

Supplementary Materials: Understanding the Heteroatom Effect on the Ullmann Copper-Catalyzed Cross-Coupling of X-Arylation (X = NH, O, S) Mechanism

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Estimation of the Activation barrier by Savént's model

The reorganization energy λ_0 according to the Marcus equation can be calculated with:

$$\lambda_0 = (332 \text{ kcal/mol}) \left(\frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{R} \right) \left(\frac{1}{\epsilon_{op}} - \frac{1}{\epsilon} \right) \quad (\text{S1})$$

where a_1 and a_2 are the radii of the reactant molecules, $R = a_1 + a_2$. ϵ_{op} is the optical dielectric constant, and ϵ is the static dielectric constant. The inner reorganization energy was estimated to be $\lambda_i \approx 0$.

The Marcus equation is:

$$\Delta G_{ET}^\ddagger = \Delta G_0^\ddagger \left(1 + \frac{\Delta G_r}{4\Delta G_0^\ddagger} \right)^2 \quad (\text{S2})$$

where ΔG_r is the reaction energy and $\Delta G_0^\ddagger$ is the intrinsic barrier. Within the Savént model, the last term is related to the reorganization energy according to:

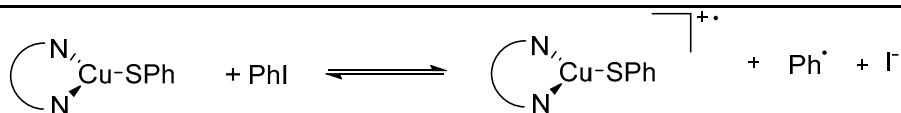
$$\Delta G_0^\ddagger = \frac{\lambda}{4} = \frac{\lambda_i + \lambda_0 + BDFE}{4} \quad (\text{S3})$$

where $BDFE$ stand for bond dissociation free energy of PhI (60.4 kcal/mol).

Single Electron Transfer

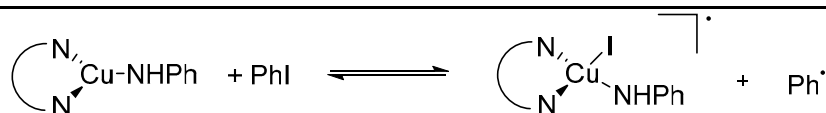
Solvent	ΔG (kcal/mol)	ϵ_{op}	ϵ	λ_0 (kcal/mol)	λ_i (kcal/mol)	λ (kcal/mol)	$\Delta G_{ET}^\ddagger$
Gas	+107.0	1.0	1.0	0.0	0.0	60.4	+116.0
Toluene	+56.2	2.24	2.37	0.9	0.0	61.3	+56.3
ACN	+24.3	35.69	1.81	19.3	0.0	79.7	+33.9
a_0 ([Cu(fen)NHPH])	5.36 Å						
a_0 (PhI)	4.31 Å						
Solvent	ΔG (kcal/mol)	ϵ_{op}	ϵ	λ_0 (kcal/mol)	λ_i (kcal/mol)	λ (kcal/mol)	$\Delta G_{ET}^\ddagger$
Gas	+118.1	1.0	1.0	0.0	0.0	60.4	+131.9
Toluene	+67.8	2.24	2.37	0.9	0.0	61.3	+67.9
ACN	+35.6	35.69	1.81	18.4	0.0	78.8	+41.5
a_0 ([Cu(fen)OPh])	5.39 Å						

ao(PhI) 4.31 Å

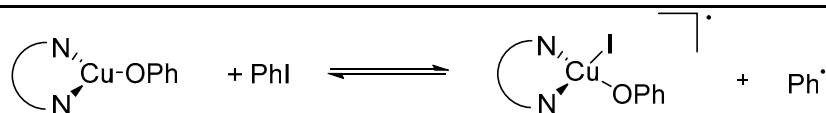


Solvent	ΔG (kcal/mol)	ϵ_{op}	ϵ	λ_o (kcal/mol)	λ_i (kcal/mol)	λ (kcal/mol)	$\Delta G_{ET}^\ddagger$
Gas	+120.1	1.0	1.0	0.0	0.0	60.4	+135.1
Toluene	+69.7	2.24	2.37	0.9	0.0	61.3	+70.0
ACN	+37.7	35.69	1.81	18.3	0.0	78.7	+43.0
ao([Cu(fen)SPh])	5.48 Å						
ao(PhI)	4.31 Å						

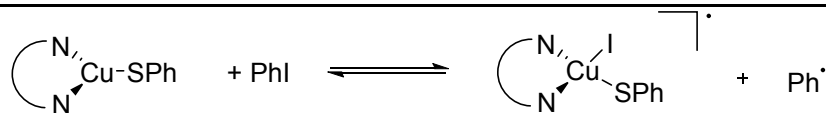
Halogen Atom Transfer



Solvent	ΔG (kcal/mol)	ϵ_{op}	ϵ	λ_o (kcal/mol)	λ_i (kcal/mol)	λ (kcal/mol)	$\Delta G_{ET}^\ddagger$
Gas	+25.2	1.0	1.0	0.0	0.0	60.4	+30.3
Toluene	+23.7	2.24	2.37	0.9	0.0	61.3	+29.5
ACN	+22.2	35.69	1.81	18.5	0.0	78.9	+32.4
ao([Cu(fen)NHPh])	5.36 Å						
ao(PhI)	4.31 Å						



Solvent	ΔG (kcal/mol)	ϵ_{op}	ϵ	λ_o (kcal/mol)	λ_i (kcal/mol)	λ (kcal/mol)	$\Delta G_{ET}^\ddagger$
Gas	+27.0	1.0	1.0	0.0	0.0	60.4	+31.6
Toluene	+27.0	2.24	2.37	0.9	0.0	61.3	+31.8
ACN	+26.3	35.69	1.81	18.4	0.0	78.8	+35.1
ao([Cu(fen)OPh])	5.39 Å						
ao(PhI)	4.31 Å						



Solvent	ΔG (kcal/mol)	ϵ_{op}	ϵ	λ_o (kcal/mol)	λ_i (kcal/mol)	λ (kcal/mol)	$\Delta G_{ET}^\ddagger$
Gas	+31.2	1.0	1.0	0.0	0.0	60.4	+34.7
Toluene	+30.8	2.24	2.37	0.9	0.0	61.3	+34.6
ACN	+30.3	35.69	1.81	18.3	0.0	78.7	+37.7
ao([Cu(fen)SPh])	5.48 Å						
ao(PhI)	4.31 Å						

Table S1. Gibbs Free Energies (kcal/mol) for Key Stationary Points in the Mechanisms of Ullmann-Type X-Arylation Reactions (X = NH, O, S) in different solvents at the PCM-[B3LYP/def2-TZVPP//B3LYP/def2-SVP] level of theory.

	PhNH ₂			PhOH			PhSH		
	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}
TS _{OA}	33.4	35.0	36.5	29.3	31.6	33.0	33.4	35.6	37.1
INT _{OA/RE}	23.7	24.7	25.7	26.1	28.3	30.1	26.2	27.3	28.0
TS _{RE}	25.3	25.1	24.9	35.0	36.1	36.7	30.2	31.5	32.5
TS _{Met}	40.2	41.5	42.7	40.1	42.4	44.5	40.2	42.0	43.9
TS _{HAT}	31.7	30.8	33.6	33.6	33.7	36.8	36.2	36.1	39.1
INT _{HAT}	27.1	25.6	24.1	29.6	29.6	29.0	33.2	32.8	32.2
TS _{SET}	109.7	52.2	30.8	117.1	63.3	38.1	126.9	64.5	39.0
INT _{SET}	102.4	51.9	19.6	113.4	63.3	30.8	114.7	64.4	32.1
Prod	-37.6	-39.9	-41.2	-27.2	-28.2	-28.5	-21.5	-22.9	-23.2

Table S2. Gibbs Free Energies (kcal/mol) for Key Stationary Points in the Mechanisms of Ullmann-Type X-Arylation Reactions (X = NH, O, S) in different solvents at the PCM-[M06/def2-TZVPP//B3LYP/def2-SVP] level of theory.

	PhNH ₂			PhOH			PhSH		
	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}
TS _{OA}	22.2	24.0	25.3	18.6	21.0	22.2	22.3	24.5	25.7
INT _{OA/RE}	18.3	20.1	21.6	19.5	22.1	24.2	18.8	20.4	21.3
TS _{RE}	20.5	20.9	21.1	29.8	31.4	32.3	24.1	25.8	27.1
TS _{Met}	34.3	36.0	37.5	35.1	37.5	39.6	36.2	38.1	40.0
TS _{HAT}	35.2	34.8	37.7	37.3	38.0	41.4	39.8	40.1	43.3
INT _{HAT}	31.8	31.1	29.9	34.5	35.2	35.2	37.7	37.9	37.9
TS _{SET}	126.6	65.1	40.4	144.1	78.4	49.7	147.5	80.2	50.8
INT _{SET}	114.5	65.0	33.8	126.2	77.3	46.2	128.3	79.0	47.6
Prod	-36.1	-37.7	-38.6	-27.1	-27.7	-27.6	-17.1	-18.1	-18.1

Table S3. Gibbs Free Energies (kcal/mol) for Key Stationary Points in the Mechanisms of Ullmann-Type X-Arylation Reactions (X = NH, O, S) in different solvents at the PCM-[TPSSH/def2-TZVPP//B3LYP/def2-SVP] level of theory.

	PhNH ₂			PhOH			PhSH		
	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}
TS _{OA}	27.1	28.3	29.5	21.4	23.4	24.6	25.5	27.5	28.9
INT _{OA/RE}	15.4	15.8	16.4	17.6	19.3	20.7	18.3	19.1	19.4
TS _{RE}	16.9	16.2	15.6	26.4	27.1	27.3	21.7	22.7	23.4
TS _{Met}	35.4	36.3	37.2	35.0	37.0	38.8	34.9	36.5	38.4
TS _{HAT}	29.6	28.4	31.3	30.8	30.8	34.2	41.1	33.3	36.7
INT _{HAT}	24.1	22.1	20.2	25.9	25.5	24.7	39.3	29.1	28.4
TS _{SET}	110.0	51.7	30.2	123.6	61.7	36.8	126.5	63.8	38.5
INT _{SET}	102.6	51.2	18.5	112.4	61.6	28.6	114.4	63.7	31.1

Prod	-35.3	-38.0	-39.5	-26.5	-27.8	-28.2	-20.0	-21.4	-21.7
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Table S4. Gibbs Free Energies (kcal/mol) for Key Stationary Points in the Mechanisms of Ullmann-Type X-Arylation Reactions (X = NH, O, S) in different solvents at the PCM-[TPSS+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP] level of theory.

