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## 1. Experimental Section

A vacuum glass Schlenk tube (25 mL) equipped with a magnetic stirring bar was evacuated and flushed with argon. The calculated amount of zinc powder and 10 mL of deoxidized acetonitrile were placed in the reactor. Then to the mixture obtained were successively added phenylacetylene and  $\text{Me}_3\text{SiCl}$  under a flow of argon. The reactor was placed in an oil bath, and the reaction was conducted at 100 °C. All manipulations with air-sensitive materials were performed with the exclusion of oxygen and moisture using Schlenk techniques or a glovebox. Acetonitrile solvent was distilled under  $\text{N}_2$  from  $\text{CaH}_2$ . Nitrogen was purified by passage through a Ag oxygen-removal column and a Davison 4 Å molecular sieve column. Phenylacetylene,  $\text{Me}_3\text{SiCl}$ , Styrene, 1-Phenyl-2-trimethylsilylacetylene, TEMPO and Toluene were purchased from TCI and the radical scavenger N-tert-Butyl- $\alpha$ -phenylnitron (PBN) from Sigma-Aldrich. All reagents were used as received without further purification.

## 2. Characterization Methods

The  $^1\text{H}$  (400MHz) and  $^{13}\text{C}$  (100MHz) NMR spectra was recorded in  $\text{CDCl}_3$  using a Bruker AVANCE III 400 MHz spectrometer and referenced to the residual protonated solvent peaks ( $^1\text{H}$   $\delta$  7.26 ppm and  $^{13}\text{C}$   $\delta$  77.16 ppm for  $\text{CDCl}_3$ ). The EPR spectra was recorded on a Bruker BioSpin GmbH X-band ( $\nu = 9.87$  GHz) digital EPR spectrometer. All EPR spectra were recorded at a microwave power of 1-10 mW and 100 kHz magnetic field modulation of 1.0 G amplitude. The GC analysis was performed on gas chromatography apparatus equipped with a FID detector and capillary column HP-5 (30 m  $\times$  0.32 mm). Products were identified by GC/MS equipped with a HP-5 column (30 m  $\times$  0.25 mm) and ion trap mass detector. The conversion yields were calculated using the internal standard calculation method with toluene as an internal standard.

## 3. Experimental results

### 3.1. Procedure for testing reaction time under different reaction temperatures

To a 25 mL Schlenk flask zinc powder (9 mmol), phenylacetylene (3 mmol),  $\text{Me}_3\text{SiCl}$  (3 mmol) and dry acetonitrile (10 mL) was added and the mixture was stirred at different reaction temperatures monitored by GC with FID detector. The yields were calculated using area normalization method.

Table S1. Time required to complete reaction under different temperatures

Entry	Temperature (°C)	Time for yield over 98% (h)
1	80	20
2	100	12
3	120	10

### 3.2. Procedure for time course reaction monitored by GC analysis

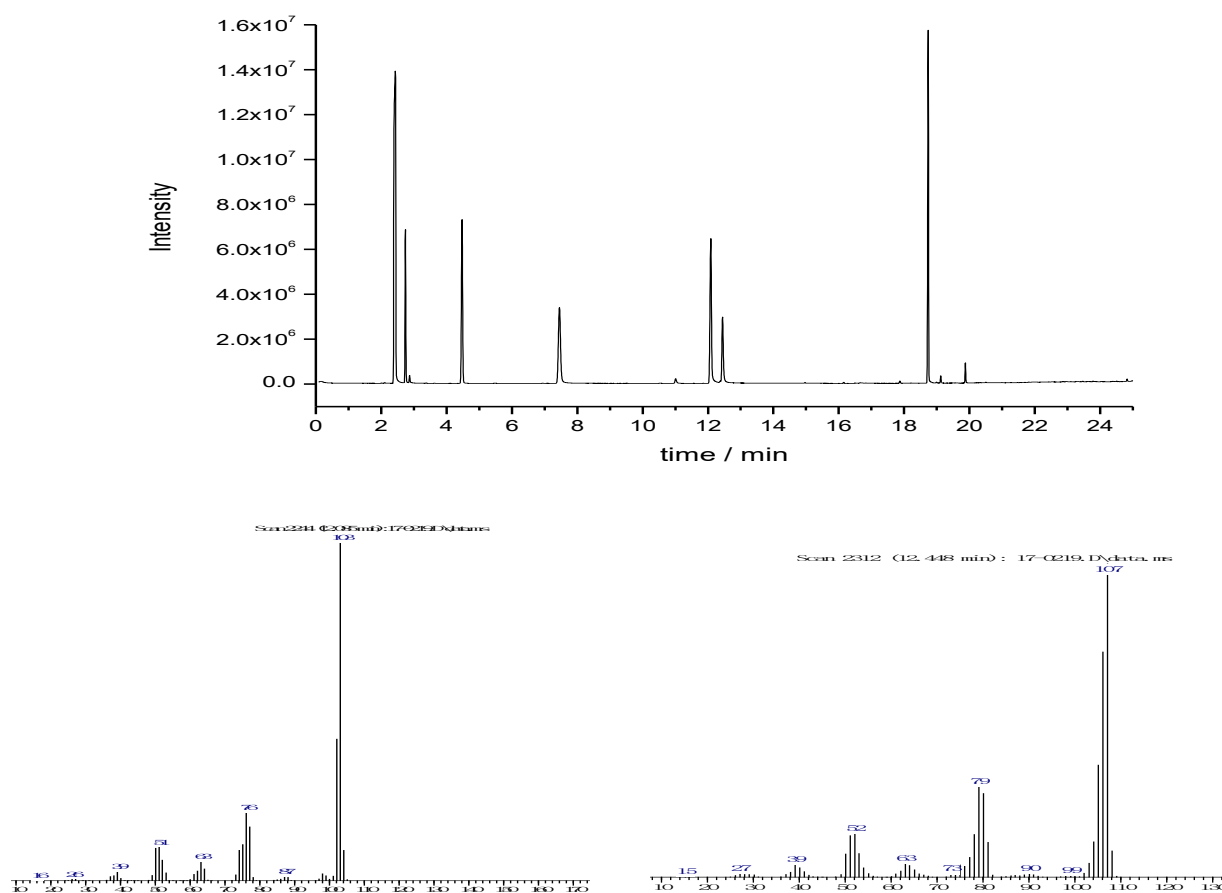
To a 25 mL Schlenk flask zinc powder (9 mmol), phenylacetylene (3 mmol),  $\text{Me}_3\text{SiCl}$  (3 mmol) and dry acetonitrile (10 mL) was added and the mixture was stirred at 100 °C. At the indicated time points, an aliquot was removed with a clean and dry syringe and analyzed by GC with FID detector using toluene as the internal standard.

Table S2. Time required to complete reaction under different temperatures

t/h	Yield (%)			c:d
	c	d	Total	
1	6	3	9	2.0
2	12	6	18	2.0
3	40	20	60	2.0
5	46	23	69	2.0
6	47	26	73	1.8
8	58	30	88	2.0
10	60	30	90	2.0
12	64	34	98	2.0
20	66	33	99	2.0

### 3.3. Procedure for deuterated experiment

To a 25 mL Schlenk flask zinc powder (9 mmol), deuterated phenylacetylene (3 mmol),  $\text{Me}_3\text{SiCl}$  (3 mmol) and dry acetonitrile (10 mL) was added and the mixture is stirred at 100 °C for 10 h. The reaction liquid was taken with a clean, dry capillary tube and diluted in acetonitrile and analyzed by GC-MS. The yields were determined by GC with FID detector using toluene as the internal standard. The peak with a retention of 12.085 min was deuterated phenylacetylene while 12.448 min for deuterated styrene.



**Figure S1** GC-MS spectra for reaction liquid using deuterated phenylacetylene.

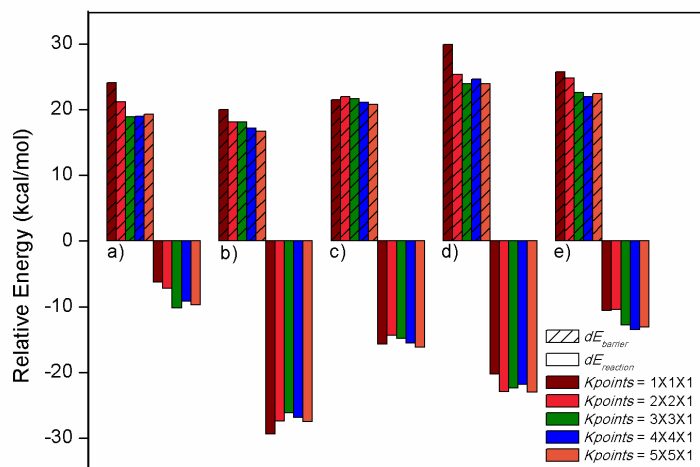
### 3.4. Procedure for acquisition of EPR spectra

To a 25 mL Schlenk flask zinc powder (3 mmol), phenylacetylene (1 mmol),  $\text{Me}_3\text{SiCl}$  (1 mmol) and dry acetonitrile (5 mL) was added and the mixture was stirred at 100 °C for 4 h. Then PBN (1 mmol) was added into the reaction liquid in the glove box, and the mixture was transferred into an sealed EPR tube. Removing from the glove box, the tube was quickly frozen in liquid nitrogen. The EPR spectrum was acquired at room temperature. For the spectra of single reactant, phenylacetylene or  $\text{Me}_3\text{SiCl}$  was used to react with zinc powder under the same conditions separately.

## 4. Benchmarking

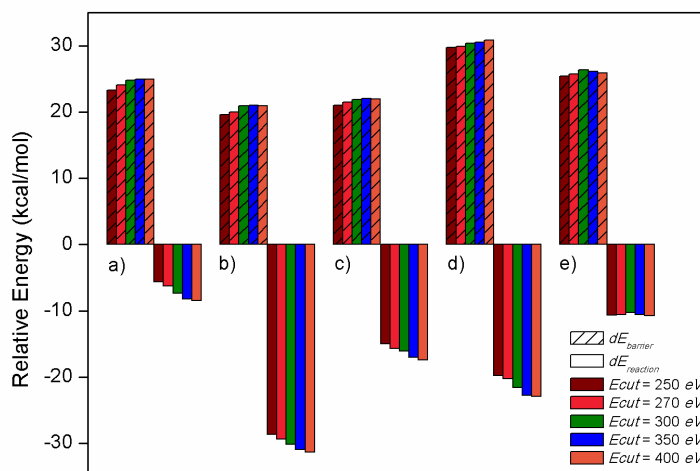
### 4.1. K-point mesh

The Kpoint was chosen  $1 \times 1 \times 1$  as a higher kpoint mesh would lead to dramatically increased calculation cost. Although the  $1 \times 1 \times 1$  kpoint would overestimate some of the energies, it had little effect on the understanding of the mechanism of zinc promoted silylation.



