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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 Me₃SiCl 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 N₂ from CaH₂. Nitrogen was purified by passage through a Ag oxygen-removal column and a Davison 4 Å molecular sieve column. Phenylacetylene, Me₃SiCl, Styrene, 1-Phenyl-2-trimethylsilylacetylene, TEMPO and Toluene were purchased from TCI and the radical scavenger N-tert-Butyl- α -phenylnitrone (PBN) from Sigma-Aldrich. All reagents were used as received without further purification.

2. Characterization Methods

The ¹H (400MHz) and ¹³C (100MHz) NMR spectra was recorded in CDCl₃ using a Bruker AVANCE III 400 MHz spectrometer and referenced to the residual protonated solvent peaks (¹H δ 7.26 ppm and ¹³C δ 77.16 ppm for CDCl₃). The EPR spectra was recorded on a Bruker BioSpin GmbH X-band (v = 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 × 0.32 mm). Products were identified by GC/MS equipped with a HP-5 column (30 m × 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), Me₃SiCl (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), Me_3SiCl (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), Me_3SiCl (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.

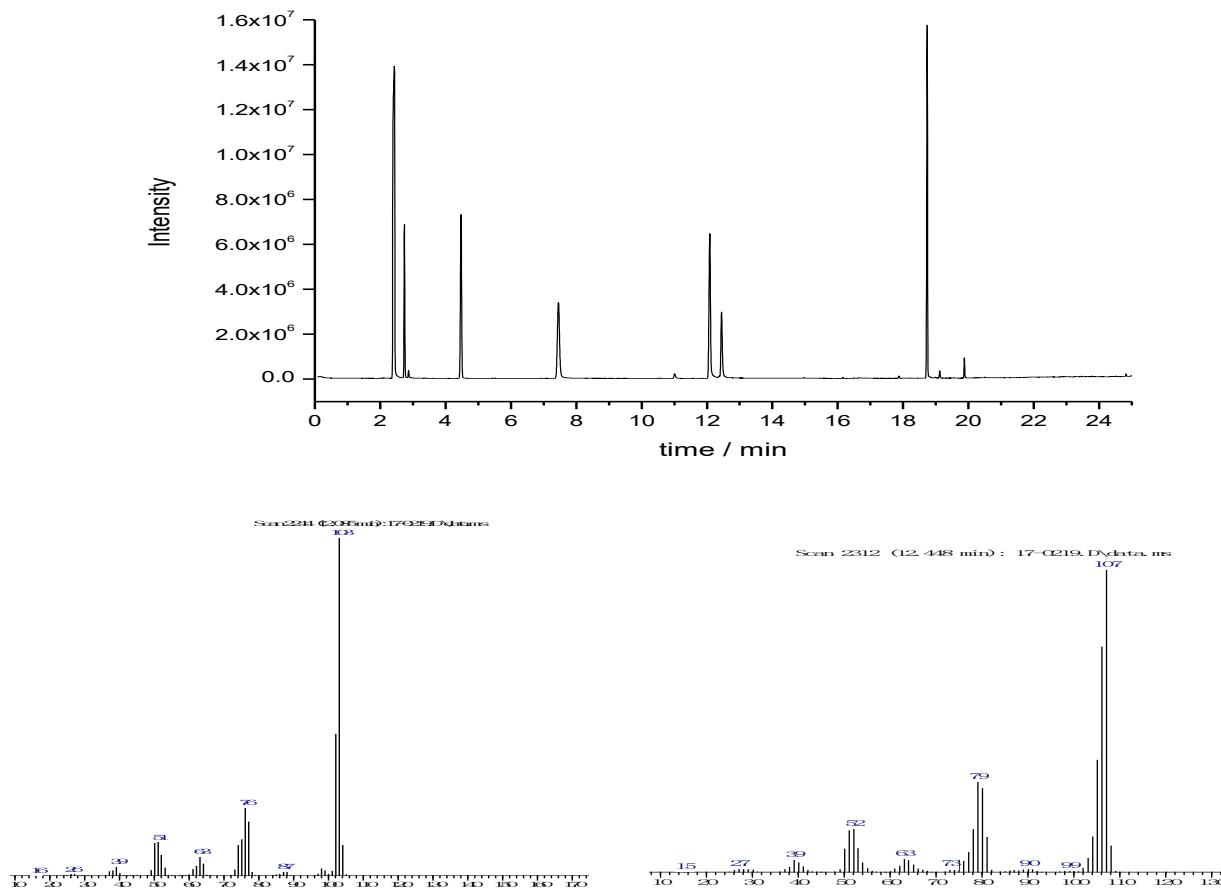


Figure S1 GC-MS spectra for reaction liquid using deuterated phenylacetylene.

3.4. Procedure for acquisition of EPR spectra

To a 25 mL Schlenk flask zinc powder (3 mmol), phenylacetylene (1 mmol), Me_3SiCl (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 Me_3SiCl 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.

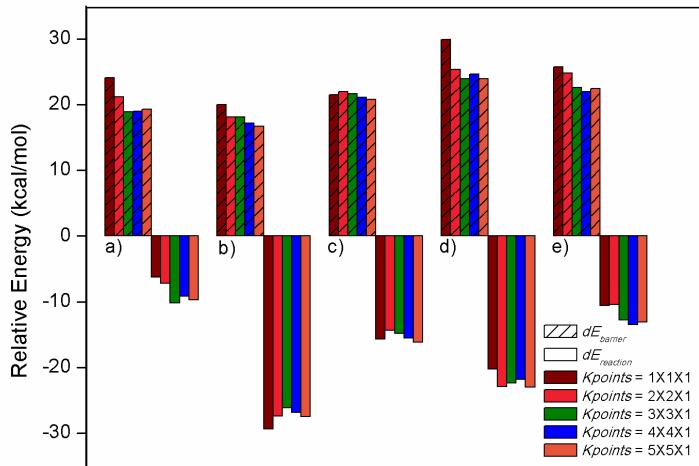


Figure S2 Reaction barriers and energies with different K-point mesh. For a) H transfer from phenylacetylene to the inner carbon of alkynyl of phenylacetylene to form trans alkene species A; b) H transfer from phenylacetylene to the intermediate A to form alkene; c) H transfer from phenylacetylene to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

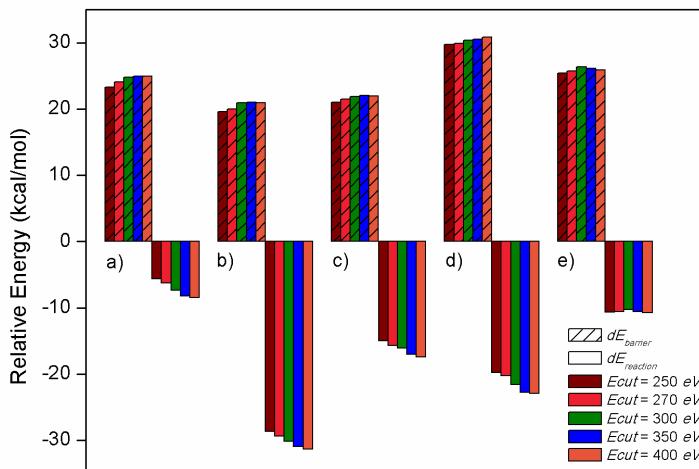


Figure S3 Reaction barriers and energies with different cutoff energy. For a) H transfer from phenylacetylene to the inner carbon of alkynyl of phenylacetylene to form trans alkene species A; b) H transfer from phenylacetylene to the intermediate A to form alkene; c) H transfer from phenylacetylene to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

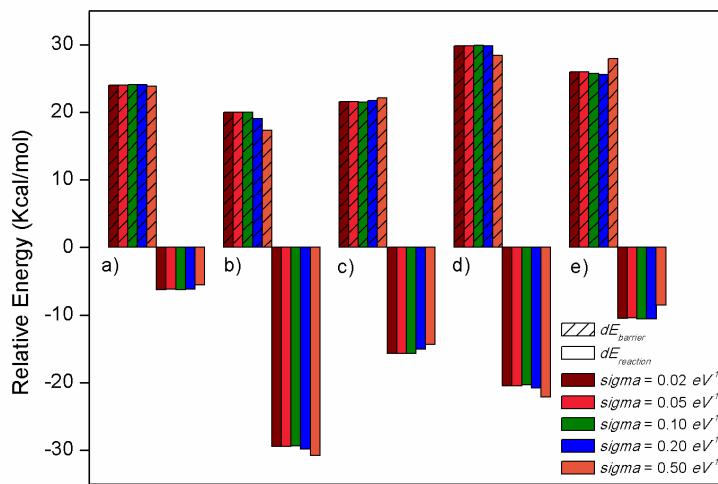


Figure S4 Reaction barriers and energies with different smearing (σ value). For a) H transfer from phenylacetylene to the inner carbon of alkynyl of phenylacetylene to form trans alkene species A; b) H transfer from phenylacetylene to the intermediate A to form alkene; c) H transfer from phenylacetylene 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

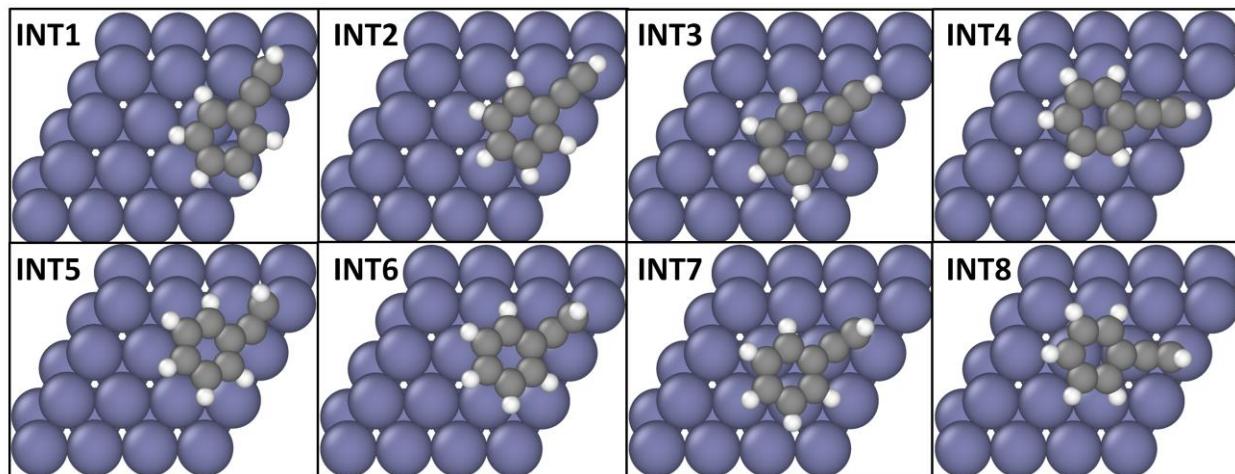


Figure S5 Alkyne-mode (INT1-4) and alkene-mode (INT5-8) adsorption of phenylacetylene on zinc surface at different sites

5.2. Mechanism of the initiation stage

5.2.1 Dissociation of Me_3SiCl on zinc surface

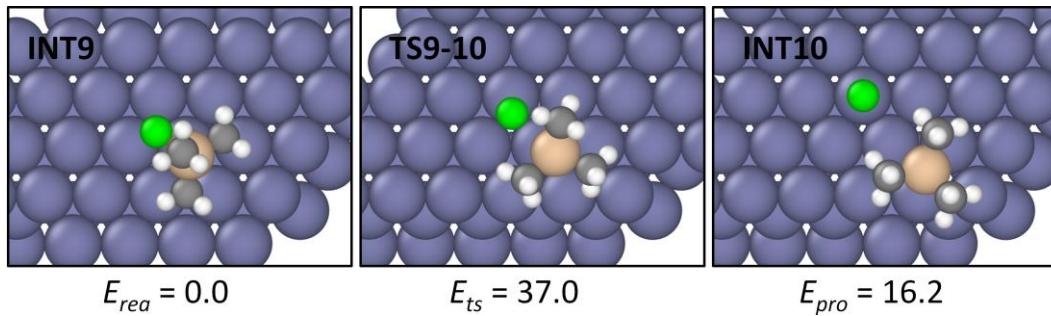


Figure S6 Dissociation pathway of Me_3SiCl on zinc surface. Energies (kcal/mol) are relative to reactant species.

5.2.2 Proposed mechanisms for the initiation between phenylacetylene and zinc

For mechanism I and II in the initiation stage, no radicals were obtained via magnetic optimization.

Mechanism I. Reported single-electron transfer from zinc to phenylacetylene

magnetization (x)		52	0.000	-0.000	0.000	0.000		107	0.000	0.000	0.000	0.000
# of ion	s	53	0.000	0.000	0.000	0.000		108	0.000	0.000	0.000	0.000
	p	54	0.000	0.000	0.000	0.000		109	0.000	-0.000	0.000	0.000
	d	55	0.000	-0.000	0.000	0.000		110	0.000	-0.000	0.000	0.000
	tot	56	0.000	-0.000	0.000	0.000		111	0.000	0.000	0.000	0.000
1	0.000	0.000	0.000	-0.000				112	0.000	0.000	-0.000	0.000
2	0.000	-0.000	0.000	-0.000				113	0.000	0.000	-0.000	0.000
3	0.000	-0.000	0.000	-0.000				114	-0.000	0.000	-0.000	0.000
4	0.000	-0.000	0.000	0.000				115	0.000	0.000	0.000	0.000
5	0.000	0.000	0.000	0.000				116	0.000	-0.000	0.000	0.000
6	0.000	-0.000	0.000	-0.000				117	0.000	0.000	0.000	0.000
7	0.000	-0.000	0.000	-0.000				118	0.000	0.000	0.000	0.000
8	0.000	-0.000	0.000	-0.000				119	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	-0.000				120	0.000	0.000	-0.000	0.000
10	0.000	-0.000	0.000	-0.000				121	0.000	0.000	-0.000	0.000
11	0.000	-0.000	0.000	0.000				122	0.000	0.000	0.000	0.000
12	0.000	-0.000	0.000	-0.000				123	0.000	0.000	0.000	0.000
13	0.000	-0.000	0.000	-0.000				124	0.000	-0.000	-0.000	-0.000
14	0.000	-0.000	0.000	-0.000				125	0.000	0.000	-0.000	0.000
15	0.000	-0.000	0.000	-0.000				126	0.000	0.000	-0.000	0.000
16	0.000	-0.000	0.000	-0.000				127	-0.000	0.000	-0.000	0.000
17	0.000	-0.000	0.000	-0.000				128	0.000	0.000	-0.000	0.000
18	0.000	-0.000	0.000	-0.000				129	-0.000	0.000	0.000	0.000
19	0.000	-0.000	0.000	-0.000				130	0.000	0.000	-0.000	0.000
20	0.000	-0.000	0.000	-0.000				131	0.000	0.000	-0.000	0.000
21	0.000	-0.000	0.000	-0.000				132	-0.000	0.000	-0.000	0.000
22	0.000	-0.000	0.000	-0.000				133	0.000	0.000	-0.000	0.000
23	0.000	-0.000	0.000	-0.000				134	0.000	0.000	-0.000	0.000
24	0.000	-0.000	0.000	-0.000				135	-0.000	0.000	0.000	-0.000
25	0.000	-0.000	0.000	-0.000				136	0.000	-0.000	0.000	0.000
26	0.000	-0.000	0.000	-0.000				137	0.000	-0.000	0.000	0.000
27	0.000	-0.000	0.000	-0.000				138	0.000	0.000	0.000	0.000
28	0.000	-0.000	0.000	-0.000				139	0.000	0.000	-0.000	0.000
29	0.000	-0.000	0.000	-0.000				140	-0.000	0.000	0.000	0.000
30	0.000	-0.000	0.000	-0.000				141	-0.000	-0.000	0.000	-0.000
31	0.000	-0.000	0.000	-0.000				142	0.000	0.000	0.000	0.000
32	0.000	-0.000	0.000	0.000				143	-0.000	-0.000	0.000	-0.000
33	0.000	-0.000	0.000	0.000				144	0.000	0.000	0.000	0.000
34	0.000	-0.000	0.000	0.000				145	-0.000	-0.000	0.000	-0.000
35	0.000	-0.000	0.000	-0.000				146	0.000	0.000	0.000	0.000
36	0.000	-0.000	0.000	-0.000				147	-0.000	-0.000	0.000	-0.000
37	0.000	-0.000	0.000	-0.000				148	0.000	0.000	0.000	0.000
38	0.000	-0.000	0.000	0.000				149	0.000	-0.000	0.000	0.000
39	0.000	0.000	0.000	0.000				150	0.000	0.000	0.000	0.000
40	0.000	0.000	0.000	0.000				151	0.000	-0.000	0.000	0.000
41	0.000	-0.000	0.000	0.000				152	0.000	-0.000	0.000	0.000
42	0.000	-0.000	0.000	0.000				153	0.000	-0.000	0.000	0.000
43	0.000	-0.000	0.000	-0.000				154	0.000	-0.000	0.000	0.000
44	0.000	-0.000	0.000	0.000				tot	0.000	-0.000	0.000	0.000
45	0.000	0.000	0.000	0.000								
46	0.000	0.000	0.000	0.000								
47	0.000	0.000	0.000	0.000								
48	0.000	-0.000	0.000	0.000								
49	0.000	-0.000	0.000	-0.000								
50	0.000	-0.000	0.000	0.000								
51	0.000	-0.000	0.000	0.000								

Mechanism II. Hydrogen transfer from the phenylacetylene dissolved in MeCN to the adsorbed phenylacetylene to form radical species

magnetization (x)		55	0.000	-0.000	-0.000	0.000		113	-0.000	0.000	-0.000	-0.000
# of ion	s	p	d	tot				56	-0.000	0.000	-0.000	0.000
1	0.000	0.000	-0.000	0.000				57	0.000	0.000	-0.000	0.000
2	0.000	0.000	-0.000	0.000				58	-0.000	0.000	-0.000	0.000
3	0.000	-0.000	-0.000	0.000				59	0.000	0.000	-0.000	0.000
4	0.000	-0.000	-0.000	0.000				60	0.000	-0.000	-0.000	0.000
5	0.000	-0.000	-0.000	0.000				61	0.000	-0.000	-0.000	0.000
6	0.000	-0.000	-0.000	0.000				62	-0.000	0.000	-0.000	-0.000
7	0.000	-0.000	-0.000	0.000				63	0.000	0.000	-0.000	0.000
8	0.000	0.000	-0.000	0.000				64	0.000	0.000	-0.000	0.000
9	0.000	-0.000	-0.000	0.000				65	0.000	0.000	-0.000	0.000
10	0.000	-0.000	-0.000	0.000				66	0.000	0.000	-0.000	0.000
11	0.000	0.000	-0.000	0.000				67	0.000	0.000	-0.000	0.000
12	0.000	0.000	-0.000	0.000				68	-0.000	0.000	-0.000	-0.000
13	-0.000	-0.000	-0.000	-0.000				69	-0.000	0.000	-0.000	0.000
14	0.000	-0.000	0.000	0.000				70	0.000	0.000	-0.000	0.000
15	0.000	-0.000	-0.000	0.000				71	-0.000	0.000	-0.000	-0.000
16	0.000	-0.000	0.000	0.000				72	0.000	-0.000	-0.000	-0.000
17	0.000	0.000	-0.000	0.000				73	-0.000	0.000	0.000	-0.000
18	0.000	0.000	0.000	0.000				74	0.000	0.000	-0.000	0.000
19	-0.000	0.000	-0.000	-0.000				75	0.000	0.000	0.000	0.000
20	-0.000	0.000	-0.000	-0.000				76	-0.000	0.000	-0.000	-0.000
21	0.000	-0.000	0.000	0.000				77	-0.000	0.000	-0.000	-0.000
22	-0.000	-0.000	0.000	-0.000				78	0.000	-0.000	-0.000	-0.000
23	0.000	-0.000	-0.000	-0.000				79	-0.000	0.000	0.000	-0.000
24	-0.000	-0.000	-0.000	-0.000				80	-0.000	0.000	0.000	-0.000
25	-0.000	-0.000	-0.000	-0.000				81	-0.000	0.000	0.000	-0.000
26	-0.000	-0.000	-0.000	-0.000				82	-0.000	-0.000	0.000	-0.000
27	0.000	-0.000	0.000	0.000				83	-0.000	0.000	0.000	-0.000
28	0.000	-0.000	0.000	-0.000				84	-0.000	0.000	-0.000	-0.000
29	0.000	-0.000	-0.000	0.000				85	-0.000	0.000	0.000	-0.000
30	0.000	-0.000	-0.000	0.000				86	-0.000	-0.000	0.000	-0.000
31	-0.000	-0.000	0.000	-0.000				87	0.000	-0.000	-0.000	0.000
32	-0.000	-0.000	0.000	-0.000				88	-0.000	-0.000	0.000	-0.000
33	0.000	-0.000	0.000	0.000				89	-0.000	-0.000	0.000	-0.000
34	0.000	-0.000	0.000	0.000				90	0.000	-0.000	-0.000	0.000
35	-0.000	-0.000	0.000	-0.000				91	-0.000	0.000	-0.000	-0.000
36	0.000	0.000	-0.000	0.000				92	-0.000	0.000	-0.000	-0.000
37	0.000	0.000	-0.000	0.000				93	-0.000	-0.000	-0.000	-0.000
38	0.000	-0.000	-0.000	0.000				94	-0.000	0.000	0.000	-0.000
39	-0.000	0.000	-0.000	-0.000				95	-0.000	-0.000	0.000	-0.000
40	-0.000	-0.000	-0.000	-0.000				96	0.000	-0.000	-0.000	-0.000
41	-0.000	-0.000	-0.000	-0.000				97	-0.000	0.000	0.000	-0.000
42	-0.000	0.000	-0.000	-0.000				98	-0.000	0.000	-0.000	-0.000
43	-0.000	0.000	-0.000	-0.000				99	-0.000	0.000	-0.000	-0.000
44	0.000	0.000	-0.000	0.000				100	-0.000	0.000	-0.000	-0.000
45	0.000	0.000	-0.000	0.000				101	-0.000	-0.000	-0.000	-0.000
46	-0.000	-0.000	-0.000	-0.000				102	0.000	0.000	-0.000	0.000
47	-0.000	-0.000	-0.000	-0.000				103	-0.000	0.000	-0.000	0.000
48	-0.000	0.000	-0.000	0.000				104	0.000	0.000	-0.000	0.000
49	-0.000	0.000	-0.000	-0.000				105	0.000	0.000	-0.000	0.000
50	0.000	0.000	-0.000	0.000				106	0.000	0.000	0.000	0.000
51	-0.000	0.000	0.000	0.000				107	0.000	0.000	-0.000	0.000
52	-0.000	0.000	0.000	-0.000				108	-0.000	0.000	0.000	-0.000
53	-0.000	-0.000	-0.000	-0.000				109	-0.000	-0.000	0.000	-0.000
54	0.000	0.000	-0.000	0.000				110	0.000	-0.000	0.000	0.000
					111	-0.000	0.000	0.000	-0.000			
					112	0.000	-0.000	0.000	0.000			
								tot	0.000	0.000	-0.000	0.000

