NO PBC

תהליך ריצה:

- מינימיזציה. 1
- עם תרמוסטט מ50 עד NVT. 2
- 1000 עם תרמוסטט מ300 עד 300 והוספת הפוטנציאל על רביעיות חשודות לאחר צעד זמן NVT .3

פרמטרים פוטנציאל:

הפעלת הפוטנציאל בכל פעם למשך 5000 צעדי זמן

ATOM1	ATOM2	F1	F2	R12
С	O	10.5	0.5	3.0
Н	O	21	1.0	1.0
С	N	21	1.0	1.5

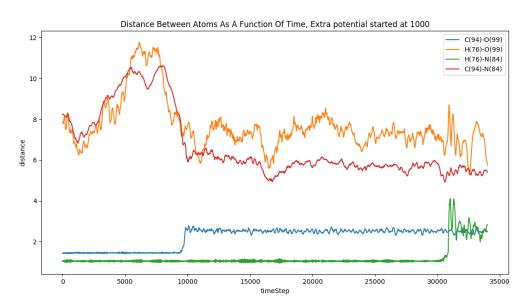
גודל תא יחידה:

xlo	xhi	ylo	yhi	zlo	zhi
-20.0	20.0	-20.0	20.0	-20.0	20.0

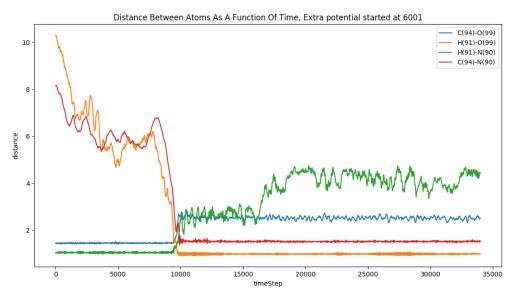
<u>הריצה:</u>

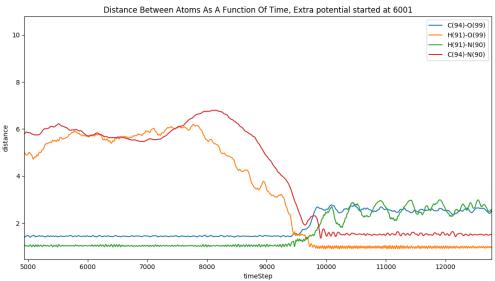
סהייכ 34,000 צעדי זמן. זוהו 5 רביעיות מתוכן 2 התרחשה ריאקציה.

