Supplementary Information

Intramolecular Hydroarylation of Aryl Propargyl Ethers Catalyzed by Indium: Mechanism and Identifying the Catalytic Species

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Table of Contents

Table S1. Calculated relative zero-point energy correction ΔZPE, electronic energy ΔE, enthalpy ΔH, entropy ΔS, Gibb's free energy ΔG and Gibb's free energy in solution (toluene) ΔG-sol for the 6-*endo* and 5-*exo* cyclization pathways at 298.15 K. (The unit of relative entropy ΔS is cal/mol-K while kcal/mol is for the rest).

	ΔZPE	Δ*E*	Δ*H*	Δ*S*	Δ*G*	ΔG_{sol}
1a-InI_3	0.0	0.0	0.0	0.0	0.0	0.0
Ts1-6	0.2	10.3	9.5	-10.8	12.7	13.0
Int1-6	1.7	0.9	0.0	-11.0	3.3	-0.4
Ts2-6e	-1.6	14.8	13.6	-16.3	18.5	18.5
Int2-6e	-1.9	-3.2	-3.8	20.8	-10.0	-15.3
Ts3-6e	-1.9	-2.3	-3.5	-13.8	0.6	1.1
Ts2-6f	-0.7	20.9	19.8	-10.8	23.0	20.5
Int2-6f	0.6	-5.4	-6.3	-11.0	-3.0	-1.2
Ts3-6f	-0.1	-1.3	-2.4	-12.2	1.2	1.4
Int3-6	2.7	-40.3	-41.3	-10.9	-38.0	-34.9
Ts1-5	0.1	17.1	16.3	-11.0	19.6	19.0
Int1-5	1.3	9.3	8.4	-11.9	11.9	6.6
Ts2-5g	-1.3	26.9	25.9	-12.8	22.6	24.2
Int2-5g	-2.6	-2.3	-2.8	22.6	-9.5	-12.3
Ts3-5g	-2.2	-3.4	-4.6	-11.0	-1.3	0.8
Ts2-5h	-1.3	26.9	25.9	-12.8	29.7	26.3
Int2-5h	2.5	-8.5	-9.8	-13.2	-5.8	-3.4
Ts3-5h	-0.3	4.3	3.1	-14.7	7.5	8.6
Int3-5	2.0	-46.0	-46.9	-11.8	-43.4	-41.3

2. A comparison between B3LYP hybrid functional and MP2 method results for the first step of 6-*endo* and 5-*exo* pathways.

The calculations were performed using the B3LYP hybrid functional and MP2 method with 6-31+G(d) basis set for H, C and O atoms whereas the effective core potential (ECP) of Hay and Wadt combined with the double-ζ valence basis set (LanL2DZ) was used for In and I atoms.

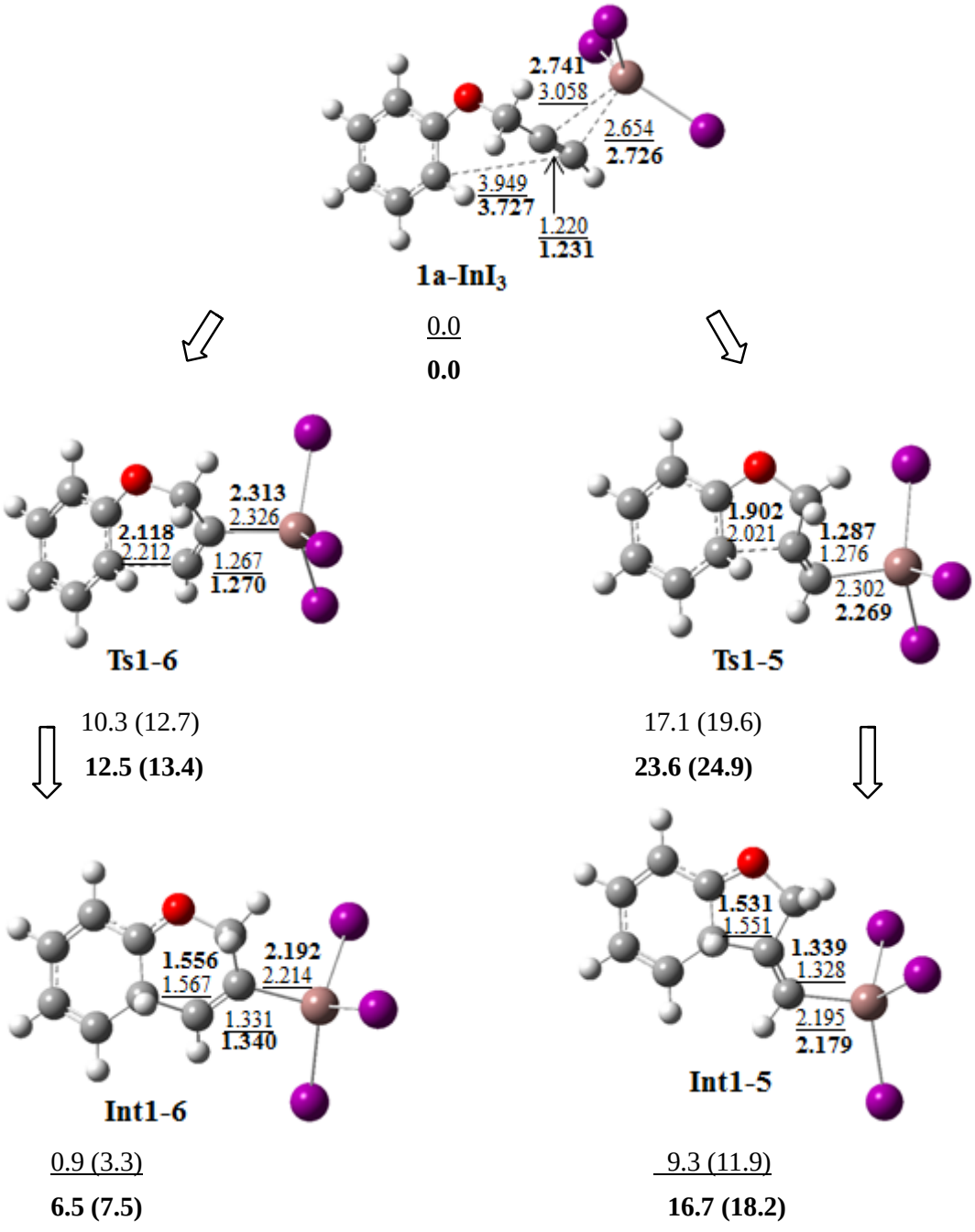


Figure S1. A comparison of geometrical parameters (Å), ZPE-corrected energy and free energy differences (in parenthesis) obtained by B3LYP (underlined) and MP2 (**bold**) for the first step of 6-*endo* and 5-*exo* pathways.

The calculation results depicted in Figure S1 show small geometric differences on the optimized structures at both theoretical levels. The major differences are found in the coordination of the catalyst to the alkyne in **1a-InI_3** and in the forming bond in **Ts1-5**, whereas other parameters differ by < 0.02 Å. The energy results show similar trends and suggest that the *endo*-cyclization should be favored from both kinetic and thermodynamic points of view. The MP2 model affords higher activation barriers for the *endo*- and *exo*-cyclizations than the DFT method. However, both theoretical levels show similar qualitative results and yield analogous energy differences in the activation barrier between the *endo*- and *exo*- processes, favoring the *endo*-route: 6.9 (B3LYP) *vs* 11.35 kcal/mol (MP2). In summary, these results do not justify the use of the computationally expensive MP2 method and support the application of the B3LYP as method of choice for the present system.

3. Calculation results with InI_2^+ as the possible catalytic species of the hydroarylation process.

We found that, if InI_2^+ was proposed as the catalytic species, the 5-*exo* and 6-*endo* pathways would have similar activation energies and form a mixture of 2*H*-chromene and benzofuran products, as suggested by B3LYP calculations (Figure S2). Furthermore, B3LYP calculations performed by coordination of InI_2^+ with a solvent molecule, toluene, give the same results as in the absence of coordination with a solvent molecule (Figure S3). In addition, calculations performed on *p*-OCH_3 and *p*-CO_2Me substituted phenyl propargyl ether, with InI_2^+ as a possible catalytic species, show slight preference for 5-*exo* than 6-*endo* cyclization. The 6-*endo* cyclization of *p*-OCH_3 substituted phenyl propargyl ether gives five membered *spiro* cyclic first intermediate then six membered fused ring which proceeds by stepwise [1,2]-H shift steps to give the final product (Table S1). However, it is reported that the hydroarylation process proceeds regioselectively to produce only the 6-*endo*-dig cyclization product.[1] To check whether this discrepancy between experiments and calculations was caused by computational methods, we performed the calculations with various methods such as MP2 method, and M06, M06-2X functionals (Table S1). All these calculations indicated similar activation energies for the 5-*exo* and 6-*endo* pathways, except the M06 functional, which favored 5-*exo* versus 6-*endo* pathways. This further supported InI_2^+ is not the real catalytic species.