Mechanism III. Hydrogen transfer from the phenylacetylene dissolved in MeCN to the adsorbed phenylacetylene to form ionic species

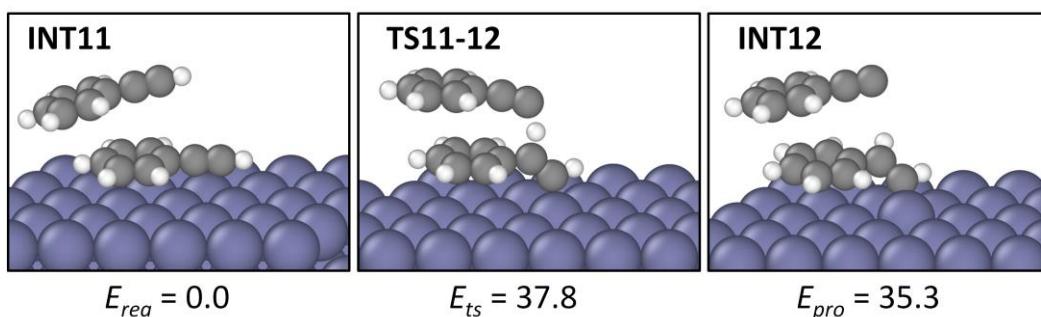


Figure S7 Pathway of hydrogen transfer between the phenylacetylene dissolved in MeCN to the adsorbed phenylacetylene. Energies (kcal/mol) are relative to reactant species.

Mechanism IV. Dissociation of phenylacetylene on zinc surface

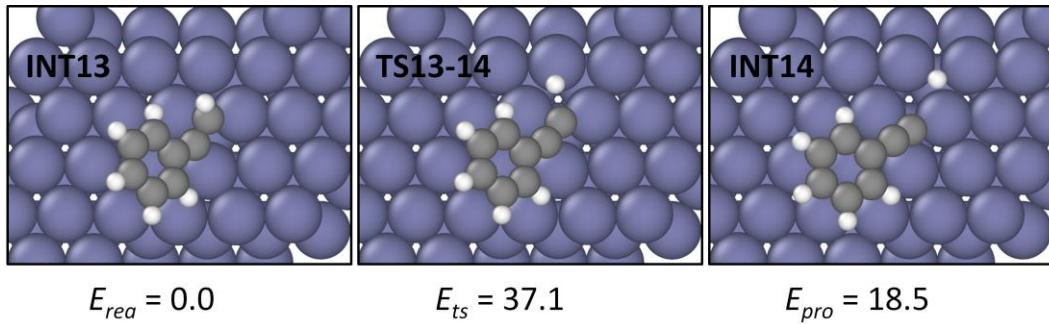


Figure S8 Dissociation pathway of phenylacetylene on zinc surface. Energies (kcal/mol) are relative to reactant species.

Mechanism V. Hydrogen transfer between adsorbed phenylacetylene on zinc surface

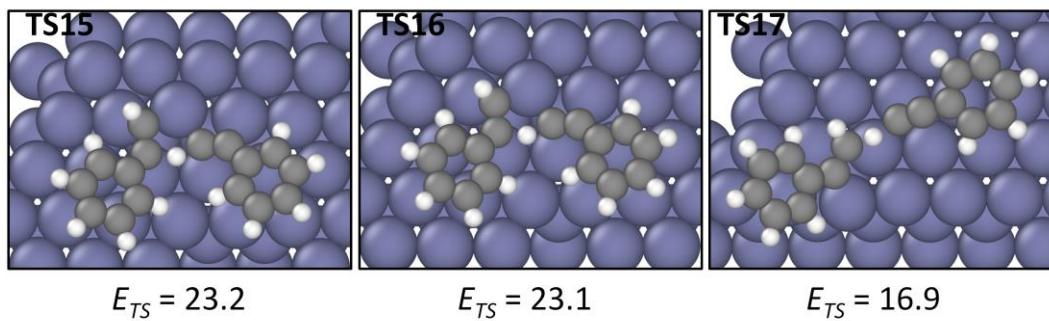


Figure S9 Transition states of the first hydrogen transfer between the adsorbed phenylacetylene on zinc surface: TS15 for intermediate A; TS16 for intermediate B; TS17 for intermediate C. Energies (kcal/mol) are relative to reactant species.

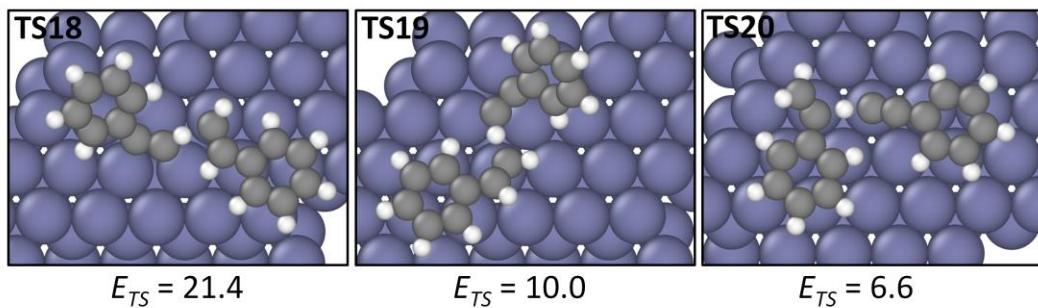


Figure S10 Transition states of the second hydrogen transfer between the adsorbed phenylacetylene and alkene moieties on zinc surface: TS18 via intermediate A; TS19 via intermediate B; TS20 via intermediate C. Energies (kcal/mol) are relative to reactant species.

5.3. Product formation pathways

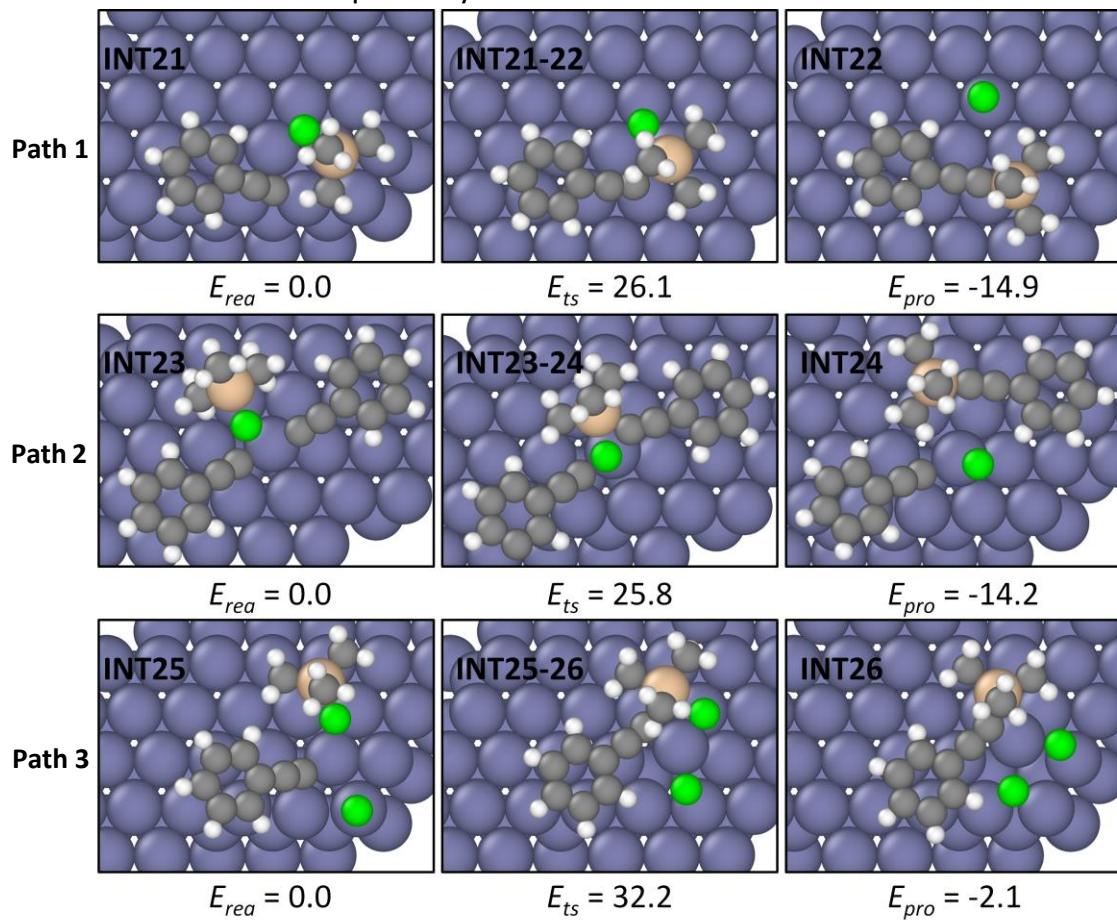


Figure S11 Reaction pathways for the formation step, path 1 via intermediate I PhC≡C-Zn; path 2 via intermediate II (PhC≡C)₂Zn; path 3 via intermediate III PhC≡CZnCl. Energies (kcal mol⁻¹) are relative to reactant species.

5.4. Bader charge analysis for the surface adsorbed species

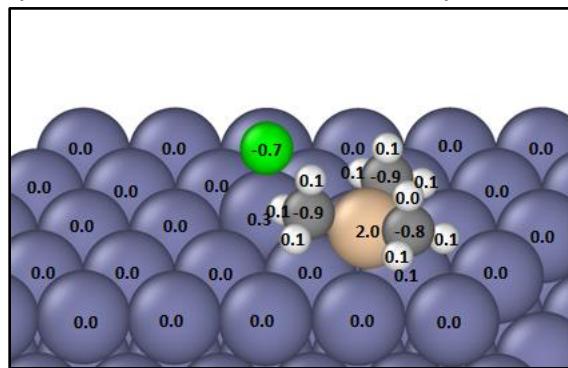


Figure S12 Bader charges distribution of dissociation products of Me₃SiCl on zinc surface.

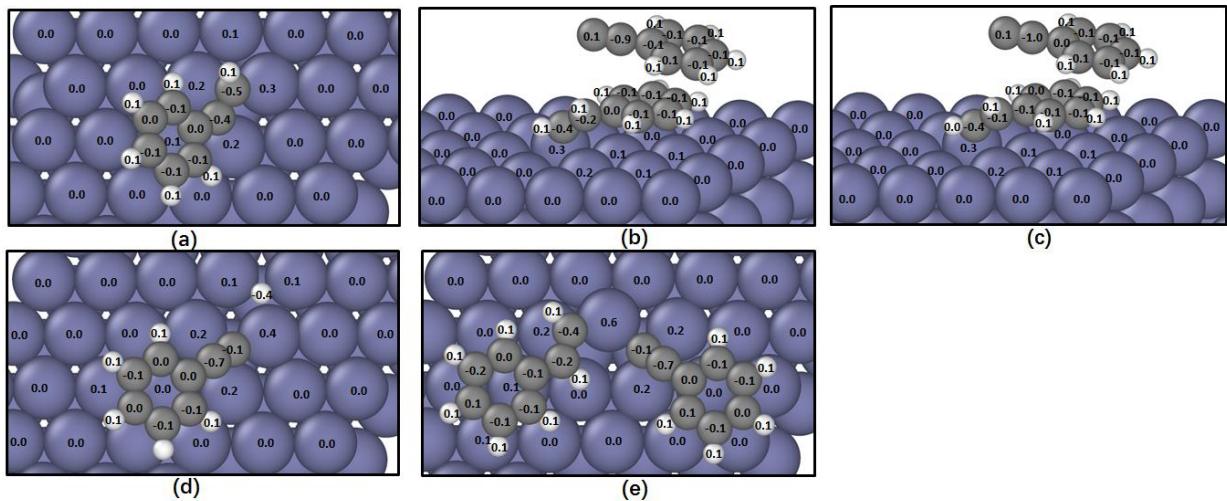


Figure S13 Bader charge distribution for the intermediates of the interaction between phenylacetylene and zinc in the initiation stage of Scheme 3. For a) alkene-mode adsorption of phenylacetylene on zinc surface; b) H transfer from phenylacetylene dissolving in the solvent to the adsorbed phenylacetylene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

6. Structure data

1.3309375969050001	3.842085896902083	4.7727620106400002	T	T	T	11.9784399999999422	6.9157499999999708	2.3863800000000821	F	F	F	
3.9928127882850002	3.842085896902083	4.7727620106400002	T	T	T	14.6483089999999764	6.9157499999999708	2.3863800000000821	F	F	F	
6.6546879804750008	3.842085896902083	4.7727620106400002	T	T	T	17.3021900000000102	6.9157499999999708	2.3863800000000821	F	F	F	
9.3165631726649991	3.842085896902083	4.7727620106400002	T	T	T	19.9640600000000390	6.9157499999999708	2.3863800000000821	F	F	F	
2.6618751921900001	6.1473374350403324	4.7727620106400002	T	T	T	23.958763450000155	9.2210100000000370	2.3863800000000821	F	F	F	
5.3237503843800003	6.1473374350403324	4.7727620106400002	T	T	T	7.9856300000000449	9.2210100000000370	2.3863800000000821	F	F	F	
7.9856255765700013	6.1473374350403324	4.7727620106400002	T	T	T	10.6475000000000790	9.2210100000000370	2.3863800000000821	F	F	F	
18.6475007687600005	6.1473374350403324	4.7727620106400002	T	T	T	13.3093799999999796	9.2210100000000370	2.3863800000000821	F	F	F	
3.9928127882850002	8.4525889731804575	4.7727620106400002	T	T	T	15.9712500000000119	9.2210100000000370	2.3863800000000821	F	F	F	
6.6546879804749999	8.4525889731804575	4.7727620106400002	T	T	T	18.633100000000039	9.2210100000000370	2.3863800000000821	F	F	F	
9.3165631726650009	8.4525889731804575	4.7727620106400002	T	T	T	21.2950000000000763	9.2210100000000370	2.3863800000000821	F	F	F	
11.9784383648550001	8.4525889731804575	4.7727620106400002	T	T	T	18.6422999543939708	1.5477000000000370	2.3863800000000821	T	T	T	
0.0000000000000000	0.0000000000000000	7.159143015959998	T	T	T	2.6698758490614742	1.5452370645077509	4.6619160972519378	T	T	T	
2.6618751921900001	0.0000000000000000	7.159143015959998	T	T	T	5.3030887192682059	1.5450609836204595	4.6626043645532338	T	T	T	
5.3237503843800003	0.0000000000000000	7.159143015959998	T	T	T	7.9966363939642198	1.5451137483343931	4.6587564838719944	T	T	T	
7.9856255765700004	0.0000000000000000	7.159143015959998	T	T	T	10.65111786594763732	1.5456869420763732	4.66091337356969722	T	T	T	
1.3309375969050001	2.3052515381401251	7.159143015959998	T	T	T	13.3150108526917901	1.5434415657382804	4.6659029182322908	T	T	T	
3.9928127882850002	2.3052515381401251	7.159143015959998	T	T	T	15.9877119335807105	1.5435858846546118	4.6569214664962075	T	T	T	
6.6546879804749999	2.3052515381401251	7.159143015959998	T	T	T	19.9712989861636409	1.5438110316323388	4.65598680296459408	T	T	T	
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2.6618751921900001	4.0150307362820504	7.159143015959998	T	T	T	6.660477356848124607	1.5481033300000000	4.66114246229956044	T	T	T	
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6.6546879804749999	6.157546144203756	7.159143015959998	T	T	T	21.3027189272636406	1.54853754199588521	4.661847075882452	T	T	T	
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## POSCAR for INT9 ##						13.316900417815730427	1.5469227413107349	4.6619639551830225	T	T	T	
Zn C Cl H Si						15.9797798600188266	1.546711387015268	4.6628994437503075	T	T	T	
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14.6483100000000006	6.157546144203756	7.159143015959998	0.0000000000000000	0.0000000000000000	0.0000000000000000	21.30155847301933	1.54662150436134993	4.6644148522794704	T	T	T	
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62..306714942944956	5..2043488590520875	4..6989950567685759	T T T	9..316563172665056	1..309379596499533	0..0000000000000000	F F	
64..306714942944956	5..2063488590520875	4..6989950567685759	T T T	1..309379596499533	1..309379596499533	0..0000000000000000	F F	
66..306714942944956	5..2083488590520875	4..6989950567685759	T T T	14..6403135574053085	1..309379596499533	0..0000000000000000	F F	
68..306714942944956	5..2103488590520875	4..6989950567685759	T T T	17..3021887492349649	1..309379596499533	0..0000000000000000	F F	
70..306714942944956	5..2123488590520875	4..6989950567685759	T T T	21..2590501537519922	1..309379596499533	0..0000000000000000	F F	
72..306714942944956	5..2143488590520875	4..6989950567685759	T T T	6..1615036726820333	1..309379596499533	0..0000000000000000	F F	
74..306714942944956	5..2163488590520875	4..6989950567685759	T T T	9..316563172665056	1..309379596499533	0..0000000000000000	F F	
76..306714942944956	5..2183488590520875	4..6989950567685759	T T T	1..309379596499533	1..309379596499533	0..0000000000000000	F F	
78..306714942944956	5..2203488590520875	4..6989950567685759	T T T	14..6403135574053085	1..309379596499533	0..0000000000000000	F F	
80..306714942944956	5..2223488590520875	4..6989950567685759	T T T	17..3021887492349649	1..309379596499533	0..0000000000000000	F F	
82..306714942944956	5..2243488590520875	4..6989950567685759	T T T	21..2590501537519922	1..309379596499533	0..0000000000000000	F F	
84..306714942944956	5..2263488590520875	4..6989950567685759	T T T	6..1615036726820333	1..309379596499533	0..0000000000000000	F F	
86..306714942944956	5..2283488590520875	4..6989950567685759	T T T	9..316563172665056	1..309379596499533	0..0000000000000000	F F	
88..306714942944956	5..2303488590520875	4..6989950567685759	T T T	1..309379596499533	1..309379596499533	0..0000000000000000	F F	
90..306714942944956	5..2323488590520875	4..6989950567685759	T T T	14..6403135574053085	1..309379596499533	0..0000000000		