רביעייה ראשונה

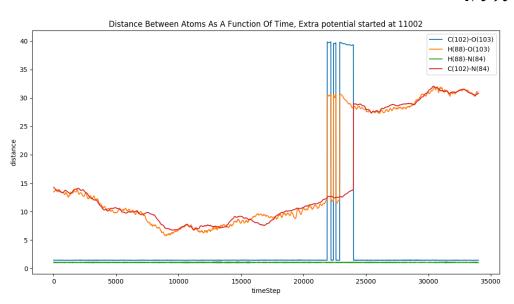


רביעייה שנייה-התרחשה ריאקציה

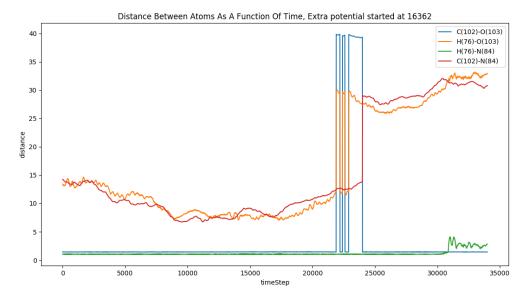




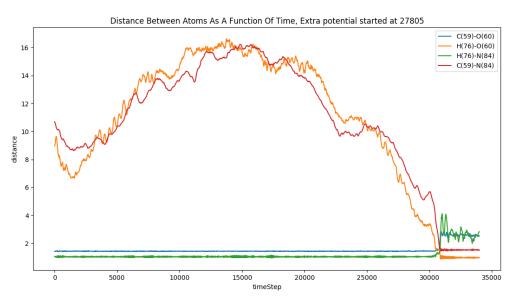
רביעייה שלישית

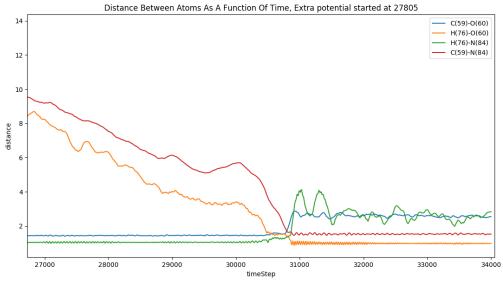


רביעייה רביעית

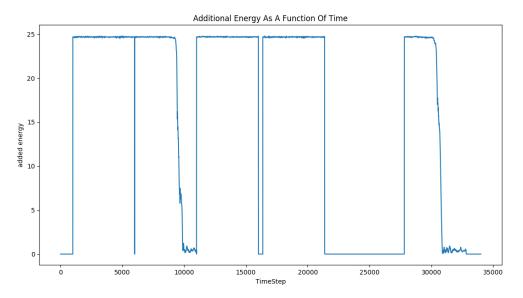


רביעייה חמישית-התרחשה ריאקציה

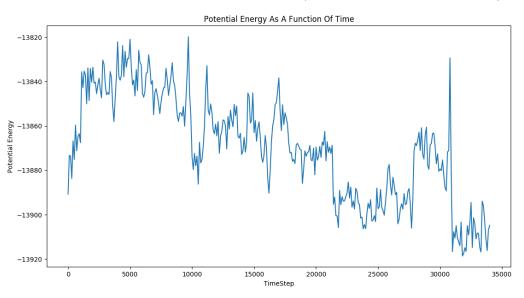




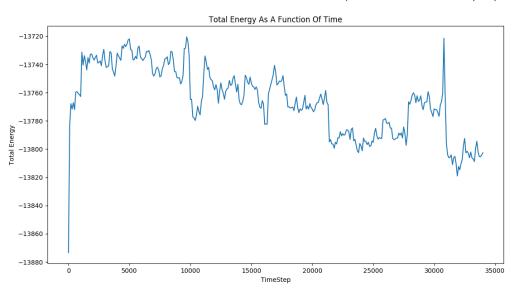
גרף אנרגיה שהפוטנציאל מוסיף כתלות בזמן



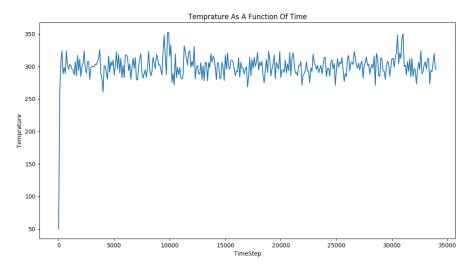
גרף אנרגיה פוטנציאלית כתלות בזמן



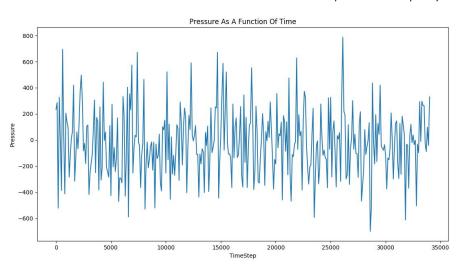
גרף סך האנרגיה כתלות בזמן



גרף טמפרטורה כתלות בזמן



גרף לחץ כתלות בזמן



SPECIES קובץ

No_Moles	No_Specs	C19H20O4	C11H18N2
2 2	1		
No_Moles	No_Specs	C19H20O4	C11H18N2
2 2	1		
No_Moles	No_Specs	C19H20O4	C11H18N2
2 2	1		
No_Moles	No_Specs	C19H20O4	C11H18N2
2 2	1		
No_Moles	No_Specs	C19H20O4	C11H18N2
2 2	1		
No_Moles	No_Specs	C19H20O4	C11H18N2
2 2	1		
No_Moles	No_Specs	C19H20O4	C11H18N2
2 2	1		
No_Moles	No_Specs	C19H20O4	C11H18N2
2 2	1		
No_Moles	No_Specs	C19H20O4	C11H18N2
2 2	1		
No_Moles	No_Specs	C19H20O4	C11H18N2
2 2	1		
ite potentia	l on the #1	fourset	
No_Moles	No_Specs	C19H20O4	C11H18N2
2	- 1		
No_Moles	No_Specs	C19H20O4	C11H18N2
2	- 1		
No_Moles	No_Specs	C19H20O4	C11H18N2
_2 2	1		
	2 2 No_Moles	2 2 1 No_Moles No_Specs 2 2 1 No_Moles No_Specs 2 2 1 No_Moles No_Specs 2 1 No_Moles No_Specs 2 2 1 tote potential on the #1 No_Moles No_Specs 2 2 1 No_Moles No_Specs 2 2 No_Moles No_Specs	2 2 1 No_Moles No_Specs C19H20O4 2 2 1 tote potential on the #1 fourset No_Moles No_Specs C19H20O4 2 2 1 No_Moles No_Specs C19H20O4