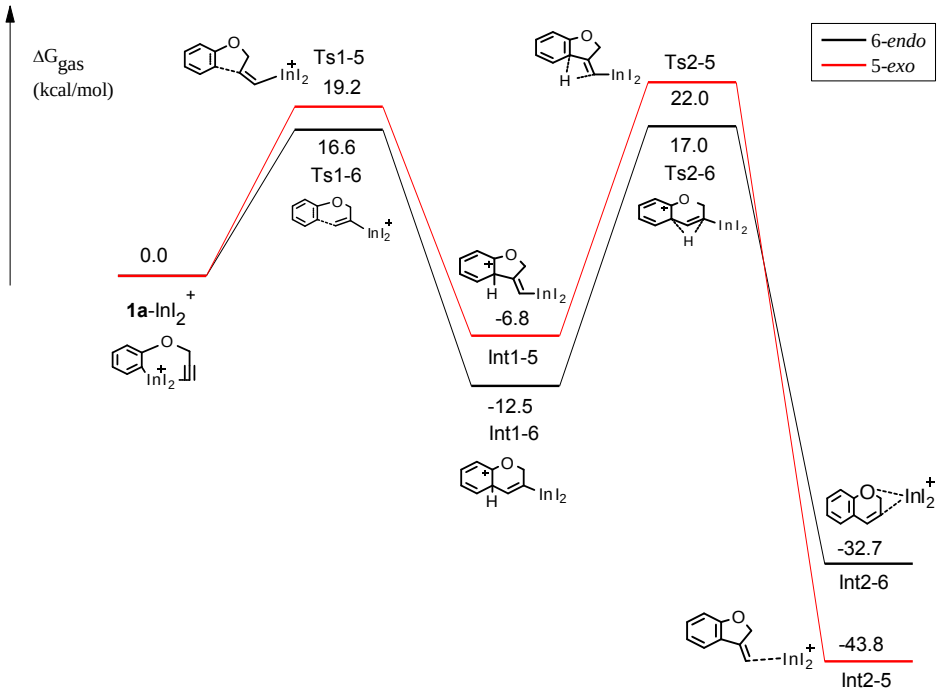


Figure S2. Comparison between potential energy surfaces of 5-*exo* and 6-*endo* pathways for the hydroarylation of **1a** using InI_3^+ as a possible catalytic species in gas phase.

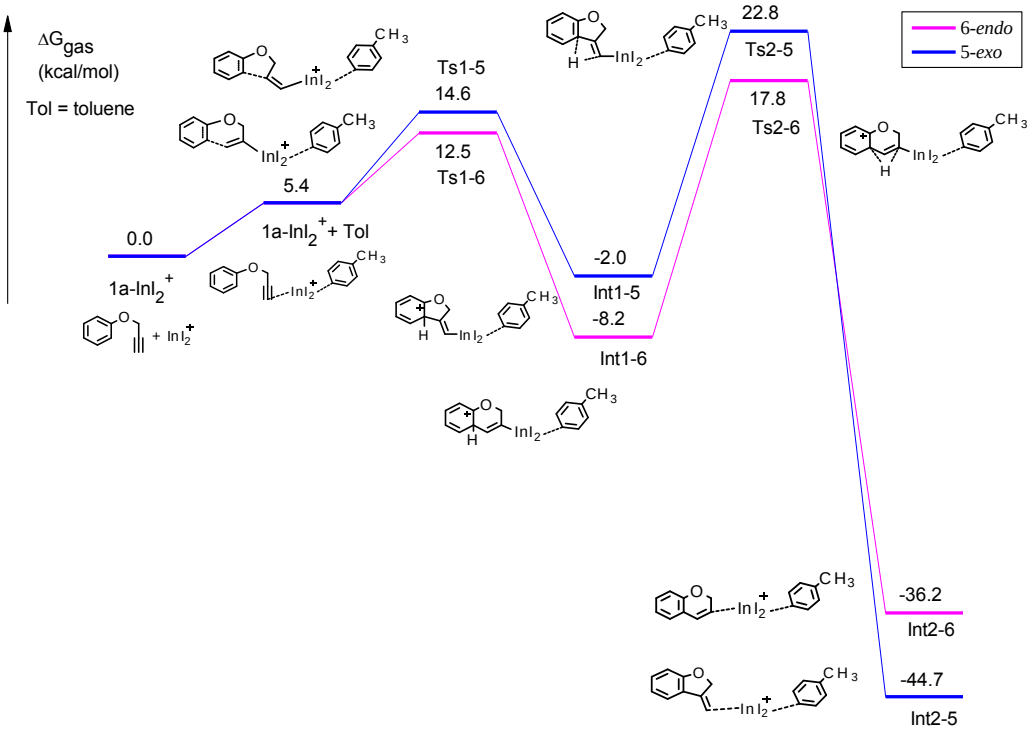


Figure S3. Comparison between potential energy surfaces of 5-*exo* and 6-*endo* pathways for the hydroarylation of **1a** using InI_2^+ coordinated to a solvent molecule as a possible catalytic species in gas phase.

Table S2. Computed relative free energies of 5-*exo* and 6-*endo* pathways for the hydroarylation of **1a** and substituted derivatives with various methods (MP2, M06, M06-2X) and B3LYP functional using InI_2^+ as a possible catalytic species in gas phase.[a]

	MP2		M06		M06-2X		B3LYP[c]		B3LYP[d]	
	5-*exo*	6-*endo*	5-*exo*	6-*endo*	5-*exo*	6-*endo*	5-*exo*	6-*endo*	5-*exo*	6-*endo*
1a-InI_3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Ts-S								4.8		
Int-S								-18.6		
Ts1-5/6	25.5	22.0	1.8	2.5	6.3	4.7	4.7	-3.9	15.6	16.5
Int1-5/6	3.8	-3.6	-23.6	-29.0	-19.6	-25.4	-16.8	-21.9	-6.5	-12
Ts2-5/6	*b*	*b*	5.0	-0.8	11.2	4.6	10.5	5.9	21.1	17.1
Int2								-6.3		
Ts3								-6.2		
Int2-5/6	-33.4		-60.8	-57.9	-56.2	-57.1	-55	-42.8	-44.2	-38.4

[a] 6-31+G(d) for H, C and O, and LanL2DZ for In and I.

[b] Ts2-5 and Ts2-6 were not found.

[c] *p*-OCH_3 substituted phenyl propargyl ether

[d] *p*-CO_2Me substituted phenyl propargyl ether

Reference

1. Alonso-Maranon, L.; Martinez, M. M.; Sarandeses, L. A.; Sestelo, J. P., Indium-catalyzed intramolecular hydroarylation of aryl propargyl ethers. *Org. Biomol. Chem.* **2015,** *13*, 379-387.