	PhNH ₂			PhOH			PhSH		
	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}
TS _{OA}	12.7	13.5	14.4	6.1	7.6	8.6	9.6	11.2	12.4
INT _{OA/RE}	-0.5	-0.8	-0.7	0.7	1.8	2.9	0.9	1.1	1.3
TS _{RE}	1.4	0.2	-0.9	10.7	10.9	10.9	4.7	5.3	5.7
TS _{Met}	22.8	23.2	23.8	22.6	24.2	25.8	22.3	23.6	25.3
TS _{HAT}	33.3	27.5	30.3	29.7	29.5	33.0	32.4	32.0	35.3
INT _{HAT}	23.3	20.9	18.6	24.4	23.7	22.9	28.1	27.2	26.4
TS _{SET}	110.2	55.4	32.5	129.1	64.6	38.8	132.9	67.3	34.6
INT _{SET}	107.7	55.3	22.2	116.2	64.5	31.6	118.8	67.2	41.0
Prod	-31.6	-34.6	-36.5	-24.1	-25.4	-26.1	-17.4	-18.8	-19.3

Table S5. Gibbs Free Energies (kcal/mol) for Key Stationary Points in the Mechanisms of Ullmann-Type X-Arylation Reactions (X = NH, O, S) in different solvents at the PCM-[PBE/def2-TZVPP//B3LYP/def2-SVP] level of theory.

	PhNH ₂			PhOH			PhSH		
	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}
TS _{OA}	24.9	25.6	26.5	18.6	20.1	21.0	22.8	24.2	25.4
INT _{OA/RE}	15.1	14.9	15.0	15.8	16.8	17.9	16.6	16.8	16.8
TS _{RE}	16.6	15.4	14.4	24.7	24.9	25.0	19.6	20.1	20.5
TS _{Met}	32.5	32.9	33.4	31.6	33.2	34.8	30.5	31.7	33.3
TS _{HAT}	34.1	32.5	34.9	35.0	34.7	37.8	37.0	36.5	39.4
INT _{HAT}	30.3	28.0	25.8	31.5	31.0	30.2	34.2	33.3	32.5
TS _{SET}	122.7	59.6	35.1	134.5	68.7	41.4	126.8	69.8	42.4
INT _{SET}	111.8	59.6	26.2	119.9	68.4	35.3	121.2	69.7	36.8
Prod	-32.0	-34.8	-36.7	-23.5	-24.8	-25.3	-17.8	-19.3	-19.8

Table S6. Gibbs Free Energies (kcal/mol) for Key Stationary Points in the Mechanisms of Ullmann-Type X-Arylation Reactions (X = NH, O, S) in different solvents at the PCM-[PBE+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP] level of theory.

	PhNH ₂			PhOH			PhSH		
	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}	ΔG_{gas}	ΔG_{tol}	ΔG_{acn}
TS _{OA}	14.9	15.6	16.5	8.7	10.1	11.1	12.6	14.1	15.3
INT _{OA/RE}	4.5	4.3	4.4	5.2	6.3	7.4	5.5	5.7	5.8
TS _{RE}	6.1	5.0	4.0	14.8	15.0	15.1	9.1	9.6	10.0
TS _{Met}	24.2	24.6	25.1	23.9	25.5	27.1	23.2	24.4	26.0

TS _{HAT}	33.2	31.7	34.1	33.8	33.5	36.8	36.3	35.8	38.7
INT _{HAT}	29.1	26.8	24.7	29.9	29.4	28.6	33.2	32.3	31.6
TS _{SET}	126.2	61.7	36.7	138.3	71.0	43.2	130.7	72.6	44.5
INT _{SET}	114.2	61.7	28.6	122.4	70.6	37.8	124.2	72.5	39.8
Prod	-32.1	-34.9	-36.8	-23.8	-25.1	-25.6	-17.3	-18.8	-19.3

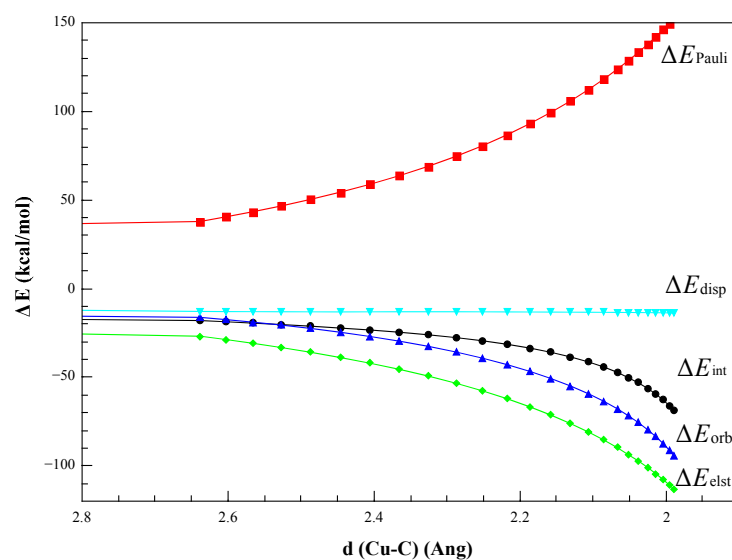


Figure S1. EDA of the interaction energy for the oxidative addition reaction of PhI (**1**) to [(phen)Cu^I(OPh)] projected onto the forming Cu-C bond. All data have been computed at the BP86+D3(BJ)/TZ2P+//B3LYP/def2-SVP level.

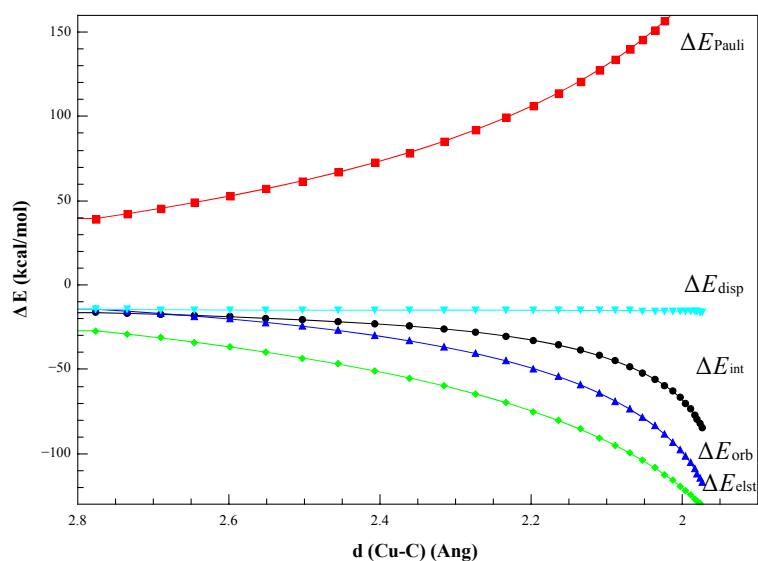


Figure S2. EDA of the interaction energy for the oxidative addition reaction of PhI (**1**) to [(phen)Cu^I(SPh)] projected onto the forming Cu-C bond. All data have been computed at the BP86+D3(BJ)/TZ2P+//B3LYP/def2-SVP level.

Cartesian coordinates (Å) and energies (au).**HI**

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -298.406660199

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -298.407496229

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -298.408407861

1 0.000000 0.000000 -1.594027

53 0.000000 0.000000 0.030076

PhI

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -529.560359051

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -529.561755658

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -529.563386024

6 0.568347 -0.000045 0.000348

6 1.256087 -1.217515 0.000350

6 2.655637 -1.209020 -0.000021

6 3.357234 0.000035 -0.000265

6 2.655510 1.209046 -0.000080

6 1.256032 1.217517 0.000235

1 0.712326 2.163553 0.000389

1 3.196601 2.158825 0.000049

1 4.449859 0.000139 -0.000625

1 3.196708 -2.158786 -0.000396

1 0.712494 -2.163668 0.000251

53 -1.561530 -0.000003 -0.000058

PhNH₂

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -287.744493783

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -287.747335585

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -287.750847934

6 0.945628 0.000119 0.008911

6 0.221623 -1.209798 0.004274

6 0.221660 1.209791 0.004075

6 -1.173238 -1.203912 -0.003271

6 -1.173394 1.203806 -0.003104

6 -1.885597 0.000044 -0.006807

1 0.764608 -2.159701 0.010292

1 0.764399 2.159843 0.009936

1 -1.710076 -2.156680 -0.007783

1 -1.710035 2.156695 -0.007684

1 -2.977785 -0.000141 -0.013415

7 2.333503 -0.000045 0.068151

1 2.796804 -0.844566 -0.246909

1 2.797470 0.844561 -0.245961

PhOH

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -307.616903114

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -307.619628787

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -307.622915767

8	-2.304643	-0.111562	0.000152
6	-0.948159	-0.027192	-0.000117
6	-0.267369	1.198913	-0.000078
6	-0.219380	-1.226399	-0.000126
6	1.130545	1.222004	-0.000143
6	1.174830	-1.190544	-0.000052
6	1.860282	0.030644	0.000232
1	-0.834470	2.135678	0.000069
1	-0.766544	-2.171402	-0.000136
1	1.649436	2.184257	-0.000085
1	1.733880	-2.130115	0.000022
1	2.952332	0.051717	0.000408
1	-2.681986	0.777805	0.000207

