032580	-1.3467420	0.8280280
3	C	-1.4377880	-0.3355600	-0.1347070
4	C	-2.4566930	-0.1277860	-1.0808220
5	C	-3.5962980	-0.9293150	-1.0821060
6	C	-3.7429550	-1.9404710	-0.1311610
7	H	-2.8627840	-2.9157400	1.5791400
8	H	-0.8469720	-1.4821950	1.5939290
9	H	-2.3448980	0.6503510	-1.8309170
10	H	-4.3688450	-0.7634830	-1.8265660
11	H	-4.6334520	-2.5615140	-0.1293750
12	C	-0.2362870	0.5331090	-0.1531640
13	C	-0.5188980	1.9944360	-0.2922940
14	C	1.3994000	-1.3216950	-0.2063800
15	C	2.6746680	-1.7574060	-0.1454720
16	C	3.8111760	-0.8267120	-0.0007290

17	C	3.4657580	0.6073260	0.0317620
18	C	2.1888920	1.0349080	-0.0428310
19	C	1.0676430	0.1001640	-0.1386760
20	H	0.5881440	-2.0279180	-0.3393960
21	H	2.9211480	-2.8119640	-0.2195050
22	H	4.2946680	1.3021590	0.1212250
23	H	1.9760900	2.0977020	-0.0194280
24	O	-0.1592830	2.7427110	-1.1546130
25	O	4.9732720	-1.2224530	0.0726220
26	O	-1.3799250	2.5684330	0.7063600
27	O	-1.4765400	1.8195530	1.8019170

16a

	Symbol	X	Y	Z
1	C	-0.9662870	-2.5926780	-2.3269920
2	C	-0.8611260	-1.5104260	-1.4551600
3	C	-1.7690050	-1.3686280	-0.3902880
4	C	-2.7639410	-2.3453550	-0.2094010
5	C	-2.8661780	-3.4224520	-1.0869310
6	C	-1.9691860	-3.5474270	-2.1495400
7	H	-0.2540990	-2.6949040	-3.1400950
8	H	-0.0539680	-0.7936990	-1.5666960
9	H	-3.4729770	-2.2490010	0.6085790
10	H	-3.6466880	-4.1627630	-0.9408620
11	H	-2.0461250	-4.3897990	-2.8301950
12	C	-1.6849140	-0.2278130	0.5576770
13	C	-1.7389350	-0.5871080	1.9986890
14	C	-1.7978670	1.5097190	-1.1950660
15	C	-1.7266500	2.8033500	-1.5687670
16	C	-1.4790780	3.8833250	-0.5934040
17	C	-1.3475170	3.4609150	0.8143430
18	C	-1.4340390	2.1665420	1.1813120
19	C	-1.6448860	1.1018700	0.2000360
20	H	-2.0043180	0.7407900	-1.9296830
21	H	-1.8663650	3.1076500	-2.6012430

22	H	-1.1709130	4.2478750	1.5404500
23	H	-1.3326010	1.8972130	2.2257130
24	O	-2.4410930	-0.1612360	2.8677150
25	O	-1.4026570	5.0625650	-0.9322010
26	O	-0.8572340	-1.6728220	2.4199220
27	O	0.2399060	-1.7908990	1.6867840
28	C	5.1385820	0.7227460	-0.8737930
29	C	3.7548370	0.8782820	-0.8435700
30	C	2.9819860	0.0436310	-0.0286530
31	C	3.5980470	-0.9411850	0.7518780
32	C	4.9855610	-1.0851800	0.7117800
33	C	5.7634400	-0.2579760	-0.0987570
34	H	5.7330170	1.3745500	-1.5077790
35	H	3.2570340	1.6370950	-1.4384680
36	H	2.9946220	-1.5873810	1.3847700
37	H	5.4569640	-1.8512890	1.3208290
38	H	6.8422530	-0.3739650	-0.1257760
39	O	1.6269360	0.2362640	-0.0342240
40	H	1.2002420	-0.3982760	0.5641510

TS(16a-17)