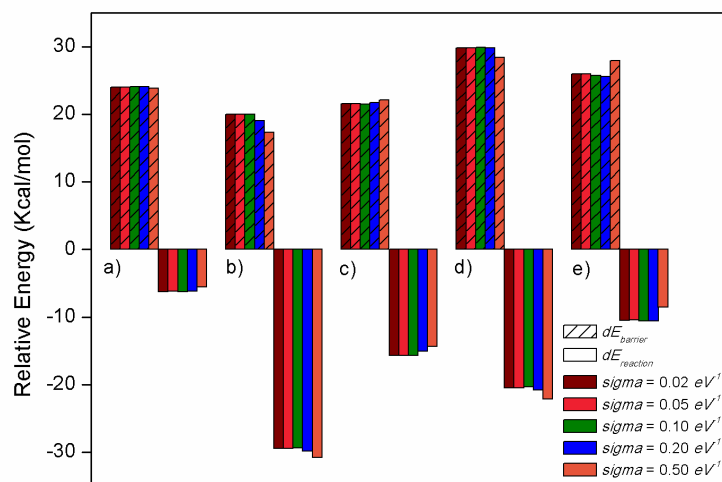
**Figure S2** Reaction barriers and energies with different K-point mesh. For a) H transfer from phenylacetylene to the inner carbon of alkynyl of phenylacetylene to form trans alkene species **A**; b) H transfer from phenylacetylene to the intermediate **A** to form alkene; c) H transfer from phenylacetylene to the outer carbon of alkynyl of phenylacetylene to form alkene species **C**; d) H transfer from phenylacetylene to the intermediate **C** to form alkene; e) Formation of phenylethynyltrimethylsilane.

#### 4.2. Cut-off energy



**Figure S3** Reaction barriers and energies with different cutoff energy. For a) H transfer from phenylacetylene to the inner carbon of alkynyl of phenylacetylene to form trans alkene species **A**; b) H transfer from phenylacetylene to the intermediate **A** to form alkene; c) H transfer from phenylacetylene to the outer carbon of alkynyl of phenylacetylene to form alkene species **C**; d) H transfer from phenylacetylene to the intermediate **C** to form alkene; e) Formation of phenylethynyltrimethylsilane.

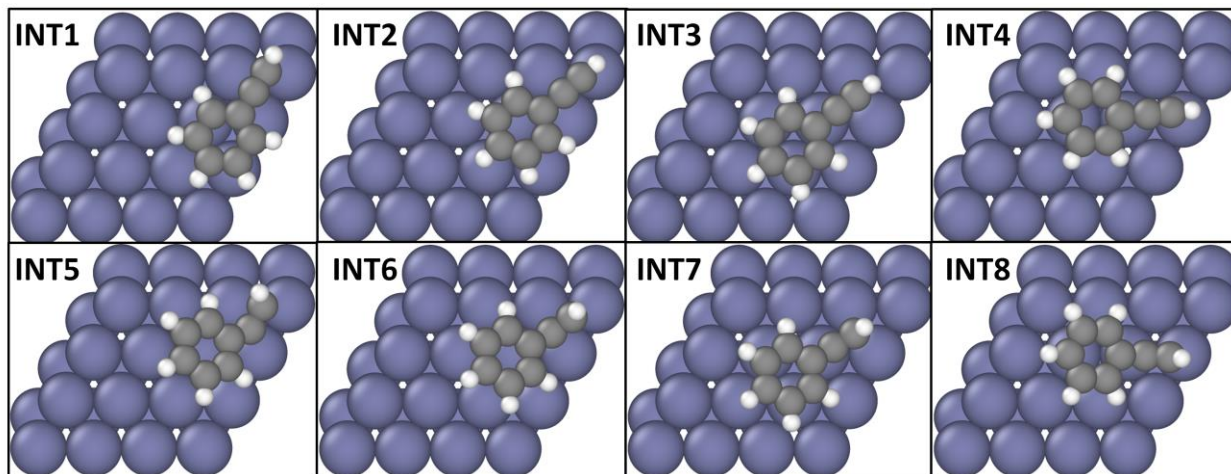
### 4.3. Smearing



**Figure S4** Reaction barriers and energies with different smearing ( $\sigma$  value). For a) H transfer from phenylacetylene to the inner carbon of alkynyl of phenylacetylene to form trans alkene species **A**; b) H transfer from phenylacetylene to the intermediate **A** to form alkene; c) H transfer from phenylacetylene to the outer carbon of alkynyl of phenylacetylene to form alkene species **C**; d) H transfer from phenylacetylene to the intermediate **C** to form alkene; e) Formation of phenylethynyltrimethylsilane.

## 5. Supplemental data

### 5.1. Adsorption modes and sites

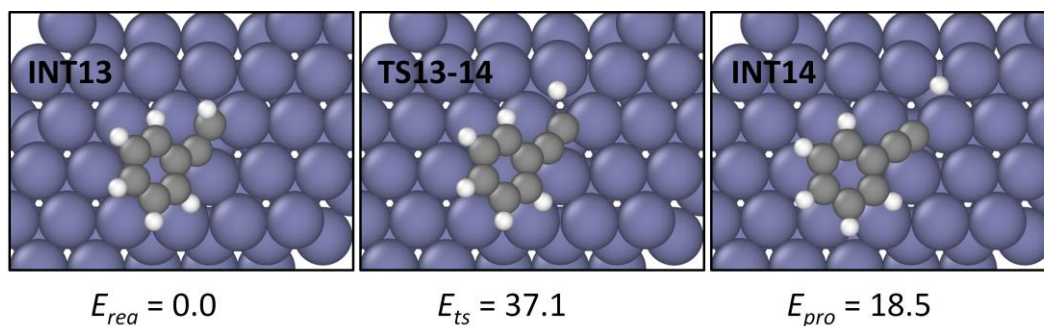


**Figure S5** Alkyne-mode (INT1-4) and alkene-mode (INT5-8) adsorption of phenylacetylene on zinc surface at different sites



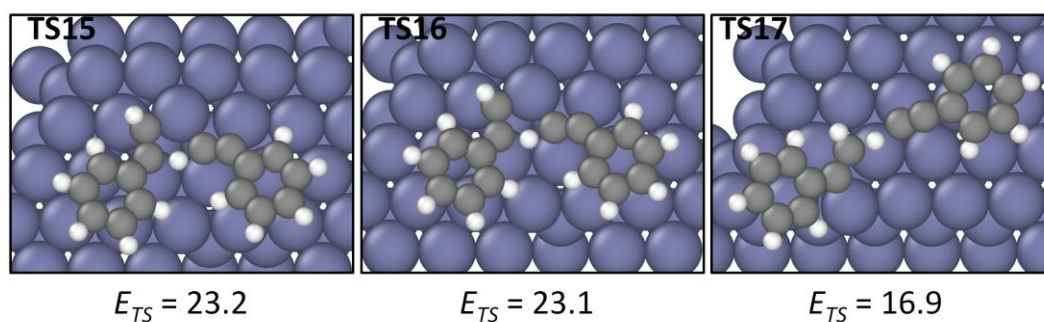




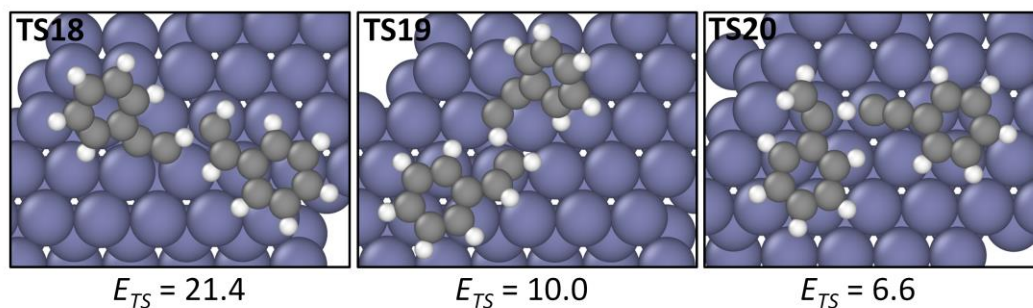


**Figure S8** Dissociation pathway of phenylacetylene on zinc surface. Energies (kcal/mol) are relative to reactant species.

**Mechanism V. Hydrogen transfer between adsorbed phenylacetylene on zinc surface**

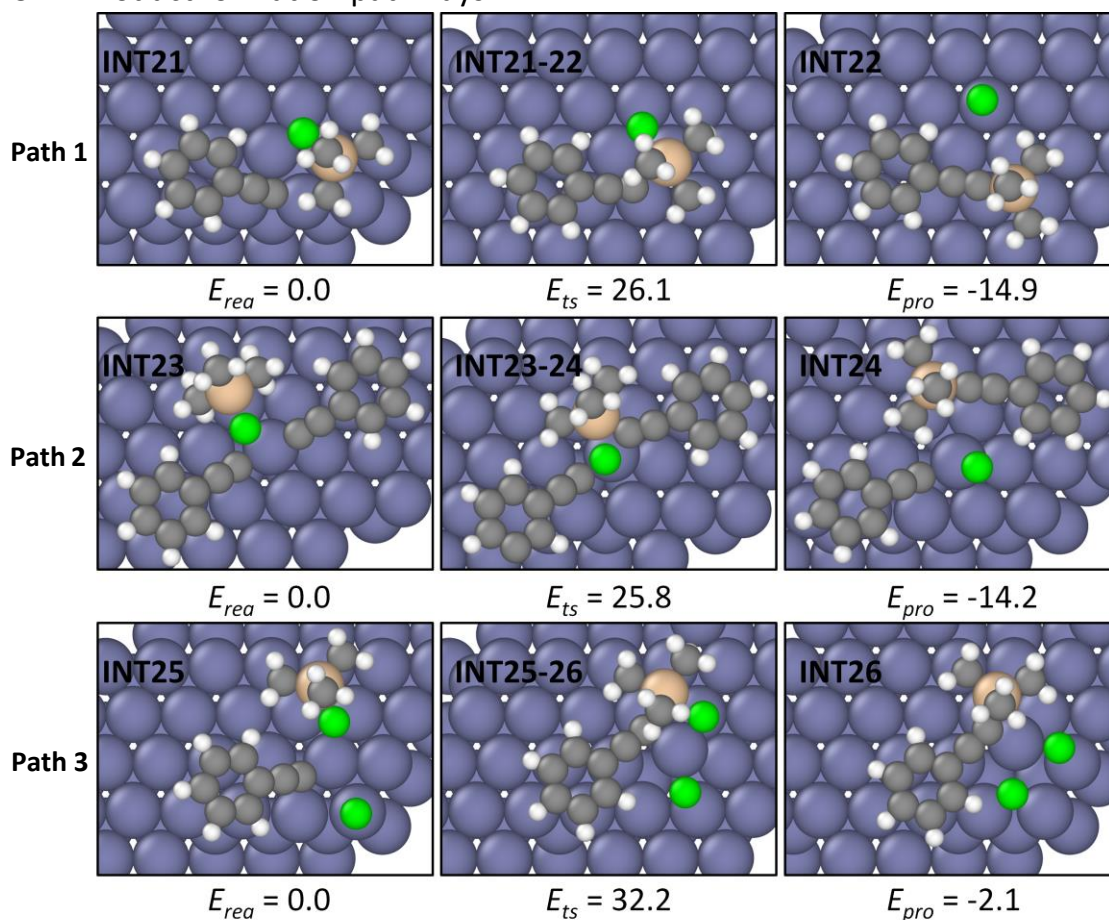


**Figure S9** Transition states of the first hydrogen transfer between the adsorbed phenylacetylene on zinc surface: TS15 for intermediate A; TS16 for intermediate B; TS17 for intermediate C. Energies (kcal/mol) are relative to reactant species.