4. Potential Energy Surface and Optimized Structures for the Hydroarylation of 1a following the Claisen Mechanism

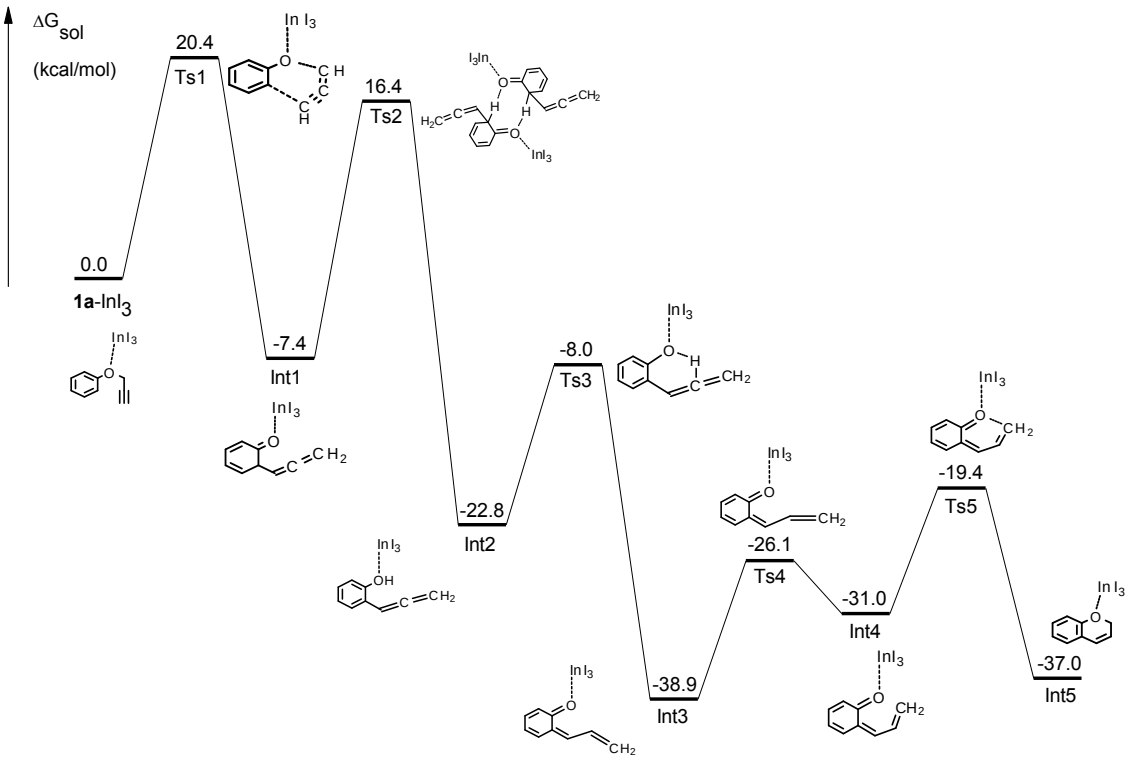
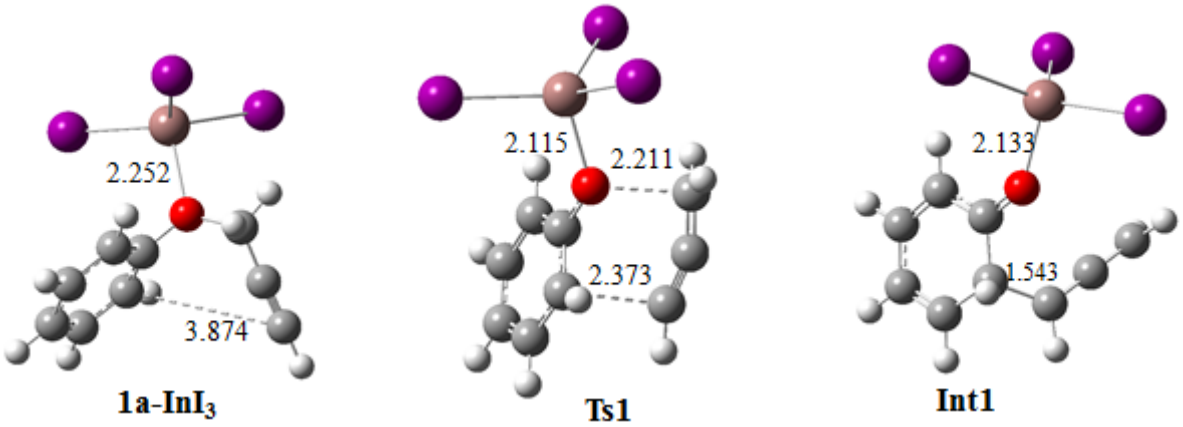
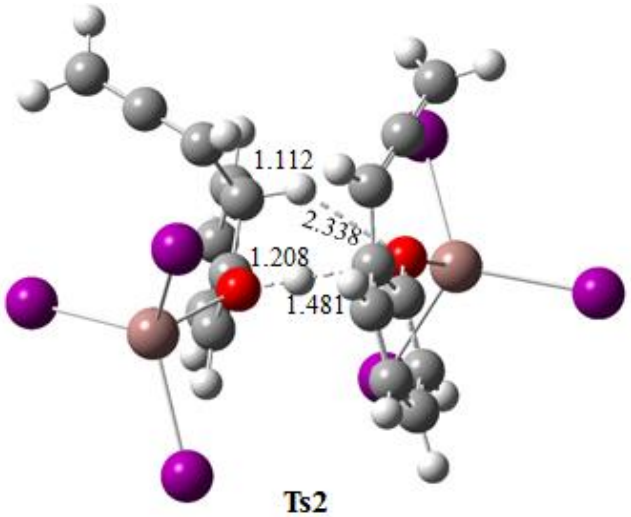
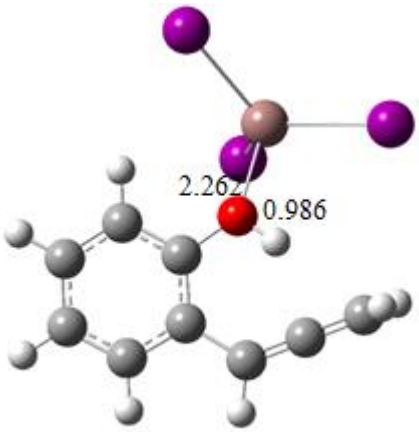


Figure S4. Potential energy surface for the hydroarylation of **1a** catalyzed by InI_3 following the Claisen mechanism.