	Symbol	X	Y	Z
1	C	4.6710640	-0.3864060	1.4917470
2	C	3.3698660	-0.0447450	1.1310120
3	C	2.8420460	-0.4561930	-0.1067700
4	C	3.6403950	-1.2432070	-0.9575650
5	C	4.9432180	-1.5745740	-0.5935950
6	C	5.4634950	-1.1465390	0.6293930
7	H	5.0619020	-0.0683810	2.4536010
8	H	2.7421380	0.5125860	1.8177770
9	H	3.2389090	-1.5748690	-1.9094300
10	H	5.5526490	-2.1697600	-1.2668460
11	H	6.4773350	-1.4120720	0.9133660
12	C	1.4550310	-0.1129310	-0.4876820
13	C	0.6719130	-1.2673860	-1.0509500

14	C	1.6348360	2.3288620	-0.0898420
15	C	1.0427390	3.5391110	0.0020330
16	C	-0.4018090	3.7227780	-0.2303820
17	C	-1.1467680	2.5087950	-0.6131580
18	C	-0.5431040	1.3060240	-0.7108340
19	C	0.8769580	1.1277870	-0.4236550
20	H	2.7043410	2.2327550	0.0600350
21	H	1.6107340	4.4344520	0.2348160
22	H	-2.2072420	2.6321780	-0.8085670
23	H	-1.1270630	0.4346780	-0.9936140
24	O	0.6797910	-1.6219040	-2.2017390
25	O	-0.9491580	4.8213110	-0.1276870
26	O	-0.0869320	-2.0093520	-0.1600150
27	O	0.0528860	-1.5715390	1.1579660
28	C	-5.1929220	-0.0322250	0.3220320
29	C	-4.1296420	-0.0760400	1.2057580
30	C	-3.1260300	-1.0718580	1.0608190
31	C	-3.2190950	-2.0093380	-0.0055450
32	C	-4.2839840	-1.9350670	-0.8910260
33	C	-5.2752210	-0.9561860	-0.7335990
34	H	-5.9623430	0.7245290	0.4390800
35	H	-4.0303140	0.6302980	2.0226420
36	H	-2.4506870	-2.7655670	-0.1150790
37	H	-4.3522890	-2.6471110	-1.7074790
38	H	-6.1073150	-0.9111690	-1.4289620
39	O	-2.1570980	-1.1021470	1.9539820
40	H	-1.2245690	-1.5074750	1.6194590

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	Symbol	X	Y	Z
1	C	-3.3514880	-1.5378790	0.9865140
2	C	-2.3495450	-0.5718780	1.0037880
3	C	-1.3255750	-0.5853690	0.0403990
4	C	-1.3497020	-1.5776390	-0.9547860
5	C	-2.3607670	-2.5370650	-0.9765950

6	C	-3.3608460	-2.5230020	-0.0038680
7	H	-4.1283290	-1.5197370	1.7446770
8	H	-2.3519330	0.1931010	1.7741540
9	H	-0.5824530	-1.5801520	-1.7225550
10	H	-2.3691580	-3.2908580	-1.7579700
11	H	-4.1479120	-3.2707440	-0.0205570
12	C	-0.2486900	0.4410010	0.0648900
13	C	-0.6906680	1.8623250	0.0590260
14	C	1.5251940	-1.2620620	0.2633880
15	C	2.8262670	-1.6184430	0.2481410
16	C	3.8998320	-0.6313040	0.0272320
17	C	3.4582340	0.7654900	-0.1380840
18	C	2.1559480	1.1182860	-0.1033580
19	C	1.0961500	0.1246590	0.0759270
20	H	0.7629290	-2.0074950	0.4553320
21	H	3.1384170	-2.6440410	0.4186640
22	H	4.2395570	1.5017500	-0.2988000
23	H	1.8708820	2.1538290	-0.2262390
24	O	-0.0891350	2.8483180	0.4591890
25	O	5.0867180	-0.9533100	-0.0056950
26	O	-1.9349140	1.9843120	-0.4760300
27	O	-2.3645150	3.3557780	-0.4596920
28	H	-1.5632860	3.7808340	-0.0645640

TS(17-18)

	Symbol	X	Y	Z
1	C	-3.0157650	-1.8782060	0.9628180
2	C	-1.8779330	-1.0815630	1.0575030
3	C	-1.5503460	-0.1928460	0.0218420
4	C	-2.3862400	-0.1045120	-1.1028270
5	C	-3.5191020	-0.9127420	-1.1941870
6	C	-3.8363340	-1.7995310	-0.1654650
7	H	-3.2667260	-2.5545160	1.7741140
8	H	-1.2537900	-1.1180500	1.9440280
9	H	-2.1377350	0.5843060	-1.9028450