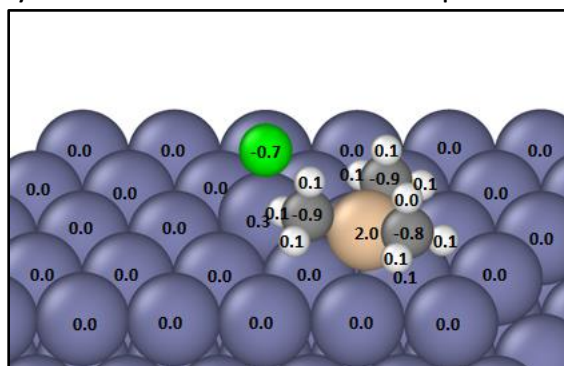
**Figure S10** Transition states of the second hydrogen transfer between the adsorbed phenylacetylene and alkene moieties on zinc surface: TS18 via intermediate A; TS19 via intermediate B; TS20 via intermediate C. Energies (kcal/mol) are relative to reactant species.

### 5.3. Product formation pathways

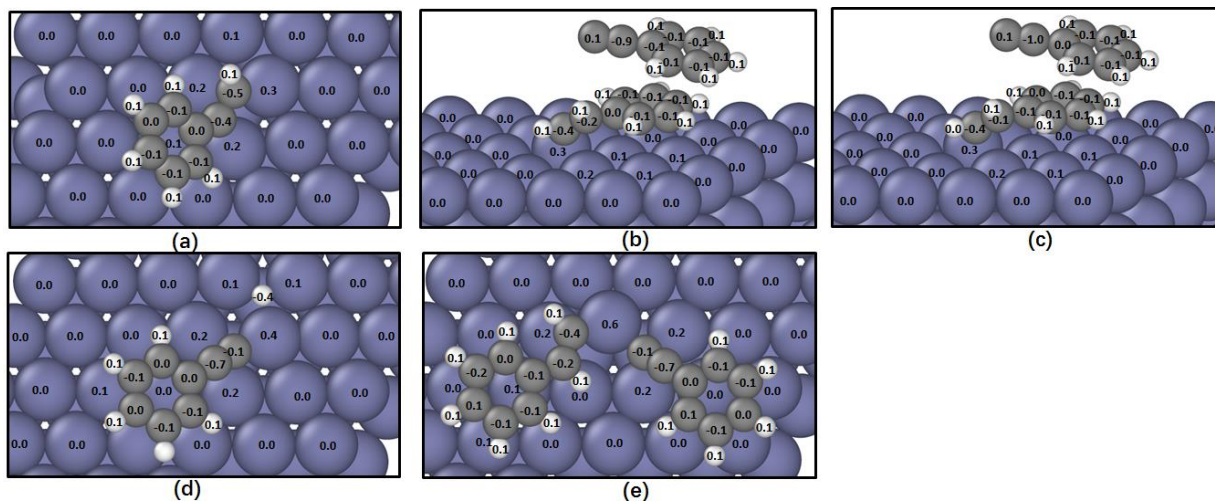


**Figure S11** Reaction pathways of for the formation step, path 1 via intermediate I  $\text{PhC}\equiv\text{C-Zn}$ ; path 2 via intermediate II  $(\text{PhC}\equiv\text{C})_2\text{Zn}$ ; path 3 via intermediate III  $\text{PhC}\equiv\text{CZnCl}$ . Energies ( $\text{kcal mol}^{-1}$ ) are relative to reactant species.

### 5.4. Bader charge analysis for the surface adsorbed species



**Figure S12** Bader charges distribution of dissociation products of  $\text{Me}_3\text{SiCl}$  on zinc surface.



**Figure S13** Bader charge distribution for the intermediates of the interaction between phenylacetylene and zinc in the initiation stage of Scheme 3. For a) alkene-mode adsorption of phenylacetylene on zinc surface; b) H transfer from phenylacetylene dissolving in the solvent to the adsorbed phenylacetylene on zinc surface to form radical species; c) H transfer from phenylacetylene dissolving in the solvent to the adsorbed phenylacetylene on zinc surface to form ion species; d) phenylacetylene dissociated on zinc surface; e) H transfer between adsorbed phenylacetylene on zinc surface.



























Table with columns: ID, Value1, Value2, Value3, Value4, Value5, Value6, Value7, Value8, Value9, Value10. Contains 1000 rows of numerical data.

### POSCAR for TS18 ###  
Zn C H

Table with columns: ID, Value1, Value2, Value3, Value4, Value5, Value6, Value7, Value8, Value9, Value10. Contains 1000 rows of numerical data.

140 16 13  
Selective dynamics

Table with columns: ID, Value1, Value2, Value3, Value4, Value5, Value6, Value7, Value8, Value9, Value10. Contains 1000 rows of numerical data.



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Selective dynamics						14.6566702133470298	11.530048856751191	7.0007917485174964	T	T	T
Cartesian						17.3273957810919725	11.492610198748203	6.986902691456320	T	T	T
18.6331299999999800	1.5368299999999688	0.0000000000000000	F	F	F	19.9994956720407515	11.4850833071601812	6.979043810252382	T	T	T
2.6618800000000453	1.5368299999999688	0.0000000000000000	F	F	F	22.6458032800277419	11.5124511045811975	7.0035842479559298	T	T	T
5.3237499999999462	1.5368299999999688	0.0000000000000000	F	F	F	1.3444969916422896	2.3211597396299806	6.972725470442326	T	T	T
7.9856299999999747	1.5368299999999688	0.0000000000000000	F	F	F	4.0081243521544883	2.319920404				



5.3237500000000599	6.1473399999999971	0.0000000000000000	F	F	F	3.9994477117661305	6.8914218467807489	6.9592251370708462	T	T	T
7.9856299999999578	6.1473399999999971	0.0000000000000000	F	F	F	6.6519346457843627	6.9080560536002844	7.0100642097442183	T	T	T
10.6474999999999920	6.1473399999999971	0.0000000000000000	F	F	F	9.3026814944918529	6.9166818057512646	7.0026100631805130	T	T	T
13.3093800000000222	6.1473399999999971	0.0000000000000000	F	F	F	11.9580312634667365	6.9306527618042386	7.0202275982735340	T	T	T
15.9712500000000546	6.1473399999999971	0.0000000000000000	F	F	F	14.6452504157008789	6.9164363920683050	7.0436040247187554	T	T	T
18.6331299999999551	6.1473399999999971	0.0000000000000000	F	F	F	17.2995223309081787	6.9126389064910114	7.011788771707924	T	T	T
22.6259400000000106	6.4525900000000416	0.0000000000000000	F	F	F	19.9735936395895415	6.8876386659873669	6.985059436667454	T	T	T
6.6546900000000839	6.4525900000000416	0.0000000000000000	F	F	F	5.3253984715715195	9.2058364965122390	6.999762064824750	T	T	T
9.3165599999999849	6.4525900000000416	0.0000000000000000	F	F	F	7.9822703302838107	9.2119404839480996	7.0025617737005250	T	T	T
11.9784400000000133	6.4525900000000416	0.0000000000000000	F	F	F	10.6436345027167789	9.2183498769835630	6.9778458204477181	T	T	T
14.6403100000000492	6.4525900000000416	0.0000000000000000	F	F	F	13.3031184869577807	9.218035329555732	6.9695621226053186	T	T	T
17.3021900000000812	6.4525900000000416	0.0000000000000000	F	F	F	15.9723807428690314	9.2013342728992367	7.0088015695090807	T	T	T
19.9640599999999786	6.4525900000000416	0.0000000000000000	F	F	F	18.6220765569655317	9.1762262070632055	7.0190760658148568	T	T	T
23.9568799999999911	10.7578400000000052	0.0000000000000000	F	F	F	21.3057408509919277	9.1626321936395208	7.0061832939400446	T	T	T
7.9856300000000617	10.7578400000000052	0.0000000000000000	F	F	F	13.2929997830250900	6.6945024960923698	6.9383499448076639	T	T	T
10.6474999999999618	10.7578400000000052	0.0000000000000000	F	F	F	9.5866223105225501	4.9632284762140264	10.4432444642533666	T	T	T
13.3093799999999938	10.7578400000000052	0.0000000000000000	F	F	F	10.8917694528622402	4.5943570006321321	10.1169985538815118	T	T	T
15.9712500000000261	10.7578400000000052	0.0000000000000000	F	F	F	11.2135534795858440	3.2275740214402919	9.95856736867373664	T	T	T
18.6331300000000581	10.7578400000000052	0.0000000000000000	F	F	F	10.2105032460779025	2.2484698876341573	10.1743324337554382	T	T	T
21.2949999999999591	10.7578400000000052	0.0000000000000000	F	F	F	8.9231217628190999	2.6320161700716202	10.5005132155333332	T	T	T
0.0000000000000000	0.0000000000000000	2.3863800000000821	F	F	F	8.59780905010480036	3.9908570584973178	10.6148640027239085	T	T	T
2.6618800000000324	0.0000000000000000	2.3863800000000821	F	F	F	13.2528646579392871	2.6324551926541067	8.5215276625907795	T	T	T
5.3237500000000644	0.0000000000000000	2.3863800000000821	F	F	F	12.4371495422662619	2.868485289449255	9.336172163702829	T	T	T
7.9856299999999631	0.0000000000000000	2.3863800000000821	F	F	F	16.0246747943064776	2.5745660006492441	10.7804115164148868	T	T	T
10.6474999999999973	0.0000000000000000	2.3863800000000821	F	F	F	15.9662460383769826	4.6311881605810949	10.8117066291318873	T	T	T
13.3093800000000275	0.0000000000000000	2.3863800000000821	F	F	F	17.9395029164092570	4.9905604424091319	10.6917529969365540	T	T	T
15.9712500000000617	0.0000000000000000	2.3863800000000821	F	F	F	9.3355353749429835	6.0237362810926944	10.5269329809307660	T	T	T
1.3309399999999771	2.3052499999999632	2.3863800000000821	F	F	F	11.6606761379142618	5.3454811394842059	9.9491310981926799	T	T	T
3.9928100000000093	2.3052499999999632	2.3863800000000821	F	F	F	10.4670118818269913	1.1951049392226121	10.0394171686857043	T	T	T
6.6546900000000422	2.3052499999999632	2.3863800000000821	F	F	F	8.1521650839795746	1.8739255697454418	10.628746655745732	T	T	T
9.3165599999999422	2.3052499999999632	2.3863800000000821	F	F	F	7.5732746166636771	4.2897803268352135	10.837827865121812	T	T	T
11.9784399999999742	2.3052499999999632	2.3863800000000821	F	F	F	14.9965384390069989	2.2449246234814191	10.9813490060546943	T	T	T
14.6403100000000066	2.3052499999999632	2.3863800000000821	F	F	F	16.7198713087458231	1.94236554957085650	11.35529333487612	T	T	T
17.3021900000000386	2.3052499999999632	2.3863800000000821	F	F	F	16.2282265268430379	2.4183636309630598	9.710497205606005	T	T	T
2.6618800000000018	4.6105000000000089	2.3863800000000821	F	F	F	14.9514423437130777	4.3043217555998563	13.3490300563965896	T	T	T
5.3237500000000342	4.6105000000000089	2.3863800000000821	F	F	F	16.0736466487287899	5.6923208334166935	13.3468763393801616	T	T	T
7.9856300000000671	4.6105000000000089	2.3863800000000821	F	F	F	16.6865432182177251	4.0475239828737237	13.679521302183161	T	T	T
10.6474999999999671	4.6105000000000089	2.3863800000000821	F	F	F	18.7485022595444626	4.4264648767596846	11.1792337029239325	T	T	T
13.3093799999999973	4.6105000000000089	2.3863800000000821	F	F	F	18.0664732135114221	6.0584188987542875	10.9172533923099994	T	T	T
15.9712500000000333	4.6105000000000089	2.3863800000000821	F	F	F	18.0380296772766693	4.8567183714771156	9.603770673636644	T	T	T
18.6331300000000653	4.6105000000000089	2.3863800000000821	F	F	F	14.8283239961888977	5.527997581505310	10.2600014083754210	T	T	T
3.9928136549999404	6.9157499999999708	2.3863800000000821	F	F	F	16.2807465359033898	4.3578904882876319	11.2616467323296199	T	T	T
6.6546900000000129	6.9157499999999708	2.3863800000000821	F	F	F	### POSCAR for TS21-22 ###					
9.3165600000000452	6.9157499999999708	2.3863800000000821	F	F	F	Zn C H Cl Si					
11.9784399999999422	6.9157499999999708	2.3863800000000821	F	F	F	1.0000000000000000					
14.6403099999999764	6.9157499999999708	2.3863800000000821	F	F	F	18.6331263450000009	0.0000000000000000	0.0000000000000000			
17.3021900000000102	6.9157499999999708	2.3863800000000821	F	F	F	6.6546879800000003	11.5262576909999996	0.0000000000000000			
19.9640600000000390	6.9157499999999708	2.3863800000000821	F	F	F	0.0000000000000000	0.0000000000000000	24.545240209999985			
5.3237536549999742	9.2210100000000370	2.3863800000000821	F	F	F	140 11 14 1					
7.9856300000000449	9.2210100000000370	2.3863800000000821	F	F	F	Selective dynamics					
10.6475000000000790	9.2210100000000370	2.3863800000000821	F	F	F	Cartesian					
13.3093799999999796	9.2210100000000370	2.3863800000000821	F	F	F	18.6331299999999800	1.5368299999999688	0.0000000000000000	F	F	F
15.9712500000000119	9.2210100000000370	2.3863800000000821	F	F	F	2.6618800000000453	1.5368299999999688	0.0000000000000000	F	F	F
18.6331300000000439	9.2210100000000370	2.3863800000000821	F	F	F	5.3237499999999462	1.5368299999999688	0.0000000000000000	F	F	F
21.2950000000000763	9.2210100000000370	2.3863800000000821	F	F	F	7.9856299999999747	1.5368299999999688	0.0000000000000000	F	F	F
18.629523894143833	1.5414770498975218	4.6668182289275411	T	T	T	10.6475000000000115	1.5368299999999688	0.0000000000000000	F	F	F
2.6698564665867015	1.54314007339439636	4.6736782120615468	T	T	T	13.3093800000000435	1.5368299999999688	0.0000000000000000	F	F	F
5.3240998427418646	1.5445469877000977	4.6803970047209482	T	T	T	15.9712499999999373	1.5368299999999688	0.0000000000000000	F	F	F
7.9747906677059764	1.5403240348418832	4.657230527474903	T	T	T	19.9640600000000106	3.8420900000000340	0.0000000000000000	F	F	F
10.6280523470900129	1.5329441968942605	4.5973023574412029	T	T	T	3.9928100000000012	3.8420900000000340	0.0000000000000000	F	F	F
13.3282186879941591	1.5392932562916440	4.7204770654172029	T	T	T	6.6546900000000324	3.8420900000000340	0.0000000000000000	F	F	F
15.9636187557231710	1.5476601008410337	4.672002095241827	T	T	T	9.3165599999999849	3.8420900000000340	0.0000000000000000	F	F	F
19.9805971652513055	3.8495726297701904	4.6537102920166173	T	T	T	11.9784400000000453	3.8420900000000340	0.0000000000000000	F	F	F
3.9966794854822414	3.8495951176722812	4.6768361998203467	T	T	T	14.6403100000000777	3.8420900000000340	0.0000000000000000	F	F	F
6.648789172178847	3.8434364329720821	4.6727295508410592	T	T	T	17.3021900000000812	3.8420900000000340	0.0000000000000000	F	F	F
9.2957645943095315	3.8485004537768654	4.6457171156926274	T	T	T	21.2949999999999804	3.8420900000000340	0.0000000000000000	F	F	F
11.9964386196381518	3.84207160435959704	4.7319324187406648	T	T	T	5.3237500000000546	6.1473399999999971	0.0000000000000000	F	F	F
14.654933002325890	3.8197432117202470	4.7575954651912014	T	T	T	7.9856299999999587	6.1473399999999971	0.0000000000000000	F	F	F
17.3279677406967565	3.84114004308987662	4.6304658983877189	T	T	T	10.6474999999999920	6.1473399999999971	0.0000000000000000	F	F	F
21.298352000294817	4.1491498027430204	4.6697769957465090	T	T	T	13.3093800000000222	6.1473399999999971	0.0000000000000000	F	F	F
5.342039638963196	6.1376216266916819	4.6715410839647884	T	T	T	15.9712500000000510	6.1473399999999971	0.0000000000000000	F	F	F
7.9984173191864372	6.1493979388264721	4.6683741899712610	T	T	T	18.6331299999999480	6.1473399999999971	0.0000000000000000	F	F	F
10.655252353160652	6.1676075523959623	4.6557399625717641	T	T	T	22.6259399999					