5.3295487568789053	4.6108749218476808	6.9958671436220330	T	T	T	13.3093759609499518	4.6105030762802253	2.3863810053199646	F	F	F
7.9917878995462779	4.6107330450619779	6.9675471726317078	T	T	T	15.9712511531400079	4.6105030762802253	2.3863810053199646	F	F	F
10.6569425206089701	4.6662078399959506	6.9782851489601088	T	T	T	18.63312645329934	4.6105030762802253	2.3863810053199646	F	F	F
15.9781043581502518	4.6085344975028155	6.98548735887178650	T	T	T	22.6259391336148781	6.9157546144283774	2.3863810053199646	F	F	F
18.6327851727839224	4.60993933489398955	6.979566474999095	T	T	T	6.6546879844750594	6.9157546144283774	2.3863810053199646	F	F	F
3.9975670963116805	6.9128195142976256	6.9984126480133195	T	T	T	9.3165631726649867	6.9157546144283774	2.3863810053199646	F	F	F
6.657857390597471	6.9142111735703264	6.977868650246038	T	T	T	11.978438364858428	6.9157546144283774	2.3863810053199646	F	F	F
9.319938924365349	6.9699725045887845	6.9821197345533639	T	T	T	14.640313557049799	6.9157546144283774	2.3863810053199646	F	F	F
11.9762700376469375	6.9095732191050319	6.9626316758814442	T	T	T	17.3021887492350288	6.9157546144283774	2.3863810053199646	F	F	F
14.6339047617313	6.9113268217979833	7.0036285764309989	T	T	T	19.946063942429534	6.9157546144283774	2.3863810053199646	F	F	F
17.3803465926701345	6.9127636298342967	6.9868271645356418	T	T	T	5.3237503843799798	9.2210861525604585	2.3863810053199646	F	F	F
19.965294626177099	6.913771536252780	6.979838663646111	T	T	T	7.98562594836700582	9.2210861525604585	2.3863810053199646	F	F	F
5.3268635120823840	9.2166951357657723	6.988866751385143	T	T	T	10.6475007687599597	9.2210861525604585	2.3863810053199646	F	F	F
7.9879959414909856	9.214384283067495	6.9890212489933615	T	T	T	13.309375969508051	9.2210861525604585	2.3863810053199646	F	F	F
10.645686551324994	6.988093443801852	6.9820910016161388	T	T	T	15.9712511531399404	9.2210861525604585	2.3863810053199646	F	F	F
13.305397341734947	9.2154563284172237	6.98911397676508879	T	T	T	18.6331265329998	9.2210861525604585	2.3863810053199646	F	F	F
15.9700152668487657	9.2178167740817762	6.9815179418488116	T	T	T	21.2950015375199087	9.2210861525604585	2.3863810053199646	F	F	F
18.633931744631380	9.2183824768156768	6.9774990037514844	T	T	T	18.6385124572772618	1.5631054844590919	4.6837540634804675	T	T	T
21.297200863603793	9.217996260825396	6.9779697227318738	T	T	T	2.66791948381944	1.564741232800803	4.6900802004222868	T	T	T
13.3132996813902108	6.46078499579151594	7.0323269982163879	T	T	T	5.3235894824646062	1.5522237857766956	4.6876794701195657	T	T	T
9.2921287416717351	6.8526595178184076	18.0588995445133072	T	T	T	7.99942644933624	1.5501697501463063	4.6566910522755071	T	T	T
10.6827267726206347	6.8809896759492218	18.142772418923572	T	T	T	10.686798890699696	1.5461505582363624	4.66071422882191090	T	T	T
11.3481358364585349	6.569675597487640	18.198569767388193	T	T	T	13.3368265948386452	1.5199483437135391	4.6801387176466425	T	T	T
10.5884676068030945	6.377181983518041	18.1680477395351999	T	T	T	15.983159823078906	1.5595417491871570	4.6942332968157796	T	T	T
9.19758033241015184	4.435203580695487	18.1069611274882796	T	T	T	19.985668745435970	3.862057197972538	4.6998635925343688	T	T	T
8.5465805533351515	6.5691253824646978	10.435233915173846	T	T	T	3.9929935392734577	3.864828503303933	4.694492669582639	T	T	T
13.9822875359380804	5.46097748919306211	18.2659640418793696	T	T	T	6.6452451904598053	3.8628682348601830	4.6431665983644441	T	T	T
12.7662432450123288	5.5098664516063476	18.2575962135981328	T	T	T	9.32562427708876872	3.859848185113146	4.6327839774618977	T	T	T
6.597817518591946	7.352319368256875	12.547322759837873	T	T	T	12.01243947526561230	3.874934321795653	4.727907923960978	T	T	T
7.9177939439194094	7.3458793943121558	12.994752794873975	T	T	T	14.646226982688628	3.863714761974859	4.7405660383051149	T	T	T
8.54463313845465349	6.130868487584776	13.3356985156629478	T	T	T	15.983159823078906	3.863714761974859	4.6942332968157796	T	T	T
7.8139712959469807	4.9302619864307439	13.2359986021815734	T	T	T	21.2959521120974593	6.1659504803644048	4.6960112629828306	T	T	T
6.494126182799988	4.9476313583642633	12.78966569828082582	T	T	T	5.311168921615788	6.1630382179224332	4.658664554998839	T	T	T
5.8842829972755082	16.555566680200551	12.4373082743878720	T	T	T	7.98678678873613462	16.5733334925940405	4.6468334917548872	T	T	T
11.0955958348226266	6.8940170351660417	14.0098947341808787	T	T	T	10.672274105268888	6.159762410526367	4.643657647253034	T	T	T
9.9166105323371934	6.1115280019672609	13.7169983586007511	T	T	T	13.33993965363074362	6.1492558586714452	4.7143054607405572	T	T	T
8.74845735911363680	7.8167518540424581	18.0152367496933975	T	T	T	15.9616486061945249	16.607691473294910	4.6380719739127043	T	T	T
11.2648076434864208	7.3383787576184027	18.1586101502805288	T	T	T	18.6415939007361728	6.1615047537463718	4.6921753693475128	T	T	T
11.101315135873593	3.416332745329934	13.23598374587604778	T	T	T	22.637450286411460529	8.48678262804211592	4.6887129996708428	T	T	T
8.6197267303120688	3.510218800184839	18.093431724023513	T	T	T	6.65528415523376	8.4855261261582366	4.6499501297206862	T	T	T
7.458293488988409	5.7161337402471711	9.999584930333481	T	T	T	9.327667742538798	8.48166982372632	4.6541645619058007	T	T	T
15.0529954140641458	5.4231904190198713	10.1302269982157054	T	T	T	12.0020595846061390	8.4847594158653463	4.6399038112181810	T	T	T
6.128392079307639698	8.2983490383743928	12.2709231128047295	T	T	T	14.657244844872007	8.4798018465004823	4.608085151373224	T	T	T
8.4829427663408926	8.27547111510356	13.0627367795363245	T	T	T	16.716710522965563	8.4657252830461864	4.7108242033097243	T	T	T
8.2996785789358540	8.9873445216231951	12.488310948827975	T	T	T	19.9820502578432938	8.4634197695815945	4.6963112627114434	T	T	T
5.94345053445455439	4.010132244842410	12.70109093828124	T	T	T	23.96364721582452	7.084833599818856	4.7035851116249461	T	T	T
4.855896972186977	6.16361445599977438	12.0743539271812184	T	T	T	10.6556569923076395	7.092381860988109	4.703871983745948	T	T	T
12.13976096923076024	6.07664733375385461	14.2547989430044719	T	T	T	13.3259853440638274	7.0771805546041398	4.691701333723592	T	T	T
140	16	12	## POSCAR for TS11-12 ##			7.99146065408673961	7.0257881914713788	7.03965833976262846			
Selective dynamics											
Cartesian											
18.63312645329934	1.5368343587600748	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
2.661875192189989	1.5368343587600748	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
6.6546879847499999	11.5262576907006000	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
0.0000000000000000	0.0000000000000000	24.5455240212799985									
14.6401663174463031	4.85288971381804504	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
13.309375960608175	6.1473374350420292	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
15.971251153139421	6.1473374350420292	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
16.473374350420292	6.1473374350420292	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
13.3021887492350182	8.4525889731804504	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
21.2950615375199868	10.7578405113205235	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
0.0000000000000000	0.0000000000000000	2.386381053199646	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
2.661875192189895	2.368381053199646	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
5.323753843799807	2.368381053199646	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
7.9856257567003508	2.368381053199646	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
10.647500768759614	2.368381053199646	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F	F	F	F	F
13.309375960580175	2.368381053199646	0.0000000000000000	0.0000000000000000	0.00000							

9.0205611952315650	8.3017140362026858	12.6842668581980522	T	T	T	17.3119658557792739	8.4497844032717015	4.6793511290550320	T	T	T
8.9583651925890617	3.9839959424614797	13.1375600578792682	T	T	T	19.9810958219462265	8.4571866266365721	4.6727324613433829	T	T	T
6.4691595952985734	3.994637685930739	12.9159754909726203	T	T	T	23.9663197837617332	10.7633839899142694	4.6902617595512117	T	T	T
5.2395326608396475	6.1611600144144081	12.5567867023454015	T	T	T	7.9938612645872258	10.7608113541032360	4.6882891955044750	T	T	T
12.371897973741505	5.8331297688770096	11.3755402128258520	T	T	T	10.6556326244618802	10.7615284012487278	4.6901514173519416	T	T	T
### POSCAR for INT12 ###											
Zn C H						13.3151595117412196	10.7652696997788890	4.678524632318620	T	T	T
1.0000000000000000	18.6331263453300018	0.0000000000000000	0.0000000000000000	0.0000000000000000	15.988771891253727	10.7802806270820679	4.6793258336538708	T	T	T	
6.6546879804749999	11.5262576987006249	0.0000000000000000	0.0000000000000000	0.0000000000000000	18.6421319479210759	10.7596049463351129	4.6855033652451975	T	T	T	
0.0000000000000000	6.6546879804749999	0.0000000000000000	24.5455240212800021	2.6524125072027213	0.0124339238645855	7.0111328560649268	T	T	T		
140 16 12	Selective dynamics				5.3117010094804238	0.0065570948452439	6.9934019574834112	T	T	T	
Cartesian					7.9720225893114662	0.0136713500493837	7.02354162627374132	T	T	T	
18.6331263453299378	1.5368343587600781	0.0000000000000000	F	F	F	10.6344091438867903	7.0180746795334744	7.0289379005925090	T	T	T
2.6618751921899000	1.5368343587600781	0.0000000000000000	F	F	F	13.2956939647766390	0.0099817678328934	7.0099805658885250	T	T	T
5.2237503843800473	1.5368343587600781	0.0000000000000000	F	F	F	15.94957631345217636	0.01791626880897645	7.0190232399928973	T	T	T
7.9856255765699720	1.5368343587600781	0.0000000000000000	F	F	F	1.3170556594915972	2.3166173557831143	7.0261414456804072	T	T	T
10.6475007687608229	1.5368343587600781	0.0000000000000000	F	F	F	3.9671000871185042	2.3197408441014784	7.02660609063643570	T	T	T
13.389375960949536	1.5368343587600781	0.0000000000000000	F	F	F	6.6325420856596142	2.3185052449762202	6.9820582566027051	T	T	T
15.97121513140081	1.5368343587600781	0.0000000000000000	F	F	F	9.2898388131781036	2.2998348898289213	6.95745308393470431	T	T	T
19.9640639414249534	1.5368343587600781	0.0000000000000000	F	F	F	11.956343956238279	2.31903873100130288	7.00309694606144871	T	T	T
3.9922817882850993	3.84208585969002354	0.0000000000000000	F	F	F	14.6107367250116074	3.375554696933545	7.0299706069376749	T	T	T
6.6546879804750656	3.84208585969002354	0.0000000000000000	F	F	F	17.2892311786550231	2.32523818795363508	7.0104439205817286	T	T	T
9.3185631726589056	3.84208585969002354	0.0000000000000000	F	F	F	2.6442964301751639	6.1688754457672026	7.0269473297873083	T	T	T
9.316563172656494000	3.84208585969002354	0.0000000000000000	F	F	F	5.2975307015791793	4.6136461003422140	7.0279134888538641	T	T	T
11.9784383648550481	3.84208585969002354	0.0000000000000000	F	F	F	7.9479099442599112	4.621138057543855	7.0072694482258822	T	T	T
14.6403135570449727	3.84208585969002354	0.0000000000000000	F	F	F	10.5948804628609997	4.6085736270991058	6.9769717587451305	T	T	T
17.3821887492350288	3.84208585969002354	0.0000000000000000	F	F	F	15.9266953695694954	4.62798844126216198	6.9777345432631295	T	T	T
21.2950615375199264	6.1473374350403116	0.0000000000000000	F	F	F	18.60029957296269693	6.1431719479175273	6.9681619922014811	T	T	T
5.32375038437998077	6.1473374350403116	0.0000000000000000	F	F	F	3.976232795361209715	6.929753943614165	7.0428220931209715	T	T	T
7.9856255765700377	6.1473374350403116	0.0000000000000000	F	F	F	6.6484959820160735	6.9280362299144615	6.98113461418346139	T	T	T
10.6475007687596140	6.1473374350403116	0.0000000000000000	F	F	F	9.3118112897481793	6.9226984635296821	7.040222145661417	T	T	T
13.389375960949536	6.1473374350403116	0.0000000000000000	F	F	F	11.9703996395626291	6.9315102847842027	7.1002361350486815	T	T	T
15.971215131394939	6.1473374350403116	0.0000000000000000	F	F	F	14.15483126580131	6.9664310282613981	6.8687704042961556	T	T	T
19.9640639414250209	6.1473374350403116	0.0000000000000000	F	F	F	17.32221070519903420	6.926479973898696	7.0245548793529850	T	T	T
21.2950615375199264	6.1473374350403116	0.0000000000000000	F	F	F	21.29715531752348427	7.00309436012198956	7.0201509222138761	T	T	T
5.32375038437998077	6.1473374350403116	0.0000000000000000	F	F	F	5.3178942184654723	6.9231786780613792	7.0394818961965075	T	T	T
7.9856255765700386	6.1473374350403116	0.0000000000000000	F	F	F	7.979508666552859	7.0218238554662981	7.0203012660729822	T	T	T
10.6475007687596120	6.1473374350403116	0.0000000000000000	F	F	F	10.6311812897481793	6.9226984635262285	7.033707819922649	T	T	T
13.389375960949536	6.1473374350403116	0.0000000000000000	F	F	F	13.2971165596058047	7.0228978664821349	7.0169999118332828	T	T	T
15.971215131394939	6.1473374350403116	0.0000000000000000	F	F	F	15.972415207618328	6.9235869229563379	7.0129834646210183	T	T	T
19.9640639414250209	6.1473374350403116	0.0000000000000000	F	F	F	18.633270876211166	7.0231780365633756	7.01269494169608167	T	T	T
21.2950615375199264	6.1473374350403116	0.0000000000000000	F	F	F	21.29715531752348427	7.00309436012198956	7.01949436012198956	T	T	T
5.32375038437998077	6.1473374350403116	0.0000000000000000	F	F	F	7.012270519903420	6.92617500081933931	6.92265493938476252	T	T	T
7.9856255765700386	6.1473374350403116	0.0000000000000000	F	F	F	8.285897440148937	6.3067538469611239	18.0520929121477618	T	T	T
13.389375960949536	6.1473374350403116	0.0000000000000000	F	F	F	9.6060349846156532	6.7651562946152285	10.0619189386316013	T	T	T
15.971215131394939	6.1473374350403116	0.0000000000000000	F	F	F	10.6737422989742541	5.8344947296847628	9.7395363401846952	T	T	T
18.6331263453299378	6.1473374350403116	0.0000000000000000	F	F	F	10.3791165596058047	4.5469640473347676	9.730365562174146393	T	T	T
21.2950615375199264	6.1473374350403116	0.0000000000000000	F	F	F	9.055232418057778	4.0169247972640019	9.72738574484571	T	T	T
5.32375038437998077	6.1473374350403116	0.0000000000000000	F	F	F	10.735722600244966	5.86151214023489681	9.1603210760895308	T	T	T
7.9856255765700386	6.1473374350403116	0.0000000000000000	F	F	F	12.047328753847776161	6.3320983791623606	9.2654539938476252	T	T	T
10.6475007687596120	6.1473374350403116	0.0000000000000000	F	F	F	6.8815113235453547	7.0479430227791775	12.93601508232818458	T	T	T
13.389375960949536	6.1473374350403116	0.0000000000000000	F	F	F	8.2491759790899825	7.0468149988513200	13.1947500624492253	T	T	T
15.971215131394939	6.1473374350403116	0.0000000000000000	F	F	F	9.010643053251160500	6.29605255136456817	10.4313262797442210	T	T	T
19.9640639414250209	6.1473374350403116	0.0000000000000000	F	F	F	8.317188447238393	5.0621975194942506	13.39887805780210810	T	T	T
21.2950615375199264	6.1473374350403116	0.0000000000000000	F	F	F	6.94924401738816593	5.0504117388165931	13.1380061603551912	T	T	T
5.32375038437998077	6.1473374350403116	0.0000000000000000	F	F	F	6.2198844748655855	6.174691510051993391	9.16025289759215962	T	T	T
7.9856255765700386	6.1473374350403116	0.0000000000000000	F	F	F	11.6448931744200174422	6.4277849785164322	13.8986598173505431	T	T	T
10.6475007687596120	6.1473374350403116	0.0000000000000000	F	F	F	8.7753670231838208	8.4329257048149374	12.0311280521388558	T	T	T
13.389375960949536	6.1473374350403116	0.0000000000000000	F	F	F	8.877536702318374956	4.140965004434964	13.563119561138167	T	T	T
15.971215131394939	6.1473374350403116	0.0000000000000000	F	F	F	6.44778876128555808	4.034282651927967	13.1049725250513255	T	T	T
19.9640639414250209	6.1473374350403116	0.0000000000000000	F	F	F	5.15146726118276402704	6.396214083779526120	10.43267149613830	T	T	T
21.2950615375199264	6.1473374350403116	0.0000000000000000	F	F	F	14.022682753776161	6.39634803791373796	9.32875841664746473	T	T	T
5.32375038437998077	6.1473374350403116	0.0000000000000000	F	F	F	6.326796493848280828	8.3291970321838558	12.747625809768849	T	T	T
7.9856255765700386	6.1473374350403116	0.0000000000000000	F	F	F	8.77536702318374956	8.4329257048149374	12.03520998504017518	T	T	T
10.64750076875961											