10	H	-4.1554170	-0.8431370	-2.0709040
11	H	-4.7234960	-2.4213770	-0.2366470
12	C	-0.3184830	0.6448610	0.0847250
13	C	-0.5325050	2.1011250	-0.3345280
14	C	1.1977290	-1.3411990	-0.1056660
15	C	2.4508950	-1.8654730	-0.1816310
16	C	3.6492020	-1.0160670	-0.1730210
17	C	3.4057280	0.4324530	-0.1040250
18	C	2.1468930	0.9376160	-0.0334850
19	C	0.9874370	0.0779970	-0.0098120
20	H	0.3319390	-1.9936480	-0.1247120
21	H	2.6149490	-2.9358110	-0.2540340
22	H	4.2791840	1.0761030	-0.1224760
23	H	2.0017870	2.0154170	-0.0023560
24	O	-0.5813710	2.5009710	-1.4779410
25	O	4.7910560	-1.4870520	-0.2279450
26	O	-0.6764880	2.8730900	0.7187620
27	O	-0.4101730	1.4286860	1.8173440
28	H	0.5180660	1.6536620	2.0206250

TS(17w-18)

	Symbol	X	Y	Z
1	C	-2.4079460	-2.5231910	0.7677890
2	C	-1.3805110	-1.5876220	0.8184120
3	C	-1.3552360	-0.5058730	-0.0833160
4	C	-2.3995170	-0.3731600	-1.0155870
5	C	-3.4157700	-1.3234310	-1.0737580
6	C	-3.4232510	-2.3987020	-0.1848100
7	H	-2.4218500	-3.3460130	1.4757680
8	H	-0.6095690	-1.6614430	1.5768180
9	H	-2.4164340	0.4678220	-1.6992860
10	H	-4.2084750	-1.2157570	-1.8072010
11	H	-4.2234680	-3.1316430	-0.2245840
12	C	-0.2480880	0.4733030	-0.0493600
13	C	-0.4901730	1.8106970	-0.7611400

14	C	1.5121380	-1.2944920	-0.3319780
15	C	2.8180230	-1.6816530	-0.3121820
16	C	3.9011200	-0.7361280	-0.0108680
17	C	3.4881270	0.6530090	0.2224940
18	C	2.1834890	1.0236620	0.1680590
19	C	1.1319560	0.0663450	-0.0803650
20	H	0.7381160	-2.0147910	-0.5684140
21	H	3.1096010	-2.7063790	-0.5189900
22	H	4.2762450	1.3690420	0.4308960
23	H	1.9145770	2.0641260	0.3202010
24	O	0.2723320	2.0743750	-1.6949220
25	O	5.0849620	-1.0910250	0.0359870
26	O	-1.4633140	2.5923110	-0.4856540
27	O	-2.4589630	2.1547320	1.1993380
28	H	-2.5015520	3.1171570	1.3152390
29	O	-0.4435450	1.0413030	1.8777710
30	H	0.2773700	1.6602180	2.0684960
31	H	-1.3524950	1.6074960	1.7305630

TS(17-17a)

	Symbol	X	Y	Z
1	C	-0.8885620	2.3771680	-2.0045830
2	C	-0.1628640	1.4503020	-1.2585680
3	C	0.7394890	1.8818090	-0.2650220
4	C	0.8731950	3.2637390	-0.0246090
5	C	0.1503180	4.1822400	-0.7808700
6	C	-0.7291870	3.7448860	-1.7740670
7	H	-1.5850710	2.0280910	-2.7610580
8	H	-0.3203280	0.3875330	-1.4100710
9	H	1.5585460	3.5996030	0.7452480
10	H	0.2768680	5.2445870	-0.5954640
11	H	-1.2917650	4.4654990	-2.3601500
12	C	1.4921280	0.8982390	0.5413370
13	C	1.4778130	1.1438840	2.0274230
14	C	2.4544360	-0.3080490	-1.4039430