11.97843999999999422	6.91574999999999708	2.3863800000000821	F	F	F	1.000000000000000			
14.64030999999999728	6.91574999999999708	2.3863800000000821	F	F	F	18.633126345000009	0.000000000000000	0.000000000000000	
17.3021900000000102	6.91574999999999708	2.3863800000000821	F	F	F	6.654687980000003	11.526257699999996	0.000000000000000	
19.9640600000000390	6.91574999999999708	2.3863800000000821	F	F	F	0.000000000000000	0.000000000000000	24.545524029999985	
5.3237536549999671	9.2210100000000370	2.3863800000000821	F	F	F	140	11	14	1
7.9856300000000395	9.2210100000000370	2.3863800000000821	F	F	F	Selective dynamics			
10.6475000000000737	9.2210100000000370	2.3863800000000821	F	F	F	Cartesian			
13.3093799999999778	9.2210100000000370	2.3863800000000821	F	F	F	18.6331299999999764	1.5368299999999688	0.000000000000000	F F F
15.9712500000000102	9.2210100000000370	2.3863800000000821	F	F	F	2.6618800000000480	1.5368299999999688	0.000000000000000	F F F
18.6331300000000439	9.2210100000000370	2.3863800000000821	F	F	F	5.3237499999999480	1.5368299999999688	0.000000000000000	F F F
21.2950000000000763	9.2210100000000370	2.3863800000000821	F	F	F	7.9856299999999809	1.5368299999999688	0.000000000000000	F F F
18.6417260284227666	1.5441048084822281	4.6676114062342435	T	T	T	10.6475000000000115	1.5368299999999688	0.000000000000000	F F F
2.6701218624964573	1.5494472224617176	4.6815234459969307	T	T	T	13.3093800000000435	1.5368299999999688	0.000000000000000	F F F
5.3277394117051449	1.548407799989997	4.670747720015254	T	T	T	15.9712499999999427	1.5368299999999688	0.000000000000000	F F F
7.9848172318576579	1.5485381830214073	4.6675519415537527	T	T	T	19.9640600000000106	3.8420900000000340	0.000000000000000	F F F
10.6448324612872209	1.5429301692885951	4.6528167062992525	T	T	T	3.9928100000000812	3.8420900000000340	0.000000000000000	F F F
13.34218511801095383	1.5600871581167628	4.6964870839981376	T	T	T	6.6546899999999989	3.8420900000000340	0.000000000000000	F F F
15.96414924201449795	1.5507828295900358	4.6754399131422346	T	T	T	9.3165600000000133	3.8420900000000340	0.000000000000000	F F F
19.9701581364774299	3.8545990648417692	4.6716091087781365	T	T	T	11.9784400000000453	3.8420900000000340	0.000000000000000	F F F
3.9980674015423063	3.8582674714666872	4.6766514423809236	T	T	T	14.6403100000000777	3.8420900000000340	0.000000000000000	F F F
6.558252122390673	3.8511897681395465	4.6728453075386218	T	T	T	17.3021900000000812	3.8420900000000340	0.000000000000000	F F F
9.3296473641385251	3.8497703699506185	4.66780732131022543	T	T	T	21.294999999999875	6.1473399999999971	0.000000000000000	F F F
11.9882153855773215	3.8475728944046991	4.6513089413337623	T	T	T	5.3237500000000599	6.1473399999999971	0.000000000000000	F F F
14.6495748179355747	3.8141705781173102	4.7234791593917260	T	T	T	7.9856299999999578	6.1473399999999971	0.000000000000000	F F F
17.3171939904204275	3.8455992138498756	4.6478522168940195	T	T	T	10.6475000000000115	6.1473399999999971	0.000000000000000	F F F
21.3008128684280009	6.1593108022508680	4.6796208197624516	T	T	T	13.3093800000000222	6.1473399999999971	0.000000000000000	F F F
5.3323891920921151	6.1533028390689437	4.6761435756428495	T	T	T	15.9712500000000546	6.1473399999999971	0.000000000000000	F F F
7.9993173483806214	6.1517194894817503	4.6700706301224590	T	T	T	18.6331299999999551	6.1473399999999971	0.000000000000000	F F F
10.6619909191039195	6.1440971828831072	4.673698564730012	T	T	T	22.6259400000000106	8.4525900000000416	0.000000000000000	F F F
13.3271510806532429	6.1589505420562884	4.6737314218169177	T	T	T	6.6546900000000839	8.4525900000000416	0.000000000000000	F F F
15.9713351884421346	6.163309637728244	4.674920555626396	T	T	T	9.3165599999999849	8.4525900000000416	0.000000000000000	F F F
18.637427063104171	6.155426254346437	4.6700996733310642	T	T	T	11.9784400000000133	8.4525900000000416	0.000000000000000	F F F
22.6326745920629584	6.4640524424509884	4.6770123842954874	T	T	T	14.6403100000000492	8.4525900000000416	0.000000000000000	F F F
6.5679892851402164	6.4606900945282693	4.6768224300700085	T	T	T	17.3021900000000812	8.4525900000000416	0.000000000000000	F F F
9.3250653627005562	6.4600565343047485	4.6738595097949611	T	T	T	19.9640599999999786	8.4525900000000416	0.000000000000000	F F F
11.9878611415205043	6.4630687389467720	4.6726630422924540	T	T	T	23.9568799999999911	10.757840000000052	0.000000000000000	F F F
14.6456038202935748	6.4602521480220046	4.6699175703568452	T	T	T	7.9856300000000617	10.757840000000052	0.000000000000000	F F F
17.3092534410639800	6.4624889112235623	4.6725294581542673	T	T	T	10.6475000000000618	10.757840000000052	0.000000000000000	F F F
19.9739711423115871	6.4638019437916174	4.6775583616107923	T	T	T	13.3093799999999938	10.757840000000052	0.000000000000000	F F F
23.956099351085662	10.7767184569528894	4.682474552738062	T	T	T	15.9712500000000261	10.757840000000052	0.000000000000000	F F F
7.9875778350592812	10.7694047879597319	4.6750394889152389	T	T	T	18.6331300000000581	10.757840000000052	0.000000000000000	F F F
10.6513840524070353	10.7727708227050165	4.6657309968359755	T	T	T	21.2949999999999591	10.757840000000052	0.000000000000000	F F F
13.3125093492302611	10.7689705203523175	4.6730451861125353	T	T	T	0.0000000000000000	0.000000000000000	2.3863800000000821	F F F
15.9754885616584126	10.7661398005350168	4.6744649147645978	T	T	T	2.6618800000000324	0.000000000000000	2.3863800000000821	F F F
18.6437779472531417	10.77070878063184476	4.6729476808804415	T	T	T	5.3237500000000644	0.000000000000000	2.3863800000000821	F F F
21.3029414642967225	10.780772796533749	4.6832536192396503	T	T	T	7.9856299999999631	0.000000000000000	2.3863800000000821	F F F
18.6169952798232750	0.0161788914542927	7.0199534653183973	T	T	T	10.6474999999999973	0.000000000000000	2.3863800000000821	F F F
2.6502395257988844	0.0118387921308438	7.0065699567991278	T	T	T	13.3093800000000275	0.000000000000000	2.3863800000000821	F F F
11.9715624284046243	11.5390772763818354	7.0162648163599606	T	T	T	15.9712500000000617	0.000000000000000	2.3863800000000821	F F F
14.6379783779038402	11.533545261359116	6.9950425627683117	T	T	T	1.3309399999999771	2.3052499999999632	2.3863800000000821	F F F
17.3031970586125787	11.5339085634389171	6.9864530312284980	T	T	T	3.9928100000000093	2.3052499999999632	2.3863800000000821	F F F
13.3146180923489919	0.0535974461750898	6.9976159203927635	T	T	T	6.6546900000000422	2.3052499999999632	2.3863800000000821	F F F
15.9402843038747246	0.046638747396359	7.0211134836001206	T	T	T	9.3165599999999422	2.3052499999999632	2.3863800000000821	F F F
19.9496808649642432	2.3212548676270930	6.9968439815051608	T	T	T	11.9784399999999742	2.3052499999999632	2.3863800000000821	F F F
3.9910489041583972	2.3156362588995338	6.9949308428102528	T	T	T	14.6403100000000666	2.3052499999999632	2.3863800000000821	F F F
6.6431791182780664	2.309582786144922	7.0079253316610526	T	T	T	17.3021900000000838	2.3052499999999632	2.3863800000000821	F F F
9.3005886685437140	2.3069913245093532	6.9825645100171698	T	T	T	2.6618800000000018	4.6105000000000089	2.3863800000000821	F F F
11.9626029390291500	2.3185496073499392	6.9123181698616243	T	T	T	5.3237500000000342	4.6105000000000089	2.3863800000000821	F F F
14.682894167543631	2.3409964409356929	6.6563133040464235	T	T	T	7.9856300000000671	4.6105000000000089	2.3863800000000821	F F F
17.2827839089125378	2.3245987460928993	6.9446783573038292	T	T	T	10.6475000000000671	4.6105000000000089	2.3863800000000821	F F F
21.2817408579145117	6.1393810920667716	7.0199357682176755	T	T	T	13.3093799999999973	4.6105000000000089	2.3863800000000821	F F F
5.3121150840642740	6.6218990425418642	7.017452631558185	T	T	T	15.9712500000000333	4.6105000000000089	2.3863800000000821	F F F
7.9840463364336207	6.617860305311696	6.9984993146179873	T	T	T	18.6331300000000653	4.6105000000000089	2.3863800000000821	F F F
10.6519312171212501	4.608342883604927	7.048238983604927	T	T	T	3.9928136549999400	6.9157499999999708	2.3863800000000821	F F F
15.9770007151697033	4.6066814513807966	6.9108660834345672	T	T	T	6.6546900000000129	6.9157499999999708	2.3863800000000821	F F F
18.6278955881608006	4.6215490782764814	7.0015352488997804	T	T	T	9.3165600000000452	6.9157499999999708	2.3863800000000821	F F F
22.612625108184616	6.9337222506754017	7.0094891834016032	T	T	T	11.9784399999999422	6.9157499999999708	2.3863800000000821	F F F
6.6529122549191529	6.9286962388085099	7.0064912609901949	T	T	T	14.6403099999999764	6.9157499999999708	2.3863800000000821	F F F
9.3216109236294589	6.9130640821716778	6.9872214093842349	T	T	T	17.3021900000000102	6.9157499999999708	2.3863800000000821	F F F
11.9783847225490376	6.9113010238809451	6.9854023738416835	T	T	T	19.9640600000000390	6.9157499999999708	2.3863800000000821	F F F
14.6371658445531985	6.9111758437556459	7.0095914241193552	T	T	T	5.3237536549999742	9.2210100000000370	2.3863800000000821	F F F
17.2946380289280057	6.9215669928079349	7.0023657184218937	T	T	T	7.9856300000000049	9.2210100000000370	2.3863800000000821	F F F
19.9523511746328666	6.9297507901742561	7.0157938317284030	T	T	T	10.6475000000000796	9.2210100000000370	2.3863800000000821	F F F
23.9450016548504010	6.9239250610645924	7.0093442773904542	T	T	T	13.3093799999999796	9.2210100000000370	2.3863800000000821	F F F
7.9784282537828357	6.9234763621432947	6.9844678942398577	T	T	T	15.9712500000000119	9.2210100000000370	2.3863800000000821	F F F
10.6437037122592546	6.9220590596711935	6.9813955738824154	T	T	T	18.6331300000000439	9.2210100000000370	2.3863800000000821	