PhSH

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -861.741511540

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -861.743581382

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -861.746099635

6	0.196443	1.213507	0.000024
6	-0.513366	0.001975	0.000072
6	0.198548	-1.209837	0.000106
6	1.594452	-1.204189	-0.000004
6	2.300896	0.002845	-0.000050
6	1.593717	1.208320	0.000008
16	-2.292521	-0.083681	-0.000084
1	-0.342757	-2.159562	0.000123
1	2.133659	-2.155163	-0.000069
1	3.393344	0.003483	-0.000139
1	2.131404	2.160221	-0.000084
1	-0.341046	2.165248	-0.000036
1	-2.518417	1.248944	0.000616

Ph₂NH

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -518.898833284

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -518.901527765

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -518.905020155

6	0.000000	1.267763	0.432647
6	-0.452436	2.360612	1.202050
6	0.477810	1.520668	-0.869155
6	-0.431754	3.655853	0.687884
6	0.479807	2.821088	-1.378097
6	0.026405	3.898223	-0.611333
1	-0.827512	2.180952	2.214071
1	0.872200	0.704641	-1.474504
1	-0.787012	4.483116	1.308169
1	0.857241	2.992409	-2.389942
1	0.033933	4.911922	-1.017952
7	0.000000	0.000000	1.017479

6	0.000000	-1.267763	0.432647
6	0.452436	-2.360612	1.202050
6	-0.477810	-1.520668	-0.869155
6	0.431754	-3.655853	0.687884
6	-0.479807	-2.821088	-1.378097
6	-0.026405	-3.898223	-0.611333
1	0.827512	-2.180952	2.214071
1	-0.872200	-0.704641	-1.474504
1	0.787012	-4.483116	1.308169
1	-0.857241	-2.992409	-2.389942
1	-0.033933	-4.911922	-1.017952
1	0.000000	0.000000	2.030002

Ph₂O

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -538.764070671

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -538.766033282

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -538.768423859

6	0.000000	1.202548	0.496672
6	-0.732675	2.246127	1.074743
6	0.751918	1.424567	-0.665033
6	-0.714008	3.512951	0.487551
6	0.755537	2.695261	-1.246554
6	0.025785	3.743564	-0.676939
1	-1.304043	2.044702	1.983013
1	1.331588	0.610584	-1.104101
1	-1.286840	4.324896	0.943043
1	1.344173	2.866656	-2.151655
1	0.035714	4.734565	-1.136538
8	0.000000	0.000000	1.160899
6	0.000000	-1.202548	0.496672
6	0.732675	-2.246127	1.074743
6	-0.751918	-1.424567	-0.665033
6	0.714008	-3.512951	0.487551
6	-0.755537	-2.695261	-1.246554
6	-0.025785	-3.743564	-0.676939
1	1.304043	-2.044702	1.983013
1	-1.331588	-0.610584	-1.104101
1	1.286840	-4.324896	0.943043
1	-1.344173	-2.866656	-2.151655
1	-0.035714	-4.734565	-1.136538

Ph₂S

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -861.741511540

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -861.743581382

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -861.746099635

6	-1.456877	0.617979	0.901449
6	-1.409620	-0.503760	0.057217
6	-2.533787	-0.837690	-0.713579
6	-3.694538	-0.061985	-0.634869
6	-3.736159	1.061631	0.194558
6	-2.611783	1.400143	0.956656
16	-0.000003	-1.605790	-0.000003

6	1.409619	-0.503768	-0.057219
6	1.456897	0.617946	-0.901483
6	2.611806	1.400107	-0.956691
6	3.736160	1.061621	-0.194551
6	3.694519	-0.061970	0.634910
6	2.533771	-0.837679	0.713608
1	2.492392	-1.703096	1.379325
1	4.565388	-0.332584	1.237709
1	4.640179	1.673232	-0.247826
1	2.637885	2.275045	-1.611745
1	0.589651	0.875976	-1.512780
1	-2.492427	-1.703127	-1.379270
1	-4.565422	-0.332622	-1.237636
1	-4.640175	1.673245	0.247836
1	-2.637849	2.275101	1.611684
1	-0.589618	0.876024	1.512721

[Cu(phen)I]

E (B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP)= -2510.37223137

E (PCM(toluene)-[B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP])= -2510.38418108

E (PCM(ACN)-[B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP])= -2510.39552099

29	-0.949875	-0.115456	0.000125
7	0.628070	1.333858	0.000148
7	0.711412	-1.366044	0.000102
6	0.548765	2.656649	0.000148
1	-0.459725	3.082524	0.000236
6	1.691035	3.484467	0.000045
1	1.572295	4.569754	0.000048
6	2.945964	2.899977	-0.000054
1	3.850689	3.513702	-0.000135
6	3.057210	1.488900	-0.000063
6	1.847060	0.747201	0.000039
6	4.311522	0.785093	-0.000162
1	5.236570	1.367218	-0.000238
6	4.354369	-0.580328	-0.000154
1	5.314050	-1.103254	-0.000222
6	1.892335	-0.700130	0.000028
6	3.147365	-1.363014	-0.000059
6	3.129859	-2.778088	-0.000045
1	4.072850	-3.331094	-0.000107
6	1.915901	-3.443369	0.000045
1	1.867653	-4.533981	0.000059
6	0.722399	-2.693669	0.000113
1	-0.253596	-3.187931	0.000171
53	-3.404028	0.003291	-0.000084

[Cu(phen)NHPh]

E (B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP)= -2499.64729312

E (PCM(toluene)-[B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP])= -2499.65690489

E (PCM(ACN)-[B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP])= -2499.66799135

29	0.633614	-0.222110	-0.035108
7	-0.752028	1.184215	-0.025812

6	-2.058292	0.792571	-0.013211
6	-2.341612	-0.624385	0.013731
7	-1.289776	-1.474742	0.016743
6	-1.519697	-2.777487	0.048203
6	-2.817913	-3.327533	0.074516
6	-3.906415	-2.470302	0.067397
6	-3.691722	-1.073519	0.036677
6	-4.754767	-0.106471	0.027070
6	-4.485709	1.231714	-0.002432
6	-3.133201	1.722116	-0.022454
6	-2.811661	3.097861	-0.049151
6	-0.480763	2.492859	-0.052316
1	0.575962	2.770891	-0.065614
1	-1.190258	4.532726	-0.086296
1	-3.611673	3.842293	-0.056841
1	-5.300558	1.960042	-0.010184
1	-5.787542	-0.464032	0.043411
1	-4.927942	-2.859473	0.085589
1	-2.949491	-4.411125	0.098666
1	-0.639781	-3.429962	0.053143
7	2.288901	-1.069303	-0.085379
6	3.546846	-0.550171	-0.029481
6	4.715367	-1.355975	-0.166036
6	5.994253	-0.807916	-0.107430
6	6.185410	0.565658	0.090747
6	5.051494	1.378789	0.231733
6	3.769380	0.842523	0.175355
1	4.592852	-2.433173	-0.323056
1	6.861039	-1.467254	-0.219303
1	7.190397	0.991668	0.136074
1	5.172033	2.455197	0.392065
1	2.894333	1.488262	0.298196
6	-1.478459	3.480109	-0.064947
1	2.320921	-2.078702	-0.214402

[Cu(phen)OPh]

E (B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP)= -2519.53070551

E (PCM(toluene)-[B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP])= -2519.54166661

E (PCM(ACN)-[B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP])= -2519.55323864

29	0.637696	0.154660	-0.000191
7	-0.939381	1.327248	-0.000263
6	-2.159724	0.717670	-0.000121
6	-2.203611	-0.730512	-0.000172
7	-1.027927	-1.389209	-0.000470
6	-1.018490	-2.710323	-0.000395
6	-2.206379	-3.473998	-0.000043
6	-3.424875	-2.816081	0.000189
6	-3.456521	-1.400758	0.000121
6	-4.667321	-0.626692	0.000353
6	-4.627118	0.738381	0.000339
6	-3.376413	1.450185	0.000128
6	-3.291315	2.861751	0.000204

6	-0.892456	2.660753	-0.000178
1	0.101885	3.113381	-0.000291
1	-1.940458	4.551902	0.000113
1	-4.206224	3.459662	0.000388
1	-5.552894	1.319142	0.000514
1	-5.625764	-1.152117	0.000548
1	-4.363874	-3.376213	0.000432
1	-2.152773	-4.564576	0.000026
1	-0.031142	-3.184925	-0.000640
8	2.224332	-0.787169	0.000151
6	3.472417	-0.383131	0.000119
6	4.524682	-1.340146	0.000317
6	5.861993	-0.949540	0.000344
6	6.218512	0.406148	0.000167
6	5.198642	1.365403	-0.000054
6	3.856722	0.984761	-0.000081
1	4.245265	-2.397236	0.000450
1	6.643483	-1.716411	0.000499
1	7.268901	0.707869	0.000209
1	5.453168	2.430456	-0.000205
1	3.062331	1.739259	-0.000295
6	-2.045172	3.465416	0.000050

[Cu(phen)SPh]

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -2842.52106118

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2842.53158968

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2842.54331467

6	3.276859	0.291064	-0.973815
6	3.421614	-0.720264	0.001695
6	4.575433	-0.678467	0.813475
6	5.527065	0.333428	0.667783
6	5.361012	1.337465	-0.292808
6	4.228175	1.304983	-1.114341
16	2.260139	-2.052566	0.193018
29	0.316436	-1.071376	0.013395
7	-1.721870	-1.402712	-0.071735
6	-2.469253	-0.270894	-0.023158
6	-3.888979	-0.286707	-0.042754
6	-4.520833	-1.549253	-0.128170
6	-3.744540	-2.695063	-0.184643
6	-2.341958	-2.575962	-0.151311
6	-1.767487	0.990942	0.059183
6	-2.505523	2.201472	0.139229
6	-3.942613	2.149883	0.119959
6	-4.605049	0.958796	0.029297
6	-1.763870	3.402385	0.234271
6	-0.380431	3.347480	0.244795
6	0.259345	2.094176	0.150613
7	-0.413680	0.954088	0.057099
1	1.351266	2.017766	0.142393
1	0.221913	4.254900	0.319714
1	-2.288953	4.359076	0.299152

