

NO PBC

תהליך ריצה:

1. מינימיזציה

2. NVT עם תרמוסטט מ50 עד 300

3. NVT עם תרמוסטט מ300 עד 300 והוספת הפוטנציאל על רביעיות חשודות לאחר צעד זמן 1000

פרמטרים פוטנציאל:

הפעלת הפוטנציאל בכל פעם למשך 5000 צעדי זמן

ATOM1	ATOM2	F1	F2	R12
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H	O	21	1.0	1.0
C	N	21	1.0	1.5

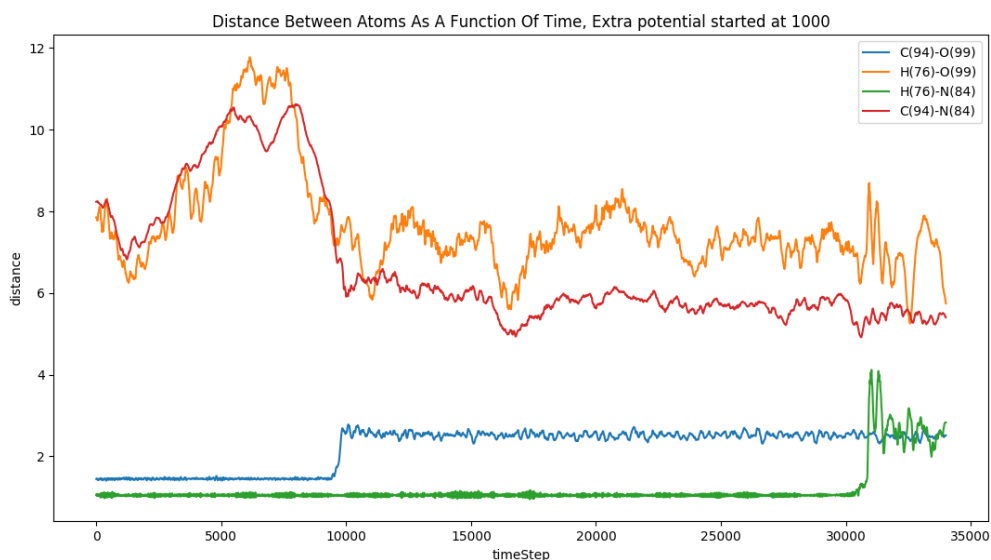
גודל תא יחידה:

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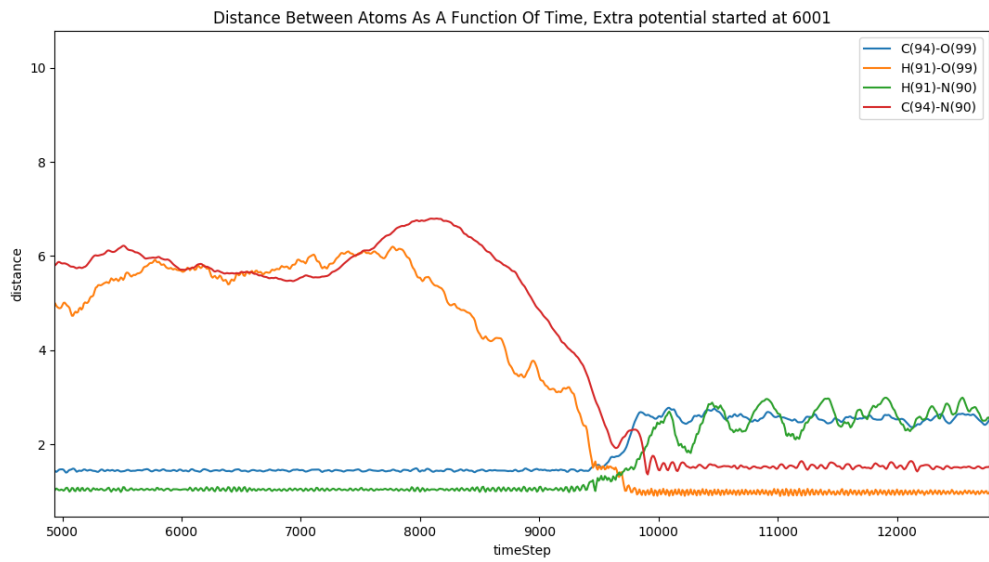
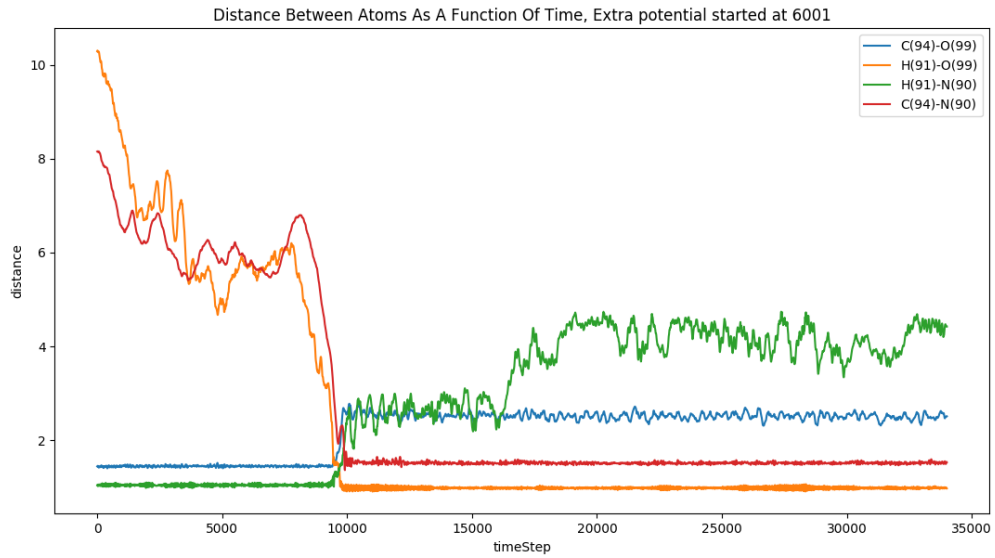
הריצה:

סה"כ 34,000 צעדי זמן. זוהו 5 רביעיות מתוכן 2 התרחשה ריאקציה.