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18.6188977920644234	0.0173753025986538	6.9795419501317877	T	T	T
2.6553935973992366	0.0132647336368995	6.9690314674125066	T	T	T
5.3231489933957211	0.0089903144310464	6.9838962836618617	T	T	T
7.9839243380543579	0.008743877520315	6.9964330325907689	T	T	T
10.6367728185443138	0.0081408913452112	6.9952599504021538	T	T	T
13.2961310880880834	0.022575497155404	7.0145974847060941	T	T	T
15.950959591726556	0.0141349457660203	6.9736331202384907	T	T	T
19.9490360027934130	2.3166838206127984	6.9846568989840945	T	T	T
3.986467616412610	2.3160337860163027	6.9758201481345843	T	T	T
6.6501274105763413	2.315729663049518	6.9862024146057982	T	T	T
9.3136591899758514	2.3208187554128307	7.0126291894654339	T	T	T
11.968834848646338	2.3291276254392801	6.9683225657591272	T	T	T
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17.2874252188342510	2.3294706697344627	6.9409709560616966	T	T	T
21.282320852396036	4.6205953645194951	6.9870341830893894	T	T	T
5.3172460930301710	4.6243783522558104	6.9976960466309353	T	T	T
7.986880376063321	4.6249872544408639	6.9864199286786350	T	T	T
10.6569654726483851	4.6218300997531816	6.9871354274579707	T	T	T
15.9405479267399990	4.6465423062867266	6.964966715054512	T	T	T
18.620472764502624	4.6276558963798138	6.9707294415957808	T	T	T
3.989454952624607	6.9290965609397928	6.9783964309758995	T	T	T
6.6531906506680885	6.921905045484851	6.9992353154600577	T	T	T
9.317342202191961	6.9274367587615142	6.9783885441787668	T	T	T
11.9893376002788443	6.9301949539049641	6.9863498497778984	T	T	T
14.6317650852875385	6.9140394615436449	6.9498311634387655	T	T	T
17.262431238761921	6.9236821485091467	7.005319394378389	T	T	T
19.9433907132448098	6.9300947810299718	6.9806785490927599	T	T	T
23.945588965742650	9.2342064946496372	6.9922748889900443	T	T	T
7.9794305338963092	9.2316423272795607	6.9843658908749058	T	T	T
10.646280892708584	9.2297414634681338	7.0160942866071494	T	T	T
13.3094609240722441	9.2198893846017231	6.9865861821898365	T	T	T
15.9504470480696554	9.212355758536540	6.9842977321918074	T	T	T
18.6214576358871824	9.2313029253837176	6.9791749544012182	T	T	T
21.2821171795425883	9.2316516087025295	6.9756707176466479	T	T	T
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9.7578761619194623	5.021226810098915	10.1112550529865324	T	T	T
11.1316814978502485	4.7854650988551919	0.0860042748106711	T	T	T
11.6265997804445860	3.462630582709682	12.166843889421843	T	T	T
10.7100692892643945	2.3896744981150153	10.1541420246963821	T	T	T
9.3379420805346562	2.6363516685133579	10.1759387024402503	T	T	T
8.8574690286099269	3.9507042703324649	10.1628091828111273	T	T	T
14.2377454332326332	3.055783089842254	10.2765850864659090	T	T	T
13.0262699019818360	3.2288206694712551	10.1761797574975876	T	T	T
16.6425485272000557	1.2129457091607618	10.4952912644513869	T	T	T
15.7108863054399421	3.0029821295325815	12.8210132988105521	T	T	T
17.0328055446186575	4.2806518632970231	10.36962505540007783	T	T	T
9.3886099968398824	6.0467842134646395	10.0796767750294016	T	T	T
11.8420831774191060	5.6140459291268484	10.0439653521221764	T	T	T
11.087171253496212	1.3668494380389847	10.1662214021119635	T	T	T
8.640555806897443	1.7979659034079931	10.1988715352149306	T	T	T
7.7830519597010426	4.1404827034219336	10.1797615207928800	T	T	T
15.9862937466307429	0.3993112051206210	10.8332142172879244	T	T	T
17.6371489737654343	1.0747208988692771	10.9445964259118362	T	T	T
16.754269424068692	1.1204708312153702	9.403390659175830	T	T	T
15.0407850883139975	2.069758924616607	13.1791434146829971	T	T	T
15.2735788799448642	3.9741255173095431	13.0912071173360847	T	T	T
16.6813672102693360	2.9013502542484556	13.329034198983872	T	T	T
17.9291883718103371	4.3500536610763236	11.0028269432363608	T	T	T
16.4951723843102052	5.2465383631234715	10.3919427510748417	T	T	T
17.367743986642028	4.1185750771925358	9.333603516996817	T	T	T
14.439592287017185	7.1308515744808227	9.9450129661479355	T	T	T
15.9426343149713432	2.8868415694598784	10.9604471265958043	T	T	T

### POSCAR for INT2 ###

Zn C H Cl Si

1.0000000000000000					
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6.6546879804749999	11.5262576907006249	0.0000000000000000	0.0000000000000000		
0.0000000000000000	0.0000000000000000	24.5455240212800021			