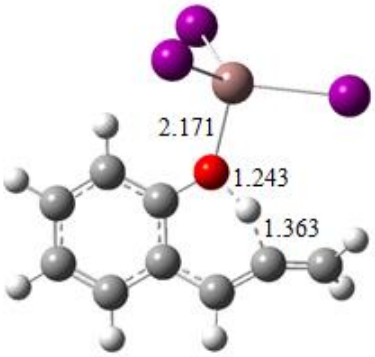




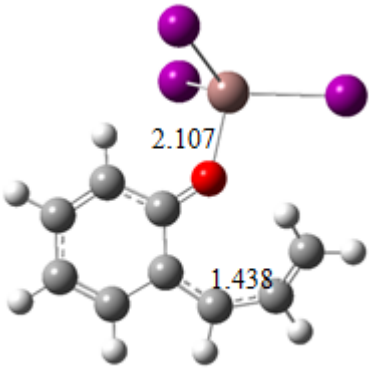
Ts2



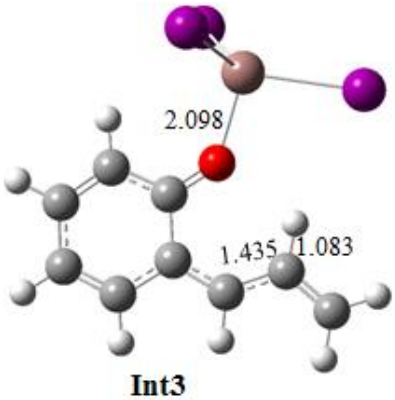
Int2



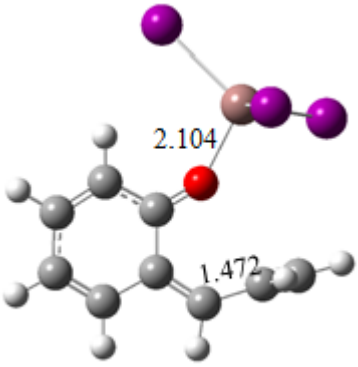
Ts3



Int4



Int3



Ts4

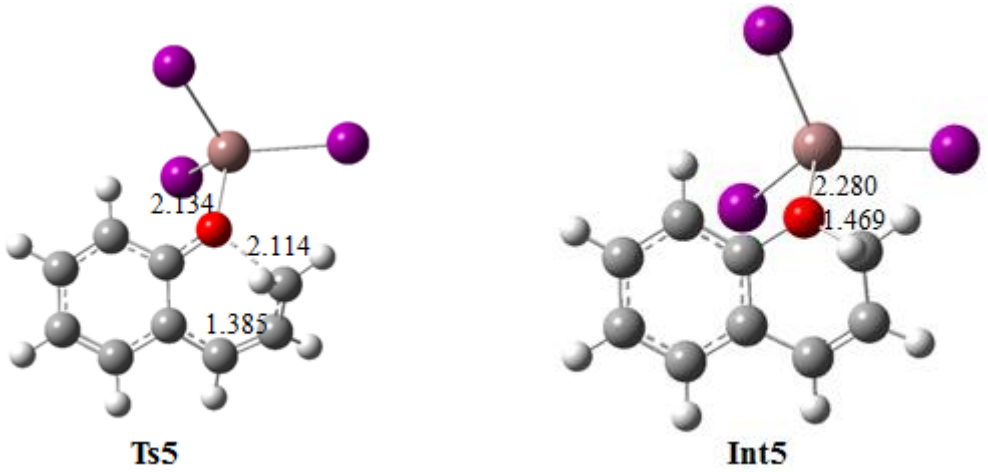
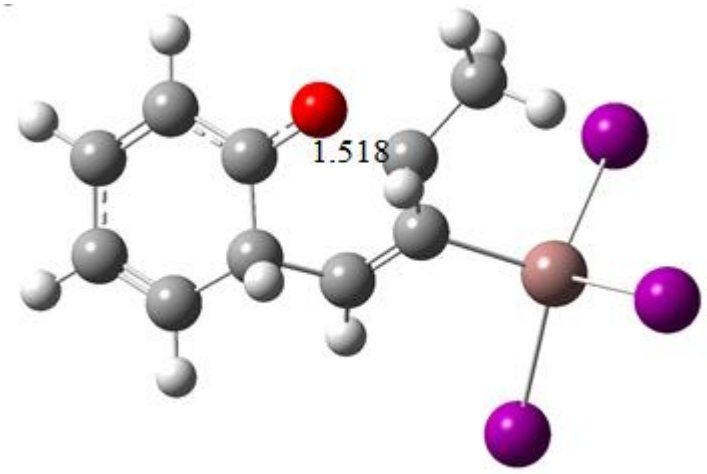
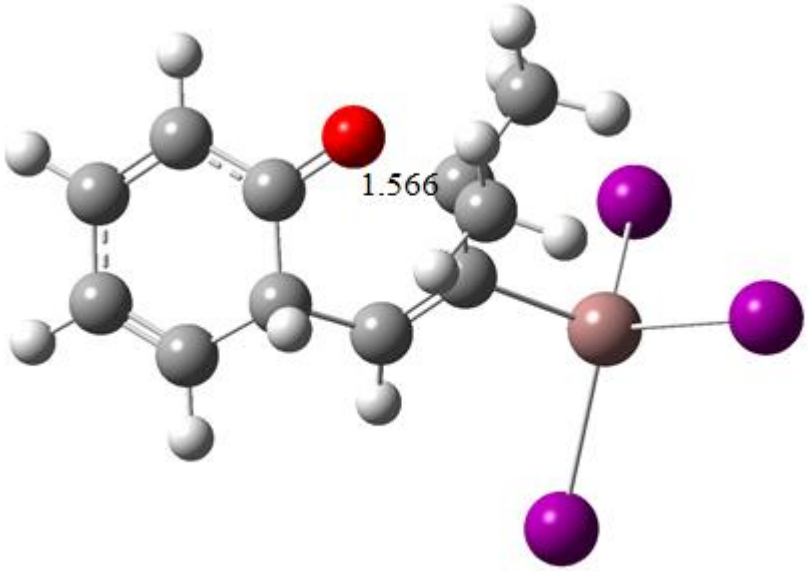


Figure S5. Optimized structures at B3LYP/6-31+G(d)/LANL2DZ level of intermediates and transition states involved in the hydroarylation of phenyl propargyl ether catalyzed by indium following the Claisen mechanism (bond lengths in Å).

5. Structures of the first intermediate showing bond breakage between O_4 and C_3



One methyl group at C_3



gem-Dimethyl group at C_3

Figure S6. Optimized structures of the first intermediate showing bond breakage between C_3 and O_4, with one methyl and *gem*-dimethyl substituents at C_3.

6. Cartesian coordinates (Å) for optimized structures in gas phase at B3LYP/6-31+G(d)/LANL2DZ level.

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.628885	-0.569028	-0.471485
2	6	0	2.755960	0.770884	-0.083242
3	6	0	1.632502	1.453367	0.382330
4	6	0	0.386745	0.818539	0.467535
5	6	0	0.274889	-0.522939	0.084868
6	6	0	1.398355	-1.215614	-0.389326
7	8	0	-0.885297	-1.259673	0.138725
8	6	0	-2.055394	-0.681189	0.714271
9	6	0	-2.740399	0.275818	-0.162645
10	6	0	-3.329498	1.053868	-0.876399
11	1	0	3.494270	-1.115126	-0.838616
12	1	0	3.717053	1.273336	-0.147444
13	1	0	1.712358	2.496080	0.679684
14	1	0	-0.475353	1.380992	0.807811
15	1	0	1.284165	-2.254885	-0.683060
16	1	0	-2.712429	-1.533394	0.912734
17	1	0	-1.813028	-0.214213	1.679172
18	1	0	-3.836931	1.742357	-1.515517

InI_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	49	0	0.000000	0.000000	0.000000
2	53	0	0.000000	2.705190	0.000000
3	53	0	2.342764	-1.352595	0.000000
4	53	0	-2.342764	-1.352595	0.000000

1a-InI_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.519179	-0.517275	-0.341947
2	6	0	-6.794453	-0.890653	0.980209

3	6	0	-5.882792	-0.567918	1.984386
4	6	0	-4.699551	0.122220	1.686654
5	6	0	-4.441636	0.492722	0.363285
6	6	0	-5.349960	0.171892	-0.653792
7	8	0	-3.322832	1.187975	-0.056043
8	6	0	-2.360335	1.592567	0.896548
9	6	0	-1.514746	0.490117	1.373169
10	6	0	-0.788378	-0.421335	1.732467
11	1	0	-7.219602	-0.763850	-1.135482
12	1	0	-7.707167	-1.428389	1.220088
13	1	0	-6.079917	-0.854703	3.014044
14	1	0	-4.005133	0.348236	2.488675
15	1	0	-5.121103	0.469684	-1.672486
16	1	0	-1.732313	2.332788	0.387641
17	1	0	-2.824245	2.089215	1.761134
18	1	0	-0.366555	-1.261446	2.247664
19	49	0	1.117987	-0.068464	-0.079449
20	53	0	0.363804	-2.052230	-1.776453
21	53	0	1.060824	2.510237	-0.975456
22	53	0	3.046382	-0.645076	1.768969

Ts1-6

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	6.009497	-0.019722	-0.759022
2	6	0	5.980548	1.134955	0.055786
3	6	0	5.015729	1.255857	1.037933
4	6	0	4.025986	0.250278	1.206748
5	6	0	4.075933	-0.903626	0.380893
6	6	0	5.068051	-1.025759	-0.609901
7	8	0	3.167727	-1.894082	0.463403
8	6	0	1.844658	-1.596434	0.942771
9	6	0	1.381252	-0.257991	0.435769
10	6	0	2.088496	0.782391	0.282632
11	1	0	6.773472	-0.115561	-1.525723
12	1	0	6.727071	1.911724	-0.079992
13	1	0	5.003997	2.117833	1.699411
14	1	0	3.451297	0.235417	2.127501

15	1	0	5.065347	-1.906392	-1.243998
16	1	0	1.229811	-2.424467	0.590330
17	1	0	1.823082	-1.581247	2.040609
18	1	0	2.239875	1.800297	-0.026490
19	49	0	-0.868913	0.065445	-0.057189
20	53	0	-1.239820	-1.782085	-2.054342
21	53	0	-1.909401	-0.658299	2.390003
22	53	0	-1.153041	2.708092	-0.756949

Int1-6

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	6.121608	-0.271075	-0.303764
2	6	0	5.865976	1.074261	0.132225
3	6	0	4.712914	1.365917	0.783951
4	6	0	3.684988	0.332258	1.067389
5	6	0	4.007987	-1.023708	0.548143
6	6	0	5.227162	-1.298804	-0.110223
7	8	0	3.136451	-1.976499	0.665433
8	6	0	1.740911	-1.634348	1.071784
9	6	0	1.321760	-0.286022	0.584537
10	6	0	2.242636	0.673937	0.558746
11	1	0	7.051636	-0.478816	-0.827136
12	1	0	6.604362	1.843818	-0.069738
13	1	0	4.499807	2.375685	1.125751
14	1	0	3.578930	0.252255	2.167598
15	1	0	5.411454	-2.302202	-0.479252
16	1	0	1.168603	-2.466726	0.661846
17	1	0	1.723366	-1.693846	2.168487
18	1	0	2.076350	1.689714	0.211971
19	49	0	-0.775518	0.060941	-0.034578
20	53	0	-2.254379	-0.603749	2.216092
21	53	0	-0.906440	2.729797	-0.767140
22	53	0	-1.155433	-1.748472	-2.101506