1	-1.702676	-3.462607	-0.187921
1	-4.199843	-3.685063	-0.250438
1	-5.612173	-1.608602	-0.147085
1	-4.498959	3.088827	0.179257
1	-5.697552	0.932807	0.014216
1	4.710585	-1.454953	1.570458
1	6.408730	0.338650	1.315887
1	6.107017	2.128422	-0.405437
1	4.088855	2.071027	-1.883870
1	2.407959	0.258276	-1.636409

I-

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -297.896555781
 E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -297.953318449
 E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -297.991986579
 53 0.000000 0.000000 0.000000

Ph•

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -231.667663370
 E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -231.668861928
 E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -231.670335776
 6 -0.000083 -1.400728 -0.000011
 6 1.229208 -0.773401 0.000015
 6 1.216447 0.633089 0.000007
 6 0.000034 1.326166 -0.000004
 6 -1.216352 0.633255 -0.000004
 6 -1.229256 -0.773368 0.000014
 1 2.171933 -1.328032 -0.000050
 1 2.162074 1.183296 -0.000013
 1 0.000175 2.418995 -0.000004
 1 -2.162023 1.183381 -0.000005
 1 -2.172147 -1.327718 -0.000021

INT_{HAT} (N)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -2797.49672298
 E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2797.50888344
 E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2797.52256488
 29 -0.421773 0.116763 -0.039873
 7 1.151590 -0.766952 1.008175
 6 2.373111 -0.200567 0.858939
 6 2.488810 0.964038 0.004095
 7 1.371860 1.412975 -0.609634
 6 1.458569 2.454018 -1.421974
 6 2.669388 3.133314 -1.669673
 6 3.821693 2.691498 -1.044018
 6 3.760643 1.572504 -0.180703
 6 4.909317 1.029238 0.491650
 6 4.800426 -0.072882 1.289752
 6 3.534090 -0.724037 1.489619
 6 3.374738 -1.880395 2.287822
 6 1.031216 -1.864637 1.744455
 1 0.032689 -2.306730 1.799924

1	1.965808	-3.354603	3.008580
1	4.243231	-2.313022	2.791358
1	5.681166	-0.484457	1.789079
1	5.878258	1.512496	0.342989
1	4.779558	3.190257	-1.214241
1	2.684480	3.987388	-2.349577
1	0.532324	2.771055	-1.912959
7	-1.787918	1.380626	0.347652
6	-3.099339	1.245023	0.695459
6	-3.994054	2.352377	0.720804
6	-5.317919	2.197249	1.118125
6	-5.804394	0.937154	1.492252
6	-4.941793	-0.169960	1.458843
6	-3.616131	-0.027220	1.071051
1	-3.621660	3.338557	0.425990
1	-5.982198	3.065734	1.133340
1	-6.846195	0.816701	1.798581
1	-5.316679	-1.159519	1.733959
1	-2.951265	-0.891732	1.017317
6	2.122099	-2.455096	2.410395
53	-0.939986	-1.795805	-1.724373
1	-1.600401	2.343119	0.059034

INT_{SET} (N)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -2499.45861147

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2499.49266389

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2499.51611121

29	-0.577918	-0.012893	-0.627058
7	0.951179	-1.358257	-0.257466
6	2.119211	-0.720493	0.010500
6	2.112902	0.724790	0.001886
7	0.939470	1.349170	-0.274108
6	0.901003	2.677097	-0.289890
6	2.036685	3.469567	-0.030148
6	3.240393	2.848499	0.252655
6	3.309536	1.434100	0.276110
6	4.512758	0.698941	0.558947
6	4.518786	-0.667136	0.566773
6	3.322055	-1.416056	0.292628
6	3.265301	-2.831189	0.285487
6	0.924257	-2.686515	-0.257659
1	-0.035660	-3.161929	-0.477812
1	1.991918	-4.554662	-0.002556
1	4.168145	-3.409756	0.496854
1	5.439188	-1.214574	0.782450
1	5.428270	1.256918	0.768332
1	4.138024	3.437363	0.457696
1	1.952114	4.557313	-0.055695
1	-0.062805	3.141576	-0.516292
7	-2.387141	-0.029555	-1.103327
6	-3.513568	-0.012473	-0.347639
6	-4.812634	-0.043505	-0.939633

6	-5.950679	-0.026343	-0.147101
6	-5.839200	0.022730	1.252464
6	-4.569166	0.054836	1.855302
6	-3.423392	0.037877	1.076035
1	-4.898867	-0.081496	-2.029333
1	-6.937603	-0.050918	-0.614620
1	-6.738468	0.036300	1.872112
1	-4.485277	0.093573	2.943823
1	-2.434094	0.064060	1.540546
6	2.066970	-3.465996	0.010451
1	-2.617133	-0.061770	-2.099510

TS_{MET}(N)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3029.18523210

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3029.19418287

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3029.20492339

6	-1.329827	2.366856	1.221115
6	-1.747536	1.994501	-0.079869
6	-2.615327	2.881016	-0.764777
6	-3.027823	4.078579	-0.183064
6	-2.601507	4.431451	1.103041
6	-1.750618	3.563067	1.798245
7	-1.358788	0.775476	-0.606317
29	0.366084	-0.138077	-0.298385
7	1.795691	-0.591643	1.137221
6	3.051843	-0.209949	0.790516
6	4.170822	-0.381483	1.648805
6	3.942679	-1.008762	2.894951
6	2.661411	-1.422788	3.220639
6	1.613170	-1.190107	2.310866
6	5.462241	0.085311	1.220320
6	5.629716	0.682898	0.003984
6	4.523591	0.849515	-0.899810
6	3.235024	0.393939	-0.510633
6	4.641830	1.437677	-2.180132
6	3.521333	1.536040	-2.988541
6	2.291005	1.040258	-2.515142
7	2.151067	0.484108	-1.318425
1	1.391275	1.096161	-3.135667
1	3.578107	1.981676	-3.983585
1	5.613849	1.804804	-2.519821
1	0.590998	-1.499504	2.546392
1	2.449448	-1.915417	4.171487
1	4.776236	-1.162184	3.585163
1	6.615288	1.038361	-0.307228
1	6.312460	-0.045255	1.894572
1	-2.959323	2.613741	-1.768232
1	-3.693390	4.745188	-0.739267
1	-2.925873	5.371411	1.556204
1	-1.407769	3.825314	2.803538
1	-0.654117	1.697026	1.758989
6	-2.868274	-0.718934	-0.100982

53	-1.217206	-2.380432	-0.846709
6	-3.957727	-0.588007	-0.969106
6	-5.235607	-0.384669	-0.433042
6	-5.436549	-0.336234	0.949349
6	-4.334632	-0.487229	1.799737
6	-3.050264	-0.682640	1.285623
1	-3.823835	-0.654786	-2.051365
1	-6.083120	-0.275694	-1.116682
1	-6.437471	-0.185452	1.359928
1	-4.469847	-0.453435	2.885066
1	-2.198277	-0.794086	1.958852
1	-1.628765	0.721861	-1.589479

TS_{OA} (N)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3029.20095705

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3029.20935418

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3029.21968227

6	1.340196	3.383102	-1.484264
6	0.977692	2.008610	-1.627962
6	1.990555	1.152912	-2.156136
6	3.250485	1.634484	-2.501566
6	3.579506	2.988629	-2.350032
6	2.601033	3.853533	-1.841180
7	-0.260904	1.534529	-1.313674
29	-0.682205	-0.103650	-0.296436
7	0.836902	-1.623390	-0.395731
6	1.919504	-1.421662	0.391861
6	3.110914	-2.186047	0.251138
6	3.120091	-3.203657	-0.729491
6	1.994272	-3.410768	-1.507436
6	0.871868	-2.585216	-1.308589
6	1.855722	-0.376633	1.394782
6	3.008974	-0.093860	2.178971
6	4.200220	-0.877527	1.997455
6	4.245481	-1.888231	1.082089
6	2.914485	0.962074	3.113515
6	1.727857	1.665396	3.224348
6	0.636963	1.289038	2.415786
7	0.692253	0.294472	1.543515
6	-2.717934	0.487255	0.198896
6	-2.803867	0.787603	1.568097
6	-3.352346	2.012282	1.966223
6	-3.853202	2.907665	1.016014
6	-3.804840	2.573544	-0.344301
6	-3.258955	1.358711	-0.761346
53	-2.774041	-1.783241	-0.304640
1	-0.317583	1.820292	2.487481
1	1.622405	2.493740	3.927711
1	3.779491	1.215456	3.732069
1	-0.028913	-2.711257	-1.917579
1	1.967068	-4.187606	-2.273835
1	4.017532	-3.812780	-0.866340

1	5.073982	-0.646770	2.612183
1	5.154433	-2.481422	0.954144
1	-3.210836	1.108717	-1.822080
1	-4.200281	3.264788	-1.093544
1	-4.293333	3.856126	1.332734
1	-3.401563	2.255392	3.031457
1	-2.441229	0.077665	2.313572
1	1.745727	0.100917	-2.315866
1	3.991370	0.939232	-2.910358
1	4.568653	3.360970	-2.627063
1	2.827149	4.917725	-1.716958
1	0.593896	4.078973	-1.085663
1	-0.845646	2.300767	-0.979529

INT_{OA/RE} (N)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3029.22161522

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3029.23091736

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3029.24202989

6	-1.250025	2.887302	-0.015785
6	-2.093713	2.082137	-0.824081
6	-3.418975	2.540958	-1.041911
6	-3.856049	3.757218	-0.522930
6	-3.004295	4.545272	0.260587
6	-1.702691	4.093291	0.513419
7	-1.622483	0.930051	-1.417522
29	-0.470783	-0.352904	-0.534012
7	1.301487	0.633009	-1.166731
6	2.309809	0.822960	-0.286886
6	3.582273	1.305972	-0.693864
6	3.751296	1.614580	-2.064196
6	2.692430	1.445777	-2.938231
6	1.472708	0.946128	-2.441623
6	2.067819	0.518646	1.107890
6	3.130861	0.656402	2.041825
6	4.411410	1.131633	1.593819
6	4.625594	1.451839	0.284068
6	2.857906	0.309829	3.386064
6	1.595572	-0.138350	3.727637
6	0.605894	-0.218853	2.724650
7	0.830420	0.108657	1.463243
6	-2.184008	-1.021177	0.132581
6	-2.669286	-0.395799	1.280983
6	-3.828945	-0.887321	1.899911
6	-4.514080	-1.971684	1.347145
6	-4.038707	-2.563474	0.172056
6	-2.871070	-2.092091	-0.442223
53	0.667711	-2.721964	-0.735282
1	-0.402472	-0.568087	2.967829
1	1.352429	-0.424264	4.752835
1	3.647714	0.395020	4.137228
1	0.604264	0.801381	-3.090968
1	2.787781	1.684144	-3.999105