15	C	3.1502960	-1.3528610	-1.9050680
16	C	3.7138550	-2.4017080	-1.0371610
17	C	3.5113010	-2.2104280	0.4110410
18	C	2.8214810	-1.1574610	0.9015420
19	C	2.2141020	-0.1587080	0.0261450
20	H	2.0770400	0.4608920	-2.0681080
21	H	3.3366440	-1.4552580	-2.9695290
22	H	3.9506970	-2.9585510	1.0634910
23	H	2.6954600	-1.0459920	1.9737760
24	O	2.0765450	2.1032740	2.5146140
25	O	4.3298940	-3.3678080	-1.4893580
26	O	0.8481650	0.3383750	2.8232960
27	O	-0.4524960	-0.9108830	1.9228480
28	H	0.1778080	-1.6369030	2.0469460
29	C	-5.0912800	-2.2970560	-0.2895660
30	C	-3.7215610	-2.4874700	-0.2317530
31	C	-2.8523750	-1.3827870	0.0085590
32	C	-3.4222690	-0.0913910	0.2195960
33	C	-4.7954380	0.0747900	0.1786980
34	C	-5.6358620	-1.0204700	-0.0795900
35	H	-5.7484920	-3.1380700	-0.4883380
36	H	-3.2703990	-3.4626520	-0.3808870
37	H	-2.7570570	0.7436560	0.4132630
38	H	-5.2265430	1.0574980	0.3436100
39	H	-6.7117090	-0.8795980	-0.1123410
40	O	-1.5602580	-1.5709260	-0.0097260
41	H	-0.8905960	-1.0385940	0.9089740

17a

	Symbol	X	Y	Z
1	C	3.6296770	1.8448450	-1.9196660
2	C	2.6767300	1.1859450	-1.1499280
3	C	3.0911030	0.2959700	-0.1355020
4	C	4.4691650	0.1156860	0.1160340
5	C	5.4096410	0.7608160	-0.6794540

6	C	4.9924010	1.6222300	-1.6983470
7	H	3.3103200	2.5443130	-2.6859570
8	H	1.6200110	1.4141790	-1.2510730
9	H	4.7753760	-0.5432810	0.9213480
10	H	6.4681780	0.6016550	-0.4993800
11	H	5.7301950	2.1347320	-2.3087980
12	C	2.1319720	-0.4292270	0.6911780
13	C	2.3640080	-0.3251490	2.1987960
14	C	0.9011880	-1.4780700	-1.1904170
15	C	-0.1568750	-2.1903270	-1.6617850
16	C	-1.2250170	-2.6564620	-0.7686070
17	C	-1.0488510	-2.3727720	0.6608590
18	C	0.0109180	-1.6604430	1.1166860
19	C	1.0172260	-1.1494090	0.2101930
20	H	1.6825400	-1.1479750	-1.8649270
21	H	-0.2617950	-2.4297780	-2.7149350
22	H	-1.8161440	-2.7462030	1.3311260
23	H	0.1014870	-1.4269200	2.1708200
24	O	3.1794050	-0.9330420	2.8625490
25	O	-2.2147380	-3.2637590	-1.1985580
26	O	1.5020770	0.5867890	2.4492650
27	O	-0.1518520	2.1525270	0.1555590
28	H	0.2408040	1.8364090	0.9829560
29	C	-5.7294390	0.2645260	-0.2014830
30	C	-4.4654440	-0.1866070	-0.5101760
31	C	-3.3135160	0.6655900	-0.2886690
32	C	-3.5321860	1.9862020	0.2709590
33	C	-4.8096470	2.4072660	0.5674940
34	C	-5.9112940	1.5576580	0.3336660
35	H	-6.5933690	-0.3722630	-0.3664330
36	H	-4.2793750	-1.1767500	-0.9147270
37	H	-2.6527780	2.6013140	0.4397970
38	H	-4.9757450	3.3957940	0.9850380
39	H	-6.9131630	1.9019210	0.5720230

40	O	-2.1506070	0.2603420	-0.5755030
41	H	-0.7613840	1.4403890	-0.1143720

TS(17a-17b)