Ts2-6e

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	5.846328	-0.026854	-0.662895
2	6	0	5.363761	1.253954	-0.292280
3	6	0	4.015706	1.506930	-0.356792
4	6	0	3.071808	0.464790	-0.695067
5	6	0	3.616665	-0.788918	-1.161184
6	6	0	4.998568	-1.032692	-1.101528
7	8	0	2.840372	-1.743579	-1.652711
8	6	0	1.373239	-1.623650	-1.607531
9	6	0	0.841781	-0.230147	-1.444091
10	6	0	1.685260	0.773061	-1.153016
11	1	0	6.914395	-0.223880	-0.617906
12	1	0	6.059082	2.023798	0.026744
13	1	0	3.614001	2.479095	-0.081473
14	1	0	2.634890	0.118112	0.554590
15	1	0	5.375918	-1.997794	-1.423527
16	1	0	1.049904	-2.067771	-2.553467
17	1	0	1.051191	-2.286311	-0.795538
18	1	0	1.340938	1.789482	-0.965332
19	49	0	-1.026795	0.038894	-0.439757
20	53	0	-1.983462	2.575193	-0.188442
21	53	0	-2.759676	-2.038702	-0.136917
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Int2-6e

Center	Atomic	Atomic	Coordinates (Angstroms)		
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3	6	0	-3.336956	1.485960	1.864386
4	6	0	-2.399023	0.456431	1.661874
5	6	0	-2.729652	-0.854127	2.076708
6	6	0	-3.954400	-1.121071	2.692213
7	8	0	-1.827775	-1.869740	1.955870
8	6	0	-0.867258	-1.741845	0.887301
9	6	0	-0.257502	-0.358220	0.807928
10	6	0	-1.050518	0.683433	1.152071
11	1	0	-5.831560	-0.296373	3.334390
12	1	0	-5.292919	2.020402	2.593204

13	1	0	-3.080824	2.498092	1.558381
14	1	0	-3.748723	0.184802	-0.535539
15	1	0	-4.172234	-2.133939	3.016771
16	1	0	-0.131310	-2.523235	1.087960
17	1	0	-1.372914	-1.988429	-0.061515
18	1	0	-0.709463	1.716528	1.089822
19	49	0	1.725873	-0.016839	0.183212
20	53	0	2.640615	2.513522	-0.158132
21	53	0	3.439666	-2.057011	-0.316003
22	53	0	-4.219256	-0.113437	-2.082340

HI

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	53	0	0.000000	0.000000	0.030311
2	1	0	0.000000	0.000000	-1.606500

Ts3-6e

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	6.214544	0.260011	-1.162204
2	6	0	5.750960	1.575174	-0.999457
3	6	0	4.397027	1.799966	-0.776467
4	6	0	3.485624	0.725814	-0.741028
5	6	0	3.971953	-0.590701	-0.929109
6	6	0	5.335435	-0.823323	-1.119832
7	8	0	3.139627	-1.663410	-0.842782
8	6	0	1.747405	-1.430813	-1.144328
9	6	0	1.209857	-0.164147	-0.505009
10	6	0	2.083720	0.888751	-0.430500
11	1	0	7.273427	0.077443	-1.325176
12	1	0	6.446262	2.408405	-1.035010
13	1	0	4.024072	2.810236	-0.623351
14	1	0	1.009042	-0.590389	1.097680
15	1	0	5.685636	-1.844193	-1.236524
16	1	0	1.635322	-1.383952	-2.239875
17	1	0	1.236980	-2.328824	-0.788886
18	1	0	1.761862	1.865763	-0.068960

19	53	0	-1.775625	2.645642	0.301170
20	53	0	0.362391	-1.213887	2.650344
21	49	0	-0.910110	0.178372	-0.401791
22	53	0	-2.639093	-1.618393	-1.451557

Ts2-6f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.395323	-0.333783	-0.076561
2	6	0	6.074362	1.027811	0.107526
3	6	0	4.763224	1.394373	0.342955
4	6	0	3.756377	0.395669	0.410750
5	6	0	4.094884	-0.980118	0.259796
6	6	0	5.423649	-1.327233	-0.017361
7	8	0	3.162553	-1.938308	0.269924
8	6	0	1.845077	-1.630302	0.821660
9	6	0	1.320050	-0.287072	0.387594
10	6	0	2.235719	0.722182	0.309463
11	1	0	7.426557	-0.617371	-0.267121
12	1	0	6.851355	1.783423	0.054850
13	1	0	4.483213	2.436936	0.469160
14	1	0	2.925187	0.661791	1.378773
15	1	0	5.666753	-2.372648	-0.176700
16	1	0	1.217967	-2.453591	0.478357
17	1	0	1.910788	-1.682285	1.919548
18	1	0	1.994931	1.753088	0.062017
19	49	0	-0.840172	0.047500	-0.040673
20	53	0	-1.980872	-0.748658	2.353396
21	53	0	-1.010739	2.758911	-0.569012
22	53	0	-1.386893	-1.637036	-2.149671

Int2-6f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.319858	-0.164068	-0.813651
2	6	0	-5.930935	1.168122	-0.632729
3	6	0	-4.621626	1.464840	-0.244659
4	6	0	-3.699925	0.436402	-0.028808

5	6	0	-4.100502	-0.886718	-0.238959
6	6	0	-5.403075	-1.200688	-0.626256
7	8	0	-3.202848	-1.918883	-0.035806
8	6	0	-1.856063	-1.621115	-0.360448
9	6	0	-1.307212	-0.313727	-0.008700
10	6	0	-2.284258	0.693218	0.445291
11	1	0	-7.337810	-0.397937	-1.112608
12	1	0	-6.644081	1.972182	-0.788726
13	1	0	-4.316055	2.497908	-0.095151
14	1	0	-1.940697	1.718002	0.256315
15	1	0	-5.677680	-2.240402	-0.775511
16	1	0	-1.240825	-2.453142	-0.000256
17	1	0	-1.716347	-1.626957	-1.469879
18	1	0	-2.226675	0.580225	1.551840
19	49	0	0.918756	0.064147	-0.035442
20	53	0	2.043038	-1.671142	-1.827236
21	53	0	0.906260	-0.795030	2.617609
22	53	0	1.293054	2.743538	-0.422249

Ts3-6f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.422609	-0.279517	-0.308678
2	6	0	-6.060137	1.074154	-0.265413
3	6	0	-4.711302	1.421444	-0.263911
4	6	0	-3.724402	0.426696	-0.319692
5	6	0	-4.103848	-0.926575	-0.377774
6	6	0	-5.453858	-1.282951	-0.359730
7	8	0	-3.173617	-1.928081	-0.377379
8	6	0	-1.840080	-1.620678	-0.815249
9	6	0	-1.305498	-0.293015	-0.366950
10	6	0	-2.279520	0.731679	-0.248671
11	1	0	-7.473025	-0.557477	-0.302959
12	1	0	-6.822964	1.845383	-0.224742
13	1	0	-4.411562	2.465728	-0.212459
14	1	0	-1.763031	0.805116	-1.325138
15	1	0	-5.723957	-2.333902	-0.384225

16	1	0	-1.215918	-2.425690	-0.418461
17	1	0	-1.776640	-1.680200	-1.915138
18	1	0	-1.973924	1.682280	0.197248
19	49	0	0.907021	0.047314	0.037403
20	53	0	1.053880	-1.341018	2.405753
21	53	0	2.161023	-1.117646	-2.111373
22	53	0	1.077804	2.794468	0.191065

Int3-6

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-5.599161	-0.001622	-0.383984
2	6	0	-5.002708	1.258315	-0.210541
3	6	0	-3.671351	1.438555	-0.562961
4	6	0	-2.911343	0.362913	-1.064004
5	6	0	-3.527116	-0.904745	-1.213089
6	6	0	-4.874915	-1.079775	-0.892365
7	8	0	-2.850847	-1.950628	-1.763365
8	6	0	-1.422851	-1.958456	-1.570314
9	6	0	-0.815360	-0.595871	-1.862397
10	6	0	-1.580482	0.509232	-1.603054
11	1	0	-6.643155	-0.143880	-0.117639
12	1	0	-5.580599	2.086204	0.188311
13	1	0	-3.198388	2.411318	-0.452837
14	1	0	0.051604	-0.526448	-2.517999
15	1	0	-5.331075	-2.053828	-1.037635
16	1	0	-1.225030	-2.298161	-0.544118
17	1	0	-1.040015	-2.715467	-2.255945
18	1	0	-1.223969	1.504648	-1.861771
19	49	0	0.801656	0.070728	0.124930
20	53	0	2.436758	-2.078063	-0.349031
21	53	0	1.744850	2.514825	-0.670134
22	53	0	-0.707118	-0.064994	2.392019