9.7852655765699711	10.7578405113205449	0.0000000000000000	F	F	13.3734476374438020	4.3315198473170726	7.0864820571485735	T	T	T
10.647508768760288	10.7578405113205449	0.0000000000000000	F	F	9.8163044186389641	5.5301972460084849	11.0879816377184011	T	T	T
13.30975690499563	10.7578405113205449	0.0000000000000000	F	F	10.799781476981120	10.1321997467827794	T	T	T	
15.9712511531400895	10.7578405113205449	0.0000000000000000	F	F	11.73927097462461	1.1593981775784116	9.570619182158699	T	T	T
16.8332163543229934	10.7578405113205449	0.0000000000000000	F	F	11.6914160922767802	7.359843276280243	9.9465937193539211	T	T	T
21.2950015375199939	10.7578405113205449	0.0000000000000000	F	F	10.7306139785905658	3.2950164381053426	10.846496269311978	T	T	T
0.0000000000000000	0.0000000000000000	2.38638108513199650	F	F	9.78034559966832	4.171214699132033	11.3669403815310384	T	T	T
2.6618751921900570	0.0000000000000000	2.38638108513199650	F	F	13.34002984635876598	6.78473946103211536	4.2557103526815804	T	T	T
5.3237508437799816	0.0000000000000000	2.38638108513199650	F	F	12.704839430399021795	5.5577708077051256	8.5484838322350541	T	T	T
7.98526557567500386	0.0000000000000000	2.38638108513199650	F	F	9.069494302194303	6.2199475675972123	11.4038928303958578	T	T	T
16.6475087687599632	0.0000000000000000	2.38638108513199650	F	F	12.7958446277707486	7.0488431015017978	9.8331181091417439	T	T	T
13.3097596095086211	0.0000000000000000	2.38638108513199650	F	F	12.427145368680085	0.0686184585296227	9.5294761841694347	T	T	T
15.9712511531399439	0.0000000000000000	2.38638108513199650	F	F	10.71462523719376	2.2402480696284168	11.126424873972982	T	T	T
1.33093759609805183	2.3052515381401570	2.38638108513199650	F	F	9.099283044983798	8.19158020374623	12.046548296285311	T	T	T
3.9921872888280572	2.3052515381401570	2.38638108513199650	F	F	13.199722843936093	7.497454256586149	9.3599874262728449	T	T	T
## POSCAR for TS13-14 ##	Zn C H	1.0000000000000000								
140	8 6	Selective dynamics								
Cartesian										
1.6331263453299343	1.5368343587600748	0.0000000000000000	F	F						
2.6618751921989980	1.5368343587600748	0.0000000000000000	F	F						
5.323750843800447	1.5368343587600748	0.0000000000000000	F	F						
7.9852655756697711	1.5368343587600748	0.0000000000000000	F	F						
10.6475087687608272	1.5368343587600748	0.0000000000000000	F	F						
14.60313575044979	1.5368343587600748	0.0000000000000000	F	F						
17.302188749234613	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531400807	1.5368343587600748	0.0000000000000000	F	F						
16.480313575044927	1.5368343587600748	0.0000000000000000	F	F						
17.302188749234613	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531399439	1.5368343587600748	0.0000000000000000	F	F						
16.615803762802333	1.5368343587600748	0.0000000000000000	F	F						
5.3237508438004477	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531400807	1.5368343587600748	0.0000000000000000	F	F						
16.480313575044927	1.5368343587600748	0.0000000000000000	F	F						
17.302188749234613	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531399439	1.5368343587600748	0.0000000000000000	F	F						
16.615803762802333	1.5368343587600748	0.0000000000000000	F	F						
5.3237508438004477	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531400807	1.5368343587600748	0.0000000000000000	F	F						
16.480313575044927	1.5368343587600748	0.0000000000000000	F	F						
17.302188749234613	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531399439	1.5368343587600748	0.0000000000000000	F	F						
16.615803762802333	1.5368343587600748	0.0000000000000000	F	F						
5.3237508438004477	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531400807	1.5368343587600748	0.0000000000000000	F	F						
16.480313575044927	1.5368343587600748	0.0000000000000000	F	F						
17.302188749234613	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531399439	1.5368343587600748	0.0000000000000000	F	F						
16.615803762802333	1.5368343587600748	0.0000000000000000	F	F						
5.3237508438004477	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531400807	1.5368343587600748	0.0000000000000000	F	F						
16.480313575044927	1.5368343587600748	0.0000000000000000	F	F						
17.302188749234613	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531399439	1.5368343587600748	0.0000000000000000	F	F						
16.615803762802333	1.5368343587600748	0.0000000000000000	F	F						
5.3237508438004477	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531400807	1.5368343587600748	0.0000000000000000	F	F						
16.480313575044927	1.5368343587600748	0.0000000000000000	F	F						
17.302188749234613	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531399439	1.5368343587600748	0.0000000000000000	F	F						
16.615803762802333	1.5368343587600748	0.0000000000000000	F	F						
5.3237508438004477	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531400807	1.5368343587600748	0.0000000000000000	F	F						
16.480313575044927	1.5368343587600748	0.0000000000000000	F	F						
17.302188749234613	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531399439	1.5368343587600748	0.0000000000000000	F	F						
16.615803762802333	1.5368343587600748	0.0000000000000000	F	F						
5.3237508438004477	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531400807	1.5368343587600748	0.0000000000000000	F	F						
16.480313575044927	1.5368343587600748	0.0000000000000000	F	F						
17.302188749234613	1.5368343587600748	0.0000000000000000	F	F						
1.6564879847799999	1.5368343587600748	0.0000000000000000	F	F						
1.3093759609499518	1.5368343587600748	0.0000000000000000	F	F						
15.9712511531399439	1.5368343587600748	0.0000000000000000	F	F						
16.615803762802333	1.5368343587600748	0.0000000000000000	F	F						
5.3237508438004477	1.5368343587600748	0.0000000000000000	F</							

7.98634477820330729	6.1471760151348809	4.6711341102509820	T T T	18.6331263453299373	10.7578405113205449	0.0000000000000000	F F F
10.642140885146544	6.1384190630541573	4.6401256586144664	T T T	21.2950015375199939	10.7578405113205449	0.0000000000000000	F F F
13.3313980666215200	6.1541625480000812	4.6964365775647750	T T T	0.0000000000000000	0.0000000000000000	2.3863810053199650	F F F
15.9959369161198422	6.1437699276945272	4.6429834971824082	T T T	2.6618751921908570	0.0000000000000000	2.3863810053199650	F F F
18.65621291512183083	6.13660262480671652	4.6607886215330119	T T T	5.3237503843799816	0.0000000000000000	2.3863810053199650	F F F
22.6501942851034279	8.4533580221618720	4.6517883811194949	T T T	7.9856255765700836	0.0000000000000000	2.3863810053199650	F F F
6.6622064741667737	8.4539943808781714	4.6640123576729557	T T T	10.6475007687599632	0.0000000000000000	2.3863810053199650	F F F
9.3157993879131737	8.4613888462642315	4.6453556056931822	T T T	13.3093759609500211	0.0000000000000000	2.3863810053199650	F F F
12.0164477052552066	8.4860816802209824	4.7756532680484627	T T T	15.97125115131399439	0.0000000000000000	2.3863810053199650	F F F
14.61422391826006	8.460586283818661	4.8373474331256165	T T T	1.309375960950185	2.3052515381401570	2.3863810053199650	F F F
17.3316686949874459	8.4395978051955147	4.621732269299768	T T T	3.9928127882850752	2.3052515381401570	2.3863810053199650	F F F
19.993029591426139	8.453629850052116	4.6362702338152546	T T T	6.6546879847499999	2.3052515381401570	2.3863810053199650	F F F
23.9776819537971314	10.7479437755164508	4.6734469274501182	T T T	9.316531726656597	2.3052515381401570	2.3863810053199650	F F F
8.0068683816790391	10.7481538827101666	4.6648286557872254	T T T	11.9784328456849823	2.3052515381401570	2.3863810053199650	F F F
16.665919972242227	14.595972321129229	4.6596794141873046	T T T	14.64003135570548042	2.3052515381401570	2.3863810053199650	F F F
13.327554806927927	10.7535061958001226	4.709966159041875941	T T T	17.3021887492349613	2.3052515381401570	2.3863810053199650	F F F
15.9775745988275031	8.47982257063622	4.6598455368497476	T T T	2.6618751921899994	4.6105030762820233	2.3863810053199650	F F F
18.6365677988910861	10.7486376164186073	4.6657479457687838	T T T	5.3237503843800473	4.6105030762820233	2.3863810053199650	F F F
21.3088540167037307	10.751368489752877	4.668233138283509	T T T	7.985625576569970	4.6105030762820233	2.3863810053199650	F F F
6.6634636837855211	11.50224233994573	4.9765158615129428	T T T	10.6475007687608289	4.6105030762820233	2.3863810053199650	F F F
2.6520624249806724	0.0137653785780955	6.9674516084905955	T T T	13.309375960949955	4.6105030762820233	2.3863810053199650	F F F
5.2994009262688540	0.015936976280244	6.9560102521160240	T T T	15.97125115131040114	4.6105030762820233	2.3863810053199650	F F F
8.0089128454820511	0.0107849662515414	7.0295581744719324	T T T	18.6331254352939343	4.6105030762820233	2.3863810053199650	F F F
10.6445674127657413	-0.028651325262175	7.032581174347841	T T T	3.9928127882850095	4.6157546144203916	2.3863810053199650	F F F
19.9745158722461262	11.483836456052480	6.957786230299882	T T T	6.6546879847499999	4.6157546144203916	2.3863810053199650	F F F
22.646634071387351	11.473981635301568	6.966777756662640	T T T	9.316531726649920	4.6157546144203916	2.3863810053199650	F F F
1.3651950173648351	2.2954435137381206	7.0132414303563113	T T T	11.9784383648550481	4.6157546144203916	2.3863810053199650	F F F
4.0022885219578355	2.3196769716574184	7.0397398421100474	T T T	14.648313557049479	4.6157546144203916	2.3863810053199650	F F F
6.648953098758982	2.3058089584825944	6.9710537966997318	T T T	17.302187492356288	4.6157546144203916	2.3863810053199650	F F F
9.30427970579666666	2.2806994939579557	7.029739995843044	T T T	19.964063941424953	4.6157546144203916	2.3863810053199650	F F F
11.930320794227872	2.215121863263841	6.9608515893615989	T T T	5.3237503843799807	4.6110061525604665	2.3863810053199650	F F F
14.712054385975957	2.1819026136763297	7.050017683736310	T T T	7.9856255765700872	4.6110061525604665	2.3863810053199650	F F F
17.3620132308049119	2.2743612083355431	7.05472138017517839	T T T	10.6475007687599614	4.6110061525604665	2.3863810053199650	F F F
2.6788822052697872	4.6545841815348482	7.047061257875349	T T T	13.3093759609500193	4.6110061525604665	2.3863810053199650	F F F
5.310674062416161	4.6114170733080268	7.059380202573625	T T T	15.97125115131399439	4.6110061525604665	2.3863810053199650	F F F
7.9366813430033076	4.5967041650327589	7.0071439327709557	T T T	18.6331263453300018	4.6110061525604665	2.3863810053199650	F F F
18.5543242048950444	4.573078375408309	6.912193964281812	T T T	21.295001752604665	4.6110061525604665	2.3863810053199650	F F F
16.0765310236758758	5.3489585858591388	6.9167565604761043	T T T	18.634638126555074	4.6157546144203916	2.3863810053199650	F F F
18.6914840613169495	4.571484990781674	6.9490482896328892	T T T	2.6747895849837068	4.61578087127888260	2.3863810053199650	F F F
3.9993965563343548	6.9126646999902128	7.0547897673548421	T T T	5.332276457949217	4.615287349871344	2.3863810053199650	F F F
6.638292416819602	6.91799835321812	7.024460088070734	T T T	7.98725465112562902	4.615287349871344	2.3863810053199650	F F F
9.2400895654576960	6.915969749833925	7.0595792073397595	T T T	10.64461014574972574	4.61534217744749263	2.3863810053199650	F F F
11.766674714488624088	9.9841025251765889	6.896911920669926	T T T	13.3242674415747074	4.5921609948408158	2.3863810053199650	F F F
14.92103366068068757	9.900154049398432	7.01187478700879	T T T	15.98865779623804866	4.516256730845375	2.3863810053199650	F F F
17.41938578415919687	6.9014188076131502	6.96500561526493882	T T T	19.9973149246719248	4.385979128928292	2.3863810053199650	F F F
20.0879951164605299	6.987602334574883	6.964191842791412	T T T	4.002658848126555074	4.38640353255966686	2.3863810053199650	F F F
5.3332746999479491	6.2895472033322991	7.0574996713519336	T T T	6.65305978055494290	4.3865467913441684	2.3863810053199650	F F F
7.979378179148214	9.2055958220526088	11.1060059518721450	T T T	9.2755750387508041	4.3859226457949217	2.3863810053199650	F F F
10.5798861018736527	2.6567573204660611	6.9956415126255376	T T T	11.974385803760952	4.38597664396973781	2.3863810053199650	F F F
13.2527557656975077	3.978205695069787	7.42007371217721	T T T	14.6771772775953	4.6494247377576263	2.3863810053199650	F F F
16.0132264588435120	9.2429088169706388	6.9810105405140349	T T T	17.34143431130834929	4.385773588921538	2.3863810053199650	F F F
18.6637759084797097	2.1198859375408369	6.9488615264951764	T T T	21.3157909133288049	4.6062796311355683	2.3863810053199650	F F F
21.3298837348033866	9.2007554368074012	6.9982727212912462	T T T	5.3275727146737928	4.61445951711564665	2.3863810053199650	F F F
13.3854740792422293	4.3264346070063899	7.0895970147671246	T T T	7.97874008434334116	4.616210427829361	2.3863810053199650	F F F
9.71561327024162587	5.49026360824058	11.1060059518721450	T T T	10.6361412601686934	4.614467260112460925	2.3863810053199650	F F F
18.7355465813232093	5.9819281591720994	18.279350001535153	T T T	13.32509418033619368	4.617889379213058689	2.3863810053199650	F F F
11.7736651720985170996	5.0888459159343277	9.7887588198704067	T T T	15.9567339538455455	4.61744088712469458	2.3863810053199650	F F F
11.780805653310916	7.33623258320575	18.1396704826714394	T T T	18.647028692363672	4.6142212402303451	2.3863810053199650	F F F
16.69917612857423874	3.250641582386703576	14.9916678346732053	T T T	22.673579582375670	4.6149948872433778	2.3863810053199650	F F F
19.696109080650184	12.7450120000000000	24.545524021280021	T T T	5.3088753890801660	4.6000278087624478	2.3863810053199650	F F F
140 8 6	Selective dynamics			5.3088753890801660	4.6000278087624478	2.3863810053199650	T T T
15.9712511513199439	1.5368343587600781	0.0000000000000000	F F F	7.9925547524424234	4.60337730940099292	2.3863810053199650	T T T
18.6331263453299373	1.5368343587600781	0.0000000000000000	F F F	10.66105982926544570	4.603396082262829	2.3863810053199650	T T T
2.6618751921899999	1.5368343587600781	0.0000000000000000	F F F	12.68499214520954	4.6033906233792688	2.3863810053199650	T T T
21.295001537519264	6.14737347350403116	0.0000000000000000	F F F	2.6657282275124787	4.6032729022644687	2.3863810053199650	T T T
5.3237503843800473	1.5368343587600781	0.0000000000000000	F F F	5.3088753890801660	4.6018867676987508	2.3863810053199650	T T T
3.9922812758809953	1.5368343587600781	0.0000000000000000	F F F	7.20233928723548779	4.60175576024482734	2.3863810053199650	T T T
19.964063941245954	3.8420858969002354	0.0000000000000000	F F F	2.900287123559294	4.6017499877697212	2.3863810053199650	T T T
6.6546879804750856	3.8420858969002354	0.0000000000000000	F F F	6.9714420873556484736	4.72335408710201878	2.3863810053199650	T T T
9.3165631726499400	3.8420858969002354	0.0000000000000000	F F F	5.3370956317565420462	4.6123751968474773	2.3863810053199650	T T T
11.9784383645845984	3.8420858969002354	0.0000000000000000	F F F	7.95			

11.5380159416923718	3.706189759336813	10.1139509112325641	T	T	T		18.6408728288012746	6.1610868066248656	4.6616949997236983	T	T	T	
10.3965729875256514	3.0539088885849535	10.5751495908909323	T	T	T		22.6227474207696666	8.4636939186710727	4.6673972746889385	T	T	T	
9.2267123421976087	3.7729029419366564	18.8076686016669168	T	T	T		6.6582529296801782	8.4722989714273123	4.6537295480841916	T	T	T	
13.4145232608852556	6.2322724789665251	8.4203172947859812	T	T	T		9.3299309234362493	8.4815447611943231	4.6623367438518677	T	T	T	
12.5780171482080796	5.7305385451507698	9.2055247550842942	T	T	T		11.9868374623938264	8.4289978403152171	4.7746443424628104	T	T	T	
8.2689189091037098	5.7166829706223895	10.7694714714307302	T	T	T		14.6473374996781917	8.4384640642029564	4.68502615225299	T	T	T	
10.297995762693070	6.8958414860108963	9.95285283959660588	T	T	T		17.3084277497456569	8.4733769745257819	4.630904676101196	T	T	T	
12.4527430049563363	3.1489958513600765	9.90896097183780575	T	T	T		19.9676105528479830	8.4606522496166927	4.6684374082074234	T	T	T	
10.4218553915003548	1.9751513009369292	10.734174836596855	T	T	T		23.9655038255750483	10.778049981021248	4.6691889489295191	T	T	T	
8.3240865342638877	3.2537760622948730	11.1448137197732571	T	T	T		7.9849263055364954	10.7875041876596853	4.6529055741475647	T	T	T	
14.6397564617258844	8.6214465651531160	7.5826259567848338	T	T	T		10.6526531374141928	10.8076443989767554	4.6135726863893813	T	T	T	
## POSCAR for TS15 ##													
Zn C H							13.2945500427016668	10.78789572357196166	4.6543138200742868	T	T	T	
1.0000000000000000	18.6331263453299982	0.0000000000000000	0.0000000000000000	F	F	F		15.9648803231190391	10.7864962998401408	4.6692388041268664	T	T	T
6.654687984749999	11.5262576987006800	0.0000000000000000	0.0000000000000000	F	F	F		18.6457872357196166	10.7677589399244046	4.6809951851323657	T	T	T
0.0000000000000000	0.0000000000000000	24.5455240212779985	F	F	F		21.3091562005681299	10.7639191781413414	4.678006539526282	T	T	T	
140 16 12	Selective dynamics						18.614687406748324	0.041558596845418	6.9570229815031368	T	T	T	
Cartesian							2.620386974853993	0.0685403183659993	6.9659681872984800	T	T	T	
18.6312363453299983	1.5368343587600748	0.0000000000000000	F	F	F		5.3237994262884634	0.0874765306057367	6.9737448815699423	T	T	T	
2.6618751921899890	1.5368343587600748	0.0000000000000000	F	F	F		7.9715799662696835	0.0845659864555983	7.0196762228405063	T	T	T	
5.323750384380047	1.5368343587600748	0.0000000000000000	F	F	F		10.6633765642376376	0.0181030352021917	7.025807572272611	T	T	T	
7.9856257565699711	1.5368343587600748	0.0000000000000000	F	F	F		19.9915056401399891	11.5162307182006224	6.9808574652859878	T	T	T	
10.6475007687608288	1.5368343587600748	0.0000000000000000	F	F	F		22.6401752776736702	11.5247593335617339	6.964737390325436	T	T	T	
15.9712515131400079	1.5368343587600748	0.0000000000000000	F	F	F		19.9495869980816569	2.3417296595729367	7.01235935455371721	T	T	T	
19.5646879847499424	3.84280858969002305	0.0000000000000000	F	F	F		17.3264804119362132	3.203586691008369	7.0365316316589187	T	T	T	
6.654687980475003548	3.84280858969002305	0.0000000000000000	F	F	F		21.278694131200061	4.630667440126884	7.0449931351240081	T	T	T	
9.3165317266549867	3.84280858969002305	0.0000000000000000	F	F	F		5.2886573264542485	6.316923318679963	7.0193968198465972	T	T	T	
11.9784387932645508017	3.84280858969002305	0.0000000000000000	F	F	F		7.784879372277816428	4.5948468847437571	6.916961688716476	T	T	T	
14.64903135570449709	3.84280858969002305	0.0000000000000000	F	F	F		10.5958866053089385	4.4138249657498993	6.9654516717751767	T	T	T	
17.30218874923501828	3.84280858969002305	0.0000000000000000	F	F	F		13.3232906124040171	4.450889413007919	6.79420286658672	T	T	T	
21.2950815375199887	6.1473374350420292	0.0000000000000000	F	F	F		16.0487466659326437	6.5466697805446676	6.8897272987564219	T	T	T	
5.3237503843799763	6.1473374350420292	0.0000000000000000	F	F	F		18.648049198982736	4.6216544473965593	7.0230444929372986	T	T	T	
7.9856257567080288	6.1473374350420292	0.0000000000000000	F	F	F		22.6046155263093948	6.91472847574887788	6.999905712078612	T	T	T	
10.6475007687602072	6.1473374350420292	0.0000000000000000	F	F	F		6.579973571936223	6.946717181987274	6.9567846677201230	T	T	T	
13.3093759660580175	6.1473374350420292	0.0000000000000000	F	F	F		9.163633054265767	7.0289985426576349	6.89548245556550642	T	T	T	
15.9712515131399421	6.1473374350420292	0.0000000000000000	F	F	F		12.0336142623506218	7.0458450441395453	7.5316717842945113	T	T	T	
18.6312363453299982	6.1473374350420292	0.0000000000000000	F	F	F		14.8278429916155995	7.1291268082055597	7.2368290565999525	T	T	T	
21.25959313613419420	6.1473374350420292	0.0000000000000000	F	F	F		17.382170249408293	6.9484241110663695	6.9193183705306485	T	T	T	
6.6546879804749941	8.4525889731840548	0.0000000000000000	F	F	F		19.97814564401132201	6.9248253639162808	7.0278027576485567	T	T	T	
5.3237503843799763	8.4525889731840548	0.0000000000000000	F	F	F		18.648049198982736	4.6216544473965593	7.0230444929372986	T	T	T	
7.9856257567080288	8.4525889731840548	0.0000000000000000	F	F	F		21.278694131200061	4.630667440126884	7.0449931351240081	T	T	T	
10.6475007687602072	8.4525889731840548	0.0000000000000000	F	F	F		6.579973571936223	6.946717181987274	6.9567846677201230	T	T	T	
13.3093759660580175	8.4525889731840548	0.0000000000000000	F	F	F		10.593717002020174	9.4186754797141425	6.8758677225988043	T	T	T	
17.30218874923501828	8.4525889731840548	0.0000000000000000	F	F	F		13.37583434997158897	10.801873498372126	6.9173597174720038	T	T	T	
19.5646879804749942	8.4525889731840548	0.0000000000000000	F	F	F		16.0354239970365007	9.3289159007365007	6.9776924641089944	T	T	T	
23.95876779799711	10.757840511320523	0.0000000000000000	F	F	F		18.65471257215165171	9.2413977036308008	7.02234383859870351	T	T	T	
7.9856257567080288	10.757840511320523	0.0000000000000000	F	F	F		21.296294446050175	9.298671204011200	7.0253463374233407	T	T	T	
10.6475007687602072	10.757840511320523	0.0000000000000000	F	F	F		7.2893947918198121	4.4124103292935166	10.5791767257953992	T	T	T	
13.3093759660580175	10.757840511320523	0.0000000000000000	F	F	F		8.2440413149722007	5.2288132506087600	6.9588236355807970	T	T	T	
15.9712515131399421	10.757840511320523	0.0000000000000000	F	F	F		9.54028704915883	4.748526545495649	6.68907588959565207	T	T	T	
18.6312363453299982	10.757840511320523	0.0000000000000000	F	F	F		9.8630350805523861	3.436564352242727	10.071052741105272	T	T	T	
21.2595081537519985	10.757840511320523	0.0000000000000000	F	F	F		8.92147982075735736	2.62363340446058458	10.7380765326457386	T	T	T	
0.0000000000000000	10.757840511320523	0.0000000000000000	F	F	F		7.6230072481922900	1.13633647213168127	10.96234324685363365	T	T	T	
2.6618751921899895	10.757840511320523	0.0000000000000000	F	F	F		10.36713671367188560	6.8900320865007600	8.5984139500198751	T	T	T	
5.3237503843800456	10.757840511320523	0.0000000000000000	F	F	F		13.79617369248171989	7.2962622266508533	10.910444721147400	T	T	T	
7.9856257567080288	10.757840511320523	0.0000000000000000	F	F	F		15.9492869845380790	5.19225919388652	10.94711644961684	T	T	T	
10.6475007687602072	10.757840511320523	0.0000000000000000	F	F	F		6.27776807180879	3.333513394995054	6.8427701594761684	T	T	T	
13.3093759660580175	10.757840511320523	0.0000000000000000	F	F	F		7.97120588403540367	5.6377628920933649	10.671155140146365	T	T	T	
17.30218874923501828	10.757840511320523	0.0000000000000000	F	F	F		10.8636184263529948	3.049237093762085	9.8861193391794499	T	T	T	
19.5646879804749942	10.757840511320523	0.0000000000000000	F	F	F		9.18757842316823145	1.613659129184468253	10.6375143676884253	T	T	T	
5.3237503843800456	10.757840511320523	0.0000000000000000	F	F	F		6.8755371624299045	2.4678962759896814	11.423923245460688	T	T	T	
7.9856257567080288	10.757840511320523	0.0000000000000000	F	F	F		9.9463627896748478	5.7386327967484784	9.3317662138746478	T	T	T	
10.6475007687602072	10.757840511320523	0.0000000000000000	F	F	F		15.69916894538051989	7.5783632791880852	10.9417786				