	Symbol	X	Y	Z
1	C	-3.8157680	-1.9024010	-1.7719880
2	C	-2.7963310	-1.3142240	-1.0330230
3	C	-3.0854010	-0.1914050	-0.2151400
4	C	-4.4189240	0.2788550	-0.1152530
5	C	-5.4199620	-0.3169260	-0.8687970
6	C	-5.1215610	-1.4045840	-1.7000240
7	H	-3.5945490	-2.7580690	-2.4024430
8	H	-1.7853950	-1.7164290	-1.0333400
9	H	-4.6377880	1.1069480	0.5493700
10	H	-6.4371080	0.0571310	-0.8070050
11	H	-5.9116710	-1.8723060	-2.2800230
12	C	-2.0378450	0.4333360	0.5339530
13	C	-2.2790070	-0.0724610	2.3759740
14	C	-0.8170550	1.7506410	-1.0971860
15	C	0.2664210	2.4694770	-1.4497820
16	C	1.3618790	2.7372870	-0.5005300
17	C	1.1489330	2.2700610	0.8819970
18	C	0.0685890	1.5455510	1.2330660
19	C	-0.9631560	1.1997150	0.2566160
20	H	-1.6050620	1.5360970	-1.8120180
21	H	0.3939330	2.8512550	-2.4579450
22	H	1.9271410	2.5133510	1.5985630
23	H	-0.0399760	1.1763160	2.2461230
24	O	-3.1837950	0.5700990	2.8271090
25	O	2.3976880	3.3120620	-0.8414820
26	O	-1.4216760	-0.9146700	2.5195470
27	O	0.1181820	-2.3095850	0.0250960
28	H	-0.2076870	-2.0079550	0.8856880
29	C	5.6160830	-0.2063330	-0.2695620
30	C	4.3361680	0.2025580	-0.5738930

31	C	3.2240380	-0.7164120	-0.4253110
32	C	3.4989470	-2.0542120	0.0646080
33	C	4.7909150	-2.4316240	0.3567060
34	C	5.8536390	-1.5187660	0.1899200
35	H	6.4496620	0.4808550	-0.3795130
36	H	4.1089080	1.2084150	-0.9139410
37	H	2.6482260	-2.7181730	0.1884060
38	H	4.9986430	-3.4337870	0.7198480
39	H	6.8676410	-1.8289360	0.4240720
40	O	2.0479860	-0.3529740	-0.7149190
41	H	0.6943780	-1.5829530	-0.2827720

17b

	Symbol	X	Y	Z
1	C	2.5170670	4.1781560	-0.5389750
2	C	1.7308390	3.0372380	-0.5837520
3	C	2.2002920	1.8267220	0.0101530
4	C	3.4681970	1.8312590	0.6672900
5	C	4.2290930	2.9896010	0.7015970
6	C	3.7644360	4.1664260	0.0997500
7	H	2.1544920	5.0922490	-1.0001500
8	H	0.7505520	3.0380950	-1.0515820
9	H	3.8276620	0.9154750	1.1241560
10	H	5.1961090	2.9787950	1.1960650
11	H	4.3682150	5.0681780	0.1321810
12	C	1.4135120	0.6794450	0.0086860
13	C	3.6427990	-2.7483220	1.3292200
14	C	1.8478450	-1.2619160	-1.4162100
15	C	1.5454070	-2.5282150	-1.7726760
16	C	0.4430080	-3.2785480	-1.1360640
17	C	-0.3009950	-2.5636060	-0.0817940
18	C	0.0020170	-1.2983060	0.2784930
19	C	1.1008590	-0.5665890	-0.3589560
20	H	2.6588870	-0.7197460	-1.8941900
21	H	2.0953560	-3.0498360	-2.5505070

22	H	-1.1136860	-3.1107980	0.3861050
23	H	-0.5686770	-0.7752200	1.0399080
24	O	4.2479020	-1.7569250	1.1837900
25	O	0.1595960	-4.4283180	-1.4742740
26	O	3.0467450	-3.7405000	1.4823060
27	O	-1.3180150	2.0123450	-1.4551450
28	H	-0.8937680	1.2225440	-1.8149080
29	C	-5.6666860	0.7977190	-0.8206210
30	C	-4.3291680	1.0420560	-0.5986050
31	C	-3.7188220	0.6725350	0.6658710
32	C	-4.5592530	0.0436800	1.6668710
33	C	-5.8928660	-0.1866640	1.4150960
34	C	-6.4553430	0.1867690	0.1758080
35	H	-6.1210990	1.0734580	-1.7674860
36	H	-3.6847740	1.5037260	-1.3411370
37	H	-4.0925150	-0.2280580	2.6079870
38	H	-6.5194700	-0.6567310	2.1670380
39	H	-7.5081400	-0.0004850	-0.0124710
40	O	-2.4941900	0.8883270	0.8967700
41	H	-1.5788720	1.7322690	-0.5556900