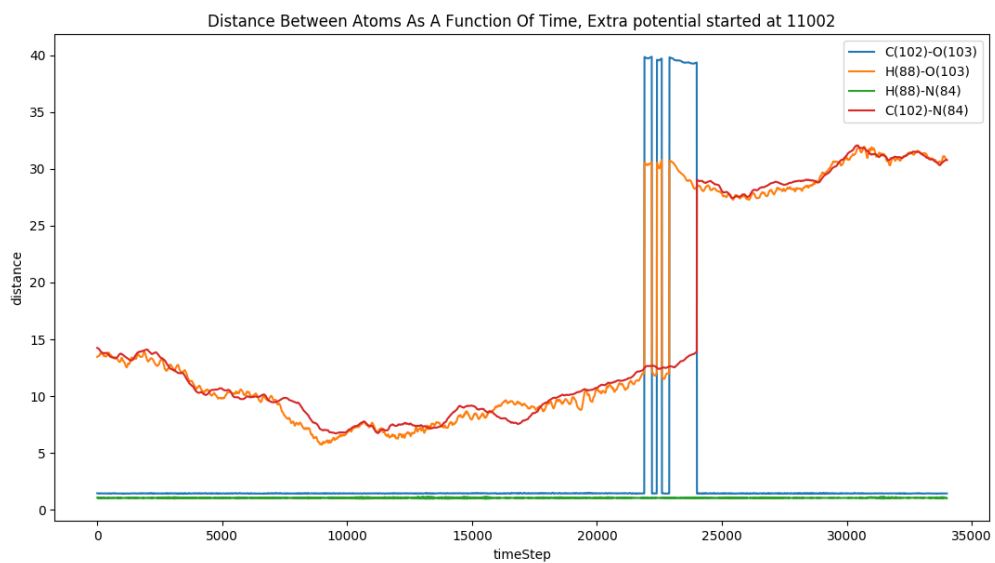
רביעייה ראשונה



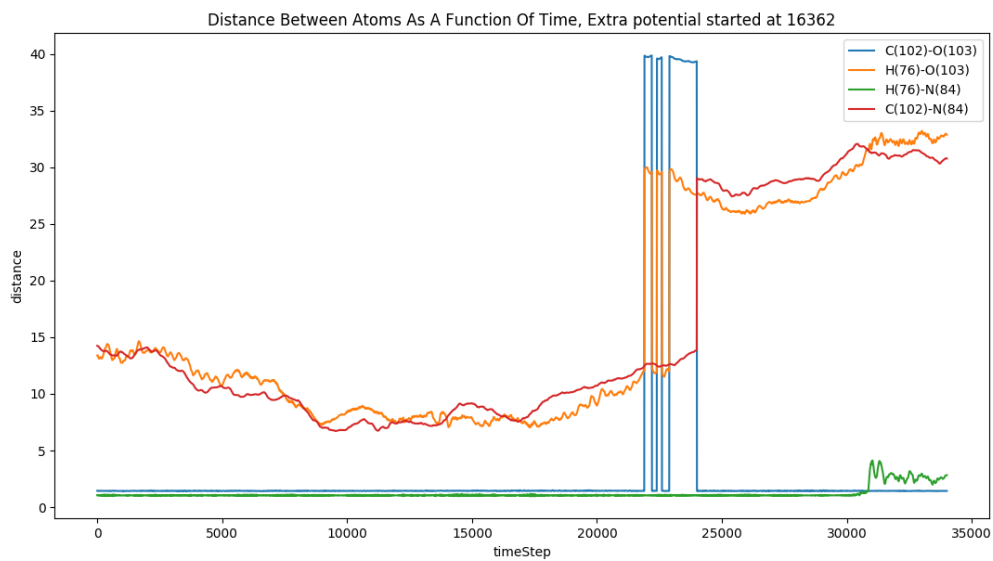