13.3093759609500157	9.2210061525604505	2.3863810053199646	F	F	F		Cartesian	18.6331299999999800	1.5368299999999688	0.000000000000000	F	F	F
15.9712511531399404	9.2210061525604505	2.3863810053199646	F	F	F			2.6618800000000453	1.5368299999999688	0.000000000000000	F	F	F
18.631263453299982	9.2210061525604505	2.3863810053199646	F	F	F			5.3237499999999462	1.5368299999999688	0.000000000000000	F	F	F
21.2950815375199087	9.2210061525604505	2.3863810053199646	F	F	F			7.9856299999999747	1.5368299999999688	0.000000000000000	F	F	F
18.6321254492534401	1.5555566860014243	4.6706108010157079	T	T	T			10.647500000000115	1.5368299999999688	0.000000000000000	F	F	F
2.64582200000545265	1.555003686221463	4.6550584322809616	T	T	T			13.3093800000000435	1.5368299999999688	0.000000000000000	F	F	F
5.2924326973184606	5.405760449599251	4.6403809373420497	T	T	T			15.9712499999999373	1.5368299999999688	0.000000000000000	F	F	F
8.0111393086660918	1.5545902445905238	4.7434229113281612	T	T	T			19.9640600000000106	3.8420900000000340	0.000000000000000	F	F	F
10.6403880216706384	1.5506582066915689	4.7284117072318255	T	T	T			3.9281000000000812	3.8420900000000340	0.000000000000000	F	F	F
13.31593858898767398	1.540748163857124	4.6626114987481781	T	T	T			6.6546899999999800	3.8420900000000340	0.000000000000000	F	F	F
15.9847024770374464	1.5446946502980547	4.66630157678376799	T	T	T			9.3156600000000151	3.8420900000000340	0.000000000000000	F	F	F
19.96266260010176785	3.8471299413995878	4.6698257112523502	T	T	T			11.9784400000000453	3.8420900000000340	0.000000000000000	F	F	F
3.9994112074178699	3.8400861306389784	4.6781295581584956	T	T	T			14.6043100000000340	3.8420900000000340	0.000000000000000	F	F	F
6.6613289518417318	3.837009638449599251	4.6636932336493127	T	T	T			17.3021899999999782	3.8420900000000340	0.000000000000000	F	F	F
5.2924326973184606	5.405760449599251	4.6403809373420497	T	T	T			21.2949999999999803	6.147339999999971	0.000000000000000	F	F	F
11.9916234876554747	3.84839332390937	4.626132034323128	T	T	T			5.2327500000000564	6.147339999999971	0.000000000000000	F	F	F
14.6499763622330023	3.846568223428424	4.64630085659913001	T	T	T			7.9856299999999587	6.147339999999971	0.000000000000000	F	F	F
17.3045075758056548	3.8518559129454744	4.6711937064190012	T	T	T			10.6474999999999971	6.147339999999971	0.000000000000000	F	F	F
21.299261341404018735	6.1479792617129124	4.6578116063677588	T	T	T			13.3093800000000222	6.147339999999971	0.000000000000000	F	F	F
5.3217042127106406	6.1489237982373755	4.6675906677686765	T	T	T			15.9712500000000216	6.147339999999971	0.000000000000000	F	F	F
7.99906938449599251	6.1567142017023073	4.661423715752392	T	T	T			18.6331299999999480	6.147339999999971	0.000000000000000	F	F	F
16.671801340674807	6.1717129501443775	4.7432767891310181	T	T	T			22.6593999999999587	8.4525900000000416	0.000000000000000	F	F	F
13.31191352196404	6.147412735110281	4.7150874866842476	T	T	T			6.6546900000000839	8.4525900000000416	0.000000000000000	F	F	F
15.9994179472248753	6.1488089085969344	4.6471921699893928	T	T	T			9.3155999999999844	8.4525900000000416	0.000000000000000	F	F	F
18.64341365758056548	6.145315759979593	4.6680087113101878	T	T	T			11.9784400000000133	8.4525900000000416	0.000000000000000	F	F	F
22.6346461342119660	6.4542996540146290	4.6594412957479404	T	T	T			14.6483100000000492	8.4525900000000416	0.000000000000000	F	F	F
6.6664344683314658	8.4637703376570652	4.6667010187694640	T	T	T			17.3021900000000812	8.4525900000000416	0.000000000000000	F	F	F
9.3311031844059151	8.482535557197387	4.6486656951362382	T	T	T			19.9645999999999644	8.4525900000000416	0.000000000000000	F	F	F
11.9799097691878731	6.4587988376752312	4.6998922353589669	T	T	T			23.9568779999999957	10.7578400000000852	0.000000000000000	F	F	F
14.639793478875565474	6.4948826203224978	4.6676208467060669	T	T	T			0.000000000000000	0.000000000000000	2.3863800000000821	F	F	F
17.3019162130736426	6.4437703464161995	4.668888124203322	T	T	T			7.985629999999971	10.7578400000000852	0.000000000000000	F	F	F
19.97331595982172112	6.489918257128115	4.6688995292866252	T	T	T			10.647499999999957	10.7578400000000852	0.000000000000000	F	F	F
22.6359846577672654	10.767868382937293	4.6682465130393990	T	T	T			13.3093799999999867	10.7578400000000852	0.000000000000000	F	F	F
7.977201817013101873	10.7802463101015588	4.6680072055038944	T	T	T			15.9712500000000261	10.7578400000000852	0.000000000000000	F	F	F
16.6430889089885383	10.7755361250427339	4.675349988698669	T	T	T			18.6331000000000510	10.7578400000000852	0.000000000000000	F	F	F
13.3117684541449837	10.7610976666713842	4.6695164141426542	T	T	T			21.2949999999999555	10.7578400000000852	0.000000000000000	F	F	F
15.9847292202334248	10.7555335053780734	4.63836629642963173	T	T	T			0.000000000000000	0.000000000000000	2.3863800000000821	F	F	F
18.642847414194696	10.7606120154732317	4.6680525581604043	T	T	T			2.6118800000000324	0.000000000000000	2.3863800000000821	F	F	F
21.3025900084665965	10.7617112906169197	4.6611256045746198	T	T	T			5.3237500000000064	0.000000000000000	2.3863800000000821	F	F	F
18.6168453251702102	0.0164283673303256	6.99972213195705278	T	T	T			7.9856299999999631	0.000000000000000	2.3863800000000821	F	F	F
2.6568138044297931	0.0179267732823280	6.9967608260545427	T	T	T			10.647499999999957	0.000000000000000	2.3863800000000821	F	F	F
11.97403599000545439	11.5170308153475691	6.999723802203519594	T	T	T			13.3093800000000222	0.000000000000000	2.3863800000000821	F	F	F
14.6359967150873615	11.4703650866856263	6.932550965536464146	T	T	T			15.97125000000000617	0.000000000000000	2.3863800000000821	F	F	F
17.335610514951063	12.42463883313259	6.96884484644676956	T	T	T			1.3093999999999754	2.3052949999999632	2.3863800000000821	F	F	F
13.32082624179171312	-0.0085333348474759	6.971963594633130181	T	T	T			3.9281000000000080	2.3052949999999632	2.3863800000000821	F	F	F
15.96371103417018735	-0.0018579899871895	7.0096241720280595	T	T	T			6.65469000000000404	2.3052949999999632	2.3863800000000821	F	F	F
19.9418349744700447	2.3082770263452135	7.0383891121858289	T	T	T			9.3165599999999387	2.3052949999999632	2.3863800000000821	F	F	F
3.961183479474404	2.308086108120393	7.02777069571234	T	T	T			11.9784400000000453	2.3052949999999632	2.3863800000000821	F	F	F
6.599331617468371	2.2883935003437958	6.9055317495462569	T	T	T			14.6483100000000066	2.3052949999999632	2.3863800000000821	F	F	F
9.4595137166004400	2.032883557166004400	7.451568201958118	T	T	T			17.3021900000000038	2.3052949999999632	2.3863800000000821	F	F	F
12.0140908570027598	2.2963842592630241	6.9491455178051940	T	T	T			2.6118800000000000	4.6105000000000089	2.3863800000000821	F	F	F
14.634842847424721	2.2872436331571497	6.942336314636462	T	T	T			5.3237500000000324	4.6105000000000089	2.3863800000000821	F	F	F
17.2884018743662971	2.30799589423731	7.025388089733946	T	T	T			7.9856300000000053	4.6105000000000089	2.3863800000000821	F	F	F
21.2696548144623740	6.1447441952370478	6.9865366016444135	T	T	T			10.647499999999957	4.6105000000000089	2.3863800000000821	F	F	F
5.2828851081238648	6.113130460406017	7.000051654264060	T	T	T			13.3093799999999593	4.6105000000000089	2.3863800000000821	F	F	F
7.8733745597777594	6.4681987018426888	6.941038171827991	T	T	T			15.97124999999994915	4.6105000000000089	2.3863800000000821	F	F	F
10.698590576593839	6.4244498682077506	6.89315199312384764	T	T	T			18.63310000000000439	4.6105000000000089	2.3863800000000821	F	F	F
13.351290168163853753	6.458863333133192	6.9811303656729801	T	T	T			23.956723453545928	6.9157499999999788	2.3863800000000821	F	F	F
15.97161406192003678	6.4020576593801251	6.995921453719797	T	T	T			6.6546900000000111	6.9157499999999788	2.3863800000000821	F	F	F
17.30823645174938012	6.4693877031711188	7.02121698113453546	T	T	T			2.65372947158323	6.9154624774499718	2.3863800000000821	F	F	F
15.9675219324242251	17.4755579322878	7.0121698113453546	T	T	T			5.315279451158220595	7.9918280000000413	2.38			

8.9511943391400788	1.9142062442975234	10.1473897817832253	T	T	T	17.3119739906613646	3.8531727694062639	4.6695638240248680	T	T	T
7.6026151882064461	1.57208424325265865	10.1602241341519157	T	T	T	21.2989133835628692	6.1537776519760854	4.6740428910049179	T	T	T
6.6195751360855262	2.5659027245389618	10.1162244262467063	T	T	T	5.3282478868660813	6.15405260804075695	4.6651893144523386	T	T	T
11.2956247459384613	4.6143559730087161	9.2348519649994181	T	T	T	8.0117494290163247	6.1714732038861655	4.698096572164125	T	T	T
10.7587369560299599	3.6055562774227181	9.9823819024359608	T	T	T	10.6483348546559924	6.1821477651942569	4.7430721138235503	T	T	T
14.6808472258508883	6.9901761576929471	11.7879229940871006	T	T	T	13.2928793831523890	6.1596710416029437	4.6983301982993411	T	T	T
13.2151834552760956	4.4454674405201118	9.8548225542215739	T	T	T	15.98313652553167065	6.15081012138262908	4.6597673892329650	T	T	T
11.7834054731648230	5.118871737797459	9.9365457285526013	T	T	T	18.6398642884259431	6.1543616047940946	4.6707474693689486	T	T	T
13.2128243067221351	10.9581135948131241	11.9255471176855625	T	T	T	22.6303997274209969	8.4571255490646645	4.6703116540920702	T	T	T
14.6712723668660736	9.172679197194537	12.8449818496943866	T	T	T	6.634605482169311	8.453953569427390	4.6655748542932973	T	T	T
10.7124667110874755	5.9527818596633875	9.0767618796237239	T	T	T	9.3165124682385372	8.4347514716786582	4.686369686159681	T	T	T
6.2380126358258585	4.6915571690894710	9.998017995593460	T	T	T	11.978291239468678	8.4331306791117129	4.6954321944019348	T	T	T
8.6367749823512625	5.3078584906878523	9.92256173753559787	T	T	T	14.6446815062470902	8.459672893581438	4.6456197597056663	T	T	T
9.7111475932374738	1.1311182378419817	10.1846256740418593	T	T	T	17.30379056280838556	8.48658454820754	4.6659559667628301	T	T	T
7.3167885597583355	2.1311802897589918	10.1817917821965693	T	T	T	19.9639122886294949	8.45834938411021498	4.6752041228846206	T	T	T
5.5644969324507788	2.2948652374328842	10.1402672795888145	T	T	T	23.963988237936102	10.76044472951673	4.66630385658463032	T	T	T
12.3821843759180208	4.748539786914141	9.3255258801677628	T	T	T	7.9921802791562643	10.757519288826399	4.6685288666899214	T	T	T
11.4407347603174792	2.9256330001019535	10.5115021978611676	T	T	T	10.6498361164508211	10.758684640792012	4.6787967354822815	T	T	T
## POSCAR for TS20 ##											
Zn C H											
1.0000000000000000											
18.6331263453299982	0.0000000000000000	0.0000000000000000	F	F	F	18.6330952376407346	10.762796976840845	4.6747160724941343	T	T	T
6.6546787980474999	11.5265267569700600	0.0000000000000000	F	F	F	21.297511136176443	6.7617070622923994	4.6687350843919330	T	T	T
0.0000000000000000	24.5455240212799985					25.2802449770878936	11.5213024346210875	6.9944376381724922	T	T	T
140 16 13						9.3040724456801751	11.5131608322615726	6.9949517676081620	T	T	T
Selective dynamics											
Cartesian											
18.6331263453299943	1.5368343587600748	0.0000000000000000	F	F	F	11.988627214293215	11.5134325046842539	7.0011467361843090	T	T	T
2.6618751912899898	1.5368343587600748	0.0000000000000000	F	F	F	19.994860446342884	11.5131929865265674	6.9804928410157032	T	T	T
5.3237503843800407	1.5368343587600748	0.0000000000000000	F	F	F	22.61737408937826	11.5300503642491129	6.9784526415686141	T	T	T
7.9856257565697971	1.5368343587600748	0.0000000000000000	F	F	F	3.979791765496559	2.301394148513162	7.01649243737262805	T	T	T
10.64750076876080272	1.5368343587600748	0.0000000000000000	F	F	F	6.6373237255806454	2.3055660399729212	7.0166061468998701	T	T	T
13.389375960949518	1.5368343587600748	0.0000000000000000	F	F	F	9.297026167254883	2.3119814521040110	7.029565411976862	T	T	T
15.9712511314007991	1.5368343587600748	0.0000000000000000	F	F	F	11.9619397131242746	2.3088738082692941	6.9895401285358831	T	T	T
19.9646639414249428	3.8420858969002305	0.0000000000000000	F	F	F	14.632803775242801	2.3061315341998951	6.9782039876876796	T	T	T
3.992812782841800	3.8420858969002305	0.0000000000000000	F	F	F	17.2924656452641408	2.3134162848550703	6.9953356435285050	T	T	T
6.6546879804750603	3.8420858969002305	0.0000000000000000	F	F	F	21.280466874045117	4.6153731406153344	7.0003811649859843	T	T	T
9.3165631726659872	3.8420858969002305	0.0000000000000000	F	F	F	5.301896226155045107	6.111109365779548	6.9807981384655557	T	T	T
11.9793759609508175	3.8420858969002305	0.0000000000000000	F	F	F	7.95957480822919216	6.1445320436252973	6.938320796516256	T	T	T
14.64931355704407909	3.8420858969002305	0.0000000000000000	F	F	F	10.630782898275618	6.110147793525122	6.9336468984812154	T	T	T
17.3028177492350174	3.8420858969002305	0.0000000000000000	F	F	F	13.303051646853322	4.95352229880626416	6.9340646908428196	T	T	T
21.2950015375190987	1.6473734530420292	0.0000000000000000	F	F	F	15.954615711267631	2.300128330524183	7.020529546082307	T	T	T
5.32375038437979807	1.6473734530420292	0.0000000000000000	F	F	F	18.216774836466321207	4.617071996728474808	6.999915644211206	T	T	T
7.9856257565700288	1.6473734530420292	0.0000000000000000	F	F	F	22.613242348658072	6.9147872452619871	6.9995833849022840	T	T	T
10.64750076876080272	1.6473734530420292	0.0000000000000000	F	F	F	6.638198774289901	6.918921956459466	6.9674448353514927	T	T	T
13.3093759609508175	1.6473734530420292	0.0000000000000000	F	F	F	9.2652848726128109	6.914848262128109	7.4751906135111970	T	T	T
15.97125115131399421	1.6473734530420292	0.0000000000000000	F	F	F	11.9927938288608625	6.9047882898832315	7.288455643538039	T	T	T
18.6331263453299928	1.6473734530420292	0.0000000000000000	F	F	F	14.6331462035999999	6.9169784039999999	7.9224741691807425	T	T	T
22.62593139136419428	4.8525889731804504	0.0000000000000000	F	F	F	17.297354092841754	6.9192215331407258	6.9942748342307155	T	T	T
6.6546879804749990	4.8525889731804504	0.0000000000000000	F	F	F	19.9518814078708041	6.9202480843871240	7.0137103875486124	T	T	T
9.3165631726659872	4.8525889731804504	0.0000000000000000	F	F	F	23.946817485825246	6.9206646657819458	7.0014032279837819	T	T	T
11.9784364784598916	4.8525889731804504	0.0000000000000000	F	F	F	7.974082786139313981	6.920339728516718503	6.9823007165178503	T	T	T
14.6493135570450331	4.8525889731804504	0.0000000000000000	F	F	F	18.6423249452993638	7.184214656851919	6.9596113382915422	T	T	T
17.3021887492349613	4.8525889731804504	0.0000000000000000	F	F	F	21.1219584273778538	9.21129584273778538	6.9572721227150387	T	T	T
19.96406394142450174	4.8525889731804504	0.0000000000000000	F	F	F	15.9571110998471164	9.2235946203299399	6.9880061697522393	T	T	T
23.95681053125751986	1.7578480511320523	0.0000000000000000	F	F	F	10.336075891569288	4.936075891569288	10.2946652051246371	T	T	T
2.6618751921900565	2.386381053199646	0.0000000000000000	F	F	F	7.9757849344938805	2.461696842609346	10.2915978233835510	T	T	T
5.3237503843799807	2.386381053199646	0.0000000000000000	F	F	F	8.5833942613203345	7.6011884686587356	10.288944280850119	T	T	T
6.6546879804749990	2.386381053199646	0.0000000000000000	F	F	F	9.214883938922550	6.54392770924460876	9.287970201608768	T	T	T
7.9856257567038035	2.386381053199646	0.0000000000000000	F	F	F	16.374481884667687487	4.760813981781564	10.1664493867271588	T	T	T
10.64750076876080272	2.386381053199646	0.0000000000000000	F	F	F	14.9982166894426264	2.3998829259153152	10.13656788259057874	T	T	T
13.3093759609508157	2.386381053199646	0.0000000000000000	F	F	F	16.3705973580158161	3.7408067104579139	10.1401851030247556	T	T	T
15.97125115131399407	2.386381053199646	0.0000000000000000	F	F	F	14.306464446454232	1.435024279540664	10.0640216125321267	T	T	T
18.631263453299982	2.386381053199646	0.0000000000000000	F	F	F	14.992171255643263	8.39988264772381	10.19032297915683	T	T	T
22.625931364187461	2.386381053199646	0.0000000000000000	F	F	F	17.446911831324491	7.998279638632151	10.2612960836124685	T	T	T
6.6546879804750594	2.386381053199646	0.0000000000000000	F	F	F	18.337127749320273344	5.6710217457604552	10.223239122873344			