1	4.716696	1.986527	-2.417592
1	5.214869	1.234651	2.327632
1	5.601312	1.817717	-0.045346
1	-2.492037	-2.583719	-1.339712
1	-4.570001	-3.411257	-0.269995
1	-5.422224	-2.349169	1.824236
1	-4.202923	-0.401231	2.805714
1	-2.179212	0.492884	1.688221
1	-4.098311	1.925407	-1.638923
1	-4.879046	4.088890	-0.721451
1	-3.352411	5.493979	0.675729
1	-1.028813	4.693469	1.131489
1	-0.234626	2.544573	0.186980
1	-2.395279	0.448175	-1.876841

TS_{RE}(N)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3029.21822593

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3029.22948718

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3029.24266196

6	-3.852666	2.060664	-0.987360
6	-2.517939	1.763824	-0.618638
6	-1.867965	2.647490	0.276135
6	-2.517683	3.783864	0.755019
6	-3.827453	4.079385	0.358997
6	-4.486290	3.209012	-0.518016
7	-1.847907	0.679313	-1.151032
29	-0.351236	-0.284104	-0.398898
7	1.230519	1.072665	-0.917332
6	2.258820	1.135988	-0.044456
6	3.452107	1.852032	-0.325044
6	3.522072	2.524290	-1.567973
6	2.450294	2.457726	-2.441687
6	1.313429	1.710665	-2.073833
6	2.120739	0.426289	1.207458
6	3.197575	0.430342	2.133472
6	4.392479	1.167134	1.820629
6	4.513350	1.851877	0.644969
6	3.024937	-0.310628	3.326003
6	1.842201	-0.997875	3.532788
6	0.829745	-0.929134	2.553619
7	0.960754	-0.231887	1.435780
6	-2.051804	-1.024948	0.298981
6	-2.454985	-0.543462	1.543183
6	-3.370312	-1.288266	2.302118
6	-3.905014	-2.474240	1.793132
6	-3.523719	-2.916214	0.520684
6	-2.598703	-2.191519	-0.240141
53	0.846812	-2.408111	-1.522566
1	-0.117522	-1.460277	2.687964
1	1.679826	-1.588055	4.436672
1	3.828500	-0.338573	4.066759
1	0.444220	1.625360	-2.733688

1	2.474413	2.966275	-3.407278
1	4.422488	3.087429	-1.827435
1	5.210062	1.164759	2.545943
1	5.427856	2.405743	0.418226
1	-2.279818	-2.558443	-1.217395
1	-3.939267	-3.841816	0.112729
1	-4.627410	-3.047314	2.379805
1	-3.676568	-0.920915	3.285771
1	-2.086494	0.412148	1.924686
1	-0.842157	2.426962	0.578602
1	-1.992476	4.451988	1.443306
1	-4.331223	4.973481	0.733468
1	-5.512401	3.421257	-0.830645
1	-4.381757	1.378614	-1.659290
1	-2.458331	0.123881	-1.746284

INT_{HAT} (O)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -2817.37758565

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2817.38879507

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2817.40157823

29	-0.228969	-0.041126	-0.002559
7	1.618772	-1.045535	0.438040
6	2.716418	-0.263850	0.303374
6	2.510885	1.118185	-0.061150
7	1.237455	1.521007	-0.247988
6	0.984323	2.782562	-0.556755
6	2.018166	3.729810	-0.719886
6	3.333637	3.332737	-0.548124
6	3.620253	1.989580	-0.202973
6	4.944522	1.469648	0.007780
6	5.141927	0.159558	0.344583
6	4.034868	-0.745336	0.506007
6	4.171138	-2.107965	0.864158
6	1.770280	-2.321367	0.766712
1	0.850687	-2.912108	0.829253
1	3.110519	-3.947952	1.267223
1	5.167009	-2.526413	1.032807
1	6.153398	-0.223440	0.501320
1	5.796150	2.144732	-0.107561
1	4.153581	4.045250	-0.672081
1	1.769422	4.760486	-0.979720
1	-0.075390	3.033857	-0.663478
8	-1.523516	1.333781	0.212700
6	-2.823226	1.328265	0.419640
6	-3.693354	1.991987	-0.484233
6	-5.061753	2.065492	-0.235961
6	-5.610577	1.469013	0.907130
6	-4.767282	0.794878	1.802063
6	-3.397521	0.721703	1.567185
1	-3.255735	2.443187	-1.378284
1	-5.712472	2.587296	-0.943759
1	-6.685581	1.522982	1.096146

1	-5.188220	0.319568	2.692790
1	-2.735943	0.191857	2.256810
6	3.039612	-2.893429	0.994436
53	-1.549183	-2.112717	-0.791191

INT_{SET} (O)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -2519.32332774
 E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2519.35799624
 E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2519.38239286

29	0.550596	-0.000158	-0.418939
7	-0.965549	1.355433	-0.177751
6	-2.152931	0.722493	0.008901
6	-2.152982	-0.722443	0.008970
7	-0.965660	-1.355488	-0.177674
6	-0.931916	-2.683853	-0.188637
6	-2.088424	-3.468559	-0.011266
6	-3.306015	-2.840068	0.181773
6	-3.369654	-1.425154	0.196506
6	-4.586679	-0.682959	0.386499
6	-4.586633	0.683217	0.386408
6	-3.369555	1.425307	0.196332
6	-3.305824	2.840217	0.181430
6	-0.931718	2.683790	-0.188854
1	0.043299	3.153798	-0.344491
1	-2.008061	4.556803	-0.029603
1	-4.219082	3.424060	0.321333
1	-5.517744	1.235980	0.530386
1	-5.517827	-1.235638	0.530559
1	-4.219304	-3.423836	0.321781
1	-2.008388	-4.556771	-0.029107
1	0.043059	-3.153939	-0.344299
8	2.342516	-0.000134	-0.823729
6	3.511726	-0.000043	-0.270323
6	4.677774	-0.000447	-1.102402
6	5.940778	-0.000363	-0.533851
6	6.087895	0.000140	0.865921
6	4.952940	0.000542	1.701269
6	3.682672	0.000446	1.151120
1	4.531831	-0.000817	-2.184511
1	6.827007	-0.000680	-1.172571
1	7.086784	0.000211	1.308038
1	5.078645	0.000934	2.786508
1	2.791203	0.000760	1.784049
6	-2.088185	3.468599	-0.011635

TS_{MET}(O)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3049.06532304
 E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3049.07399234
 E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3049.08398199

6	0.911776	2.202852	-1.554195
6	1.497562	1.879403	-0.309131
6	2.249523	2.876907	0.352071

6	2.399655	4.144669	-0.211032
6	1.803026	4.456690	-1.438731
6	1.055920	3.477259	-2.103615
8	1.351296	0.663730	0.228475
29	-0.331295	-0.422955	0.250750
7	-1.924361	-0.857150	-1.050285
6	-3.106510	-0.360766	-0.606921
6	-4.325988	-0.535242	-1.314301
6	-4.277294	-1.281667	-2.514360
6	-3.066416	-1.800764	-2.942352
6	-1.909102	-1.561004	-2.177123
6	-5.531235	0.049328	-0.790167
6	-5.520784	0.767064	0.371635
6	-4.306902	0.950816	1.120807
6	-3.100915	0.376557	0.637958
6	-4.237816	1.674608	2.333835
6	-3.022741	1.789283	2.988590
6	-1.885287	1.169117	2.435601
7	-1.924294	0.478757	1.302404
1	-0.912307	1.234587	2.931655
1	-2.934319	2.343462	3.925021
1	-5.141384	2.135559	2.741346
1	-0.937541	-1.954249	-2.491427
1	-2.993534	-2.383736	-3.862538
1	-5.192463	-1.441856	-3.090316
1	-6.442474	1.211620	0.755611
1	-6.461595	-0.089082	-1.346769
1	2.704770	2.630997	1.313235
1	2.986299	4.902349	0.316891
1	1.918959	5.453098	-1.872639
1	0.586269	3.707859	-3.064592
1	0.332206	1.432087	-2.069484
6	3.000915	-0.471514	0.104461
53	1.418055	-2.340312	0.710480
6	3.868290	-0.144738	1.144269
6	5.204878	0.132017	0.831260
6	5.657127	0.091795	-0.492039
6	4.754287	-0.225110	-1.512433
6	3.413623	-0.507659	-1.224622
1	3.517131	-0.120120	2.176870
1	5.896378	0.380287	1.642028
1	6.701790	0.308962	-0.726038
1	5.088618	-0.256426	-2.553644
1	2.710495	-0.753631	-2.021813

TS_{OA} (O)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3049.09082209

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3049.09952737

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3049.11042309

6	1.999321	-1.210911	-2.603957
6	0.854866	-1.627663	-1.863154
6	0.866116	-2.971424	-1.384049