140 19 1 1

Selective dynamics

Cartesian

18.6331263453299378	1.5368343587600781	0.0000000000000000	F	F	F
2.6618751921899908	1.5368343587600781	0.0000000000000000	F	F	F
5.3237503843800473	1.5368343587600781	0.0000000000000000	F	F	F
7.9856255765699720	1.5368343587600781	0.0000000000000000	F	F	F
10.6475007687600289	1.5368343587600781	0.0000000000000000	F	F	F
13.3093759609499536	1.5368343587600781	0.0000000000000000	F	F	F
15.9712511531400014	1.5368343587600781	0.0000000000000000	F	F	F
19.9640639414249534	3.8420858969002354	0.0000000000000000	F	F	F
3.9928127882850095	3.8420858969002354	0.0000000000000000	F	F	F
6.6546879804750656	3.8420858969002354	0.0000000000000000	F	F	F
9.3165631726649902	3.8420858969002354	0.0000000000000000	F	F	F
11.978438364850481	3.8420858969002354	0.0000000000000000	F	F	F
14.6403135704497727	3.8420858969002354	0.0000000000000000	F	F	F
17.30218874292350288	3.8420858969002354	0.0000000000000000	F	F	F
21.2950015375199264	6.1473734350403116	0.0000000000000000	F	F	F
5.3237503843799807	6.1473734350403116	0.0000000000000000	F	F	F
7.9856255765700377	6.1473734350403116	0.0000000000000000	F	F	F
10.6475007687599614	6.1473734350403116	0.0000000000000000	F	F	F
13.3093759609500193	6.1473734350403116	0.0000000000000000	F	F	F
15.9712511531399439	6.1473734350403116	0.0000000000000000	F	F	F
18.6331263453300018	6.1473734350403116	0.0000000000000000	F	F	F
22.6259391336149456	4.452588971804700	0.0000000000000000	F	F	F
6.6546879804749999	4.452588971804700	0.0000000000000000	F	F	F
9.3165631726650560	4.452588971804700	0.0000000000000000	F	F	F
11.9784383648549806	4.452588971804700	0.0000000000000000	F	F	F
14.6403135704503385	4.452588971804700	0.0000000000000000	F	F	F
17.30218874292349649	4.452588971804700	0.0000000000000000	F	F	F
19.9640639414250209	4.452588971804700	0.0000000000000000	F	F	F
23.9568767297093185	10.7578405113205449	0.0000000000000000	F	F	F
7.9856255765699711	10.7578405113205449	0.0000000000000000	F	F	F
10.6475007687600289	10.7578405113205449	0.0000000000000000	F	F	F
13.3093759609499536	10.7578405113205449	0.0000000000000000	F	F	F
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18.6331263453299343	10.7578405113205449	0.0000000000000000	F	F	F
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0.0000000000000000	0.0000000000000000	2.386318053199650	F	F	F
2.6618751921900570	0.0000000000000000	2.386318053199650	F	F	F

5.3237503843799816	0.0000000000000000	2.386318053199650	F	F	F
7.9856255765700386	0.0000000000000000	2.386318053199650	F	F	F
10.6475007687599632	0.0000000000000000	2.386318053199650	F	F	F
13.3093759609500211	0.0000000000000000	2.386318053199650	F	F	F
15.9712511531399439	0.0000000000000000	2.386318053199650	F	F	F
1.3309375960950185	2.3052515381401570	2.386318053199650	F	F	F
3.9928127882850752	2.3052515381401570	2.386318053199650	F	F	F
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9.3165631726650577	2.3052515381401570	2.386318053199650	F	F	F
11.9784383648549824	2.3052515381401570	2.386318053199650	F	F	F
14.640313570450402	2.3052515381401570	2.386318053199650	F	F	F
17.30218874292349613	2.3052515381401570	2.386318053199650	F	F	F
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7.9856255765699720	4.6105030762802333	2.386318053199650	F	F	F
10.6475007687600289	4.6105030762802333	2.386318053199650	F	F	F
13.3093759609499536	4.6105030762802333	2.386318053199650	F	F	F
15.9712511531400014	4.6105030762802333	2.386318053199650	F	F	F
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3.9928127882850095	6.9157546144203916	2.386318053199650	F	F	F
6.6546879804750656	6.9157546144203916	2.386318053199650	F	F	F
9.3165631726649920	6.9157546144203916	2.386318053199650	F	F	F
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17.30218874292350288	6.9157546144203916	2.386318053199650	F	F	F
19.9640639414249534	6.9157546144203916	2.386318053199650	F	F	F
5.3237503843799807	9.2210061525604665	2.386318053199650	F	F	F
7.9856255765700377	9.2210061525604665	2.386318053199650	F	F	F
10.6475007687599614	9.2210061525604665	2.386318053199650	F	F	F
13.3093759609500193	9.2210061525604665				

11.0794475316642060	3.3255726901596723	9.3376250880295224	T	T	T	18.6331263453300018	9.2210061525604665	2.3863810053199650	F	F	F
12.2190206895351814	8.9838642359872836	10.3245031057095993	T	T	T	21.2950015375199229	9.2210061525604665	2.3863810053199650	F	F	F
17.0638242662513058	8.2185123275180043	10.1901575252686030	T	T	T	18.6582074105635130	1.5441383775583029	4.66099767263032	T	T	T
17.1434015570639318	6.8094785536601234	10.0845741452053712	T	T	T	2.6669405408048132	1.5524221518133099	4.67392986098687	T	T	T
18.4174551894013021	6.1995227567577773	10.1343246954632263	T	T	T	5.2996676537881173	1.5540778829266413	4.667159210583197	T	T	T
19.5683017334208209	6.9768975472579235	10.2597673574752264	T	T	T	7.934111288263094	1.5486245761069735	4.640730227381315	T	T	T
19.4761478884671035	8.370092980249980	10.3496418617758209	T	T	T	10.6456598012546415	1.5496592581467219	4.6603726893489558	T	T	T
14.9714747480345345	5.437276848520613	9.4235533605858848	T	T	T	13.3540256326592637	1.5535160648810198	4.690153441821997	T	T	T
15.9794674517059399	6.051362956293110	9.8090583390334700	T	T	T	16.0047553878597348	1.5370011713911393	4.659012935367784	T	T	T
12.9786392045577070	8.396713266251084	10.4994444509147904	T	T	T	19.9745827939738874	3.8547499361009407	4.668616903136789	T	T	T
11.1074051664891993	8.4831176195417370	12.9518404454798954	T	T	T	3.9932307252291532	3.8592211095526881	4.672009681587710	T	T	T
10.1456927559105097	7.0984347458301755	10.3614401040873414	T	T	T	6.6524280884408507	3.8532533047096131	4.675590654611013	T	T	T
15.4788055501747586	11.0454704711370866	10.5761674300507895	T	T	T	9.3159227201117538	3.8535262642583090	4.6409812833104818	T	T	T
10.9149220519721624	0.7360196724965455	9.9572737171244946	T	T	T	11.9977469632709939	3.8589599162432875	4.7034326582543793	T	T	T
8.7210954933441958	4.4534233184749157	9.8871045103742574	T	T	T	14.6229230021891166	3.8585835222713479	4.6950467239739030	T	T	T
6.632330834931974	3.2356076350792780	10.4806064295067891	T	T	T	17.3053497053545478	3.8469370530166049	4.6595188355418005	T	T	T
6.682349221307510	0.7654294120665068	10.8033678996185998	T	T	T	21.3032132021794602	3.61648066368379366	4.6701401527822517	T	T	T
18.1443447870180563	10.0697709966249231	10.3930046798989368	T	T	T	5.3281553457186579	3.61605141569850037	4.6745046963532273	T	T	T
16.08196065210628614	6.6910718105515674	10.1414869077879395	T	T	T	7.9943822211721143	3.61605198708742819	4.67829024965146680	T	T	T
18.4898653610628614	5.1148959897257477	10.0477084220198486	T	T	T	10.6677682040925532	3.61522829280718400	4.675856325183269	T	T	T
20.5458312826937295	6.4920777349500263	10.2736354004610199	T	T	T	13.3108547808426273	3.61020460388559981	4.751877422428211	T	T	T
20.3789412668727508	8.9759552878459754	10.4289309981774974	T	T	T	15.983701636388970	3.61474149197130119	4.6551498779902412	T	T	T
13.7959431006566220	8.6715836326492575	11.1814084826520398	T	T	T	18.6545812191757552	3.61632754843104536	4.641337219147849	T	T	T
12.5876117958594129	9.3149943964953543	10.0323207669352925	T	T	T	22.6394168912048315	3.4622054933905186	4.6791878820128989	T	T	T
13.3924200057058904	7.7540834347501919	7.7091681338007287	T	T	T	6.6671932548965795	3.4613694677429429	4.666607795730408	T	T	T
11.9728260399728939	8.653188857408630	13.6078351706159832	T	T	T	9.3346210089515438	3.4595149583952261	4.677027892294773	T	T	T
10.3401838507385206	7.9361967738924477	13.5170515051535727	T	T	T	11.9859848301066503	3.4774688501651809	4.647849843244864	T	T	T
10.694594350441688	9.4609412758548044	12.6606756282577748	T	T	T	14.6222524374215475	3.4733465786547146	4.658830886953785	T	T	T
9.7317371184605044	8.0033975901228533	9.8896851392754748	T	T	T	17.3115440266170495	3.4626248729691635	4.6618645854021343	T	T	T
9.3549972305206488	6.6223731857788515	10.95808851217183087	T	T	T	19.9778873095243199	3.4657804578061171	4.6738981149926149	T	T	T
10.4428857314915700	6.4064454321865988	9.5587898208956474	T	T	T	23.9720188665432019	3.4626248729691635	4.6782627495796257	T	T	T
12.3833527530177214	5.6889782449415085	12.1114578904281700	T	T	T	7.9982935010914566	3.7655742656232878	4.683518054068846	T	T	T
11.6131145246756695	7.5291190028126108	11.4312647367033495	T	T	T	10.6468319424554885	3.763913464821943	4.6769919266437009	T	T	T
### POSCAR for INT3-24 ###						13.2979023232387945	3.7845415059295089	4.6631196218439088	T	T	T
Zn C H Cl Si						15.9725768404836810	3.767299057685850	4.6703110723479062	T	T	T
1.0000000000000000						18.6477095243477962	3.7754050505952002	4.6602827147878649	T	T	T
18.6331263453300018	0.0000000000000000	0.0000000000000000				21.3107486169998275	3.7682738915637177	4.6815494263638482	T	T	T
6.6546879804749999	11.526257697006249	0.0000000000000000				18.6398199471727288	3.0052766521238537	6.9989060290057301	T	T	T
0.0000000000000000	0.0000000000000000	24.545524021280021				2.6637761459903677	3.0177917364503341	4.0189067929813636	T	T	T
5.3096423429027260	0.0236528638503508					5.3096423429027260	0.0236528638503508	7.0022367086177892	T	T	T
7.9617991314066243	0.0025337270984548					17.2702172457638845	11.5043724549607074	7.0134308284173921	T	T	T
19.9868823053718110	11.4858034405609981					19.9868823053718110	11.4858034405609981	9.580295184504308	T	T	T
15.9780546976065327	0.0123355291164431					15.9780546976065327	0.0123355291164431	7.0154833783364996	T	T	T
19.9584296164361206	2.3197245964016511					19.9584296164361206	2.3197245964016511	7.015231202724448	T	T	T
3.9770277211151324	2.3249588531525847					3.9770277211151324	2.3249588531525847	7.038102562397932	T	T	T
6.6217143053252396	2.3070956382451615					6.6217143053252396	2.3070956382451615	7.019571037193657	T	T	T
9.2420665575123540	2.28926652570888239					9.2420665575123540	2.28926652570888239	6.8418983052682054	T	T	T
12.0086919843162452	2.1693292299905114					12.0086919843162452	2.1693292299905114	7.0191073274859788	T	T	T
14.6760439394223194	2.3430115614817866					14.6760439394223194	2.3430115614817866	6.959299053772863	T	T	T
17.3208378814586617	2.3048271232587503					17.3208378814586617	2.3048271232587503	9.580295184504308	T	T	T
21.2802596802514650	4.6195121226795068					21.2802596802514650	4.6195121226795068	7.0137203264149975	T	T	T
5.2973607737731108	4.6243529934571663					5.2973607737731108	4.6243529934571663	7.0138078351352773	T	T	T
7.9438381931627724	4.6220760191470518					7.9438381931627724	4.6220760191470518	6.9769552782762267	T	T	T
10.531683945687639	4.7046363091497385					10.531683945687639	4.7046363091497385	6.9685645680092063	T	T	T
15.9256967122917025	4.6158018787748585					15.9256967122917025	4.6158018787748585	6.9450395712985058	T	T	T
18.6187134542033661	4.6341952930913761					18.6187134542033661	4.6341952930913761	6.970274683638589	T	T	T
22.6164490316256952	6.9264071436776895					22.6164490316256952	6.9264071436776895	7.0003158892612523	T	T	T
6.6471465910414733	6.9272152901131170					6.6471465910414733	6.9272152901131170	7.0040127154769921	T	T	T
9.0983845081710079	6.9632466245860059					9.0983845081710079	6.9632466245860059	7.0266680132123130	T	T	T
11.9896230377822258	6.9651524602155409					11.9896230377822258	6.9651524602155409	6.9295812370204804	T	T	T
14.6551754002284151	6.990427846627807					14.6551754002284151	6.990427846627807	6.9511606475719182	T	T	T
17.3069891494496616	6.929122944587076					17.3069891494496616	6.929122944587076	6.9310811984776572	T	T	T
19.9632133948696762	6.9196062442783752					19.9632133948696762	6.9196062442783752	7.0219356571504505	T	T	T
23.9546224739784961	9.2267257195208607					23.9546224739784961	9.2267257195208607	7.0102380365088686	T	T	T
7.9802631318525830	2.400998511794623					7.9802631318525830	2.400998511794623	7.004918415376167	T	T	T
10.6472880781571408	9.245853537830129					10.6472880781571408	9.245853537830129	6.998618655177253	T	T	T
13.3009289662006296	2.677909423752407					13.3009289662006296	2.677909423752407	6.962987773824137	T	T	T
15.964849473737402	9.2395137582195996					15.964849473737402	9.2395137582195996	6.988445665751598	T	T	T
18.6265750888704424	9.2163435747268618					18.6265750888704424	9.2163435747268618	6.996658887398150	T	T	T
21.3000131168362294	9.2086567235875574					21.3000131168362294	9.2086567235875574	6.9941270224377901	T	T	T
13.6533992066594063	4.9967211394128439					13.6533992066594063	4.9967211394128439	7.113932728091585	T	T	T
9.0310929151371244	0.5477758166019372					9.0310929151371244	0.5477758166019372	10.457945945768624	T	T	T
10.1859485574345516	2.137137969332492					10.1859485574345516	2.137137969332492	10.0892862942840686	T	T	T
10.1381343044800073	2.6273145326380303					10.1381343044800073	2.6273145326380303	9.8662239628116613	T	T	T
8.9209299298799143	3.197070832513140					8.9209299298799143	3.197070832513140	10.056120030639642	T	T	T
7.7726505518047269	2.6203922938235129					7.7726505518047269	2.6203922938235129	10.4244925863278155	T	T	T
7.8209103918071010	1.2344392992556039					7.820910391					