רביעייה שנייה-התרחשה ריאקציה



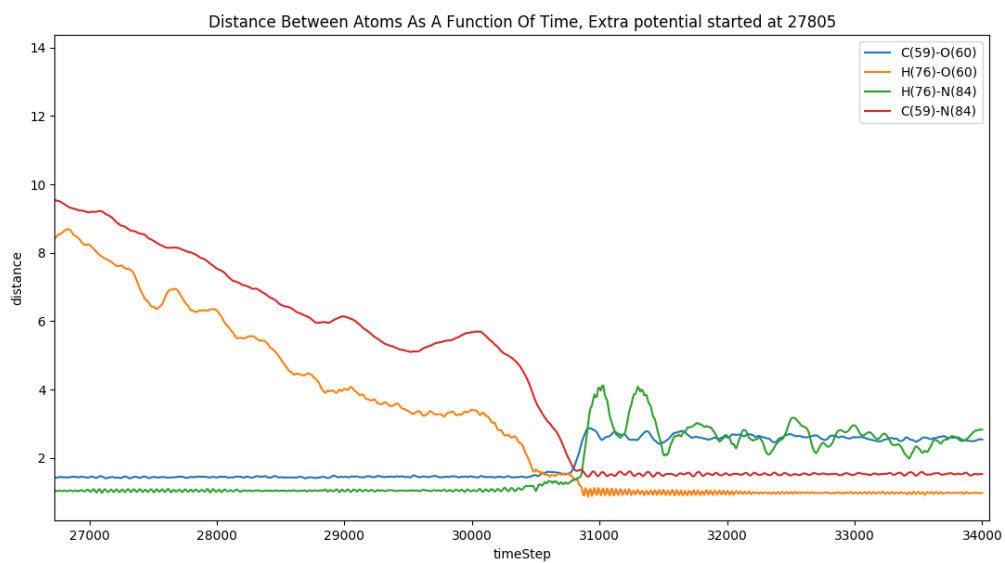
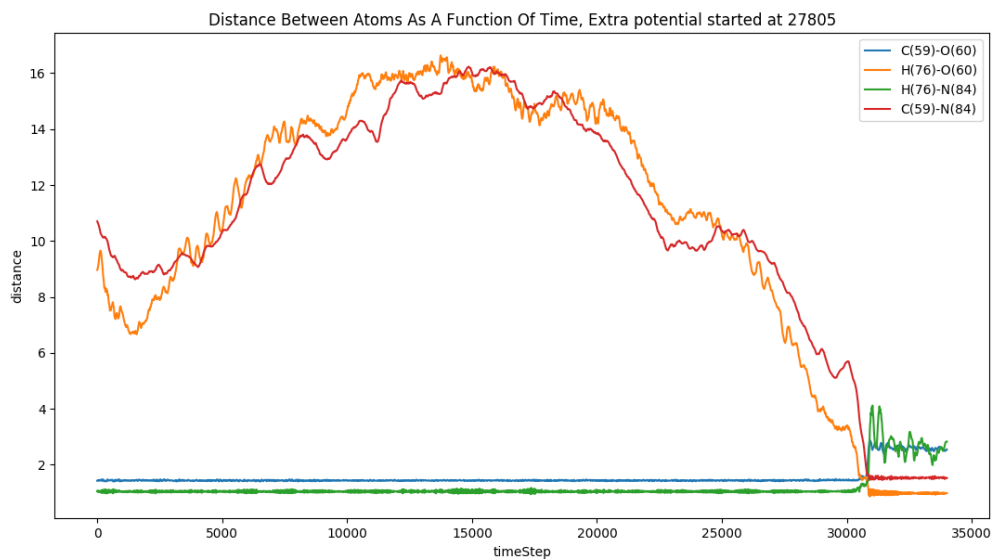
רביעייה שלישית