6	1.937294	-3.828689	-1.637557
6	3.049701	-3.394097	-2.370122
6	3.063954	-2.076952	-2.850164
8	-0.154658	-0.823569	-1.654520
29	-0.633109	-0.012333	0.122177
7	1.212530	-0.319436	1.097450
6	2.099828	0.690741	0.943885
6	3.459207	0.574642	1.334969
6	3.869084	-0.659507	1.893674
6	2.950818	-1.683453	2.029316
6	1.621544	-1.469661	1.612467
6	1.630945	1.920270	0.341519
6	2.540569	2.994911	0.146780
6	3.907069	2.848160	0.567229
6	4.346685	1.687797	1.137333
6	2.036454	4.163744	-0.470327
6	0.709556	4.210175	-0.857685
6	-0.112454	3.090108	-0.615172
7	0.331051	1.989863	-0.028161
6	-2.602201	0.328831	-0.298343
6	-3.129169	1.544813	0.159115
6	-3.963787	2.283546	-0.689581
6	-4.293750	1.792345	-1.956575
6	-3.780060	0.560761	-2.382268
6	-2.944219	-0.190857	-1.552398
53	-2.371166	-1.271342	1.570167
1	-1.166673	3.094388	-0.908268
1	0.290909	5.092917	-1.344778
1	2.701963	5.014198	-0.640905
1	0.869382	-2.257338	1.707184
1	3.236580	-2.652043	2.442856
1	4.909021	-0.792969	2.202904
1	4.592700	3.685269	0.413789
1	5.389873	1.582707	1.445711
1	-2.506065	-1.130334	-1.889172
1	-4.028821	0.175571	-3.374843
1	-4.959154	2.363107	-2.609163
1	-4.371189	3.237519	-0.342889
1	-2.901937	1.911619	1.161907
1	-0.010016	-3.318885	-0.828008
1	1.901684	-4.857618	-1.263746
1	3.884658	-4.070257	-2.570896
1	3.921270	-1.721766	-3.431876
1	2.005712	-0.187533	-2.990297

INT_{OA/RE} (O)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3049.09810529

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3049.10694815

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3049.11732839

6	0.087817	3.319642	-0.567897
6	0.430298	2.226351	-1.408698
6	1.713760	2.246776	-2.016663

6	2.592810	3.310127	-1.809578
6	2.238023	4.377171	-0.975787
6	0.979018	4.369742	-0.358426
8	-0.419045	1.249898	-1.662806
29	-0.768353	-0.203808	-0.436966
7	1.053268	-1.097650	-0.950844
6	2.090810	-1.004900	-0.088893
6	3.353672	-1.595291	-0.368603
6	3.497096	-2.272488	-1.601308
6	2.426831	-2.333962	-2.475461
6	1.210604	-1.730459	-2.104673
6	1.900077	-0.273746	1.147869
6	2.980315	-0.169147	2.066208
6	4.237262	-0.795377	1.759794
6	4.417103	-1.476739	0.591161
6	2.752754	0.571798	3.249636
6	1.519740	1.161574	3.455276
6	0.515808	0.998096	2.477276
7	0.697319	0.298492	1.370028
6	-2.507580	0.574631	0.003159
6	-2.925530	0.688638	1.328266
6	-4.077746	1.437397	1.616007
6	-4.809294	2.029748	0.584338
6	-4.386104	1.879824	-0.740796
6	-3.227627	1.150960	-1.040025
53	-1.862995	-2.466167	0.086795
1	-0.466843	1.461359	2.607449
1	1.313207	1.749120	4.351850
1	3.556373	0.676311	3.983439
1	0.339081	-1.772944	-2.763014
1	2.505135	-2.844570	-3.436830
1	4.453914	-2.737809	-1.852375
1	5.053236	-0.707357	2.481524
1	5.378796	-1.942498	0.362162
1	-2.873192	1.076500	-2.069210
1	-4.951031	2.344237	-1.554168
1	-5.712987	2.601646	0.810443
1	-4.409542	1.532336	2.654039
1	-2.395180	0.181211	2.135692
1	1.981067	1.419135	-2.678472
1	3.568192	3.307858	-2.305783
1	2.930012	5.207191	-0.812749
1	0.687441	5.201845	0.289787
1	-0.897917	3.316461	-0.096863

TS_{RE}(O)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3049.08330425

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3049.09384856

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3049.10613456

6	-3.419110	2.498911	-1.092261
6	-2.179091	1.978935	-0.659504
6	-1.372115	2.769465	0.185643

6	-1.782986	4.051067	0.559576
6	-3.001664	4.567353	0.107829
6	-3.814472	3.782464	-0.720825
8	-1.807280	0.771466	-1.103705
29	-0.383166	-0.368286	-0.413171
7	1.340190	0.676856	-1.159157
6	2.368520	0.846927	-0.299203
6	3.630221	1.347767	-0.718245
6	3.768380	1.694586	-2.082868
6	2.695609	1.531627	-2.941026
6	1.490294	1.008358	-2.432419
6	2.164744	0.483215	1.088453
6	3.249261	0.592024	2.001183
6	4.514082	1.098055	1.541754
6	4.694903	1.467486	0.240034
6	3.015632	0.182940	3.335061
6	1.768953	-0.299101	3.689151
6	0.755280	-0.351157	2.709882
7	0.942416	0.037540	1.458599
6	-2.273306	-0.729206	0.166692
6	-2.583130	-0.263750	1.438887
6	-3.630070	-0.888122	2.137364
6	-4.368488	-1.908084	1.536079
6	-4.069274	-2.304390	0.224232
6	-3.027860	-1.702176	-0.485380
53	0.491010	-2.774294	-0.896693
1	-0.241415	-0.727811	2.960627
1	1.557300	-0.634484	4.706232
1	3.823757	0.245476	4.068710
1	0.624691	0.848815	-3.082540
1	2.770096	1.790470	-3.998790
1	4.723034	2.084453	-2.445968
1	5.334032	1.179933	2.259739
1	5.660497	1.851587	-0.098383
1	-2.789328	-2.008870	-1.503933
1	-4.651674	-3.094686	-0.257156
1	-5.190371	-2.382704	2.077349
1	-3.872398	-0.550755	3.149023
1	-2.046546	0.577096	1.883319
1	-0.421534	2.363663	0.537334
1	-1.142749	4.652700	1.211066
1	-3.319393	5.570469	0.402380
1	-4.771731	4.174772	-1.075398
1	-4.043884	1.874070	-1.733918

INT_{HAT} (S)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3140.36056009

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3140.37189159

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3140.38462831

7	1.548919	1.448411	-0.411134
6	2.734481	0.933603	-0.012238
6	3.954539	1.651886	-0.114670

6	3.887512	2.958017	-0.655514
6	2.665223	3.469227	-1.055050
6	1.509096	2.673691	-0.915201
6	2.737091	-0.410355	0.522309
6	3.960963	-1.002557	0.929619
6	5.178219	-0.244758	0.817544
6	5.175027	1.027412	0.319674
6	3.900922	-2.326803	1.425163
6	2.682216	-2.980162	1.480129
6	1.521354	-2.307385	1.047218
7	1.552546	-1.060676	0.597723
29	-0.107481	0.078005	-0.077547
53	-1.371377	-1.743427	-1.388914
16	-1.539936	1.741371	0.425588
6	-3.202201	1.238908	0.737886
6	-4.258527	2.045831	0.267692
6	-5.584749	1.720476	0.557167
6	-5.882764	0.579074	1.308707
6	-4.840777	-0.233821	1.772263
6	-3.514016	0.092330	1.496020
1	0.522905	3.043764	-1.211789
1	2.581327	4.472631	-1.476570
1	4.801701	3.549375	-0.754082
1	0.542384	-2.796480	1.043055
1	2.604802	-4.004887	1.848094
1	4.818346	-2.822969	1.752778
1	6.107217	1.591956	0.238323
1	6.113215	-0.710485	1.138790
1	-4.022964	2.929999	-0.328857
1	-6.391362	2.358485	0.185694
1	-6.921696	0.320609	1.529112
1	-5.065224	-1.131812	2.354305
1	-2.703653	-0.544506	1.854624

INT_{SET} (S)

E (B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP)= -2842.31093804

E (PCM(toluene)-[B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP])= -2842.34548460

E (PCM(ACN)-[B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP])= -2842.36967220

29	0.404029	0.000099	-0.759017
7	-1.075373	1.355462	-0.301978
6	-2.225976	0.722368	0.045419
6	-2.225865	-0.722418	0.045366
7	-1.075171	-1.355291	-0.302077
6	-1.041997	-2.683502	-0.316906
6	-2.162895	-3.468628	0.017988
6	-3.342872	-2.840437	0.375671
6	-3.405008	-1.425428	0.398366
6	-4.584576	-0.683375	0.753598
6	-4.584680	0.682883	0.753653
6	-3.405228	1.425152	0.398480
6	-3.343337	2.840180	0.375903
6	-1.042438	2.683669	-0.316687

1	-0.097341	3.152465	-0.604178
1	-2.086441	4.556811	-0.009659
1	-4.228606	3.424224	0.640020
1	-5.487380	1.235403	1.024087
1	-5.487191	-1.236055	1.023988
1	-4.228036	-3.424664	0.639738
1	-2.085705	-4.556835	-0.010025
1	-0.096815	-3.152099	-0.604434
16	2.432978	0.000169	-1.542616
6	3.588311	0.000064	-0.231606
6	4.962958	0.000209	-0.575496
6	5.933588	0.000142	0.421901
6	5.556295	-0.000065	1.771400
6	4.197333	-0.000222	2.123198
6	3.219356	-0.000158	1.135306
1	5.250075	0.000368	-1.629125
1	6.991142	0.000253	0.148672
1	6.320539	-0.000118	2.552019
1	3.906011	-0.000400	3.176094
1	2.162049	-0.000296	1.411596
6	-2.163471	3.468591	0.018272

TS_{MET}(S)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3372.05447635

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3372.06361764

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3372.07388411

6	-3.476461	-0.165390	1.111104
6	-2.964581	-1.023728	0.138808
6	-3.795181	-1.839161	-0.632010
6	-5.177985	-1.770978	-0.427030
6	-5.721019	-0.914682	0.537929
6	-4.863184	-0.115450	1.300091
53	-0.873522	-2.236262	0.921554
29	0.472763	-0.190573	-0.268987
7	2.301863	-0.693015	-1.235610
6	3.377404	-0.172141	-0.597810
6	4.708060	-0.360546	-1.058590
6	4.881751	-1.120608	-2.238501
6	3.771334	-1.643023	-2.880185
6	2.492554	-1.404069	-2.339507
6	3.138020	0.594054	0.606163
6	4.238420	1.134112	1.324356
6	5.572327	0.924660	0.828664
6	5.797172	0.212102	-0.314321
6	3.949937	1.855506	2.505944
6	2.632685	2.002527	2.907111
6	1.610091	1.437533	2.121257
7	1.851544	0.759714	1.004276
16	-1.461448	0.270877	-1.382606
6	-2.006026	1.931386	-1.122208
6	-1.181846	2.909081	-0.528580
6	-1.641821	4.214315	-0.344219