18.6331263453300018	6.1473374350403116	0.0000000000000000	F	F	F	17.3246243390996955	6.9757012705460744	7.032816109973334	T	T	T
12.6259391336149456	8.452588971804700	0.0000000000000000	F	F	F	19.9722459786525981	6.9190321560250343	6.9942580216906531	T	T	T
6.6546879804749999	8.452588971804700	0.0000000000000000	F	F	F	5.3388823593515706	9.2025480373817690	6.976645896405979	T	T	T
9.3165631726650560	8.452588971804700	0.0000000000000000	F	F	F	7.9952876711891465	9.2073494669122839	6.986138541305701	T	T	T
11.9784383645849806	8.452588971804700	0.0000000000000000	F	F	F	10.6387780413905730	9.2316006442781351	6.9896154326668732	T	T	T
14.6403135750450385	8.452588971804700	0.0000000000000000	F	F	F	13.2978292199118755	9.2551188286289570	6.9584993689899360	T	T	T
17.3021887492349649	8.452588971804700	0.0000000000000000	F	F	F	15.9582952122984238	9.2532129731794300	6.9460683692644682	T	T	T
19.9640639414250209	8.452588971804700	0.0000000000000000	F	F	F	18.6274328140107883	9.2249784939496031	7.009192875783757	T	T	T
23.9568767297099185	10.7578405113205449	0.0000000000000000	F	F	F	21.3008601638036055	9.2118877275809948	6.9873782745157973	T	T	T
7.9856255765699711	10.7578405113205449	0.0000000000000000	F	F	F	13.13036424221209048	4.7209886388425364	6.8436821338172553	T	T	T
10.6475007687600289	10.7578405113205449	0.0000000000000000	F	F	F	10.8462960822770818	2.2464016496923485	10.5910414246343514	T	T	T
13.3093759609499536	10.7578405113205449	0.0000000000000000	F	F	F	12.1615644610376730	2.3711555760168421	10.1488571687441414	T	T	T
15.9712511531400096	10.7578405113205449	0.0000000000000000	F	F	F	12.6928655341785745	3.6541440856733618	9.8960868503124040	T	T	T
18.6331263453299343	10.7578405113205449	0.0000000000000000	F	F	F	11.9038281807103719	4.800445417963615	10.1470051301508146	T	T	T
21.2950015375199939	10.7578405113205449	0.0000000000000000	F	F	F	10.59307196755232104	4.6582418975391171	10.5862990265816617	T	T	T
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	10.0551083011344105	3.809611722394610	10.7926482117853944	T	T	T
2.6618715921900570	0.0000000000000000	2.3863810053199650	F	F	F	14.7193396118745294	3.9264073747282340	8.218975531130294	T	T	T
5.3237503843790816	0.0000000000000000	2.3863810053199650	F	F	F	13.8775007287341534	3.7975724367269534	9.1395627239229782	T	T	T
7.9856255765790386	0.0000000000000000	2.3863810053199650	F	F	F	13.845167397594716	6.5383423356425645	10.650004263496670	T	T	T
10.6475007687599532	0.0000000000000000	2.3863810053199650	F	F	F	16.7142064008043576	9.718152559430082	10.6502905226126760	T	T	T
13.3093759609500111	0.0000000000000000	2.3863810053199650	F	F	F	15.7888156077816174	7.9858064961733901	13.0011451310556359	T	T	T
15.9712511531399430	0.0000000000000000	2.3863810053199650	F	F	F	10.4265078921118468	1.252772039759238	10.7520995127171348	T	T	T
1.3309375960950185	2.3052515381401570	2.3863810053199650	F	F	F	12.7708382776572194	1.4889529257026857	9.95372644473266	T	T	T
3.9928127882850752	2.3052515381401570	2.3863810053199650	F	F	F	12.3173353058189612	5.7876673044599229	9.938198062150498	T	T	T
6.6546879804749999	2.3052515381401570	2.3863810053199650	F	F	F	9.9784816078132899	5.5446918911109231	10.742862572924788	T	T	T
9.3165631726650577	2.3052515381401570	2.3863810053199650	F	F	F	9.0167711011896419	3.2733881978369683	11.1068093908331799	T	T	T
11.9784383648549824	2.3052515381401570	2.3863810053199650	F	F	F	13.7618843021027857	8.5541987554485797	9.514385156694228	T	T	T
14.6403135750450402	2.3052515381401570	2.3863810053199650	F	F	F	13.4577964047383465	9.4933070449149035	11.0346470269418564	T	T	T
17.3021887492349613	2.3052515381401570	2.3863810053199650	F	F	F	13.2118986865488353	7.7266176037277017	11.033221052899574	T	T	T
2.6618715921899044	4.6105030762802333	2.3863810053199650	F	F	F	16.5748891505067739	9.9171265879672195	9.530236018722586	T	T	T
5.3237503843800473	4.6105030762802333	2.3863810053199650	F	F	F	17.7766885727292838	9.4841076054000002	10.7726098712584758	T	T	T
7.9856255765699720	4.6105030762802333	2.3863810053199650	F	F	F	16.454515784486125	10.6217140337425917	11.163017917127576	T	T	T
10.6475007687600289	4.6105030762802333	2.3863810053199650	F	F	F	15.4447332406356228	8.8634159038812843	13.5686209823013997	T	T	T
13.3093759609499536	4.6105030762802333	2.3863810053199650	F	F	F	16.8361553050204762	7.7885579285013939	13.2668821583053780	T	T	T
15.9712511531400114	4.6105030762802333	2.3863810053199650	F	F	F	15.1822266724039210	7.1193760063385758	13.2989013584226345	T	T	T
18.6331263453299343	4.6105030762802333	2.3863810053199650	F	F	F	17.36978013260192747	2.1451258378716442	9.8347337059219289	T	T	T
3.9928127882850095	6.9157546144203916	2.3863810053199650	F	F	F	16.3125306561598800	6.5566216384724818	10.218656173417436	T	T	T
6.6546879804750665	6.9157546144203916	2.3863810053199650	F	F	F	15.6215677881399628	8.3086914062051580	11.1733824660978059	T	T	T
9.3165631726649920	6.9157546144203916	2.3863810053199650	F	F	F	### POSCAR for TS25-26 ###					
11.9784383648550481	6.9157546144203916	2.3863810053199650	F	F	F	Zn C H Cl Si					
14.6403135750449727	6.9157546144203916	2.3863810053199650	F	F	F	1.0000000000000000					
17.3021887492350288	6.9157546144203916	2.3863810053199650	F	F	F	18.6331263453299982	0.0000000000000000	0.0000000000000000	F	F	F
19.9640639414249534	6.9157546144203916	2.3863810053199650	F	F	F	6.6546879804749999	11.5262576907006000	0.0000000000000000	F	F	F
5.3237503843798007	9.2210061525604665	2.3863810053199650	F	F	F	0.0000000000000000					
7.9856255765700377	9.2210061525604665	2.3863810053199650	F	F	F	140 11 14 2 1					
10.6475007687599614	9.2210061525604665	2.3863810053199650	F	F	F	Selective dynamics					
13.3093759609500193	9.2210061525604665	2.3863810053199650	F	F	F	Cartesian					
15.9712511531399439	9.2210061525604665	2.3863810053199650	F	F	F	18.6331263453299343	1.5368343587600748	0.0000000000000000	F	F	F
18.6331263453300018	9.2210061525604665	2.3863810053199650	F	F	F	2.6618715921899890	1.5368343587600748	0.0000000000000000	F	F	F
21.2950015375199229	9.2210061525604665	2.3863810053199650	F	F	F	5.3237503843800447	1.5368343587600748	0.0000000000000000	F	F	F
18.6463280365353304	1.5420485391749164	4.6815288533023818	T	T	T	7.9856255765699711	1.5368343587600748	0.0000000000000000	F	F	F
2.6800802279040870	1.5386163423239006	6.65417440835814308	T	T	T	10.6475007687600272	1.5368343587600748	0.0000000000000000	F	F	F
5.3254555678254762	1.5552816329689279	4.670446034932194	T	T	T	13.3093759609499518	1.5368343587600748	0.0000000000000000	F	F	F
7.9681936936843085	1.5528923173841203	4.6618096720761750	T	T	T	15.9712511531400079	1.5368343587600748	0.0000000000000000	F	F	F
10.6088018284182795	1.5442623203095972	4.6458304496679839	T	T	T	19.9640639414249428	3.8420858969022305	0.0000000000000000	F	F	F
13.3139959483356627	1.5507660918775057	4.6674292120709699	T	T	T	3.9928127882847373	3.8420858969022305	0.0000000000000000	F	F	F
16.0324873280363782	1.5576298717992343	4.7461421857015731	T	T	T	6.6546879804750603	3.8420858969022305	0.0000000000000000	F	F	F
19.9624986424377013	3.8420658497291322	4.6692785289143970	T	T	T	9.3165631726649867	3.8420858969022305	0.0000000000000000	F	F	F
3.9993772992639025	8.8546271183406187	4.6617930416880222	T	T	T	11.9784383648550428	3.8420858969022305	0.0000000000000000	F	F	F
6.6565341341317676	8.857385302620212	4.6716916027702631	T	T	T	14.6403135750449709	3.8420858969022305	0.0000000000000000	F	F	F
9.3097744767164844	3.8595180072943812	4.6819371009777328	T	T	T	17.3021887492350182	3.8420858969022305	0.0000000000000000	F	F	F
11.9644015980595260	3.8349308506985091	4.6276709030717471	T	T	T	21.2950015375199887	6.1473374350403116	0.0000000000000000	F	F	F
14.6611295076369892	3.8362802774330875	4.6680776541092124	T	T	T	5.3237503843799763	6.1473374350403116	0.0000000000000000	F	F	F
17.3079363602251703	3.8056919671762666	4.767129010932922	T	T	T	7.9856255765700288	6.1473374350403116	0.0000000000000000	F	F	F
21.3025115602008911	6.1593340771066032	4.6484542878198090	T	T	T	10.6475007687599561	6.1473374350403116	0.0000000000000000	F	F	F
5.3290634293058119	6.1569749116073851	4.6669215561739890	T	T	T	13.3093759609500175	6.1473374350403116	0.0000000000000000	F	F	F
7.986374704888127	6.1543424764943300	4.6740708930636616	T	T	T	15.9712511531399421	6.1473374350403116	0.0000000000000000	F	F	F
10.644902543470228	6.1559888229062927	4.6677783570398802	T	T	T	18.6331263453299982	6.1473374350403116	0.0000000000000000	F	F	F
13.3201712901438469	6.1684246129948432	4.6468897897482444	T	T	T	22.6259391336149420	8.452588971804504	0.0000000000000000	F	F	F
15.9814020191479322	6.1261823713381052	4.7161004795829680	T	T	T	6.6546879804749901	8.452588971804504	0.0000000000000000	F	F	F
18.6481161129883724	6.1465542830315743	4.659355575539722	T	T	T	9.3165631726650524	8.452588971804504	0.0000000000000000	F	F	F
22.6352103212066282	4.4644768567614008	4.6700572076355291	T	T	T	11.9784383648549806	8.452588971804504	0.0000000000000000	F	F	F
6.6660596710999096	4.4610202988452663	4.6711681535394973	T	T	T	14.6403135750450311	8.452588971804504	0.0000000000000000	F	F	F
9.3217206984811281	4.4581649970640809	4.665606929488786	T	T	T	1					