# Timestep No. 1300 3	_Moles 2 2	No_Specs 1	C19H20O4	C11H18N2
# Timestep No.		_	C19H20O4	C11H18N2
1400 3	2 2	1	~	
# Timestep No. 1500 3	_Moles 2 2	No_Specs 1	C19H20O4	C11H18N2
# Timestep No.			C19H20O4	C11H18N2
1600 3	2 2	1	GLOYYOO L	GUIVANA
# Timestep No. 1700 3	2 2	No_Specs 1	C19H20O4	C11H18N2
# Timestep No.			C19H20O4	C11H18N2
1800 3	2 2	1 N- C	C10H20O4	CHILLIANO
# Timestep No. 1900 3	2 2	No_Specs 1	C19H20O4	C11H18N2
# Timestep No	_	No_Specs	C19H20O4	C11H18N2
2000 3 # Timestep No.	2 2 Moles	1 No_Specs	C19H20O4	C11H18N2
2100 3	2 2	1	C17112004	CITITION2
# Timestep No.		— *.	C19H20O4	C11H18N2
2200 3 # Timestep No.	2 2 Moles	1 No_Specs	C19H20O4	C11H18N2
2300 3	2 2	1		
# Timestep No. 2400 3	_Moles 2 2	No_Specs	C19H20O4	C11H18N2
# Timestep No.		_	C19H20O4	C11H18N2
2500 3	2 2	1	C10H20C4	CHILIPANA
# Timestep No. 2600 3	_Moles 2 2	No_Specs 1	C19H20O4	C11H18N2
# Timestep No.	_Moles	No_Specs	C19H20O4	C11H18N2
2700 3 # Timestep No.	2 2 Moles	1 No_Specs	C19H20O4	C11H18N2
2800 3	2 2	1 1	C19H20O4	CIIIII0N2
# Timestep No.		- 1	C19H20O4	C11H18N2
2900 3 # Timestep No.	2 2 Moles	1 No_Specs	C19H20O4	C11H18N2
3000 3	2 2	1		CITITION2
# Timestep No.		-	C19H20O4	C11H18N2
3100 3 # Timestep No.	2 2 Moles	1 No_Specs	C19H20O4	C11H18N2
3200 3	2 2	1		
# Timestep No. 3300 3	_Moles 2 2	No_Specs	C19H20O4	C11H18N2
# Timestep No.		No_Specs	C19H20O4	C11H18N2
3400 3	2 2	1	C10112004	CHIHONA
# Timestep No. 3500 3	2 2	No_Specs 1	C19H20O4	C11H18N2
# Timestep No.		- 1	C19H20O4	C11H18N2
3600 3 # Timestep No.			C19H20O4	C11H18N2
3700 3	2 2	1 1	C19112004	CITITION2
# Timestep No	_	No_Specs	C19H20O4	C11H18N2
3800 3 # Timestep No.	2 2 Moles	l No_Specs	C19H20O4	C11H18N2
3900 3	2 2	1		
# Timestep No. 4000 3	_Moles 2 2	No_Specs	C19H20O4	C11H18N2
# Timestep No.		-	C19H20O4	C11H18N2
4100 3	2 2	1	C10H20C4	CHILIPANA
# Timestep No. 4200 3	_Moles 2 2	No_Specs 1	C19H20O4	C11H18N2
# Timestep No.	_Moles	No_Specs	C19H20O4	C11H18N2
4300 3 # Timestep No.	2 2 Moles	1 No_Specs	C19H20O4	C11H18N2
4400 3	2 2	No_Specs	C131120U4	C111110142
# Timestep No.	_	- 1	C19H20O4	C11H18N2
4500 3 # Timestep No	2 2 Moles	1 No_Specs	C19H20O4	C11H18N2
4600 3	2 2	1		
# Timestep No. 4700 3	_Moles 2 2	No_Specs	C19H20O4	C11H18N2
# Timestep No.		No_Specs	C19H20O4	C11H18N2
4800 3	2 2	1	C10H20C4	CHILIPANA
# Timestep No. 4900 3	_Moles 2 2	No_Specs 1	C19H20O4	C11H18N2
# Timestep No.	_Moles	- 1	C19H20O4	C11H18N2
5000 3 # Timestep No.	2 2 Moles	1 No_Specs	C19H20O4	C11H18N2
5100 3	2 2	1	C17112004	CITIION
# Timestep No.	_Moles	No_Specs	C19H20O4	C11H18N2

```
5200
# Timestep No_Moles No_Specs C19H20O4 C11H18N2
5300
      3
           2 2
                     1
                         C19H20O4
                                   C11H18N2
# Timestep No_Moles
                No_Specs
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
# Timestep No_Moles No_Specs C19H20O4 C11H18N2
5800 3 2 2
                    1
# Timestep No_Moles
                 No_Specs
                         C19H20O4 C11H18N2
5900 3 2 2
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
                     1
# Timestep No_Moles No_Specs
                         C19H20O4
                                   C11H18N2
6500 3
         2 2
                     1
                         C19H20O4 C11H18N2
# Timestep No_Moles
                 No_Specs
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
                     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
                 No_Specs C19H20O4
                                   C11H18N2
# Timestep No_Moles
7400 3 2 2
                    1
# Timestep No_Moles No_Specs C19H20O4 C11H18N2
7500
           2 2
                     1
# Timestep No_Moles No_Specs 7600 3 2 2 1
                         C19H20O4
                                   C11H18N2
# Timestep No_Moles
                 No_Specs
                         C19H20O4 C11H18N2
7700 3
                     1
# Timestep No_Moles No_Specs C19H20O4 C11H18N2
         2. 2.
7800 3
                     1
# Timestep No_Moles
                No_Specs
                         C19H20O4
                                   C11H18N2
7900 3 2 2
                     1
                No_Specs C19H20O4 C11H18N2
# Timestep No_Moles
8000 3 2 2
                     1
# Timestep No_Moles No_Specs
                         C19H20O4
                                   C11H18N2
         2 2