Ts1-5

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-6.064516	1.355178	0.310132
2	6	0	-5.565876	2.105046	-0.785271
3	6	0	-4.576057	1.576250	-1.585640
4	6	0	-4.012646	0.296578	-1.288054
5	6	0	-4.494168	-0.393367	-0.135256
6	6	0	-5.543732	0.111943	0.641586
7	8	0	-3.791410	-1.455470	0.297358
8	6	0	-2.478937	-1.463145	-0.296062
9	6	0	-2.132560	-0.037998	-0.627555
10	6	0	-1.178072	0.808847	-0.654341
11	1	0	-6.853036	1.778061	0.926845
12	1	0	-5.991498	3.079033	-1.006060
13	1	0	-4.238476	2.105355	-2.472493
14	1	0	-3.661523	-0.281948	-2.142551
15	1	0	-5.875071	-0.435949	1.517577
16	1	0	-1.792263	-1.888199	0.441343
17	1	0	-2.475498	-2.081373	-1.201808
18	1	0	-1.171761	1.837308	-0.993192
19	49	0	0.904274	0.086964	0.011349
20	53	0	1.443166	-1.948113	-1.783312
21	53	0	0.564941	-0.849257	2.585429
22	53	0	2.413787	2.365562	-0.264039

Int1-5

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-6.204982	1.310451	-0.049581
2	6	0	-5.396049	2.257315	-0.773914
3	6	0	-4.173125	1.903070	-1.248344
4	6	0	-3.687698	0.512713	-1.083071
5	6	0	-4.493545	-0.322392	-0.160848
6	6	0	-5.789806	0.030596	0.256827
7	8	0	-3.850886	-1.358217	0.281559
8	6	0	-2.425931	-1.298171	-0.172334
9	6	0	-2.250332	0.132074	-0.642715
10	6	0	-1.137604	0.857504	-0.659458
11	1	0	-7.176139	1.640575	0.311451
12	1	0	-5.782964	3.259668	-0.928117

13	1	0	-3.561251	2.596675	-1.818132
14	1	0	-3.813924	0.041247	-2.086322
15	1	0	-6.374961	-0.639001	0.878022
16	1	0	-1.824748	-1.593015	0.688590
17	1	0	-2.329829	-2.039032	-0.973786
18	1	0	-1.197226	1.876010	-1.048004
19	49	0	0.837439	0.133257	-0.033406
20	53	0	1.181091	-2.228351	-1.498161
21	53	0	0.560186	-0.490494	2.674820
22	53	0	2.696234	2.094205	-0.581162

Ts2-5g

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-5.910336	-0.558874	-0.569869
2	6	0	-5.117759	-1.649159	-1.028687
3	6	0	-3.768060	-1.489927	-1.230586
4	6	0	-3.148777	-0.233583	-0.871686
5	6	0	-4.019614	0.874111	-0.577370
6	6	0	-5.388678	0.708950	-0.344817
7	8	0	-3.390366	2.037974	-0.548241
8	6	0	-1.988257	1.849277	-0.954236
9	6	0	-1.843583	0.376942	-1.311973
10	6	0	-0.725456	-0.313972	-1.572722
11	1	0	-6.974368	-0.719570	-0.415971
12	1	0	-5.593309	-2.605722	-1.220827
13	1	0	-3.142293	-2.314380	-1.559710
14	1	0	-2.670934	-0.551106	0.309139
15	1	0	-6.012395	1.548820	-0.058236
16	1	0	-1.815317	2.523662	-1.796597
17	1	0	-1.373787	2.167704	-0.107001
18	1	0	-0.873121	-1.386286	-1.729994
19	49	0	1.059883	0.017636	-0.472162
20	53	0	-1.158609	-0.865141	1.835089
21	53	0	1.869194	2.536709	0.237072
22	53	0	2.970685	-1.920883	-0.470788

Int2-5g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.421607	-0.965106	-0.000615
2	6	0	-5.581027	-2.093748	-0.000391
3	6	0	-4.194908	-1.940522	-0.000061
4	6	0	-3.657859	-0.646829	0.000189
5	6	0	-4.516943	0.463053	0.000033
6	6	0	-5.904445	0.332980	-0.000456
7	8	0	-3.858051	1.652864	0.000271
8	6	0	-2.436772	1.374744	0.000832
9	6	0	-2.284103	-0.144196	0.000551
10	6	0	-1.135089	-0.860507	0.000580
11	1	0	-7.499556	-1.104118	-0.000901
12	1	0	-6.016421	-3.088692	-0.000448
13	1	0	-3.542972	-2.810295	-0.000001
14	1	0	-6.546821	1.207666	-0.000650
15	1	0	-2.005508	1.846844	-0.887633
16	1	0	-2.006377	1.846299	0.890008
17	1	0	-1.229959	-1.947261	0.000418
18	49	0	0.840392	-0.181332	0.000203
19	53	0	1.541310	2.449369	-0.000216
20	53	0	2.898866	-1.947619	-0.000103

Ts3-5g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.130785	0.503922	-1.658313
2	6	0	-5.322092	-0.472025	-2.276145
3	6	0	-3.965894	-0.555733	-1.976996
4	6	0	-3.423692	0.348339	-1.049269
5	6	0	-4.251411	1.312646	-0.446232
6	6	0	-5.611956	1.412634	-0.734759
7	8	0	-3.589071	2.118286	0.420651
8	6	0	-2.207888	1.689455	0.453898
9	6	0	-2.082993	0.536498	-0.528929
10	6	0	-0.966848	-0.219822	-0.769426
11	1	0	-7.187513	0.551255	-1.907754
12	1	0	-5.764185	-1.161035	-2.989479

13	1	0	-3.338747	-1.305994	-2.450913
14	1	0	-1.006844	-1.299243	0.621019
15	1	0	-6.230772	2.164765	-0.256632
16	1	0	-1.583686	2.552630	0.202068
17	1	0	-1.976264	1.377799	1.479469
18	1	0	-1.080430	-1.008570	-1.516601
19	49	0	1.055664	0.268039	-0.396076
20	53	0	-0.875551	-2.396176	1.979430
21	53	0	1.808326	2.371820	1.144938
22	53	0	3.009392	-1.094272	-1.675719

Ts2-5h

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-6.454908	1.275797	0.009750
2	6	0	-5.602109	2.388719	-0.166215
3	6	0	-4.232990	2.212272	-0.292747
4	6	0	-3.731663	0.891424	-0.246701
5	6	0	-4.594366	-0.214180	-0.046391
6	6	0	-5.971414	-0.030888	0.076656
7	8	0	-3.965396	-1.389821	0.072630
8	6	0	-2.518945	-1.194369	0.000581
9	6	0	-2.281373	0.306864	-0.180710
10	6	0	-1.097759	0.979694	-0.218052
11	1	0	-7.523761	1.443625	0.107708
12	1	0	-6.022582	3.388567	-0.198153
13	1	0	-3.562887	3.054961	-0.434961
14	1	0	-2.916866	0.668938	-1.232939
15	1	0	-6.626628	-0.879696	0.240367
16	1	0	-2.079558	-1.561019	0.932837
17	1	0	-2.138324	-1.785115	-0.837485
18	1	0	-1.168252	2.048191	-0.438673
19	49	0	0.919961	0.100230	0.006072
20	53	0	0.925822	-1.679520	-2.139509
21	53	0	0.818629	-1.221051	2.443054
22	53	0	2.738513	2.148436	-0.164569

Int2-5h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.157444	-0.333254	-0.948758
2	6	0	5.360467	-1.439430	-1.273049
3	6	0	3.964260	-1.319254	-1.301035
4	6	0	3.388665	-0.089728	-0.994097
5	6	0	4.200831	1.000944	-0.675897
6	6	0	5.589473	0.909977	-0.643953
7	8	0	3.495995	2.146094	-0.428285
8	6	0	2.093281	1.794940	-0.362639
9	6	0	1.947114	0.384817	-0.999687
10	6	0	0.908395	-0.549088	-0.383303
11	1	0	7.238989	-0.439635	-0.929936
12	1	0	5.825821	-2.393878	-1.501634
13	1	0	3.347515	-2.178847	-1.554464
14	1	0	1.618055	0.492715	-2.049380
15	1	0	6.198574	1.771844	-0.390371
16	1	0	1.799165	1.786562	0.693255
17	1	0	1.534857	2.574185	-0.884815
18	1	0	0.958303	-1.530372	-0.860344
19	49	0	-1.169804	0.016144	-0.272805
20	53	0	-2.015082	2.551340	0.190369
21	53	0	1.304435	-1.059553	1.772946
22	53	0	-3.078568	-1.872955	-0.646976