TS(17b-18)

	Symbol	X	Y	Z
1	C	0.8172250	4.5532010	-0.4752960
2	C	0.3270800	3.2712870	-0.6818140
3	C	1.0463560	2.1404760	-0.2113980
4	C	2.2707100	2.3678210	0.4850550
5	C	2.7398030	3.6582730	0.6828460
6	C	2.0218280	4.7608410	0.2056590
7	H	0.2549230	5.4031570	-0.8513230
8	H	-0.6029190	3.1148000	-1.2121010
9	H	2.8288700	1.5210760	0.8688840
10	H	3.6750010	3.8062820	1.2148870
11	H	2.3951090	5.7677660	0.3642370
12	C	0.6005450	0.8039040	-0.3288030

13	C	4.1367540	-1.4938830	1.8632480
14	C	2.4193260	-0.5396330	-1.3212690
15	C	2.9833750	-1.7506760	-1.5909940
16	C	2.3386340	-3.0095130	-1.2060010
17	C	1.0643770	-2.8762970	-0.4917130
18	C	0.5193960	-1.6599290	-0.2097740
19	C	1.1682140	-0.4335400	-0.6074180
20	H	2.9066630	0.3785310	-1.6375120
21	H	3.9259400	-1.8298060	-2.1244850
22	H	0.5773980	-3.7992990	-0.1923840
23	H	-0.4171490	-1.5867910	0.3382030
24	O	4.4211310	-0.3725960	1.6817760
25	O	2.8331550	-4.1163510	-1.4738820
26	O	3.8597390	-2.6106350	2.0594700
27	O	-1.1366110	0.8642960	-1.1070280
28	H	-1.0487330	0.1545330	-1.7625830
29	C	-5.9047010	0.0124110	-0.7965540
30	C	-4.5456600	0.1950280	-0.6454440
31	C	-3.8619600	-0.3229480	0.5146830
32	C	-4.6485230	-1.0161470	1.5046520
33	C	-6.0053000	-1.1895630	1.3272800
34	C	-6.6448410	-0.6806300	0.1806210
35	H	-6.4112260	0.4082420	-1.6717900
36	H	-3.9617100	0.7410260	-1.3800630
37	H	-4.1270580	-1.3982930	2.3757930
38	H	-6.5873680	-1.7201270	2.0748230
39	H	-7.7137360	-0.8178490	0.0517330
40	O	-2.6024390	-0.1858890	0.6803930
41	H	-1.7496680	0.4832510	-0.3675440

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	Symbol	X	Y	Z
1	C	3.0301280	-1.6161960	0.6789420
2	C	1.8057520	-0.9530380	0.7063160
3	C	1.6497440	0.2813260	0.0495590

4	C	2.7596180	0.8480390	-0.6045720
5	C	3.9790640	0.1787410	-0.6325530
6	C	4.1174530	-1.0564400	0.0053770
7	H	3.1384670	-2.5644190	1.1964450
8	H	0.9753410	-1.3723790	1.2633040
9	H	2.6503400	1.8087130	-1.0949770
10	H	4.8239980	0.6210980	-1.1514950
11	H	5.0712910	-1.5750730	-0.0136660
12	C	0.3764250	1.0178720	0.0848660
13	C	-1.1462120	-0.8879360	-0.3841710
14	C	-2.4004190	-1.3932850	-0.4706330
15	C	-3.5894130	-0.6023220	-0.1272970
16	C	-3.3197410	0.7793990	0.3055790
17	C	-2.0621280	1.2766670	0.3720360
18	C	-0.8975110	0.4758590	0.0431020
19	H	-0.3012920	-1.4927660	-0.6944940
20	H	-2.5772100	-2.4038770	-0.8252810
21	H	-4.1811440	1.3744200	0.5925440
22	H	-1.9245240	2.2863700	0.7572880
23	O	-4.7357000	-1.0558840	-0.1951400
24	O	0.5801730	2.3562200	0.1729530
25	H	-0.2476090	2.8231020	-0.0114800