8100 3
                     1
# Timestep No_Moles
                No_Specs
                         C19H20O4
                                   C11H18N2
8200 3 2 2
                     1
# Timestep No_Moles
                                   C11H18N2
                 No_Specs
                         C19H20O4
8300 3
         2 2
                     1
# Timestep No_Moles
                 No_Specs C19H20O4 C11H18N2
8400 3
         2 2
# Timestep No_Moles
                 No_Specs C19H20O4
                                   C11H18N2
8500 3 2 2
                     - 1
# Timestep No_Moles
                 No_Specs C19H20O4 C11H18N2
8600
                     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
                 No_Specs C19H20O4 C11H18N2
# Timestep No_Moles
8900 3
           2 2
                     1
# Timestep No_Moles No_Specs C19H20O4 C11H18N2
```

```
9000
# Timestep No_Moles No_Specs C19H20O4 C11H18N2
9100 3 2 2
                           1
# Timestep No_Moles No_Specs C19H20O4
                                             C11H18N2
9200 3 2 2
                           1
# Timestep No_Moles
                     No_Specs C19H20O4
                                             C11H18N2
9300 3 2 2
                           1
# Timestep No_Moles
                     No_Specs C19H20O4
                                            C11H18N2
9400 3 2 2
                           1
# Timestep No_Moles
9500 3 2 2
                      No_Specs C19H20O4
                                             C11H18N2
Reaction happens
# Timestep No_Moles No_Specs C19H20O4 C30H38O4N2 9600 2 2 1 1
# Timestep No_Moles No_Specs C19H20O4
                                             C30H38O4N2
9700 2 2 1
                           1
# Timestep No_Moles No_Specs C19H20O4
                                             C30H38O4N2
9800 2 2 1
                           1
# Timestep No_Moles No_Specs C19H20O4
                                             C30H38O4N2
9900 2 2 1
                           1
# Timestep No_Moles No_Specs C19H20O4 C30H38O4N2 10000 2 2 1 \, 1
# Timestep No_Moles No_Specs C19H20O4
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4 C30H38O4N2 10200 2 2 1 1
# Timestep No_Moles No_Specs C19H20O4 10300 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4 10400 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4 C30H38O4N2 10500 2 2 1 1
# Timestep No_Moles No_Specs C19H20O4 10600 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4
10700 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4 10800 2 2 1 1
                                             C30H38O4N2
# Timestep 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_Specs C19H20O4 11000 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4
11100 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4
11200 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4 11300 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4 11400 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4
11500 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles 11600 2 2 1
                     No_Specs C19H20O4
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4
11700 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4 C30H38O4N2 11800 2 2 1 1
# Timestep No_Moles No_Specs C19H20O4
11900 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles
12000 2 2 1
                      No_Specs
                                C19H20O4
                                             C30H38O4N2
                          1
# Timestep No_Moles No_Specs C19H20O4 C30H38O4N2 12100 2 2 1 1
# Timestep No_Moles
12200 2 2 1
                     No_Specs C19H20O4
                                             C30H38O4N2
                           1
# Timestep No_Moles No_Specs C19H20O4 12300 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4
12400 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles No_Specs C19H20O4 12500 2 2 1 1
                                             C30H38O4N2
# Timestep No_Moles
12600 2 2 1
                               C19H20O4
                                             C30H38O4N2
                      No_Specs
                           1
# Timestep No_Moles
                      No_Specs
                                 C19H20O4
                                             C30H38O4N2
```