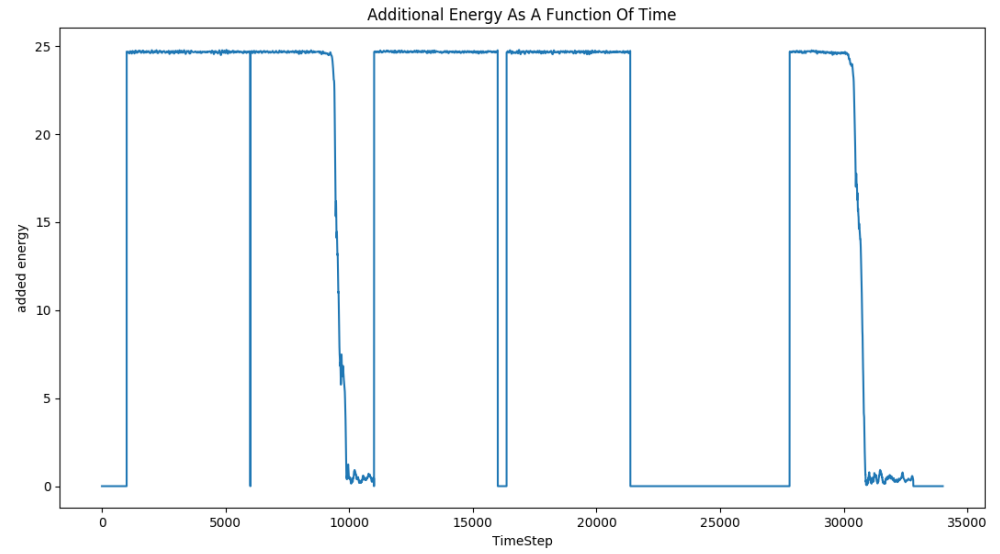
רביעייה רביעית



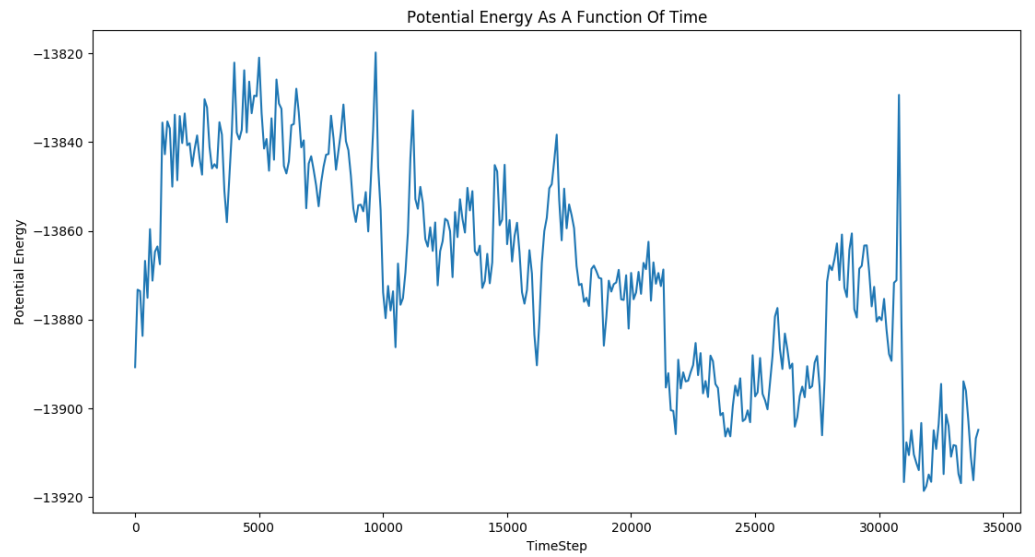
רביעייה חמישית-התרחשה ריאקציה



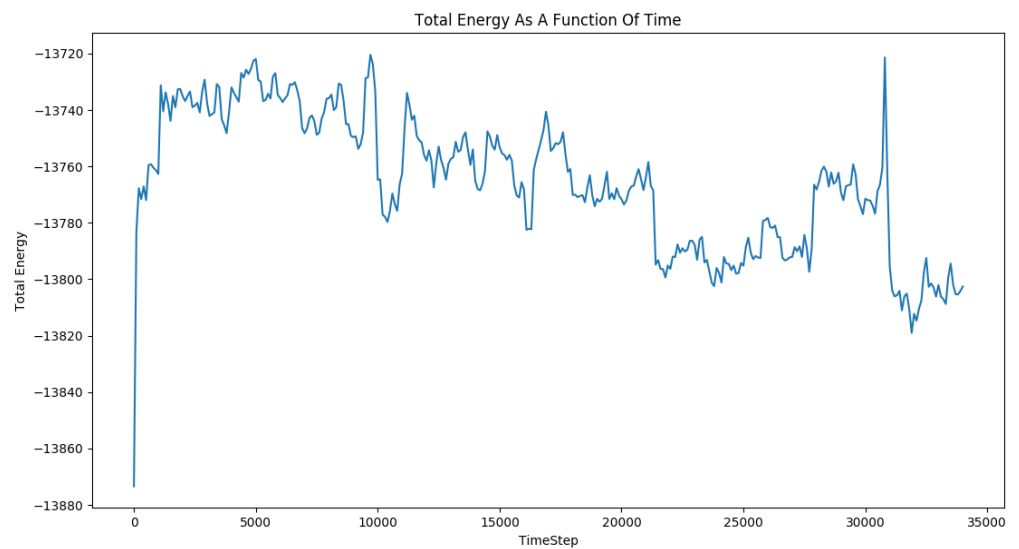
גרף אנרגיה שהפוטנציאל מוסיף כתלות בזמן



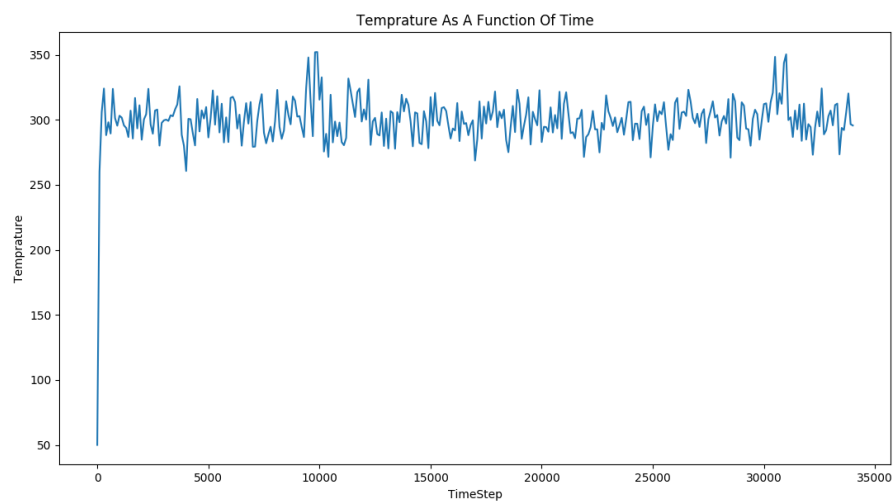
גרף אנרגיה פוטנציאלית כתלות בזמן



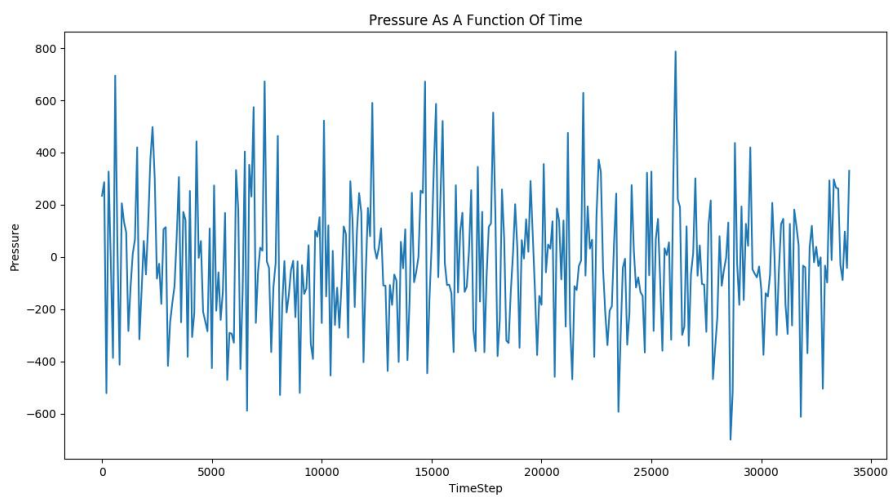
גרף סך האנרגיה כתלות בזמן



גרף טמפרטורה כתלות בזמן



גרף לחץ כתלות בזמן



קובץ SPECIES

START					
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
0	3	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
100	3	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
200	3	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
300	3	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
400	3	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
500	3	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
600	3	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
700	3	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
800	3	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
900	3	2	2	1	
Start operate potential on the #1 fourset					
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
1000	3	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
1100	3	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C11H18N2	
1200	3	2	2	1	

[illegible]