5. 3237500000000599	6. 147339999999999971	0. 0000000000000000	F	F	3. 999447717611305	6. 8912418476870489	6. 9972521309708462	T	T
7. 9856299999999995	6. 147339999999999971	0. 0000000000000000	F	F	6. 6519346457843627	9. 0080565603602844	7. 0106420977442183	T	T
10. 64749999999999920	6. 147339999999999971	0. 0000000000000000	F	F	9. 3026014944918529	9. 6168188575612146	7. 020210631805130	T	T
13. 309380000000222	6. 147339999999999971	0. 0000000000000000	F	F	11. 9580312654667365	9. 3606527618042386	7. 02227598273540	T	T
9. 9712500000008546	6. 147339999999999971	0. 0000000000000000	F	F	14. 6452584157008788	9. 6146346392680385	7. 0436490247187554	T	T
18. 63312999999999551	6. 147339999999999971	0. 0000000000000000	F	F	17. 299522339081787	9. 61236984916114	7. 18178873170097	T	T
22. 625940000000106	6. 45259000000000416	0. 0000000000000000	F	F	19. 973593635895941	6. 887633866597389	6. 985095443666745	T	T
6. 6546900000000839	6. 45259000000000416	0. 0000000000000000	F	F	25. 532598471571519	9. 2058346495122390	6. 98734940048876639	T	T
9. 3165599999999995	6. 45259000000000416	0. 0000000000000000	F	F	7. 9822073032838107	9. 119404839489986	7. 0025617737095250	T	T
11. 978440000000133	6. 45259000000000416	0. 0000000000000000	F	F	16. 64363450827167789	9. 2183489768935630	6. 9774852404477181	T	T
14. 648310000000492	6. 45259000000000416	0. 0000000000000000	F	F	13. 303118486957795	9. 101835329555732	6. 9695652122650318	T	T
17. 302190000000812	6. 45259000000000416	0. 0000000000000000	F	F	15. 9723807482690314	9. 201334272899367	6. 888015695098807	T	T
19. 9640599999999786	6. 45259000000000416	0. 0000000000000000	F	F	18. 620765556955313	9. 1762262978672055	7. 019876058184586	T	T
21. 29568799999999911	10. 7578400000000852	0. 0000000000000000	F	F	21. 3057488509919277	9. 1626321936395208	7. 0018329394004146	T	T
7. 9856380000000617	10. 7578400000000852	0. 0000000000000000	F	F	23. 299987382305980	6. 4945824968923698	6. 98334940048876639	T	T
10. 6474999999999918	10. 7578400000000852	0. 0000000000000000	F	F	9. 5866223105255501	9. 4632284762142064	10. 443224464253396	T	T
13. 30937999999999938	10. 7578400000000852	0. 0000000000000000	F	F	18. 8917694528622420	9. 549357008632131	10. 116988538815111	T	T
17. 971250000000261	10. 7578400000000852	0. 0000000000000000	F	F	11. 213557495858443	2. 3277549214402919	9. 958576368673366	T	T
18. 633130000000581	10. 7578400000000852	0. 0000000000000000	F	F	20. 1959032460779925	2. 248468973431573	10. 1743324375554082	T	T
21. 2949999999999951	10. 7578400000000852	0. 0000000000000000	F	F	8. 923152176281999	6. 6231916700716202	10. 508591321535333	T	T
24. 2999999999999951	10. 7578400000000852	0. 0000000000000000	F	F	8. 5978895814898936	3. 9988570584973178	6. 187464992739587	T	T
26. 61880000000234	0. 0000000000000000	2. 3863800000000821	F	F	8. 358664579392871	2. 6324551926541067	8. 52127665597795	T	T
5. 3237500000000644	0. 0000000000000000	2. 3863800000000821	F	F	12. 437149542266219	2. 8684852889449255	9. 3361722163702829	T	T
7. 98562999999999631	0. 0000000000000000	2. 3863800000000821	F	F	16. 824674794386477	2. 5745660664942441	10. 88411516414886	T	T
10. 6474999999999973	0. 0000000000000000	2. 3863800000000821	F	F	15. 966246038376982	6. 431181605109949	13. 08811760629318873	T	T
13. 3093800000000275	0. 0000000000000000	2. 3863800000000821	F	F	17. 93590216914093	9. 995664424491319	10. 6971259969306354	T	T
17. 971250000000617	0. 0000000000000000	2. 3863800000000821	F	F	9. 335535374942993	6. 02373628109544	10. 526693286630976	T	T
1. 33093999999999771	2. 30524999999999632	0. 0000000000000000	F	F	11. 600671731942616	9. 5454813194942059	9. 94131098129679	T	T
3. 992810000000093	2. 30524999999999632	0. 0000000000000000	F	F	10. 4670118812896911	9. 19514939226211	10. 039471168657943	T	T
6. 6546900000000442	2. 30524999999999632	0. 0000000000000000	F	F	8. 1521650930975476	1. 87392545697454418	10. 62874644565574573	T	T
9. 3165599999999942	2. 30524999999999632	0. 0000000000000000	F	F	5. 737241661663771	2. 4897882036852135	10. 837287856212812	T	T
11. 9784399999999742	2. 30524999999999632	0. 0000000000000000	F	F	14. 996538439069989	2. 2449424623481491	10. 9813949060546943	T	T
14. 6403100000000666	2. 30524999999999632	0. 0000000000000000	F	F	16. 719871386758231	1. 9423655497855650	11. 355329933487612	T	T
17. 3021900000008382	2. 30524999999999632	0. 0000000000000000	F	F	16. 2282265268430837	2. 4183636389630598	9. 7184972056086005	T	T
2. 6618800000000818	0. 0000000000000000	2. 3863800000000821	F	F	15. 941542343710377	4. 03423715559985613	10. 34983080000000000	T	T
5. 3237500000000342	6. 1610500000000089	0. 0000000000000000	F	F	16. 07364684787899	5. 623208334166953	13. 3468763339348016	T	T
7. 9856300000000671	6. 1610500000000089	0. 0000000000000000	F	F	16. 6854532182217251	4. 0572453828737	13. 67452310218161	T	T
10. 647499999999671	6. 1610500000000089	0. 0000000000000000	F	F	18. 748502539544626	4. 426644875695846	11. 17233702929325	T	T
13. 3093799999999974	6. 1610500000000089	0. 0000000000000000	F	F	18. 0646732135114221	6. 058418897542875	10. 9172533392309994	T	T
17. 9712500000000333	6. 1610500000000089	0. 0000000000000000	F	F	18. 03829677266693	5. 64571837314771156	9. 6037760673636464	T	T
18. 633130000000653	6. 1610500000000089	0. 0000000000000000	F	F	14. 8283239961888977	5. 5279797581505310	10. 26000104038754210	T	T
19. 9928100000000449	6. 1610500000000089	0. 0000000000000000	F	F	16. 2807465539833898	4. 357894882876319	11. 2616467323296199	T	T
## POSCAR for TS21-22 ##									
Zn	C	H	Cl	Si	1.	0.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000
18. 6331263545000000453	1. 8372803340000000	1. 0000000000000000	1. 0000000000000000	1. 0000000000000000	18.	16. 6331263545000000453	1. 5368299999999968	1. 0000000000000000	0.0000000000000000
6. 65468798000000003	6. 65468798000000003	11. 5622576909999996	11. 5622576909999996	11. 5622576909999996	6. 5548800000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000	24.	54.552402099999985			
Selective dynamics									
Cartesian									
1. 633129999999999800	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
2. 26188000000000453	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
5. 32374999999999442	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
7. 98562999999999747	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
10. 64750000000000115	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
13. 309380000000004435	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
15. 97238000000000115	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
18. 9640600000000106	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
19. 9640600000000106	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
21. 29499999999999884	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
2. 32750000000000564	1. 5373399999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
5. 78862999999999587	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
8. 78562999999999587	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
10. 6474999999999951	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
13. 30938000000000222	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
15. 97125000000000510	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
18. 63313000000000510	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
21. 29499999999999551	1. 5368299999999968	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
2. 0800000000000000	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
2. 66188000000000324	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
5. 32375000000000644	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
7. 98562999999999587	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
10. 6474999999999951	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
13. 30938000000000222	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
15. 97125000000000617	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
18. 63313000000000617	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	0. 0000000000000000	F	F	F	F	F
21. 29499999999999551	0. 0000000000000000	0. 000000000000000							

11.978439999999942	6.915749999999708	2.3863800000000821	F F F	1.000000000000000	18.6331263450000009	0.000000000000000	0.000000000000000
14.640309999999728	6.915749999999708	2.3863800000000821	F F F	6.6546879800000003	11.526257698999996	0.000000000000000	0.000000000000000
17.3021900000000102	6.915749999999708	2.3863800000000821	F F F	0.000000000000000	0.000000000000000	24.545524020999985	
19.9640600000000390	6.915749999999708	2.3863800000000821	F F F				
5.3237536549999671	9.2218100000000370	2.3863800000000821	F F F	140 11 14 1 1			
7.9856300000000395	9.2218100000000370	2.3863800000000821	F F F	Selective dynamics			
10.6475000000000373	9.2218100000000370	2.3863800000000821	F F F	Cartesian			
13.389379999999778	9.2218100000000370	2.3863800000000821	F F F	18.633129999999764	1.5368299999999688	0.000000000000000	F F F
15.9712500000000102	9.2218100000000370	2.3863800000000821	F F F	2.6618800000000480	1.5368299999999688	0.000000000000000	F F F
18.6313100000000439	9.2218100000000370	2.3863800000000821	F F F	5.3237499999999488	1.5368299999999688	0.000000000000000	F F F
21.2950000000000763	9.2218100000000370	2.3863800000000821	F F F	7.9856299999999899	1.5368299999999688	0.000000000000000	F F F
18.641726028422766	5.144018462342345	T T T		10.6475000000000115	1.5368299999999688	0.000000000000000	F F F
2.6761218624964573	1.549447224071774	T T T		13.309380000000035	1.5368299999999688	0.000000000000000	F F F
5.3277394117851449	1.548407799089997	T T T		15.9712499999999427	1.5368299999999688	0.000000000000000	F F F
7.9841872318576579	1.548531830214073	T T T		19.9640600000000106	3.8428900000000340	0.000000000000000	F F F
10.6448324612872209	1.54293169285951	T T T		3.9928100000000812	3.8428900000000340	0.000000000000000	F F F
13.3421951181095383	1.5600871581167828	T T T		6.6546899999999889	3.8428900000000340	0.000000000000000	F F F
15.9614942420149795	1.5507852895009358	T T T		9.3165600000000133	3.8428900000000340	0.000000000000000	F F F
19.9781518364774299	3.85459964617692	T T T		11.9781518364774299	3.8428900000000340	0.000000000000000	F F F
3.9988674015423063	4.6765144223809236	T T T		14.6483100000000777	3.8428900000000340	0.000000000000000	F F F
6.6588207471466872	4.6765144223809236	T T T		17.3021899999999978	3.8428900000000340	0.000000000000000	F F F
9.3296473614385251	3.8497736956906185	T T T		21.2949999999999875	6.1473399999999971	0.000000000000000	F F F
11.998215385577321	3.8475728934064991	T T T		5.3237500000000599	6.1473399999999971	0.000000000000000	F F F
14.6495748179355747	3.8147195718173102	T T T		7.9856299999999578	6.1473399999999971	0.000000000000000	F F F
17.3179399042074275	3.8458592126894195	T T T		10.6473999999999971	6.1473399999999971	0.000000000000000	F F F
21.3008128688428089	6.15913188022508680	T T T		13.3093800000000222	6.1473399999999971	0.000000000000000	F F F
5.3323091920921151	6.15533020390689437	T T T		15.9712500000000546	6.1473399999999971	0.000000000000000	F F F
7.9993137483806214	6.15171948948171503	T T T		18.6331299999999951	6.1473399999999971	0.000000000000000	F F F
10.6619908191039195	6.1440971828831072	T T T		22.6529400000000106	6.1545900000000416	0.000000000000000	F F F
13.327105080653243	6.158956504262984	T T T		6.6546900000000541	8.4525900000000416	0.000000000000000	F F F
15.9713351884421436	6.163309633772824	T T T		10.6473999999999849	8.4525900000000416	0.000000000000000	F F F
18.6374270613610417	6.15542652453463475	T T T		11.9784400000000133	8.4525900000000416	0.000000000000000	F F F
22.6326745920629584	6.4846524424509984	T T T		14.6493100000000492	8.4525900000000416	0.000000000000000	F F F
6.6579909281542073	4.6768242300700885	T T T		17.3021900000000812	8.4525900000000416	0.000000000000000	F F F
9.3250653627005562	4.6768242300700885	T T T		19.9640599999999786	8.4525900000000416	0.000000000000000	F F F
11.987811415205043	4.6630687389467720	T T T		23.9568799999999911	10.7578400000000852	0.000000000000000	F F F
14.6456308202935748	4.68062512482200146	T T T		7.98563000000000617	10.7578400000000852	0.000000000000000	F F F
17.3892534410639800	4.6824887112235623	T T T		10.6474999999999618	10.7578400000000852	0.000000000000000	F F F
19.9739117411311517	4.6830819437916176	T T T		13.309379999999998	10.7578400000000852	0.000000000000000	F F F
23.956099351085662	10.776718359288941	T T T		15.9712500000000261	10.7578400000000852	0.000000000000000	F F F
7.987577835059281	10.769440778359731	T T T		18.6331000000000581	10.7578400000000852	0.000000000000000	F F F
16.6513840524070533	10.772778227050165	T T T		21.2949999999999591	10.7578400000000852	0.000000000000000	F F F
13.3125934932032611	10.7689705203523175	T T T		0.000000000000000	0.000000000000000	2.3863800000000821	F F F
15.974885616584126	10.7661398005350168	T T T		2.6118800000000324	0.000000000000000	2.3863800000000821	F F F
18.643779947251317	10.77077836148476	T T T		5.2327500000000644	0.000000000000000	2.3863800000000821	F F F
21.308291464296725	10.780772795633749	T T T		7.9856299999999563	0.000000000000000	2.3863800000000821	F F F
18.6169592798232758	0.0161788914524927	T T T		10.6474999999999973	0.000000000000000	2.3863800000000821	F F F
2.650295811085662	0.018115788914524927	T T T		13.3093800000000227	0.000000000000000	2.3863800000000821	F F F
11.9715624248046243	11.5390772763818356	T T T		15.9712500000000617	0.000000000000000	2.3863800000000821	F F F
14.637093492302611	10.535330687399121	T T T		1.3093800000000999	2.3052499999999632	0.000000000000000	F F F
17.3031970586125787	11.5339085634389171	T T T		3.9928100000000993	2.3052499999999632	0.000000000000000	F F F
13.3146189923489991	0.0359574461750089	T T T		6.5546900000000442	2.3052499999999632	0.000000000000000	F F F
15.9402830387472426	0.0466638747396359	T T T		7.9856300000000644	2.3052499999999632	0.000000000000000	F F F
19.94968086496424232	2.321254867620930	T T T		10.6473999999999974	2.3052499999999632	0.000000000000000	F F F
3.991048904158379	2.31563625895338	T T T		14.6403100000000666	2.3052499999999632	0.000000000000000	F F F
6.64317918278064764	2.309852786144922	T T T		17.3021900000000386	2.3052499999999632	0.000000000000000	F F F
9.30958668865437140	2.3069913245093532	T T T		2.6118800000000098	4.6105000000000089	0.000000000000000	F F F
11.9626293902915000	2.3185946373499932	T T T		5.3237500000000342	4.6105000000000089	0.000000000000000	F F F
14.6892894167543631	2.304998440935692	T T T		7.9856300000000671	4.6105000000000089	0.000000000000000	F F F
17.2827039089125378	2.3245087387469999	T T T		10.6474999999999971	4.6105000000000089	0.000000000000000	F F F
21.28112712712571	4.61938219926380599	T T T		13.3093799999999978	4.6105000000000089	0.000000000000000	F F F
5.3121565084261462740	7.00174522631558185	T T T		15.9712500000000333	4.6105000000000089	0.000000000000000	F F F
7.9840446336433267	6.178636835511696	T T T		18.6331000000000653	4.6105000000000089	0.000000000000000	F F F
10.6519331271212501	6.998493146179873	T T T		2.6118800000000098	4.6105000000000089	0.000000000000000	F F F
15.9770007151697033	6.066861541308766	T T T		3.9928100000000129	4.6105000000000089	0.000000000000000	F F F
18.6278955881608008	6.215459072476814	T T T		6.5546900000000129	4.6105000000000089	0.000000000000000	F F F
22.621622510818616	6.9337225067451807	T T T		9.3165000000000452	4.6105000000000089	0.000000000000000	F F F
6.652912251915129	6.928652362838599	T T T		11.9784399999999942	4.6105000000000089	0.000000000000000	F F F
9.3216109236294598	6.913064821716776	T T T		14.6403099999999978	4.6105000000000089	0.000000000000000	F F F
11.978384725490387	6.9113021032889451	T T T		17.3021900000000102	4.6157499999999978	0.000000000000000	F F F
14.637165844551985	6.9117584375356459	T T T		21.2949999999999978	4.6157499999999978	0.000000000000000	F F F
17.2946380288200857	6.912569928793499	T T T		0.000000000000000	4.6157499999999978	0.000000000000000	F F F
19.9523511746328666	6.929759701970142561	T T T		7.9856300000000449	4.6157499999999978	0.000000000000000	F F F
23.9450165485048018	6.9439736214064924	T T T		10.6475000000000070	4.6157499999999978	0.000000000000000	F F F
7.978428457382783857	4.6162061249606272	T T T		13.3225873025882007	4.61548253646607713	0.000000000000000	F F F
10.6437093122592546	4.28457158389349	T T T		15.9671518081424328	4.6156197496089411	0.000000000000000	F F F
13.302585188790560129	2.020278751745173	T T T		19.9691279797307297	4.6158521140815917	0.000000000000000	F F F
14.34921271231043	2.020278751745173	T T T		4.0019296919190243	3.857924171163359	0.000000000000000	F F F
18.7838125099976683	3.0094326625458234	T T T		6.6628075129556777	4.605071291962114623	0.000000000000000	F F F
14.165281243918896	2.92329631161462	T T T		7.9932214759745997	3.8475035423791089	0.000000000000000	F F F
19.6981192340627654	4.4280072						