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	Symbol	X	Y	Z
1	C	4.9906130	0.0030400	0.2067480
2	C	3.6861830	0.3185330	-0.1664830
3	C	2.6761510	-0.6590290	-0.1143010
4	C	3.0101420	-1.9634690	0.2938140
5	C	4.3114540	-2.2705740	0.6766490
6	C	5.3044330	-1.2877970	0.6363190
7	H	5.7643580	0.7625570	0.1517000
8	H	3.4546870	1.3130980	-0.5309540
9	H	2.2348150	-2.7210690	0.3088720
10	H	4.5547980	-3.2770300	1.0031850

11	H	6.3215220	-1.5303970	0.9296200
12	C	1.2895430	-0.3816190	-0.5486440
13	C	1.0734000	1.8427520	0.5860850
14	C	0.4105450	3.0216660	0.7605940
15	C	-0.7336570	3.3950590	-0.0723370
16	C	-1.1201880	2.4170360	-1.0918940
17	C	-0.4611310	1.2314100	-1.2370210
18	C	0.6613690	0.8917900	-0.4105010
19	H	1.8928480	1.5848010	1.2484700
20	H	0.6966630	3.7215720	1.5393130
21	H	-1.9460700	2.6887690	-1.7415700
22	H	-0.7695140	0.5327440	-2.0074730
23	O	-1.3378210	4.4706770	0.0747880
24	O	0.6877260	-1.3928070	-1.0893480
25	H	-0.4263620	-1.4234620	-1.1237150
26	C	-4.9647060	-1.8272140	0.2154040
27	C	-3.9298730	-2.0444020	-0.6707760
28	C	-2.6274010	-1.4922400	-0.4250840
29	C	-2.4421650	-0.7088610	0.7641070
30	C	-3.4931640	-0.5134420	1.6425480
31	C	-4.7578170	-1.0626460	1.3794490
32	H	-5.9454030	-2.2494600	0.0169200
33	H	-4.0586680	-2.6343100	-1.5720260
34	H	-1.4677150	-0.2761930	0.9577490
35	H	-3.3406290	0.0812840	2.5381440
36	H	-5.5772800	-0.8941580	2.0708310
37	O	-1.6862080	-1.7202070	-1.2775790

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	Symbol	X	Y	Z
1	C	-5.8896730	-1.2389710	-0.6068960
2	C	-4.5894860	-0.7361580	-0.5684160
3	C	-4.3244090	0.4894830	0.0629690
4	C	-5.3838950	1.2080590	0.6409670
5	C	-6.6764040	0.6954060	0.6167310

6	C	-6.9312760	-0.5298460	-0.0070340
7	H	-6.0891310	-2.1811090	-1.1081300
8	H	-3.7888660	-1.2837430	-1.0547390
9	H	-5.1683550	2.1655240	1.1028170
10	H	-7.4878710	1.2502270	1.0776790
11	H	-7.9417300	-0.9270560	-0.0308760
12	C	-2.9677000	1.1146820	0.0818030
13	C	-1.6480960	-1.0276840	0.5660140
14	C	-0.4677820	-1.7308720	0.5346030
15	C	0.7188120	-1.1643160	-0.0826720
16	C	0.6176330	0.1791300	-0.6295040
17	C	-0.5675630	0.8660220	-0.5646950
18	C	-1.7264450	0.2730600	0.0038150
19	H	-2.5243510	-1.4570060	1.0394960
20	H	-0.3771040	-2.7236170	0.9628310
21	H	1.5108030	0.6047810	-1.0763270
22	H	-0.6519330	1.8773310	-0.9474280
23	O	1.7901870	-1.8269600	-0.1300900
24	O	-2.8378230	2.3313240	0.1764340
25	H	3.2052770	-0.9868460	-0.9352340
26	C	6.9049680	1.1860500	-0.2258490
27	C	5.8108560	0.8575310	-1.0223390
28	C	4.8562420	-0.0557810	-0.5555910
29	C	5.0096230	-0.6335280	0.7125880
30	C	6.1112900	-0.2955430	1.4990820
31	C	7.0646150	0.6138250	1.0392000
32	H	7.6399760	1.8948260	-0.5976480
33	H	5.6769480	1.2931440	-2.0073410
34	H	4.2685690	-1.3420320	1.0722350
35	H	6.2215890	-0.7498380	2.4801120
36	H	7.9197890	0.8725470	1.6557790
37	O	3.8049510	-0.3456670	-1.3715810