Ts3-5h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.377482	-0.583360	-0.900920
2	6	0	5.552970	-1.707530	-1.089545
3	6	0	4.164187	-1.575736	-1.064634
4	6	0	3.621677	-0.307861	-0.840690
5	6	0	4.457741	0.800629	-0.653847
6	6	0	5.846513	0.689377	-0.678265
7	8	0	3.780354	1.966045	-0.457173
8	6	0	2.382522	1.643080	-0.302765
9	6	0	2.226827	0.195664	-0.791480
10	6	0	1.016540	-0.547671	-0.709842

11	1	0	7.456820	-0.707395	-0.922518
12	1	0	6.001190	-2.683083	-1.250798
13	1	0	3.524600	-2.443135	-1.206694
14	1	0	1.707050	0.162764	-1.879742
15	1	0	6.478200	1.558269	-0.525934
16	1	0	2.132140	1.689194	0.764155
17	1	0	1.790706	2.381260	-0.844459
18	1	0	1.153276	-1.602789	-0.968391
19	49	0	-1.025020	-0.023903	-0.042975
20	53	0	-1.501536	2.663450	0.145554
21	53	0	0.187736	-1.234235	2.206624
22	53	0	-2.915249	-1.515096	-1.318415

Int3-5

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	5.555461	-0.839446	0.316552
2	6	0	4.584474	-1.821492	0.621075
3	6	0	3.314097	-1.452201	1.034903
4	6	0	3.019830	-0.076776	1.147880
5	6	0	4.010487	0.883866	0.841969
6	6	0	5.290792	0.524417	0.419379
7	8	0	3.587288	2.154643	1.007684
8	6	0	2.213974	2.101582	1.451181
9	6	0	1.848248	0.639825	1.551008
10	1	0	6.541701	-1.159378	-0.009164
11	1	0	4.837668	-2.871984	0.519090
12	1	0	2.561395	-2.201994	1.255692
13	1	0	6.035407	1.277515	0.185230
14	1	0	2.149170	2.613841	2.417300
15	1	0	1.593960	2.637317	0.720560
16	49	0	-0.826655	-0.045824	-0.004450
17	53	0	0.217938	-2.135635	-1.448255
18	53	0	-0.718112	2.413716	-1.247023
19	53	0	-3.179506	-0.580144	1.306110
20	6	0	0.603389	0.165898	1.943951
21	1	0	-0.057483	0.846457	2.480506
22	1	0	0.524548	-0.878205	2.245873

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.290499	-0.060138	1.232052
2	6	0	5.023337	0.172299	0.064048
3	6	0	4.412518	0.773620	-1.040637
4	6	0	3.068181	1.151007	-0.983022
5	6	0	2.361243	0.909060	0.190214
6	6	0	2.943857	0.308242	1.303434
7	8	0	0.985469	1.267067	0.228306
8	6	0	0.671185	2.485167	0.996519
9	6	0	1.298152	3.670598	0.432758
10	6	0	1.801496	4.678479	-0.003749
11	1	0	4.760053	-0.538050	2.087074
12	1	0	6.067977	-0.121524	0.012679
13	1	0	4.978657	0.947588	-1.951233
14	1	0	2.571016	1.614099	-1.828767
15	1	0	2.355757	0.115305	2.195926
16	1	0	-0.418308	2.566635	0.959654
17	1	0	0.980438	2.317728	2.032886
18	1	0	2.245560	5.567508	-0.395065
19	49	0	-0.612018	-0.291477	-0.071417
20	53	0	0.550433	-2.154841	-1.666384
21	53	0	-0.991535	-0.923070	2.570886
22	53	0	-2.514725	1.325958	-1.179782

Ts1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.255401	0.709612	0.865967
2	6	0	-5.138109	0.447498	-0.210676
3	6	0	-4.691095	-0.251283	-1.316511
4	6	0	-3.356384	-0.724234	-1.366793
5	6	0	-2.447684	-0.388045	-0.317303
6	6	0	-2.939458	0.288859	0.830043
7	8	0	-1.196001	-0.796768	-0.415722
8	6	0	-1.056063	-2.946716	0.082404
9	6	0	-2.353743	-3.205662	-0.219578

10	6	0	-3.514182	-2.960184	-0.586825
11	1	0	-4.617369	1.258050	1.731479
12	1	0	-6.162497	0.806124	-0.165797
13	1	0	-5.356295	-0.447733	-2.153382
14	1	0	-2.946347	-1.131885	-2.284505
15	1	0	-2.262593	0.491791	1.654629
16	1	0	-0.264560	-3.151749	-0.634421
17	1	0	-0.757525	-2.769715	1.113539
18	1	0	-4.551897	-3.122633	-0.788833
19	49	0	0.637662	0.178229	-0.012672
20	53	0	0.257822	2.777167	-0.756844
21	53	0	0.932428	-0.279688	2.694974
22	53	0	2.276813	-1.367486	-1.581344

Int1

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-4.045210	1.690965	0.321898
2	6	0	-5.111710	1.141049	-0.482935
3	6	0	-4.854512	0.129859	-1.339479
4	6	0	-3.486215	-0.471196	-1.484374
5	6	0	-2.406926	0.178164	-0.637733
6	6	0	-2.756158	1.240181	0.261518
7	8	0	-1.233646	-0.255951	-0.778742
8	6	0	-2.251830	-3.366495	0.527370
9	6	0	-2.930640	-2.675252	-0.350647
10	6	0	-3.588797	-1.992730	-1.252544
11	1	0	-4.282531	2.502567	1.006053
12	1	0	-6.112238	1.550425	-0.381495
13	1	0	-5.645460	-0.304960	-1.945958
14	1	0	-3.160948	-0.337405	-2.531350
15	1	0	-1.980380	1.679393	0.879091
16	1	0	-1.277528	-3.784893	0.280637
17	1	0	-2.627190	-3.535994	1.534624
18	1	0	-4.286279	-2.500000	-1.918650
19	49	0	0.720492	0.076275	0.007821
20	53	0	1.221146	2.610915	-0.917931
21	53	0	0.342159	-0.088913	2.729338

22	53	0	2.069328	-1.997592	-1.140741

Ts2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.816992	-3.592538	1.181734
2	6	0	-0.905210	-2.506291	2.021574
3	6	0	-0.026275	-1.370026	1.899334
4	6	0	1.113560	-2.584076	0.082070
5	6	0	0.211461	-3.625753	0.214398
6	6	0	1.049695	-1.447266	0.926191
7	8	0	1.860841	-0.423804	0.798868
8	6	0	0.017830	-0.445675	3.078011
9	6	0	1.050629	0.211714	3.558466
10	6	0	2.041525	0.871835	4.097296
11	1	0	-1.519141	-4.415388	1.266225
12	1	0	-1.670251	-2.471707	2.792453
13	1	0	1.894419	-2.637026	-0.669966
14	1	0	0.295943	-4.482408	-0.449195
15	1	0	-0.923960	-0.379048	3.626556
16	1	0	2.272015	1.898571	3.817822
17	1	0	2.698556	0.404470	4.829415
18	6	0	0.786146	2.984430	-1.748154
19	6	0	0.634336	3.084551	-0.399318
20	6	0	-0.145878	2.093100	0.387096
21	6	0	-0.646823	0.966052	-1.808878
22	6	0	-0.800503	1.022975	-0.433494
23	8	0	-1.517829	0.094082	0.209970
24	6	0	-1.110474	2.713990	1.408439
25	6	0	-1.628778	3.911419	1.295485
26	6	0	-2.165882	5.099449	1.200798
27	6	0	0.153879	1.917252	-2.444646
28	1	0	1.402825	3.688765	-2.295949
29	1	0	1.115927	3.878178	0.162602
30	1	0	-1.112482	0.165772	-2.374342
31	1	0	-1.361184	2.084769	2.259257
32	1	0	-3.115461	5.242982	0.688291
33	1	0	-1.690982	5.977588	1.634281

34	1	0	0.290145	1.842249	-3.519547
35	1	0	0.621930	1.550893	0.981830
36	1	0	-0.887060	-0.591055	0.979753
37	49	0	-3.711065	-0.298079	-0.099823
38	53	0	-4.468112	-0.582806	2.508316
39	53	0	-4.500771	2.016108	-1.326497
40	53	0	-3.693971	-2.492345	-1.718867
41	49	0	3.680592	-0.123549	-0.079555
42	53	0	4.252801	2.446414	0.759517
43	53	0	5.413472	-2.076840	0.710762
44	53	0	3.139304	-0.146209	-2.822082