12700 2 2 # Timestep No_M	2 1 1 loles No_Specs	C19H20O4	C30H38O4N2
	2 1 1	C19H20O4	C30H38O4N2
12900 2 2 # Timestep No_M	2 1 1	C19H20O4	C30H38O4N2
13000 2 2 # Timestep No_M	2 1 1 loles No_Specs	C19H20O4	C30H38O4N2
# Timestep No_M	- 1	C19H20O4	C30H38O4N2
# Timestep No_M	- 1	C19H20O4	C30H38O4N2
# Timestep No_M	- 1	C19H20O4	C30H38O4N2
# Timestep No_M		C19H20O4	C30H38O4N2
# Timestep No_M	2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	C19H20O4	C30H38O4N2
# Timestep No_M		C19H20O4	C30H38O4N2
# Timestep No_M		C19H20O4	C30H38O4N2
# Timestep No_M		C19H20O4	C30H38O4N2
# Timestep No_M		C19H20O4	C30H38O4N2
# Timestep No_M		C19H20O4	C30H38O4N2
	2 1 1	C19H20O4	C30H38O4N2
	2 1 1	C19H20O4	C30H38O4N2
	2 1 1	C19H20O4	C30H38O4N2
	2 1 1	C19H20O4	C30H38O4N2
	2 1 1	C19H20O4	C30H38O4N2
	2 1 1	C19H20O4	C30H38O4N2
# Timestep No_M 14800 2 2 # Timestep No_M	2 1 1	C19H20O4 C19H20O4	C30H38O4N2 C30H38O4N2
	2 1 1	C19H20O4	C30H38O4N2
	2 1 1		C30H38O4N2
	2 1 1	C19H20O4	C30H38O4N2
	2 1 1	C19H20O4	C30H38O4N2
	2 1 1	C19H20O4	C30H38O4N2
15400 2 2 # Timestep No_M	2 1 1 loles No_Specs	C19H20O4	C30H38O4N2
# Timestep No_M	- 1	C19H20O4	C30H38O4N2
# Timestep No_M		C19H20O4	C30H38O4N2
# Timestep No_M	- 1	C19H20O4	C30H38O4N2
# Timestep No_M	2 1 1 1 loles No_Specs 2 1 1	C19H20O4	C30H38O4N2
# Timestep No_M		C19H20O4	C30H38O4N2
# Timestep No_M		C19H20O4	C30H38O4N2
# Timestep No_M		C19H20O4	C30H38O4N2
		formest	
# Timestep No_M 16300 2		C19H20O4	C30H38O4N2
# Timestep No_M		C19H20O4	C30H38O4N2