18.6356357659195737	10.7708884697002301	4.6672275527001794	T	T	T	5.3237503843799816	0.0000000000000000	2.3863810053199650	F	F	F
21.293808482605348	10.772750565478329	4.6654819088880215	T	T	T	7.9856255765700836	0.0000000000000000	2.3863810053199650	F	F	F
18.6188977920644234	0.0173753029586538	6.9795419561317877	T	T	T	10.6475087687599632	0.0000000000000000	2.3863810053199650	F	F	F
2.6553935973992360	0.01326473336368995	6.9690314674125506	T	T	T	13.30937596095080211	0.0000000000000000	2.3863810053199650	F	F	F
5.3231489939357211	0.0089963144310464	6.9838962836618617	T	T	T	15.9712511531399439	0.0000000000000000	2.3863810053199650	F	F	F
7.9839243380543579	0.0087436707520315	6.9964338325907689	T	T	T	1.33093759609508185	2.30525153814901570	2.3863810053199650	F	F	F
10.6367728185443138	0.0081408931432112	6.995209594921538	T	T	T	3.9928127882850752	2.30525153814901570	2.3863810053199650	F	F	F
13.2961310880888034	0.0225574975155484	7.014597487690941	T	T	T	6.6546879847949999	2.30525153814901570	2.3863810053199650	F	F	F
15.9509559091726556	0.0141349457662023	6.9736331202384987	T	T	T	9.3165631726650577	2.30525153814901570	2.3863810053199650	F	F	F
19.9498360027934138	2.3166838206127984	6.9846568989849945	T	T	T	11.97813834648549824	2.30525153814901570	2.3863810053199650	F	F	F
3.9864676716412618	2.31603378601630287	6.9758201481345843	T	T	T	14.6483135758450462	2.30525153814901570	2.3863810053199650	F	F	F
6.650127405176341	6.2357269653049518	6.9862821446057982	T	T	T	17.3021878492349613	2.30525153814901570	2.3863810053199650	F	F	F
9.31365918758514	2.3201875514238078	7.0126921894654339	T	T	T	2.66157151921899994	6.6105030762802333	2.3863810053199650	F	F	F
11.9688334846846338	2.3291276254329801	6.96832325657591272	T	T	T	5.32375038437998075	4.6105030762802333	2.3863810053199650	F	F	F
14.627483570216288	2.331456494759781	6.94867837649661397	T	T	T	7.9856255765697925	4.6105030762802333	2.3863810053199650	F	F	F
17.287425188342518	2.32947665697344627	6.949479765960616966	T	T	T	10.64750876875280289	4.6105030762802333	2.3863810053199650	F	F	F
21.2823320582396936	4.6285053645194951	6.9870341838989894	T	T	T	13.30937596099958	4.6105030762802333	2.3863810053199650	F	F	F
5.3172460930301710	4.6243783522558104	6.9976969406309353	T	T	T	15.9712511531406114	4.6105030762802333	2.3863810053199650	F	F	F
7.98688373696321	4.6249872544408639	6.986419286786350	T	T	T	18.633083764953309943	4.6105030762802333	2.3863810053199650	F	F	F
10.6565654726481851	6.6318300997531818	6.9871354274579707	T	T	T	3.992812788285095	6.91575456144283916	2.3863810053199650	F	F	F
15.9405479267399995	4.6465249902672626	6.964964957659154512	T	T	T	6.65468794642293916	6.91575456144283916	2.3863810053199650	F	F	F
18.6204724276450264	6.627655896379818	6.9707294415597808	T	T	T	9.3165631726649920	6.91575456144283916	2.3863810053199650	F	F	F
3.98945589525624607	6.9296865695039728	6.978396439758995	T	T	T	11.97843836459548481	6.91575456144283916	2.3863810053199650	F	F	F
6.6531096506608885	6.9219050454584581	6.9992325315605077	T	T	T	14.649313575049727	6.91575456144283916	2.3863810053199650	F	F	F
9.31724221919161	6.92743765785715142	6.97383854417876768	T	T	T	17.3021878492350057	6.91575456144283916	2.3863810053199650	F	F	F
11.9893376082788443	6.9301949539094641	6.983439487779884	T	T	T	19.964063941249534	6.91575456144283916	2.3863810053199650	F	F	F
14.6317650852875385	6.91408394615436449	7.6498311634387655	T	T	T	5.3237503843799807	9.2210061525604665	2.3863810053199650	F	F	F
17.2624312387671921	6.9236821845801467	7.00531943378389	T	T	T	7.985625576570670837	9.2210061525604665	2.3863810053199650	F	F	F
19.94339071823448989	6.93008784192099729	6.988678495987959	T	T	T	10.64750876875280289	9.2210061525604665	2.3863810053199650	F	F	F
23.9455859745742607	9.294246466469372	6.992274888990443	T	T	T	13.3093759609509000	9.2210061525604665	2.3863810053199650	F	F	F
7.979438338963092	9.21634272795670	6.9843658986794985	T	T	T	15.9712511531399439	9.2210061525604665	2.3863810053199650	F	F	F
18.6462808978502485	9.2977414634618338	7.0160942866071494	T	T	T	18.6331265453300000	9.2210061525604665	2.3863810053199650	F	F	F
13.309460294072441	2.1928983846017231	6.985681621898395	T	T	T	21.295051375199229	9.2210061525604665	2.3863810053199650	F	F	F
15.9504470448696599	9.21235575586353409	6.984297321918074	T	T	T	18.652563092339999	15.4484789527136315	4.66351596385777051	T	T	T
18.624576358871824	2.231032952388371676	6.9791749544121808	T	T	T	2.662235683930232	5.5341776669748274	4.6672251537463536	T	T	T
21.2821171795425883	9.2316516087025295	6.9756707176466479	T	T	T	5.2967621418011026	5.5050681906397231	4.6658556750230771	T	T	T
13.5183719872951201	4.6513664567526161	6.975149755989444	T	T	T	7.939517987198766851	5.5044786181366808	4.6377967318285949	T	T	T
9.75787616194623	5.021226810988991	18.112556528965324	T	T	T	10.645021986688707	5.51613164798876	4.6618845162681804	T	T	T
11.1316814978502485	4.7854655098885551	18.0860042748106711	T	T	T	13.3447805229500000	5.51562212598291341	4.6905070559734740	T	T	T
11.6265997804445860	4.3626305257598682	12.8210132988105521	T	T	T	17.305671018682949849	5.54307513572432930	4.66330175244409421	T	T	T
17.710692892643945	2.919883846017231	6.985681621898395	T	T	T	19.975215761202613	3.8566502276711336	4.6676500236474983	T	T	T
9.3379420805346526	6.6363516685133579	10.17593872042240503	T	T	T	3.9195304788475868	6.9156121342446663	4.6759100088908196	T	T	T
8.8574690286099269	3.950740723324649	10.162899182111273	T	T	T	6.64866716828568	3.8511363951862882	4.6717339733144580	T	T	T
14.237745433226323	3.0575583098042524	10.2765858964659099	T	T	T	9.3111196829868386	3.8534489766721234	4.63146739485162	T	T	T
13.0262699019183860	3.22886696449712551	10.176177574975876	T	T	T	11.961614648919875	3.8592592825154659	4.7181726737416669	T	T	T
16.624585272008557	1.2129457016967613	10.495291264513869	T	T	T	14.626152227112744	3.864802828232408	4.726238858235247	T	T	T
15.710883053499421	3.0629812459325185	12.8210132988105521	T	T	T	17.305671018682949849	4.83418335134397	4.6516655250755363	T	T	T
17.02305146166161	4.286052918627038	10.3696250955040000	T	T	T	21.3021878381597321	4.854770874493560	4.6685750566212434	T	T	T
9.38866399683898824	6.046784213464395	10.0796767759770824016	T	T	T	5.3261377793306881	6.15473254462246208	4.6757953551888400	T	T	T
11.8420813121531051	5.1640422469812191608	10.15414224698121221764	T	T	T	7.9914464418478487	6.1502221537020400000	4.6746472097455845	T	T	T
11.0871721253496212	3.1668494303089487	10.1662214021119635	T	T	T	10.6677413921762092	6.1471591747732965	4.6747146529435989	T	T	T
8.6408555806897443	1.79795930932191051	10.18871353215321903	T	T	T	13.3150846383042546	6.0911368388334900	4.67308731424080000	T	T	T
7.7830519570104264	4.1404827834219334	10.17976152979288000	T	T	T	15.980043382193219321	6.1300667872193211	4.683418114126593	T	T	T
15.086293746463017429	0.39931120512610	10.8332142172789244	T	T	T	18.6523315967731849	6.1587781207313554	4.6442009963544546	T	T	T
17.637148973654338	1.0747488982771	10.944595291862771	T	T	T	22.6384478249493000	4.8547708774493298	4.6677008768822598	T	T	T
16.754269424068692	1.12847481312153702	9.4033906591751830	T	T	T	6.6623052993851819	4.8539567359351498	4.672566720206925	T	T	T
15.047588833499573	2.2975899240616607	13.1791434146629971	T	T	T	9.335024860320400000	4.8544386000000000	4.6714102746051145	T	T	T
15.2735787944486482	3.974125173095431	13.0912071173360847	T	T	T	11.9949228329934953	4.66110254729521086	4.6630365217439858	T	T	T
16.681367210269321	2.90133625042332623	10.29130264932363608	T	T	T	14.628697210279416570	4.689113424827907297	4.6611224023072310	T	T	T
17.92918837103371	5.24633836231347317	10.1797613018755721	T	T	T	19.974891101575175	5.461214762386462344	4.6760228488445298	T	T	T
14.36777439866420828	4.118575077192538	9.3333603516968817	T	T	T	7.991921482041812	5.78383771491338	4.6781392743348551	T	T	T
14.4393592287017185	7.1308515744880227	9.4540512906147935	T	T	T	10.6496530547087209	7.0079442208498455	4.672272098159639	T	T	T
15.9426334174931432	8.2886415694598784	10.9608471265958043	T	T	T	13.3088628894695957	7.007427743098386	4.6709378584346055	T	T	T
140	19	19	1	1	Selective dynamics		</td				

11.0794475316642060	3.3255726901596723	9.3376250880295224	T	T	T	18.6331263453300018	9.2210061525604665	2.3863810053199650	F	F	F
18.2190206895351814	8.9838642359872836	18.3245031057095993	T	T	T	21.2950015375199229	9.2210061525604665	2.3863810053199650	F	F	F
17.0638242662513058	8.2185123275180043	18.198157525686030	T	T	T	18.6582874195635139	1.544138377558329	4.6609978767263032	T	T	T
17.1434015570639318	8.6098478535661234	18.0845741452053712	T	T	T	2.6669405408848132	1.5524221518133099	4.6739239860098687	T	T	T
18.4174551894013021	6.1959527575677773	18.1343426954632623	T	T	T	5.2996676537881173	1.5540778829266413	4.6671592105853197	T	T	T
19.5683017334208209	9.7678975472579235	18.2597673574752264	T	T	T	7.9341311288263094	1.5486245761069733	4.6407382227381315	T	T	T
19.4761478848761035	8.3700392900249986	18.3494618617750209	T	T	T	10.6456598012546415	1.5496592581467219	4.6603726893490558	T	T	T
14.9714747480345345	5.4372768486526613	9.4235533605858848	T	T	T	13.3540256326592637	1.5535160648810189	4.6901534148821997	T	T	T
15.9794674517059399	6.0513629562093119	9.8099583399334700	T	T	T	16.0047553878597348	1.5370011713911393	4.6590129355367784	T	T	T
12.9786392045577078	8.3967132662515844	18.4994442569147904	T	T	T	19.974582793973874	3.8547499361069487	4.66867169813136789	T	T	T
11.1074051664891993	8.4831176195417370	12.9518404454798954	T	T	T	3.9932307252291532	3.8592211095526081	4.6720096815857710	T	T	T
10.1456927559105097	7.098434748021755	18.36144018040873414	T	T	T	6.6524288844088407	3.853253084696131	4.6755906546110113	T	T	T
15.4788655501747586	11.0454784711370864	18.5761743005087595	T	T	T	9.3159227201117538	3.8535262642583099	4.640981283104818	T	T	T
10.914229519721624	0.736061274956455	9.957727171244946	T	T	T	11.99774695327097397	3.85895916245823875	4.7034326582543793	T	T	T
8.7210954933441958	4.4543233184749157	9.8871845103742574	T	T	T	14.6229230812091166	3.858532222713479	4.6950467239387930	T	T	T
6.6362330433941973	3.2356076350792648	18.4866664295867891	T	T	T	17.3053497835454573	3.8469378053166494	4.65951883554180885	T	T	T
6.6828439221307518	7.0675429412065698	18.893367896185909	T	T	T	21.303212021794692	6.16480663268792366	4.6701401527822517	T	T	T
18.144347870180563	10.0697709966249231	18.393046709889368	T	T	T	5.3281553457186579	6.1605141569850037	4.6745046963532273	T	T	T
16.6819606521694638	8.691701510515674	18.1414869778778935	T	T	T	7.99438227911211143	6.161059878742819	4.6782902496514680	T	T	T
18.489865361860814	5.1148958752575477	18.047784229198486	T	T	T	10.667782849952552	6.1522862928071846	4.6758556325183269	T	T	T
20.5458132629372508	6.492677344060263	18.2736354894604199	T	T	T	13.319854782642673	6.1024608358855981	4.718774222483211	T	T	T
20.3789412668727508	9.795598784859759	18.4289309981774974	T	T	T	15.983707163638806	6.147414919713019	4.6551498779902412	T	T	T
13.7959431006566216	8.671583626492575	11.1814808426520398	T	T	T	18.654581217157552	6.1632754843104536	4.644137219147849	T	T	T
12.5876117958954192	9.3149943694953543	10.0323207669325925	T	T	T	22.63941689120488313	6.4822054933995186	4.679187882028989	T	T	T
13.3924200570589804	7.75408343474501919	9.709161338007287	T	T	T	6.6671932458965374	8.461369467294249	4.67666077975384088	T	T	T
11.972863099728939	6.6531885374408630	13.6078351796159832	T	T	T	9.3346210089515438	8.459514950395261	4.6770278982249773	T	T	T
10.3401830507385206	7.9361967738924477	13.5170515951535727	T	T	T	11.9859848301066503	8.4774688501651809	4.6478498342424864	T	T	T
18.6945943304461688	9.4696412758564042	12.6686756282577848	T	T	T	14.6225285610457457	8.47334657847146	4.6588830886953785	T	T	T
9.731731184605044	0.8633975901228533	9.8896851392754748	T	T	T	17.311540266170495	6.4626248729691635	4.6616458548421343	T	T	T
9.3549972305205206	6.6232731857885518	10.9580885127183087	T	T	T	19.97788730954523199	6.4857084578061171	4.673891149926149	T	T	T
10.4422887314915700	6.464645321856948	9.558789820856474	T	T	T	23.9702188665432012	10.759388123216785	4.6782627495796527	T	T	T
12.388352301721624	5.6889782449415085	12.1114578984281700	T	T	T	7.99886304805191456	10.7655792988727	4.6833518585468846	T	T	T
11.613145246756695	7.529119008216608	11.431264736703495	T	T	T	10.6468319424554885	10.7763913468421943	4.6769917264637009	T	T	T
## POSCAR for INT3-24 ##						13.2979023232387985	10.7845415098295880	4.66311196218439088	T	T	T
Zn C H Cl Si						15.9725768404836818	10.77629907585850	4.67031108723479062	T	T	T
Cartesian						18.6477095243477962	10.7754050505952002	4.6602827147878649	T	T	T
Selective dynamics						21.310748616999827	10.7682738915637177	4.6815494263638842	T	T	T
1.0000000000000000	18.6331263453300018	0.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000	18.6477095243477962	10.7763918423216785	4.6833518585468846	T	T	T
6.5646879804794999	11.5262576987006249	0.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000	10.6468319424554885	10.7763913468421943	4.6769917264637009	T	T	T
140 19 19 1 1						12.0077309232387985	10.7845415098295880	4.66311196218439088	T	T	T
1.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000	24.545524021280021	10.759388123216785	4.6782627495796527	T	T	T
18.6312316453299378	1.5368343587600781	0.0000000000000000	F	F	F	19.9886823857318111	11.485803440569981	7.025352720327984	T	T	T
2.661751921899908	1.5368343587600781	0.0000000000000000	F	F	F	6.6217143853252390	2.3294588513525847	7.038102562397932	T	T	T
5.3237503843800472	1.5368343587600781	0.0000000000000000	F	F	F	9.240657953257188	2.309756382459165	7.01957103817013957	T	T	T
7.9856255765697927	1.5368343587600781	0.0000000000000000	F	F	F	10.5188657953257188	2.3098665257588732	6.8418983032652054	T	T	T
15.971251151310400114	1.5368343587600781	0.0000000000000000	F	F	F	12.00869198431624529	2.3102355291164831	6.910732124869788	T	T	T
16.546879804794999	1.5368343587600781	0.0000000000000000	F	F	F	14.7604421394142493	2.310272123585783	6.9592905337722863	T	T	T
13.992812782850905	3.4208585969002354	0.0000000000000000	F	F	F	16.341928043362033	2.31082837881458617	6.9580295184504308	T	T	T
6.6546879804790506	3.4208585969002354	0.0000000000000000	F	F	F	19.228082357562054	2.31082837881458617	6.9512251226795968	T	T	T
7.9856255765700386	3.4208585969002354	0.0000000000000000	F	F	F	21.280837881458617	2.31082837881458617	6.94174561226795968	T	T	T
10.64750076876002809	3.4208585969002354	0.0000000000000000	F	F	F	23.164493124376952	2.31082837881458617	6.927252901131174	T	T	T
13.3093759609499536	10.757840513205449	0.0000000000000000	F	F	F	24.9886308512107097	2.31082837881458617	6.92663246024586059	T	T	T
15.971251151310400114	10.757840513205449	0.0000000000000000	F	F	F	11.1813473509332492	2.31082837881458617	6.92695123722824317	T	T	T
18.6331263453299343	10.757840513205449	0.0000000000000000	F	F	F	18.10047586147374374	2.31082837881458617	6.929351752819596	T	T	T
21.2950051357199399	10.757840513205449	0.0000000000000000	F	F	F	7.77265051887402769	2.31082837881458617	6.92665586833798150	T	T	T
2.6616751921899908	10.757840513205449	0.0000000000000000	F	F	F	17.306998149496616	2.31082837881458617	6.9130811984776572	T	T	T
22.62593193361349456	10.757840513205449	0.0000000000000000	F	F	F	19.9616242242735219	2.31082837881458617	6.91062442242735219	T	T	T
8.45258897318407400	10.757840513205449	0.0000000000000000	F	F	F	21.0968062442735219	2.31082837881458617	6.9097251795286067	T	T	T
6.6546879804794999	10.757840513205449	0.0000000000000000	F	F	F	23.1644927437694861	2.31082837881458617	6.9049198511201217	T	T	T
11.27337503843799816	10.757840513205449	0.0000000000000000	F	F	F	11.2737448116695821	2.31082837881458617	6.9249958325324005	T	T	T
7.9856255765700386	10.757840513205449	0.0000000000000000	F	F	F	18.573535188205348	2.31082837881458617	6.8264232954826487	T	T	T
10.64750076876002809	10.757840513205449	0.0000000000000000	F	F	F	17.243852939688988	2.31082837881458617	6.821107638441899	T	T	T
13.30937596094995028	10.757840513205449	0.0000000000000000	F	F	F	16.9952866467637939	2.31082837881458617	6.8349299562481425	T	T	T
15.971251151310400114	10.757840513205449	0.0000000000000000	F	F	F	18.10047586147374374	2.31082837881458617	6.908845567			