Int2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-3.816778	-2.074451	-0.822242
2	6	0	-4.983940	-1.316370	-0.702063
3	6	0	-4.898970	0.071949	-0.639056
4	6	0	-3.663423	0.746694	-0.684022
5	6	0	-2.509202	-0.052930	-0.792485
6	6	0	-2.574723	-1.439425	-0.868520
7	8	0	-1.226999	0.527966	-0.828702
8	6	0	-1.628595	3.856386	-0.898005
9	6	0	-2.643897	3.037332	-0.763202
10	6	0	-3.667298	2.217745	-0.626700
11	1	0	-3.863941	-3.157677	-0.881083
12	1	0	-5.954224	-1.802373	-0.661871
13	1	0	-5.805543	0.665481	-0.551598
14	1	0	-1.282179	1.507044	-0.933581
15	1	0	-1.664210	-2.018868	-0.981026
16	1	0	-1.043402	4.189071	-0.041496
17	1	0	-1.329467	4.240824	-1.872851
18	1	0	-4.647098	2.669777	-0.466805
19	49	0	0.717177	-0.133163	0.120675
20	53	0	-0.065224	-0.523975	2.697985
21	53	0	1.484901	-2.319183	-1.320904
22	53	0	2.025330	2.196486	-0.473598

Ts3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.164617	-1.512390	0.060353
2	6	0	-5.233195	-0.597883	0.044881
3	6	0	-4.965210	0.759833	0.008319
4	6	0	-3.634487	1.240059	0.038242
5	6	0	-2.565728	0.293548	0.076621
6	6	0	-2.842700	-1.078217	0.042227
7	8	0	-1.295294	0.768256	0.090169
8	6	0	-1.317550	4.180057	0.326983
9	6	0	-2.074353	3.143691	-0.049204
10	6	0	-3.342379	2.638246	-0.116828
11	1	0	-4.366766	-2.579573	0.081946
12	1	0	-6.258114	-0.955714	0.044115
13	1	0	-5.778128	1.480611	-0.034959
14	1	0	-1.380945	1.977664	-0.182112
15	1	0	-2.030946	-1.796891	0.040480
16	1	0	-1.607967	4.836424	1.149120
17	1	0	-0.325700	4.334556	-0.091696
18	1	0	-4.148570	3.270783	-0.495976
19	49	0	0.655615	-0.179828	0.002402
20	53	0	0.567153	-1.673594	-2.290541
21	53	0	2.196450	2.083747	-0.129313
22	53	0	0.726504	-1.585701	2.345523

Int3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.617839	-2.571684	-0.001235
2	6	0	4.896330	-1.929805	-0.001269
3	6	0	4.957895	-0.567470	-0.001079
4	6	0	3.763434	0.247984	-0.000826
5	6	0	2.454914	-0.429678	-0.000748
6	6	0	2.444288	-1.859116	-0.000997
7	8	0	1.380574	0.266520	-0.000436
8	6	0	3.334045	3.968518	-0.000322
9	6	0	2.941622	2.672111	-0.000473

10	6	0	3.923393	1.625529	-0.000691
11	1	0	3.574355	-3.658017	-0.001412
12	1	0	5.801011	-2.529268	-0.001451
13	1	0	5.918784	-0.058559	-0.001126
14	1	0	1.889235	2.418062	-0.000492
15	1	0	1.486787	-2.368754	-0.000987
16	1	0	4.385251	4.251444	-0.000370
17	1	0	2.606873	4.775185	-0.000155
18	1	0	4.958898	1.970826	-0.000766
19	49	0	-0.697041	-0.025773	0.000139
20	53	0	-1.170401	-1.425073	2.314508
21	53	0	-1.459164	2.612634	-0.000044
22	53	0	-1.172574	-1.425458	-2.313535

Ts4

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-3.995278	2.178547	-0.320554
2	6	0	-5.142915	1.370927	-0.629624
3	6	0	-4.983590	0.038850	-0.849568
4	6	0	-3.676490	-0.591077	-0.757928
5	6	0	-2.494923	0.269438	-0.503969
6	6	0	-2.727115	1.663375	-0.258888
7	8	0	-1.333738	-0.240756	-0.546352
8	6	0	-2.000375	-3.331348	0.432066
9	6	0	-2.416841	-2.830404	-0.734828
10	6	0	-3.586825	-1.951406	-0.894466
11	1	0	-4.138998	3.241738	-0.143077
12	1	0	-6.123903	1.832484	-0.680225
13	1	0	-5.837444	-0.595704	-1.073594
14	1	0	-1.920614	-3.122766	-1.663400
15	1	0	-1.873148	2.301194	-0.056276
16	1	0	-2.468199	-3.069362	1.377473
17	1	0	-1.154248	-4.010393	0.469952
18	1	0	-4.517846	-2.459946	-1.160743
19	49	0	0.663771	0.075678	0.032306
20	53	0	0.438949	-0.365136	2.733791
21	53	0	1.917459	-1.861503	-1.440541

22	53	0	1.272378	2.664359	-0.673924

Int4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.981157	-1.780067	-0.408806
2	6	0	-5.130030	-0.933965	-0.412656
3	6	0	-4.955851	0.418905	-0.396224
4	6	0	-3.642698	1.031449	-0.399176
5	6	0	-2.471371	0.141161	-0.408957
6	6	0	-2.706988	-1.267856	-0.392534
7	8	0	-1.283120	0.629605	-0.413930
8	6	0	-1.403279	3.446343	-0.884759
9	6	0	-2.625363	3.453440	-0.298629
10	6	0	-3.625084	2.420157	-0.285072
11	1	0	-4.115607	-2.858824	-0.417732
12	1	0	-6.124730	-1.367881	-0.419246
13	1	0	-5.819246	1.079375	-0.385720
14	1	0	-2.968956	4.392721	0.132990
15	1	0	-1.850469	-1.932850	-0.398663
16	1	0	-0.796787	4.347379	-0.885233
17	1	0	-1.007166	2.583240	-1.399010
18	1	0	-4.621764	2.834462	-0.124206
19	49	0	0.631293	-0.120111	0.045709
20	53	0	0.306258	-1.145920	2.570113
21	53	0	1.152932	-1.975519	-1.914327
22	53	0	2.123588	2.181695	-0.122024

Ts5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.943244	1.714470	-0.619734
2	6	0	5.048491	0.845486	-0.723358
3	6	0	4.815482	-0.505992	-0.851881
4	6	0	3.497680	-1.042531	-0.947051
5	6	0	2.371482	-0.128538	-0.898243
6	6	0	2.642091	1.236850	-0.661646
7	8	0	1.106105	-0.538143	-1.027040

8	6	0	1.184501	-2.489151	-1.837176
9	6	0	2.128044	-3.105123	-1.018315
10	6	0	3.323851	-2.448938	-0.776483
11	1	0	4.104424	2.783559	-0.508736
12	1	0	6.061072	1.233335	-0.675506
13	1	0	5.649293	-1.203309	-0.881554
14	1	0	1.889409	-4.031672	-0.501934
15	1	0	1.812563	1.932615	-0.594638
16	1	0	0.149226	-2.819685	-1.852937
17	1	0	1.505928	-1.892024	-2.681804
18	1	0	4.135797	-2.987620	-0.288959
19	49	0	-0.602077	0.103684	0.079124
20	53	0	-1.327062	2.490283	-1.068615
21	53	0	-2.393614	-1.931459	-0.402349
22	53	0	0.354942	0.228916	2.646975

Int5

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	3.991053	1.541704	-0.762918
2	6	0	4.921627	0.513506	-0.586944
3	6	0	4.528356	-0.818825	-0.725335
4	6	0	3.200640	-1.146649	-1.038088
5	6	0	2.291113	-0.086888	-1.197244
6	6	0	2.657584	1.245132	-1.068919
7	8	0	0.931214	-0.406210	-1.429574
8	6	0	0.769612	-1.549627	-2.337385
9	6	0	1.541752	-2.731344	-1.823484
10	6	0	2.715052	-2.516160	-1.206366
11	1	0	4.295246	2.579305	-0.661731
12	1	0	5.953085	0.749767	-0.342074
13	1	0	5.250250	-1.620089	-0.587801
14	1	0	1.133385	-3.725729	-1.977503
15	1	0	1.923589	2.032708	-1.206351
16	1	0	-0.302904	-1.735062	-2.389766
17	1	0	1.123008	-1.209893	-3.320969
18	1	0	3.320791	-3.335915	-0.829188
19	49	0	-0.617655	0.112111	0.160628

20	53	0	-1.325182	2.597856	-0.732385
21	53	0	-2.498887	-1.837887	-0.241144
22	53	0	0.813092	-0.055893	2.470913