16400	2 2 1	1		
	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
16500	2 2 1	1		
	No_Moles 2 2 1	No_Specs 1	C19H20O4	C30H38O4N2
	No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1	1 N- C	C10112004	C20H29O4N2
	No_Moles 2 2 1	No_Specs	C19H20O4	C30H38O4N2
	No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	I No_Specs	C19H20O4	C30H38O4N2
17000	2 2 1	1		
# Timestep 17100	No_Moles 2 2 1	No_Specs	C19H20O4	C30H38O4N2
	No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1	1	C10112004	C201/200 (N/2
	No_Moles 2 2 1	No_Specs	C19H20O4	C30H38O4N2
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
17500	2 2 1	1	C1711200+	C3011300-112
_	No_Moles 2 2 1	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
17700	2 2 1	1	G10770001	G201720.0 (172
	No_Moles 2 2 1	No_Specs	C19H20O4	C30H38O4N2
	No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	1 No_Specs	C19H20O4	C20U29O4N2
	2 2 1	1	C19H20O4	C30H38O4N2
	No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
18200	2 2 1	1		
	No_Moles 2 2 1	No_Specs	C19H20O4	C30H38O4N2
	No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No Space	C19H20O4	C30H38O4N2
	2 2 1	No_Specs	C19H20O4	C30H30O4N2
# Timestep	_	No_Specs	C19H20O4	C30H38O4N2
18600 # Timestep	2 2 1 No_Moles	l No_Specs	C19H20O4	C30H38O4N2
18700	2 2 1	1		
# Timestep 18800	No_Moles 2 2 1	No_Specs	C19H20O4	C30H38O4N2
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
18900 # Timestep	2 2 1	1 No_Specs	C19H20O4	C30H38O4N2
	No_Moles 2 2 1	No_specs	C19H20O4	C30H30O4N2
# Timestep		No_Specs	C19H20O4	C30H38O4N2
19100 # Timestep	2 2 1 No Moles	1 No_Specs	C19H20O4	C30H38O4N2
19200	2 2 1	1		
# Timestep 19300	No_Moles 2 2 1	No_Specs	C19H20O4	C30H38O4N2
# Timestep		No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No Moles	No Space	C10H20O4	C20U29O4N2
	2 2 1	No_Specs 1	C19H20O4	C30H38O4N2
	No_Moles	No_Specs	C19H20O4	C30H38O4N2
19600 # Timestep	2 2 1 No_Moles	I No_Specs	C19H20O4	C30H38O4N2
19700	2 2 1	1		
# Timestep 19800	No_Moles 2 2 1	No_Specs	C19H20O4	C30H38O4N2
	No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1	1 No Space	C10112004	C201129Q4N/2
# Timestep 20000	No_Moles 2 2 1	No_Specs	C19H20O4	C30H38O4N2
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No Moles	No Specs	C19H20O4	C30H38O4N2
20200	2 2 1	1		
# Timestep	No_Moles	No_Specs	C19H20O4	C30H38O4N2
# Timestep 20200	2 2 1	No_Specs	C19H20O4	C30H38O4N2