9.3189370569119898	11.5194694560480961	7.0157805114829976	T	T	T
11.9845297785290867	11.5142471236457187	7.0265658981665222	T	T	T
7.9749512323006080	0.0118350890018299	7.0208529874170473	T	T	T
10.6430984987391604	0.0073865187250623	7.0112375421320037	T	T	T
19.9525251082589961	11.4858504397462013	7.0113291907918383	T	T	T
22.6242890898472240	11.4776350973443790	6.9292742995023016	T	T	T
1.3824061672697940	2.3061548935126734	7.02055870080432661	T	T	T
4.0086194525974506	2.3058659416892127	7.0227723494382035	T	T	T
6.6458196647376218	2.3148341416132312	7.0354222492509848	T	T	T
9.2900280782646441	2.3104334476364889	6.9781445952023526	T	T	T
11.9274551529604960	2.3217704158579369	6.9669314006040155	T	T	T
14.5074411341343588	2.259673514138137	6.9325984679055725	T	T	T
17.4516356614748105	2.2520264925236848	7.0014595174124210	T	T	T
2.7330179772166043	4.6295759677130572	6.9433307604784016	T	T	T
5.3526501801229145	4.6095946665144254	7.0206245543716550	T	T	T
7.9649506320296801	4.6005698826595856	7.0436900316576052	T	T	T
10.5732827340060100	4.6187556663362734	6.9736237393262597	T	T	T
16.0347806265357953	5.5668879672695910	8.6476061591100599	T	T	T
18.7614778001395166	4.6149975307382860	7.1474340495205393	T	T	T
4.0163362120095136	6.9068562427575015	6.9603774284119035	T	T	T
6.6553378534731777	6.9027033738987527	7.011168358970431	T	T	T
9.3068502587085771	6.9252423431764640	7.0322189207318131	T	T	T
11.9749330969013847	6.9360512156123777	7.0193226933997259	T	T	T
14.6253080613180875	6.892005762868330	6.987604642336499	T	T	T
17.3092735264931932	6.9561525166479834	6.89072909909292982	T	T	T
19.9872596217516403	6.9367522534859889	6.9598612348584163	T	T	T
5.3262236645137175	9.1973673742862374	6.9741087583633012	T	T	T
7.9887216284247300	9.2058260135291707	7.0214986687922011	T	T	T
10.6444360098229112	9.2236348162067081	7.0218648550695004	T	T	T
13.156616789177988	9.2152436942054425	6.9731614699313225	T	T	T
15.9587615625196815	9.2537657528210620	6.9136733173005815	T	T	T
18.6361355196359533	9.2145121464085248	7.0070201845282609	T	T	T
21.2924093348640540	9.201678576008164	7.0104693097805200	T	T	T
13.1938051835279744	4.6358330734604154	6.8671470439443567	T	T	T
11.9318060715435141	2.0717324500775987	10.4321864824868111	T	T	T
12.9897672187474225	2.9721509793100238	10.5007461804208884	T	T	T
12.7519895398666865	4.3559871531860290	10.3368923888964765	T	T	T
11.4243961171216206	4.8129764219381963	10.1464032439378489	T	T	T
10.3715673117246361	3.9026696906141671	10.128393532337977	T	T	T
10.6223426479399621	2.5313142209618675	10.2537149037293904	T	T	T
14.6794681259419484	6.1775288982133718	10.2693387985324716	T	T	T
13.7993787611690060	5.2975119415773628	10.3438018831997542	T	T	T
13.6953711612672535	8.9414030738016699	10.7343226033255821	T	T	T
16.7252317765969067	8.548509549233569	10.4805106767349852	T	T	T
15.2686274198246110	7.3690356769354617	12.9239567713544421	T	T	T
12.1289070673508892	1.0031356946229670	10.5213030444791293	T	T	T
14.0065435610653868	2.6173500145457633	10.6542078617282137	T	T	T
11.2381199601984854	5.8798410316594456	10.0258135351651170	T	T	T
9.3509915940690256	4.2619079584171073	9.9944045882084556	T	T	T
9.796908746500151	1.8200275939426815	10.2085626224907760	T	T	T
13.6278561328463006	9.1234875069463577	9.6491300893215755	T	T	T
13.8415854877211970	9.9126225752870027	11.2312957658355863	T	T	T
12.7412284033758514	8.5099205967165030	11.0682928126650264	T	T	T
16.6327921310331064	8.8009917850822284	9.4345757843123454	T	T	T
17.5681814159680023	7.8469334306353389	10.5354525013550031	T	T	T
16.9598564804696537	9.4342104375348033	11.0907202928757407	T	T	T
15.4909950680765522	8.2719466769378958	13.5120801856603379	T	T	T
16.0782759303369716	6.6420878991963352	13.0835002885447835	T	T	T
14.3297163865156847	6.9302733200732884	13.2905335641727564	T	T	T
15.8802680946709904	3.0863201468133514	8.7655757143510673	T	T	T
18.1310724025881349	5.3041971302210547	9.7101444589085688	T	T	T
15.1349499467354427	7.8031924686908098	11.108553656161025	T	T	T

### POSCAR for INT5 ###

Zn C H

1.0000000000000000	0.0000000000000000	0.0000000000000000
18.6331263453299982	0.0000000000000000	0.0000000000000000
6.6546879804749999	11.5262576907006000	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.5455240212799985

140 16 13

Selective dynamics

Cartesian

18.6331263453299982	1.5368343587600748	0.0000000000000000	F	F	F
2.6618751921899890	1.5368343587600748	0.0000000000000000	F	F	F
5.3237503843800447	1.5368343587600748	0.0000000000000000	F	F	F
7.9856255765699711	1.5368343587600748	0.0000000000000000	F	F	F
10.6475007687600272	1.5368343587600748	0.0000000000000000	F	F	F
13.3093759609499518	1.5368343587600748	0.0000000000000000	F	F	F

### POSCAR for TS25-26 ###

Zn C H

1.0000000000000000	0.0000000000000000	0.0000000000000000
18.6331263453299982	0.0000000000000000	0.0000000000000000
6.6546879804749999	11.5262576907006000	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.5455240212799985

140 16 13

Selective dynamics

Cartesian

18.6331263453299982	1.5368343587600748	0.0000000000000000	F	F	F
2.6618751921899890	1.5368343587600748	0.0000000000000000	F	F	F
5.3237503843800447	1.5368343587600748	0.0000000000000000	F	F	F
7.9856255765699711	1.5368343587600748	0.0000000000000000	F	F	F
10.6475007687600272	1.5368343587600748	0.0000000000000000	F	F	F
13.3093759609499518	1.5368343587600748	0.0000000000000000	F	F	F

### POSCAR for INT26 ###

Zn C H

1.0000000000000000	0.0000000000000000	0.0000000000000000
18.6331263453299982	0.0000000000000000	0.0000000000000000
6.6546879804749999	11.5262576907006000	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.5455240212799985

140 16 13

Selective dynamics

Cartesian

18.6331263453299982	1.5368343587600748	0.0000000000000000	F	F	F
2.6618751921899890	1.5368343587600748	0.0000000000000000	F	F	F
5.3237503843800447	1.5368343587600748	0.0000000000000000	F	F	F
7.9856255765699711	1.5368343587600748	0.0000000000000000	F	F	F
10.6475007687600272	1.5368343587600748	0.0000000000000000	F	F	F
13.3093759609499518	1.5368343587600748	0.0000000000000000	F	F	F