6	-2.940131	4.569262	-0.727199
6	-3.771191	3.603036	-1.305150
6	-3.311368	2.300776	-1.508457
1	1.595869	-1.805750	-2.821002
1	3.870510	-2.235629	-3.791681
1	5.888318	-1.289796	-2.629911
1	0.560335	1.542938	2.409731
1	2.374527	2.549922	3.815670
1	4.766970	2.286664	3.090299
1	6.815669	0.060319	-0.680621
1	6.408543	1.349799	1.389457
1	-3.961279	1.553606	-1.969129
1	-4.788601	3.867057	-1.607278
1	-3.301032	5.589894	-0.576555
1	-0.981132	4.960421	0.107067
1	-0.169103	2.630741	-0.227802
1	-3.380335	-2.510029	-1.386135
1	-5.833293	-2.402614	-1.034373
1	-6.801371	-0.872800	0.694907
1	-5.267903	0.559800	2.059819
1	-2.814596	0.461560	1.710870

TS_{OA}(S)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3372.07555058

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3372.08394928

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3372.09490473

6	3.242863	1.290941	-0.137230
6	2.727406	0.038101	0.228794
6	3.234390	-0.652127	1.340475
6	4.200890	-0.034808	2.135379
6	4.690717	1.238038	1.811076
6	4.209732	1.896595	0.676775
29	0.657175	-0.035416	-0.018416
53	2.194629	-1.303565	-1.727061
7	-0.061280	2.133807	0.118863
6	-1.361556	2.212103	-0.245298
6	-2.149322	3.376141	-0.027710
6	-1.524748	4.469162	0.616740
6	-0.202161	4.361741	1.006453
6	0.494271	3.166701	0.732362
6	-3.520940	3.393386	-0.456347
6	-4.083521	2.303640	-1.055860
6	-3.326328	1.100870	-1.269677
6	-1.965772	1.051171	-0.864101
6	-3.872296	-0.063456	-1.859203
6	-3.078416	-1.184751	-2.010617
6	-1.741276	-1.138765	-1.570770
7	-1.204939	-0.058266	-1.020011
16	0.057221	-0.833987	2.116919
1	1.542811	3.053002	1.024122
1	0.308303	5.181491	1.515744
1	-2.095083	5.382540	0.805814

1	-1.089132	-2.010243	-1.671935
1	-3.469226	-2.103519	-2.450930
1	-4.917033	-0.066411	-2.180900
1	-4.108880	4.299175	-0.287692
1	-5.128665	2.323918	-1.374882
1	2.835357	-1.630647	1.608429
1	4.572305	-0.557155	3.021076
1	5.456392	1.706058	2.434593
1	4.600808	2.880241	0.401303
1	2.900333	1.789615	-1.045584
6	-1.365188	-1.858020	1.845851
6	-1.257415	-3.118441	1.215979
6	-2.373195	-3.942353	1.047514
6	-3.632357	-3.535356	1.504306
6	-3.757044	-2.291049	2.132868
6	-2.642773	-1.464779	2.300675
1	-0.273108	-3.445533	0.871267
1	-2.255803	-4.917089	0.563886
1	-4.503831	-4.183561	1.379414
1	-4.733061	-1.961386	2.502117
1	-2.743652	-0.497617	2.799228

INT_{OA/RE}(S)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3372.08991502

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3372.10003862

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3372.11235591

6	1.814441	2.751479	1.025378
6	1.232271	2.661165	-0.255028
6	2.064729	2.826171	-1.380476
6	3.432204	3.069525	-1.229832
6	3.998727	3.144093	0.047137
6	3.183397	2.983884	1.173477
16	-0.528047	2.474987	-0.445470
29	-0.910687	0.210587	-0.279252
7	0.861958	-0.402041	-1.169656
6	1.841582	-0.948850	-0.414592
6	3.027481	-1.476291	-0.994516
6	3.156377	-1.402643	-2.400163
6	2.145093	-0.828910	-3.148856
6	1.005768	-0.337584	-2.486646
6	1.663780	-0.998141	1.022847
6	2.679140	-1.586268	1.827028
6	3.862809	-2.114340	1.206331
6	4.030848	-2.059125	-0.146477
6	2.461112	-1.616097	3.224078
6	1.297119	-1.078637	3.741066
6	0.357303	-0.514292	2.852896
7	0.532381	-0.477956	1.542865
6	-2.707278	0.837554	0.177613
6	-3.139320	0.787268	1.502070
6	-4.413603	1.269770	1.827710
6	-5.246530	1.793604	0.835008

6	-4.801124	1.834017	-0.488826
6	-3.527102	1.356938	-0.824332
53	-1.973021	-2.139838	-0.630288
1	-0.569011	-0.077138	3.238440
1	1.096007	-1.083236	4.814087
1	3.214642	-2.062076	3.878677
1	0.184948	0.120175	-3.044876
1	2.211812	-0.755049	-4.235644
1	4.054298	-1.800133	-2.880447
1	4.630237	-2.562127	1.842750
1	4.934472	-2.461422	-0.611031
1	-3.190602	1.398500	-1.862304
1	-5.445369	2.238307	-1.274833
1	-6.240885	2.167101	1.092712
1	-4.752878	1.229093	2.866817
1	-2.509753	0.365303	2.287129
1	1.619810	2.778061	-2.376938
1	4.058877	3.206020	-2.115698
1	5.068568	3.335384	0.164569
1	3.615935	3.053713	2.175545
1	1.171999	2.648346	1.902277

TS_{RE}(S)

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -3372.08540355

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3372.09519461

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -3372.10703750

6	1.499226	2.506943	0.999151
6	0.980288	2.969539	-0.223674
6	1.692412	3.966109	-0.921775
6	2.882853	4.482780	-0.406362
6	3.395900	4.013190	0.807351
6	2.696863	3.021976	1.502515
16	-0.572118	2.434507	-0.912366
29	-0.761506	0.220660	-0.377305
7	1.129098	-0.287933	-1.073519
6	1.937870	-1.038468	-0.289154
6	3.196970	-1.511960	-0.747220
6	3.591592	-1.153967	-2.056848
6	2.753024	-0.375393	-2.832898
6	1.519311	0.038811	-2.298096
6	1.486092	-1.380619	1.042781
6	2.292596	-2.225220	1.854359
6	3.562047	-2.683684	1.360982
6	3.999300	-2.334097	0.116495
6	1.784368	-2.576893	3.126633
6	0.547040	-2.100984	3.518634
6	-0.163974	-1.252542	2.644402
7	0.296218	-0.891937	1.457275
6	-2.468835	0.904676	0.304156
6	-2.513618	1.235198	1.658374
6	-3.744131	1.573974	2.241246
6	-4.903639	1.615568	1.464625

6	-4.830703	1.323706	0.098425
6	-3.611147	0.972822	-0.492640
53	-1.804907	-2.059016	-1.199192
1	-1.145490	-0.861223	2.928211
1	0.117381	-2.363920	4.487122
1	2.370667	-3.227079	3.781377
1	0.829354	0.662689	-2.872639
1	3.026202	-0.080917	-3.847571
1	4.554459	-1.498807	-2.442811
1	4.172090	-3.322641	2.004403
1	4.966042	-2.686403	-0.251555
1	-3.571087	0.727789	-1.554833
1	-5.732240	1.356090	-0.519787
1	-5.859888	1.887979	1.918279
1	-3.781476	1.828161	3.304460
1	-1.606825	1.266817	2.264866
1	1.303299	4.336100	-1.873834
1	3.416035	5.257765	-0.964222
1	4.329317	4.416852	1.207150
1	3.082548	2.646619	2.454763
1	0.959815	1.741039	1.558425

CsI

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -318.057316828
 E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -318.080525881
 E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -318.102996421
 55 0.000000 0.000000 1.674504
 53 0.000000 0.000000 -1.737692

Cs₂CO₃

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -304.370408467
 E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -304.397735207
 E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -304.426573123
 6 -0.000026 1.194229 0.000789
 8 0.000051 -0.145096 0.001720
 8 -1.124518 1.803582 0.001843
 55 -2.773546 -0.316941 -0.000253
 8 1.124386 1.803736 -0.002403
 55 2.773561 -0.316934 -0.000002

CsHCO₃

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -284.759611446
 E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -284.780093226
 E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -284.799680602
 6 2.149235 -0.173330 -0.000048
 8 1.467897 1.131936 0.000149
 8 3.363945 -0.118641 -0.000140
 1 2.193110 1.773090 -0.000072
 8 1.316384 -1.110820 0.000158
 55 -1.168624 0.000856 -0.000018

KI

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -897.828566289
 E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -897.854989366
 E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -897.880220997
 55 0.000000 0.000000 1.674504
 53 0.000000 0.000000 -1.737692

KOtBu

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -833.152812784
 E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -833.170717073
 E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -833.187415422
 6 -1.068675 0.000020 0.000000
 6 -1.607649 1.359704 0.514099
 1 -2.710939 1.412496 0.534191
 1 -1.233757 1.542737 1.535562
 1 -1.233973 2.172711 -0.130936
 6 -1.607383 -1.125144 0.920539
 1 -1.233604 -0.973035 1.947106
 1 -2.710666 -1.169088 0.956362
 1 -1.233442 -2.101224 0.568236
 6 -1.607527 -0.234714 -1.434603
 1 -2.710814 -0.243890 -1.490438
 1 -1.233771 0.558450 -2.103843
 1 -1.233701 -1.199777 -1.816168
 8 0.304658 0.000157 -0.000022
 19 2.549727 0.000009 -0.000006