13.3183970801741491	4.7552596011845489	12.0310904347869077	T	T	T	7.997630848179765	10.7580948695767358	4.6774790901513565	T	T	T
12.8831280966184334	6.8472630043866838	11.2406544883598620	T	T	T	10.6473046183205486	10.7714996584598826	4.6725345112170125	T	T	T
## POSCAR for INT24 ##											
Zn	C	H	Cl	Si		13.3036786402766474	10.7676932526025556	4.6652419914097436	T	T	T
1.0000000000000000						15.9728192437521699	10.7629455441844826	4.6714637254586568	T	T	T
18.6331263453300018	0.0000000000000000	0.0000000000000000				18.6429918473174942	10.7705028112286989	4.6643904729628733	T	T	T
6.6546879804749999	11.5262576987006249	0.0000000000000000				21.30840461364501965	10.7660389030831852	4.6759135328624186	T	T	T
0.0000000000000000	0.0000000000000000	24.545524021280021				6.6689839611555426	11.5175457234147487	6.9886492610640438	T	T	T
140	19	19	1	1		2.6662926018375721	0.0035863751334369	6.9965012084869930	T	T	T
Selective dynamics						5.3146885810408611	0.00282629681038596	6.9836497411399139	T	T	T
Cartesian						14.616246639961509	11.5083410179156571	7.0226129320367638	T	T	T
18.631263453299378	1.5368343587600781	0.0000000000000000	F	F	F	17.2726793998591113	11.4967313137667670	6.9954176480254431	T	T	T
2.6618751921899908	1.5368343587600781	0.0000000000000000	F	F	F	19.985824068184891	11.4842466210060746	7.0291483823614564	T	T	T
5.3237503843800473	1.5368343587600781	0.0000000000000000	F	F	F	22.6432836572827914	11.5221481835835373	6.9946547889011695	T	T	T
7.9856255765699728	1.5368343587600781	0.0000000000000000	F	F	F	1.336188573989678	2.305522747575260	7.0234553013990197	T	T	T
10.6475007687680289	1.5368343587600781	0.0000000000000000	F	F	F	3.9769720783287867	2.3809947784201761	7.0355229742246230	T	T	T
13.3093759609499536	1.5368343587600781	0.0000000000000000	F	F	F	6.61272699759892	2.290578605776816	7.0099767824215483	T	T	T
14.6493135570449729	1.5368343587600781	0.0000000000000000	F	F	F	9.2265660576984052	2.269360849576197	6.8393026525041920	T	T	T
15.9712511513400114	1.5368343587600781	0.0000000000000000	F	F	F	12.022732717630347	2.178805908941686	6.9447651639734271	T	T	T
19.5646839414249534	3.8420858969002354	0.0000000000000000	F	F	F	14.70699731429024873	2.2977171474255148	6.9322418879300036	T	T	T
3.9922817880580005	3.8420858969002354	0.0000000000000000	F	F	F	17.33880178886031852	2.281229425948285	6.9627742233345983	T	T	T
6.6546879804749999	3.8420858969002354	0.0000000000000000	F	F	F	21.2913759804739873	4.614635441848614	7.0223199607072654	T	T	T
9.3165631726469902	3.8420858969002354	0.0000000000000000	F	F	F	5.2975182453084368	6.159839756227179	7.0076156804799868	T	T	T
11.9784383648550481	3.8420858969002354	0.0000000000000000	F	F	F	7.9332391845455363	4.6048309831373881	6.9796696299261737	T	T	T
14.6493135570449729	3.8420858969002354	0.0000000000000000	F	F	F	10.5182315363140471	6.98575535464949	6.912507073155258	T	T	T
17.3021887492350209	3.8420858969002354	0.0000000000000000	F	F	F	16.167415412392134	5.4981180646047546	6.9626579565500723	T	T	T
21.2950815375192964	1.647373450403116	0.0000000000000000	F	F	F	18.6476160561133754	6.170312316359396	6.9684587741692559	T	T	T
5.3237503843799807	1.647373450403116	0.0000000000000000	F	F	F	22.617038322418508	6.9209455126875312	7.0322547426095152	T	T	T
7.9856255765699728	1.647373450403116	0.0000000000000000	F	F	F	6.64517607687560289	6.9141072624781656	6.983773895646684	T	T	T
10.6475007687599614	1.647373450403116	0.0000000000000000	F	F	F	9.2962878604882054	6.95996736356146210	7.011672083035883	T	T	T
13.309375960949950193	1.647373450403116	0.0000000000000000	F	F	F	12.0023166052745009	6.9305988353098015	6.9627433860781878	T	T	T
15.9712511513139493	1.647373450403116	0.0000000000000000	F	F	F	14.6220209189584971	6.8918419821503441	7.0518350915272334	T	T	T
18.631263453300018	1.647373450403116	0.0000000000000000	F	F	F	17.298211109835531	6.92526861372933093	6.9904313372575988	T	T	T
22.6259391361494956	1.647373450403116	0.0000000000000000	F	F	F	6.919055618772999	6.9998879310173994	7.0559937533099194	T	T	T
6.6546879804749999	1.647373450403116	0.0000000000000000	F	F	F	5.3240173433970668	9.2152557561134397	6.9981238032022336	T	T	T
9.3165631726505806	1.647373450403116	0.0000000000000000	F	F	F	7.9797049924876129	6.2296287608649941	6.9974849358061508	T	T	T
11.9784383648549806	1.647373450403116	0.0000000000000000	F	F	F	10.6466535645605713	9.2329671586347875	6.9739095810092380	T	T	T
14.6493135570450385	1.647373450403116	0.0000000000000000	F	F	F	13.3148763912709151	9.2263652092643103	7.020131617702722	T	T	T
17.3021887492349649	1.647373450403116	0.0000000000000000	F	F	F	15.954624757867361	9.2057813779673156	7.010597965557995	T	T	T
19.5640639414250209	1.647373450403116	0.0000000000000000	F	F	F	18.6224458305988391	9.2144926465352896	6.9952304646047546	T	T	T
23.9568767297901985	1.6473734504031205	0.0000000000000000	F	F	F	21.2982635234011724	9.206560372867578	6.97217908952296168	T	T	T
7.9856255765699728	1.6473734504031205	0.0000000000000000	F	F	F	17.3855275576085779	9.174621942163227907	8.1519645969914940	T	T	T
10.6475007687599632	1.6473734504031205	0.0000000000000000	F	F	F	8.37346221158357836	1.429282335059250	10.4441333878648849	T	T	T
13.3093759609499536	1.6473734504031205	0.0000000000000000	F	F	F	9.63654236483649578	1.7059276663289749	10.0775364284247519	T	T	T
15.9712511513400096	1.6473734504031205	0.0000000000000000	F	F	F	19.1160853759052117	9.1429765122661903	10.2116793746547216	T	T	T
18.631263453299343	1.6473734504031205	0.0000000000000000	F	F	F	20.6938456720952117	9.16908456252917211	9.9260942552917211	T	T	T
21.2950815375192964	1.6473734504031205	0.0000000000000000	F	F	F	7.533812632132622	9.35625443085988391	10.4380962392391122	T	T	T
2.6618751921899907	2.386381053199650	0.0000000000000000	F	F	F	7.317669742473411	2.15105297006064933	10.6038926335165726	T	T	T
7.9856255765699728	2.386381053199650	0.0000000000000000	F	F	F	11.91201809051946020	3.81395642367361	8.4142645778873568	T	T	T
5.3237503843799816	2.386381053199650	0.0000000000000000	F	F	F	13.7853067285000000	4.64261942163227907	8.1519645969914940	T	T	T
7.9856255765699728	2.386381053199650	0.0000000000000000	F	F	F	10.647500768760289	5.12482333059250	10.4441333878648849	T	T	T
10.647500768760289	2.386381053199650	0.0000000000000000	F	F	F	19.116431935199650	9.12418130931793973	10.321649863595326	T	T	T
13.3093759609499536	2.386381053199650	0.0000000000000000	F	F	F	19.116431935199650	9.12418130931793973	10.321649863595326	T	T	T
15.9712511513139493	2.386381053199650	0.0000000000000000	F	F	F	18.7088417782868832	9.117080218772999	10.321649863595326	T	T	T
1.3309759804950183	2.386381053199650	0.0000000000000000	F	F	F	18.7088417782868832	9.117080218772999	10.321649863595326	T	T	T
7.9856255765699728	2.386381053199650	0.0000000000000000	F	F	F	18.7088417782868832	9.117080218772999	10.321649863595326	T	T	T
10.647500768760289	2.386381053199650	0.0000000000000000	F	F	F	19.116431935199650	9.12418130931793973	10.321649863595326	T	T	T
13.3093759609499536	2.386381053199650	0.0000000000000000	F	F	F	18.7088417782868832	9.117080218772999	10.321649863595326	T	T	T
15.9712511513139493	2.386381053199650	0.0000000000000000	F	F	F	18.7088417782868832	9.117080218772999	10.321649863595326	T	T	T
18.631263453299343	2.386381053199650	0.0000000000000000	F	F	F	18.7088417782868832	9.117080218772999	10.321649863595326	T	T	T
21.2950815375192964	2.386381053199650	0.0000000000000000	F	F	F	18.7088417782868832	9.117080218772999	10.321649863595326	T	T	T
2.6618751921899907	2.386381053199650	0.0000000000000000	F	F	F	18.7088417782868832	9.117080218772999	10.321649863595326	T	T	T
7.9856255765699728	2.386381053199650	0.0000000000000000	F	F	F	18.7088417782868832	9.117080218772999	10.321649863595326	T	T	T
10.647500768760289	2.386381053199650	0.0000000000000000	F	F	F	19.116431935199650	9.12418130931793973	10.321649863595326	T	T	T
13.3093759609499536	2.386381053199650	0.0000000000000000	F	F	F	18.7088417782868832	9.117080218772999	10.321649863595326	T	T	T
15.9712511513139493	2.386381053199650	0.0000000000000000	F	F	F	18.7088					

18.6331263453300018	6.1473374350403116	0.0000000000000000	F	F	F	17.3246243390996995	6.9757012705460744	7.0328161099973334	T	T	T
22.6259391336149456	8.4525889731804700	0.0000000000000000	F	F	F	19.9722459786525981	6.9190321560250343	6.9942580216906531	T	T	T
6.6546879804749999	8.4525889731804700	0.0000000000000000	F	F	F	5.3388823593515706	9.2025480373817690	6.9766458964059579	T	T	T
9.3165631726650560	8.4525889731804700	0.0000000000000000	F	F	F	7.9952876711891463	9.2074394669122839	6.9861358413505701	T	T	T
11.9784383648549806	8.4525889731804700	0.0000000000000000	F	F	F	10.6387788413905730	9.2316006442781351	6.98961534246068732	T	T	T
14.6493135570450385	8.4525889731804700	0.0000000000000000	F	F	F	13.2978292199118755	9.2551188286289570	6.9584993689899060	T	T	T
17.3021887492349649	8.4525889731804700	0.0000000000000000	F	F	F	15.9582952122984238	9.2532129737194300	6.9460683692644682	T	T	T
19.9646639414250209	8.4525889731804700	0.0000000000000000	F	F	F	18.6274328140107883	9.2249784939496631	7.0891928725837576	T	T	T
23.95687672707090185	10.7578485113205449	0.0000000000000000	F	F	F	21.3008601638836055	9.2118877275809048	6.9873782745157973	T	T	T
7.9856255165697110	10.7578485113205449	0.0000000000000000	F	F	F	13.1036342421209040	4.7299886388425364	6.8436821338172553	T	T	T
10.6475007686508289	10.7578485113205449	0.0000000000000000	F	F	F	10.8462968022770818	2.2464816496923485	10.5910414246343514	T	T	T
13.309375960949536	10.7578485113205449	0.0000000000000000	F	F	F	12.16156464821168421	10.1488571687441453	7.07551557601618421	T	T	T
15.9712511513400096	10.7578485113205449	0.0000000000000000	F	F	F	12.6928655341785745	6.53641440856733618	9.8960858503124040	T	T	T
18.6331263453299332	10.7578485113205449	0.0000000000000000	F	F	F	11.9038281870107319	4.8004451473963615	10.1470051301508146	T	T	T
21.2950815375199939	10.7578485113205449	0.0000000000000000	F	F	F	10.5930719675321304	4.6582418975391171	10.5862998265816617	T	T	T
0.0000000000000000	0.0000000000000000	2.3863810053199650	F	F	F	10.0551083311344105	3.3089617122394610	10.7926482117853944	T	T	T
2.6618751912908570	0.0000000000000000	2.3863810053199650	F	F	F	14.793396118745294	3.926407374283240	8.218987531130294	T	T	T
5.323750843799816	0.0000000000000000	2.3863810053199650	F	F	F	13.877500728741534	3.7975724367269534	9.1395627239229782	T	T	T
7.985625516569703086	0.0000000000000000	2.3863810053199650	F	F	F	13.845167594795947	8.5833423356425645	10.6500004263496670	T	T	T
10.6475007687595962	0.0000000000000000	2.3863810053199650	F	F	F	16.7142664008436576	9.71025255934330882	10.6229926256212765	T	T	T
13.3093759609508211	0.0000000000000000	2.3863810053199650	F	F	F	15.77888156877618370	7.98856049617333901	13.0011453191508359	T	T	T
15.9712511513139493	0.0000000000000000	2.3863810053199650	F	F	F	10.4265946440857118468	1.2527720397579238	10.7520961527171348	T	T	T
1.3309375960950185	2.3052515318401570	2.3863810053199650	F	F	F	12.7708328776572192	1.488952927026857	9.953726144473266	T	T	T
2.6618751912908570	2.3052515318401570	2.3863810053199650	F	F	F	12.317335051889162	5.7876673044599229	9.9381986210840598	T	T	T
6.6546879804749999	2.3052515318401570	2.3863810053199650	F	F	F	9.9784816078132895	5.5446918911199231	10.7428695275924788	T	T	T
9.3165631726650570	2.3052515318401570	2.3863810053199650	F	F	F	9.016771101896419	2.3733881978369683	11.106089398331799	T	T	T
11.9784383648549824	2.3052515318401570	2.3863810053199650	F	F	F	13.7618843021027857	8.5541987554485797	9.5514385156694228	T	T	T
14.6463135570450842	2.3052515318401570	2.3863810053199650	F	F	F	13.457794464914783463	9.4933070449149635	11.0346470269418564	T	T	T
17.3021887492349613	2.3052515318401570	2.3863810053199650	F	F	F	13.2118986864858335	7.7266176032777917	11.0332211052899574	T	T	T
2.6618751912908570	2.3052515318401570	2.3863810053199650	F	F	F	16.5748891505667799	9.91726587972195	9.5302361018722586	T	T	T
5.32375084379980473	6.610503076280233	2.3863810053199650	F	F	F	17.776685727298236	9.4841076054000000	10.7726009782548758	T	T	T
7.9856255765700377	6.610503076280233	2.3863810053199650	F	F	F	16.4541571784486120	10.621714037425917	11.163017491127576	T	T	T
10.64750076876280238	6.610503076280233	2.3863810053199650	F	F	F	15.4447323496356228	8.8634159038812843	10.5686029832013997	T	T	T
13.3093759609508211	6.610503076280233	2.3863810053199650	F	F	F	16.836153580204726	7.788579285913939	13.2668825183053780	T	T	T
15.9712511513140014	6.610503076280233	2.3863810053199650	F	F	F	15.1822667240939210	7.1193760063389578	13.298901358426345	T	T	T
18.633126345329932	6.610503076280233	2.3863810053199650	F	F	F	17.3697013260192747	2.1451258378716442	9.8347337059219289	T	T	T
3.9992737596236959	6.610503076280233	2.3863810053199650	F	F	F	16.312506216384724818	10.2158560173417436	10.321506216384724818	T	T	T
6.6546879804765065	6.61057464142403914	2.3863810053199650	F	F	F	15.6215778813996128	8.30861194620951580	11.17338246689705699	T	T	T
9.3165631726649929	6.61057464142403914	2.3863810053199650	F	F	F	11.9784383648550481	1.0000000000000000	1.0000000000000000	T	C	Si
11.9784383648550481	6.61057464142403914	2.3863810053199650	F	F	F	18.631263453299982	0.0000000000000000	0.0000000000000000	Zn	C	H
14.646313557044727	6.61057464142403914	2.3863810053199650	F	F	F	16.6546879804749999	11.5262576907065000	0.0000000000000000	P	S	CO
17.3021887492349613	6.61057464142403914	2.3863810053199650	F	F	F	14.00 11 14 2 1	140 11 14 2 1	140 11 14 2 1	140 11 14 2 1	140 11 14 2 1	140 11 14 2 1
16.64750076876280237	6.61057464142403914	2.3863810053199650	F	F	F	Selective dynamics					
Cartesian											
15.9712511513139493	2.3863810053199650	2.3863810053199650	F	F	F	18.631263453299982	1.5368343587600748	0.0000000000000000	F	F	F
18.631263453299982	2.3863810053199650	2.3863810053199650	F	F	F	2.6618751921898990	1.5368343587600748	0.0000000000000000	F	F	F
21.290581015560300018	2.3863810053199650	2.3863810053199650	F	F	F	5.323750834356228	1.5368343587600748	0.0000000000000000	F	F	F
22.91061525604665	2.3863810053199650	2.3863810053199650	F	F	F	7.9856255765699711	1.5368343587600748	0.0000000000000000	F	F	F
2.68002279040842	2.3863810053199650	2.3863810053199650	F	F	F	10.647500802279040842	1.5368343587600748	0.0000000000000000	F	F	F
1.552892173841203	2.3863810053199650	2.3863810053199650	F	F	F	1.592887627970904079	1.5368343587600748	0.0000000000000000	F	F	F
10.64750076876280238	2.3863810053199650	2.3863810053199650	F	F	F	13.9928127882847373	3.8240858969082385	0.0000000000000000	F	F	F
13.5076691875199087	2.3863810053199650	2.3863810053199650	F	F	F	6.6546879804749999	3.8240858969082385	0.0000000000000000	F	F	F
16.3262330356227	2.3863810053199650	2.3863810053199650	F	F	F	1.5368243309650014	3.8240858969082385	0.0000000000000000	F	F	F
1.552892173841203	2.3863810053199650	2.3863810053199650	F	F	F	1.5368243309650014	3.8240858969082385	0.0000000000000000	F	F	F
11.9784383648549824	2.3863810053199650	2.3863810053199650	F	F	F	17.3021874472350982	3.8240858969082385	0.0000000000000000	F	F	F
14.646313557044727	2.3863810053199650	2.3863810053199650	F	F	F	12.65398813361875184	3.8240858969082385	0.0000000000000000	F	F	F
17.3021874472350982	3.8240858969082385	3.8240858969082385	F	F	F	1.5368243309650014	3.8240858969082385	0.0000000000000000	F	F	F
14.646313557044727	3.8240858969082385	3.8240858969082385	F	F	F	1.5368243309650014	3.8240858969082385	0.0000000000000000	F	F	F
17.3021874472350982	3.8240858969082385	3.8240858969082385	F	F	F	1.5368243309650014	3.8240858969082385	0.0000000000000000	F	F	F
14.646313557044727	3.8240858969082385	3.8240858969082385	F	F	F	1.5368243309650014	3.8240858969082385	0.0000000000000000	F	F	F
17.3021874472350982	3.8240858969082385	3.8240858969082385	F	F	F	1.5368243309650014	3.8240858969082385	0.0000000000000000	F	F	F
14.646313557044727	3.8240858969082385	3.8240858969082385	F	F	F	1.5368243309650014	3.8240858969082385	0.0000000000000000	F	F	F
17.3021874472350982	3.8240858969082385	3.8240858969082385	F	F	F	1.5368243309650014	3.8240858969082385	0.0000000000000000	F	F	F
14.646313557044727	3.8240858969082385	3.8240858969082385	F	F	F	1.5368243309650014	3.8240858969082385	0.0000000000000000	F	F	F
17.3021874472350982</td											

5.3237503843799798	9.2210061525604505	2.3863810053199646	F F F		0.0000000000000000	0.0000000000000000	24.5455240212800021
7.98562557657080359	9.2210061525604505	2.3863810053199646	F F F		0.0000000000000000	0.0000000000000000	24.5455240212800021
10.64750076875959597	9.2210061525604505	2.3863810053199646	F F F		0.0000000000000000	0.0000000000000000	24.5455240212800021
13.30937508905080157	9.2210061525604505	2.3863810053199646	F F F		0.0000000000000000	0.0000000000000000	24.5455240212800021
15.9712511513199404	9.2210061525604505	2.3863810053199646	F F F		0.0000000000000000	0.0000000000000000	24.5455240212800021
18.6331263453299982	9.2210061525604505	2.3863810053199646	F F F		0.0000000000000000	0.0000000000000000	24.5455240212800021
21.2950815375199087	9.2210061525604505	2.3863810053199646	F F F		0.0000000000000000	0.0000000000000000	24.5455240212800021
18.6336512179045819	1.5535116509199881	4.6692910248321411	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
2.655363488636419	1.5550564076902962	4.68033723808962352	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
5.3244226721337622	1.55499620641764	4.6811565829599537	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
7.9771629174439891	1.5475743785183376	4.6751529146047162	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
10.6530130868604095	1.53978708813957666	4.6682788013957666	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
13.294648136708253976	1.5444925712915774	4.6551278385253970	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
15.9912942795986135	1.5146680679638562	4.7125670859506954	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
19.9667733148955516	3.8511233689680164	4.6508296376254049	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
4.0026830124421568	3.85541829112808424	4.6687638128080168	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
6.6589905696181989	3.8521871936328249	4.6716058328081608	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
9.310959618515838	3.8422287421825705	4.6670370358140012	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
11.96217353555690854	3.83571501842130880	4.617966173909899	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
14.687123024571707	3.854994812370380	4.739128668213978	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
17.288039781204571707	3.8409316294219745	4.769548875432594	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
21.2956715292363299	6.1542480985183141	4.6751182661684178	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
5.33316919519689805	6.1542335899159631	4.6738478313066851	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
7.9926494275231887	6.1458178903527241	4.6755345989379830	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
10.6658594161548945	6.1388024974966791	4.6705780410823573	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
13.3629192597292636	6.1455034614325169	4.721968427653827	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
15.9668495265470786	6.1145622514275058	4.7567409649242842	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
18.63520981112648263	6.138671075124953	4.66815138478084425	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
22.6356673235735768	6.4865116606897330	4.6883485446469538	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
6.6621632005644446	4.8546434477388911	4.678289607765817	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
9.3333224106759207	4.844935663044545	4.67645377314852802	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
11.993210767267697	8.4424498902217443	4.65755720538826	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
14.6519453390938654	8.441114081813758	4.6720599933575304	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
17.3087303642305596	7.7748915454569439	4.6738822337776016	T T T		0.0000000000000000	0.0000000000000000	24.5455240212800021
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 ### POSCAR for INT25 ###

Zn C H

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6.6546879804749999 11.5262576907006000 0.0000000000000000 0.0000000000000000

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140 16 13

Selective dynamics

Cartesian

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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

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POSCAR for TS25-26

Zn C H

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0.0000000000000000 0.0000000000000000 24.5455240212799985

140 16 13

Selective dynamics

Cartesian

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2.6618751921899890 1.5368343587600748 0.0000000000000000 F F F

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7.9856255765699711 1.5368343587600748 0.0000000000000000 F F F

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POSCAR for INT26

Zn C H

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6.6546879804749999 11.5262576907006000 0.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 24.5455240212799985

140 16 13

Selective dynamics

Cartesian

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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

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140 16 13

Selective dynamics

Cartesian

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