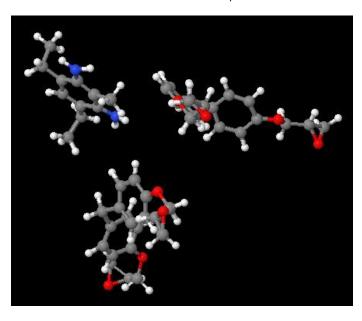
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-	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
20700 # Timestep	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
20800 # Timestep	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
20900 # Timestep	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
21000 # Timestep	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
21100 # Timestep	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
21200	2 2 1	1		
	otential on #4	fourset		
	No_Moles	No_Specs	C19H20O4	C30H38O4N2
	No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
_	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
# Timestep	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
-	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
# Timestep	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
	2 2 1 No_Moles	No_Specs	C19H20O4	C30H38O4N2
24000 # Timestep	_	No_Specs	C19H20O4	C30H38O4N2
24100	2 2 1	1		

# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
24200 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
24300 2 2 1	1	017112001	0.5011.500 17.2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
24400 2 2 1	l No Smaas	C10H20O4	C201129 O 4N2
# Timestep No_Moles 24500 2 2 1	No_Specs	C19H20O4	C30H38O4N2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
24600 2 2 1	1		
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
24700 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
24800 2 2 1	1	017112001	0.5011.500 17.2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
24900 2 2 1	1	G10H2004	C201120 O AV2
# Timestep No_Moles 25000 2 2 1	No_Specs 1	C19H20O4	C30H38O4N2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
25100 2 2 1	1		
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
25200 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
25300 2 2 1	1 1	C19112004	C301130O41V2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
25400 2 2 1	1	CIOTICO C	C201/200 (A/2
# Timestep No_Moles 25500 2 2 1	No_Specs	C19H20O4	C30H38O4N2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
25600 2 2 1	1		
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
25700 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
25800 2 2 1	No_specs	C19H20O4	C30H36O4N2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
25900 2 2 1	1	G10770001	GAONAGO INA
# Timestep No_Moles 26000 2 2 1	No_Specs	C19H20O4	C30H38O4N2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
26100 2 2 1	1		
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
26200 2 2 1 # Timestep No_Moles	I No_Specs	C19H20O4	C30H38O4N2
26300 2 2 1	1 1	C19112004	C301130O41V2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
26400 2 2 1	1	G10770001	G0077000 DV0
# Timestep No_Moles 26500 2 2 1	No_Specs	C19H20O4	C30H38O4N2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
26600 2 2 1	1		
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
26700 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
26800 2 2 1	No_specs	C171120U4	COULDOOTIVE
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
26900 2 2 1	1 N- C	C10112004	C201129Q4N12
# Timestep No_Moles 27000 2 2 1	No_Specs 1	C19H20O4	C30H38O4N2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
27100 2 2 1	1		
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
27200 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
27300 2 2 1	No_specs	C171120U4	C3011300-7172
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
27400 2 2 1	1	C10112001	C201/200 (N)2
# Timestep No_Moles 27500 2 2 1	No_Specs	C19H20O4	C30H38O4N2
# 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 f	ourset	
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
27800 2 2 1	1		
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
27900 2 2 1	1		