HOtBu

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -233.796573497
 E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -233.798617325
 E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -233.801114375
 6 -0.006168 0.000074 0.017673
 6 -1.492889 0.003807 -0.344105
 1 -1.636696 0.004078 -1.435485
 1 -1.987432 -0.885121 0.076472
 1 -1.983001 0.895279 0.076304
 6 0.681229 -1.266238 -0.515236
 1 0.201327 -2.164052 -0.096260
 1 0.633791 -1.324621 -1.614553
 1 1.746513 -1.282899 -0.226757
 6 0.687857 1.262667 -0.515306
 1 0.640289 1.321590 -1.614596
 1 0.212979 2.162947 -0.095908
 1 1.753356 1.273553 -0.227312
 8 0.030161 0.000022 1.447438
 1 0.957420 -0.002789 1.720438

[Cu(phen)₂]⁺

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -2784.25153188
 E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2784.28223278
 E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2784.30251536
 7 1.583404 0.959420 -0.961003
 6 2.784264 0.511172 -0.512027

6	4.019532	1.006261	-1.007997
6	3.963869	2.005097	-2.008597
6	2.732705	2.451582	-2.455844
6	1.562390	1.898395	-1.901624
6	5.251349	0.482204	-0.483048
6	5.251302	-0.482370	0.483207
6	4.019433	-1.006363	1.008099
6	2.784214	-0.511209	0.512073
6	3.963670	-2.005196	2.008696
6	2.732462	-2.451617	2.455885
6	1.562202	-1.898367	1.901611
7	1.583311	-0.959394	0.960992
29	-0.000001	0.000075	-0.000064
1	0.577503	-2.234994	2.238839
1	2.654103	-3.220726	3.226412
1	4.890879	-2.413913	2.418185
1	0.577725	2.235075	-2.238899
1	2.654421	3.220694	-3.226375
1	4.891118	2.413765	-2.418042
1	6.193246	-0.873440	0.874968
1	6.193331	0.873225	-0.874766
7	-1.583351	-0.960999	-0.959402
6	-2.784235	-0.512060	-0.511185
6	-4.019475	-1.008110	-1.006262
6	-3.963756	-2.008753	-2.005051
6	-2.732568	-2.455964	-2.451503
6	-1.562283	-1.901663	-1.898332
6	-2.784241	0.512086	0.511151
6	-5.251322	-0.483192	-0.482242
1	-4.890982	-2.418259	-2.413710
1	-2.654241	-3.226527	-3.220579
1	-0.577599	-2.238906	-2.234988
6	-4.019488	1.008079	1.006268
6	-3.963783	2.008724	2.005057
6	-2.732600	2.455989	2.451472
6	-1.562308	1.901743	1.898261
7	-1.583363	0.961079	0.959330
1	-4.891014	2.418189	2.413745
1	-2.654284	3.226555	3.220546
1	-0.577629	2.239030	2.234886
6	-5.251328	0.483107	0.482286
1	-6.193282	-0.874971	-0.873255
1	-6.193293	0.874844	0.873329

[Cu(NHPh)₂]-

E (B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP)= -2214.97397662

E (PCM(toluene)-[B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP])= -2215.01189022

E (PCM(ACN)-[B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP])= -2215.04115794

6	-3.171373	-0.939912	-0.199553
6	-2.905745	0.442319	0.067487
6	-4.062003	1.286261	0.130233
6	-5.349982	0.790415	-0.054430

6	-5.580620	-0.568127	-0.313478
6	-4.463357	-1.417829	-0.381554
7	-1.648125	0.898920	0.245578
29	-0.000153	0.000348	0.229171
7	1.647843	-0.898125	0.245359
6	2.905693	-0.442139	0.067376
6	4.061601	-1.286530	0.130440
6	5.349801	-0.791201	-0.054105
6	5.581009	0.567203	-0.313354
6	4.464086	1.417332	-0.381765
6	3.171895	0.939944	-0.199875
1	-2.315734	-1.619624	-0.256731
1	-4.607296	-2.485819	-0.583085
1	-6.593830	-0.952809	-0.457878
1	-6.197440	1.483644	0.005475
1	-3.915156	2.353924	0.331356
1	3.914315	-2.354104	0.331707
1	6.196981	-1.484751	0.006032
1	6.594394	0.951456	-0.457665
1	4.608470	2.485233	-0.583447
1	2.316509	1.619951	-0.257287
1	-1.642695	1.900620	0.427259
1	1.641882	-1.899801	0.427205

[Cu(OPh)₂]-

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -2254.74628765

E (PCM(toluene)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2254.78502097

E (PCM(ACN)-[B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP])= -2254.81429798

6	-2.811259	0.720356	-0.751382
6	-2.793499	-0.260969	0.284046
6	-4.042268	-0.512584	0.929637
6	-5.204611	0.163042	0.565757
6	-5.196197	1.124376	-0.455913
6	-3.982420	1.389172	-1.104938
8	-1.728877	-0.912462	0.653044
29	-0.000002	-0.816566	-0.000016
8	1.728870	-0.912419	-0.653100
6	2.793496	-0.260957	-0.284065
6	4.042242	-0.512471	-0.929742
6	5.204589	0.163131	-0.565826
6	5.196203	1.124331	0.455969
6	3.982451	1.389019	1.105086
6	2.811287	0.720227	0.751495
1	-1.869174	0.936663	-1.265471
1	-3.946747	2.135645	-1.906690
1	-6.111328	1.652574	-0.738214
1	-6.140464	-0.063464	1.089829
1	-4.050239	-1.261636	1.726767
1	4.050196	-1.261421	-1.726967
1	6.140422	-0.063293	-1.089970
1	6.111336	1.652511	0.738297
1	3.946800	2.135387	1.906937

1 1.869219 0.936442 1.265656

[Cu(SPh)₂]⁻

E (B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP)= -2900.71548153

E (PCM(toluene)-[B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP])= -2900.75446013

E (PCM(ACN)-[B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP])= -2900.78481743

6 -2.717580 0.631347 -0.838623
 6 -3.004108 -0.061341 0.362170
 6 -4.290338 0.133848 0.921875
 6 -5.230618 0.969753 0.318602
 6 -4.928679 1.647598 -0.869140
 6 -3.661527 1.467118 -1.437334
 16 -1.869184 -1.136788 1.180919
 29 -0.000012 -1.106050 0.000047
 16 1.869206 -1.136965 -1.180750
 6 3.004115 -0.061386 -0.362150
 6 4.290375 0.133673 -0.921833
 6 5.230647 0.969670 -0.318673
 6 4.928670 1.647742 0.868929
 6 3.661490 1.467392 1.437102
 6 2.717553 0.631526 0.838506
 1 -1.733471 0.502712 -1.297878
 1 -3.399996 1.986133 -2.365496
 1 -5.665433 2.303422 -1.341837
 1 -6.214489 1.093933 0.784010
 1 -4.538224 -0.389473 1.849546
 1 4.538292 -0.389824 -1.849396
 1 6.214541 1.093744 -0.784062
 1 5.665415 2.303642 1.341535
 1 3.399929 1.986583 2.365157
 1 1.733423 0.502994 1.297745

[Cu(phen)]⁺

E (B3LYP+D3(BJ)/def2-TZVPP//B3LYP/def2-SVP)= -2212.28284134

29 0.000293 -2.291754 0.000437
 7 1.397060 -0.846941 -0.000713
 6 0.728157 0.342434 -0.000330
 6 -0.728250 0.342327 -0.000284
 7 -1.397033 -0.847077 -0.000429
 6 -2.726095 -0.856576 -0.000292
 6 -3.491543 0.324413 -0.000113
 6 -2.837548 1.542041 0.000056
 6 -1.421200 1.582137 -0.000019
 6 -0.682361 2.814215 0.000188
 6 0.681848 2.814271 0.000268
 6 1.420885 1.582312 0.000057
 6 2.837257 1.542557 0.000278
 6 2.726165 -0.856106 -0.000596
 1 3.216056 -1.833485 -0.001133
 1 4.580885 0.262857 0.000229
 1 3.400603 2.479044 0.000671
 1 1.236928 3.754969 0.000478

1	-1.237488	3.754875	0.000291
1	-3.401066	2.478440	0.000195
1	-4.581037	0.262282	-0.000082
1	-3.215769	-1.834059	-0.000490
6	3.491388	0.324986	-0.000017

PhNH⁻

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -287.141243716

7	2.392763	-0.133471	0.000122
6	1.072170	-0.033674	-0.000554
6	0.296775	1.199079	-0.000029
6	-1.092924	1.218059	0.000045
6	-1.855424	0.035401	-0.000017
6	-1.143010	-1.184096	0.000098
6	0.241645	-1.229273	0.000019
1	0.851854	2.147328	0.000258
1	-1.607393	2.189782	0.000179
1	-2.949477	0.059533	-0.000039
1	-1.701859	-2.130718	0.000255
1	0.770020	-2.189289	0.000201
1	2.772119	0.824692	0.000926

PhO⁻

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -307.045286937

8	2.349126	-0.000275	0.000057
6	1.091350	0.000278	-0.000020
6	0.286909	-1.214722	-0.000199
6	-1.103330	-1.203151	-0.000216
6	-1.834281	0.000074	-0.000033
6	-1.103359	1.202894	0.000187
6	0.287271	1.214865	0.000208
1	0.840585	-2.161529	-0.000332
1	-1.645899	-2.159446	-0.000374
1	-2.929162	-0.000071	-0.000049
1	-1.645553	2.159398	0.000348
1	0.839661	2.162423	0.000393

PhS⁻

E (B3LYP+D3(BJ))/def2-TZVPP//B3LYP/def2-SVP)= -630.026980700

6	0.162204	1.204793	-0.000002
6	-0.610391	0.000081	0.000028
6	0.162294	-1.204791	-0.000055
6	1.555762	-1.202357	0.000032
6	2.282014	0.000026	0.000039
6	1.555828	1.202278	-0.000079
16	-2.339566	-0.000020	0.000009
1	-0.387698	-2.150920	-0.000134
1	2.092652	-2.159780	0.000034
1	3.376690	-0.000072	0.000090
1	2.092564	2.159783	0.000001
1	-0.387416	2.151136	0.000095