5200	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
5300	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
5400	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
5500	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
5600	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
5700	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
5800	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
5900	3	2	2	1		
End of potential on #1 fourset, start operate potential on the #2 fourset						
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
6000	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
6100	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
6200	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
6300	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
6400	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
6500	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
6600	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
6700	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
6800	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
6900	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
7000	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
7100	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
7200	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
7300	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
7400	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
7500	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
7600	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
7700	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
7800	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
7900	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
8000	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
8100	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
8200	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
8300	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
8400	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
8500	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
8600	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
8700	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
8800	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2
8900	3	2	2	1		
# Timestep		No_Moles		No_Specs	C19H20O4	C11H18N2

9000	3	2	2	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C11H18N2	
9100	3	2	2	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C11H18N2	
9200	3	2	2	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C11H18N2	
9300	3	2	2	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C11H18N2	
9400	3	2	2	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C11H18N2	
9500	3	2	2	1		
Reaction happens						
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
9600	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
9700	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
9800	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
9900	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
10000	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
10100	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
10200	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
10300	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
10400	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
10500	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
10600	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
10700	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
10800	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
10900	2	2	1	1		
End of potential on #2 fourset, start operate potential on the #3 fourset						
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
11000	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
11100	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
11200	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
11300	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
11400	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
11500	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
11600	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
11700	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
11800	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
11900	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
12000	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
12100	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
12200	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
12300	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
12400	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
12500	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	
12600	2	2	1	1		
# Timestep	No_Moles	No_Moles	No_Specs	C19H20O4	C30H38O4N2	

12700	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
12800	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
12900	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
13000	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
13100	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
13200	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
13300	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
13400	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
13500	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
13600	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
13700	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
13800	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
13900	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
14000	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
14100	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
14200	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
14300	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
14400	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
14500	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
14600	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
14700	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
14800	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
14900	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
15000	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
15100	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
15200	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
15300	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
15400	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
15500	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
15600	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
15700	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
15800	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
15900	2	2	1	1		
End of potential on #3 fourset						
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
16000	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
16100	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
16200	2	2	1	1		
start operate potential on the #4 fourset						
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		
16300	2	2	1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2		

[illegible]

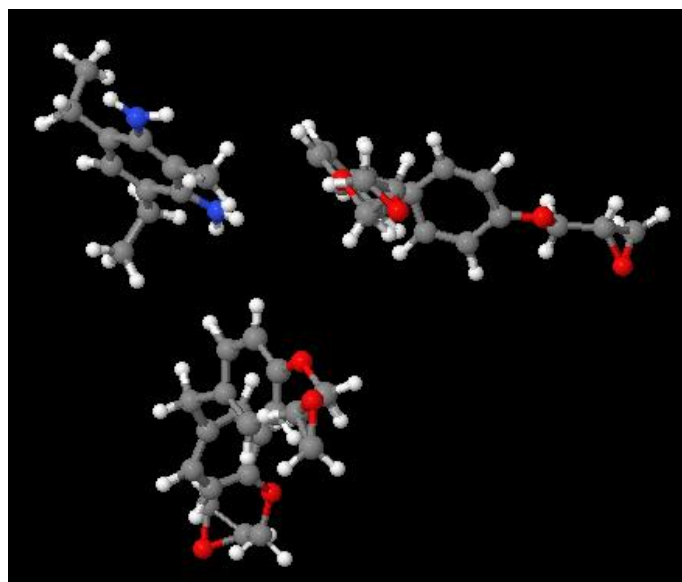
# Timestep	No_Moles	No_Specs		
20400	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
20500	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
20600	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
20700	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
20800	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
20900	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
21000	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
21100	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
21200	2	2	1	
End of potential on #4 fourset				
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
21300	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
21400	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
21500	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
21600	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
21700	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
21800	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
21900	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
22000	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
22100	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
22200	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
22300	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
22400	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
22500	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
22600	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
22700	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
22800	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
22900	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
23000	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
23100	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
23200	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
23300	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
23400	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
23500	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
23600	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
23700	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
23800	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
23900	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
24000	2	2	1	
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
24100	2	2	1	

# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
24200	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
24300	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
24400	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
24500	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
24600	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
24700	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
24800	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
24900	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
25000	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
25100	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
25200	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
25300	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
25400	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
25500	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
25600	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
25700	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
25800	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
25900	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
26000	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
26100	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
26200	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
26300	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
26400	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
26500	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
26600	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
26700	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
26800	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
26900	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
27000	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
27100	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
27200	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
27300	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
27400	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
27500	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
27600	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
27700	2 2 1	1		
start operate potential on the #5 fourset				
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
27800	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
27900	2 2 1	1		

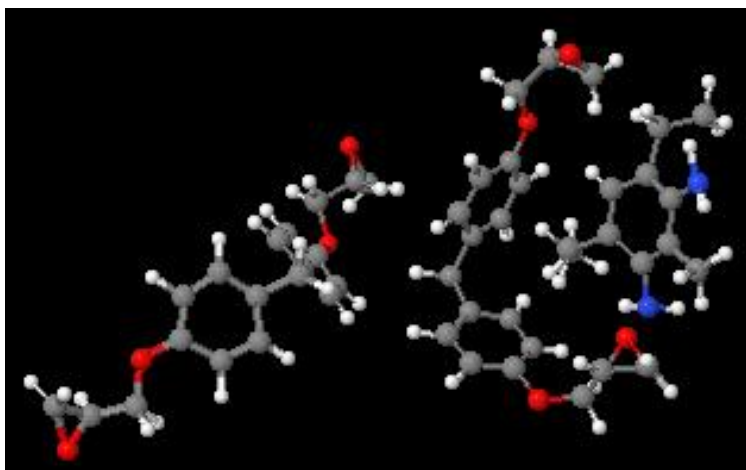
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
28000	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
28100	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
28200	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
28300	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
28400	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
28500	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
28600	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
28700	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
28800	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
28900	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
29000	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
29100	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
29200	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
29300	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
29400	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
29500	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
29600	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
29700	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
29800	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
29900	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
30000	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
30100	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
30200	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
30300	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
30400	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
30500	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
30600	2 2 1	1		
Reaction happens				
# Timestep	No_Moles	No_Specs	C49H58O8N2	
30700	1 1 1			
# Timestep	No_Moles	No_Specs	C49H58O8N2	
30800	1 1 1			
# Timestep	No_Moles	No_Specs	C49H58O8N2	
30900	1 1 1			
# Timestep	No_Moles	No_Specs	C49H58O8N2	
31000	1 1 1			
# Timestep	No_Moles	No_Specs	C49H58O8N2	
31100	1 1 1			
# Timestep	No_Moles	No_Specs	C49H58O8N2	
31200	1 1 1			
# Timestep	No_Moles	No_Specs	C49H58O8N2	
31300	1 1 1			
# Timestep	No_Moles	No_Specs	C49H58O8N2	
31400	1 1 1			
# Timestep	No_Moles	No_Specs	C49H58O8N2	
31500	1 1 1			
# Timestep	No_Moles	No_Specs	C49H58O8N2	
31600	1 1 1			
# Timestep	No_Moles	No_Specs	C49H58O8N2	
31700	1 1 1			

# Timestep	No_Moles	No_Specs	C49H58O8N2
31800	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
31900	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
32000	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
32100	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
32200	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
32300	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
32400	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
32500	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
32600	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
32700	1 1 1		
End of potential on #5 fourset			
# Timestep	No_Moles	No_Specs	C49H58O8N2
32800	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
32900	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
33000	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
33100	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
33200	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
33300	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
33400	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
33500	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
33600	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
33700	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
33800	1 1 1		
# Timestep	No_Moles	No_Specs	C49H58O8N2
33900	1 1 1		
End of run			
# Timestep	No_Moles	No_Specs	C49H58O8N2
34000	1 1 1		

מצב התחלתי (3 מולקולות)



לאחר ריאקציה ראשונה (2 מולקולות)



מצב סופי (מולקולה אחת)