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Symbol	X	Y	Z

1	C	5.7097990	-1.4478690	0.9942870
2	C	4.4967470	-0.7589400	0.8078660
3	C	4.4340680	0.3572780	-0.0692700
4	C	5.6158540	0.7894600	-0.7129050
5	C	6.8144620	0.0993760	-0.5141590
6	C	6.8694970	-1.0214320	0.3280440
7	H	5.7546510	-2.3036350	1.6605650
8	H	3.6277100	-1.0687690	1.3600550
9	H	5.5477980	1.6469750	-1.3562160
10	H	7.7107720	0.4523460	-1.0156000
11	H	7.8140660	-1.5395890	0.4845090
12	C	3.1872880	1.1398730	-0.2592700
13	C	1.6490640	-0.8893860	-0.4090440
14	C	0.3778260	-1.4449970	-0.3452790
15	C	-0.7183680	-0.6288070	-0.0299530
16	C	-0.5315570	0.7462330	0.1761810
17	C	0.7382870	1.2896720	0.0891740
18	C	1.8588490	0.4818260	-0.1776950
19	H	2.4877520	-1.5269650	-0.6532720
20	H	0.2191760	-2.5005530	-0.5094810
21	H	-1.3948020	1.3691590	0.4089120
22	H	0.8909370	2.3554540	0.2291310
23	O	-1.9562310	-1.1851040	0.0960290
24	O	3.2780220	2.3426570	-0.4734550
25	H	-2.5645030	-0.6002160	0.4672840
26	C	-7.2813530	0.5265610	0.4635570
27	C	-6.0569690	0.8111130	1.0200280
28	C	-4.8599150	0.2380680	0.4653880
29	C	-4.9712270	-0.5805240	-0.7236510
30	C	-6.2403590	-0.8476000	-1.2256450
31	C	-7.3925850	-0.2853300	-0.6545760
32	H	-8.2094980	0.9459010	0.8985070
33	H	-5.9119060	1.4858430	1.8964340
34	H	-4.0825390	-1.0118090	-1.1443410

35	H	-6.3107410	-1.4435440	-2.1477810
36	H	-8.3798410	-0.5241900	-1.0713800
37	O	-3.7462260	0.4444650	1.0217020

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	Symbol	X	Y	Z
1	C	3.0092180	-1.6430460	0.6805570
2	C	1.8023460	-0.9434070	0.6467770
3	C	1.7287060	0.3135670	0.0275540
4	C	2.8885700	0.8618380	-0.5425140
5	C	4.0865530	0.1544390	-0.5255230
6	C	4.1493140	-1.1009000	0.0865290
7	H	3.0588450	-2.6091100	1.1742250
8	H	0.9245950	-1.3623890	1.1271880
9	H	2.8260020	1.8477690	-0.9906350
10	H	4.9745650	0.5818190	-0.9819290
11	H	5.0861030	-1.6503250	0.1061110
12	C	0.4839480	1.1550220	0.0231150
13	C	-1.1226150	-0.7578880	-0.5304060
14	C	-2.4144330	-1.2677500	-0.5826490
15	C	-3.4813200	-0.5066120	-0.0907990
16	C	-3.2463390	0.7722280	0.4345500
17	C	-1.9543040	1.2776790	0.4647410
18	C	-0.8674130	0.5185130	0.0010680
19	H	-0.3071880	-1.3490880	-0.9323940
20	H	-2.6189150	-2.2459700	-1.0042260
21	H	-4.0770630	1.3656340	0.8108530
22	H	-1.7588960	2.2735200	0.8477120
23	O	-4.7248810	-1.0566590	-0.1535740
24	O	0.5859110	2.3787610	0.0388860
25	H	-5.3696840	-0.4307780	0.2026010