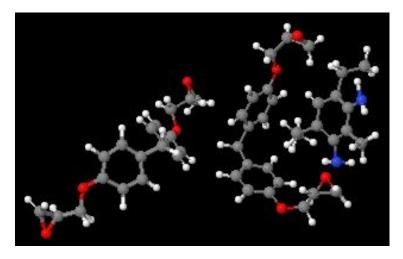
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# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
28100 2 2 1	1	01711200.	
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
28200 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C20H28O4N2
28300 2 2 1	No_specs	C19H20O4	C30H38O4N2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
28400 2 2 1	1	G10770001	G20372000 0372
# Timestep No_Moles 28500 2 2 1	No_Specs	C19H20O4	C30H38O4N2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
28600 2 2 1	1		
# Timestep No_Moles 28700 2 2 1	No_Specs	C19H20O4	C30H38O4N2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
28800 2 2 1	1		
# Timestep No_Moles 28900 2 2 1	No_Specs	C19H20O4	C30H38O4N2
28900 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
29000 2 2 1	1		
# Timestep No_Moles 29100 2 2 1	No_Specs	C19H20O4	C30H38O4N2
29100 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
29200 2 2 1	1		
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
29300 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
29400 2 2 1	1		
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
29500 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
29600 2 2 1	1	C17112004	C30130041V2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
29700 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
29800 2 2 1	1	C17112004	C30113004112
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
29900 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
30000 2 2 1	No_specs	C19H20O4	C30H36O4IN2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
30100 2 2 1 # Timestep No_Moles	1 No_Specs	C19H20O4	C30H38O4N2
30200 2 2 1	No_specs	C19H20O4	C30H36O4IN2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
30300 2 2 1		C10H20O4	C201129C4N2
# Timestep No_Moles 30400 2 2 1	No_Specs	C19H20O4	C30H38O4N2
# Timestep No_Moles	No_Specs	C19H20O4	C30H38O4N2
30500 2 2 1 # Timesten No Moles	1 No. Carre	C10112004	C20H29O4N2
# Timestep No_Moles 30600 2 2 1	No_Specs	C19H20O4	C30H38O4N2
	•		
Reaction happens	No. C.	CANTIERON	
# Timestep No_Moles 30700 1 1 1	No_Specs	C49H58O8N	<u> </u>
# Timestep No_Moles	No_Specs	C49H58O8N	2
30800 1 1 1	•		
# Timestep No_Moles 30900 1 1 1	No_Specs	C49H58O8N	2
# Timestep No_Moles	No_Specs	C49H58O8N	2
31000 1 1 1	•		
# Timestep No_Moles 31100 1 1 1	No_Specs	C49H58O8N	2
31100 1 1 1 # Timestep No_Moles	No_Specs	C49H58O8N2	2
31200 1 1 1	•		
# Timestep No_Moles	No_Specs	C49H58O8N	2
31300 1 1 1 # Timestep No_Moles	No_Specs	C49H58O8N	2
31400 1 1 1	•		
# Timestep No_Moles	No_Specs	C49H58O8N	2
31500 1 1 1 # Timestep No_Moles	No_Specs	C49H58O8N	2
31600 1 1 1	•		
# Timestep No_Moles	No_Specs	C49H58O8N	2
31700 1 1 1			

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# Timestep No_Moles
31800 1 1 1
                         No_Specs C49H58O8N2
# Timestep No_Moles No_Specs C49H58O8N2
31900 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2 32000 1 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2 32100 1 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2 32200 1 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2 32300 1 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2 32400 1 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2
32500 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2 32600 1 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2 32700 1 1 1 1
End of potential on #5 fourset
# Timestep No_Moles No_Specs C49H58O8N2 32800 1 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2 32900 1 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2
33000 1 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2
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33200 1 1 1
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# Timestep No_Moles No_Specs C49H58O8N2
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# Timestep No_Moles No_Specs C49H58O8N2 33600 1 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2 33700 1 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2
33800 1 1 1
# Timestep No_Moles No_Specs C49H58O8N2
33900 1 1 1 1
End of run
# Timestep No_Moles No_Specs C49H58O8N2
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מצב התחלתי (3 מולקולות)



לאחר ריאקציה ראשונה (2 מולקולות)



מצב סופי (מולקולה אחת)

