תהליך ריצה:

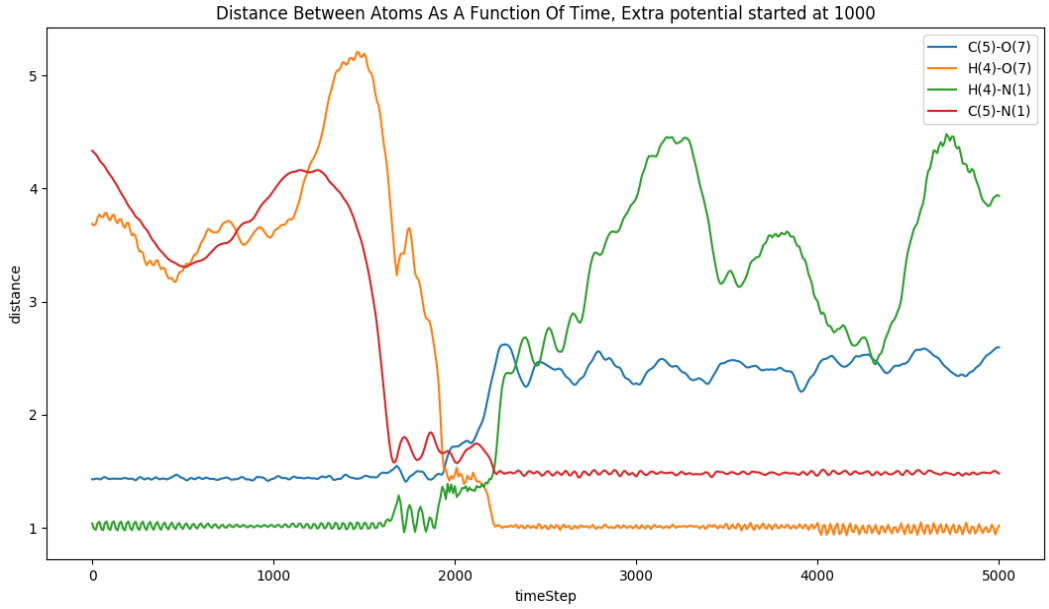
1. מינימיזציה
2. NVT עם תרמוסטט מ50 עד 300
3. ~~NVT עם תרמוסטט מ300 עד 300~~(הרחיק בין המולקולות ולכן הורדתי את השלב הזה)
4. הוספת הפוטנציאל על רביעיות חשודות לאחר צעד זמן 1000, NVT עם תרמוסטט מ300 עד 300

ריצה 1-אפוקסי ואמוניה (סה"כ 11 אטומים)

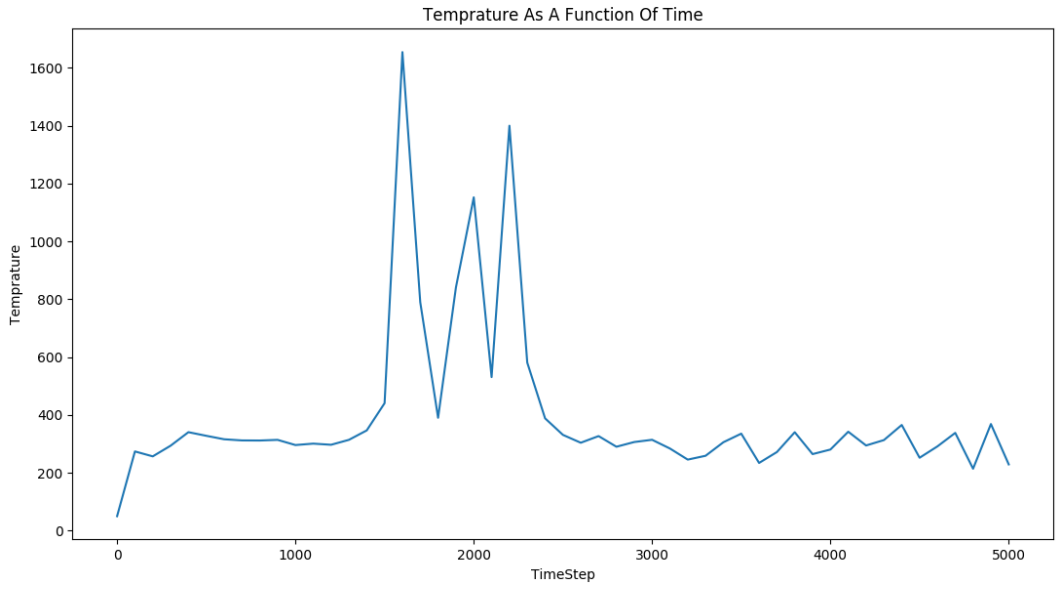
ריצה של 5,000 צעדי זמן, לאחר 1000 צעדי זמן חיפוש אחר רביעייה חשודה והפעלת הפוטנציאל למשך 3000 צעדי זמן עליה עם הפרמטרים:

TYPE1	TYPE2	F1	F2	R12
C	O	2.5	0.5	1.95
O	H	12.5	0.75	1.1
C	N	15	0.75	1.5

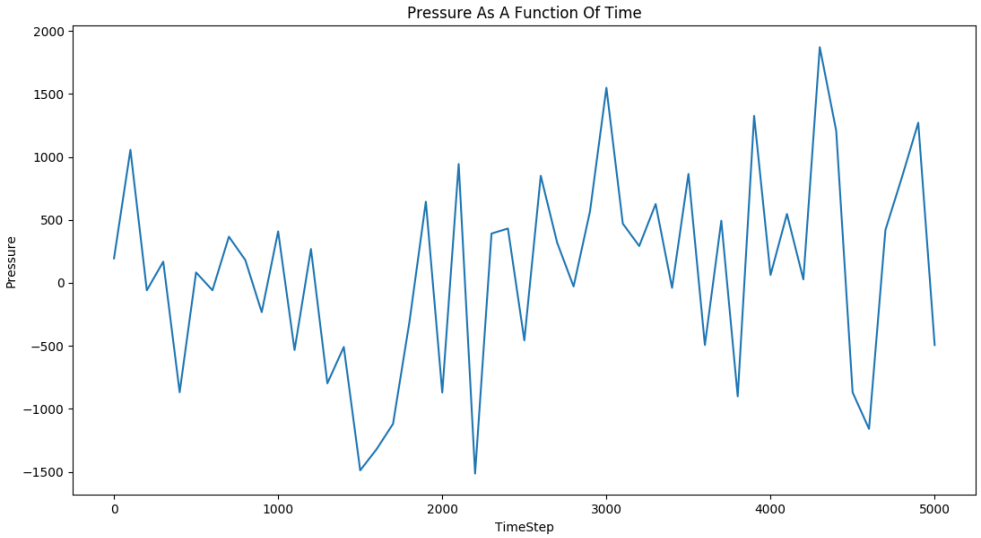
בצעד זמן 1000 נמצאה רביעייה אחת חשודה שהגיעה לריאקציה



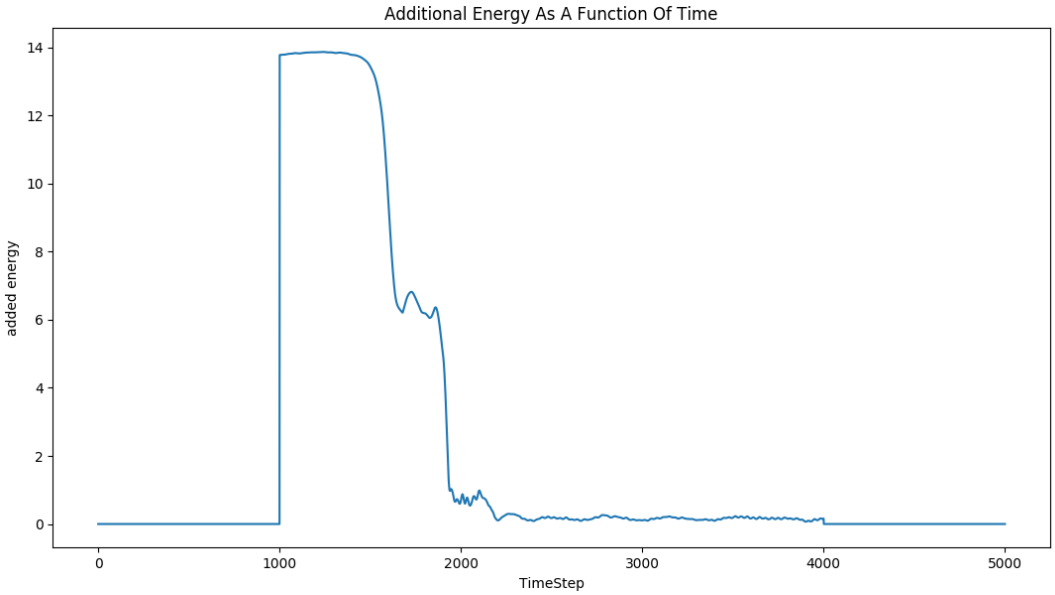
גרף טמפרטורה כתלות בזמן



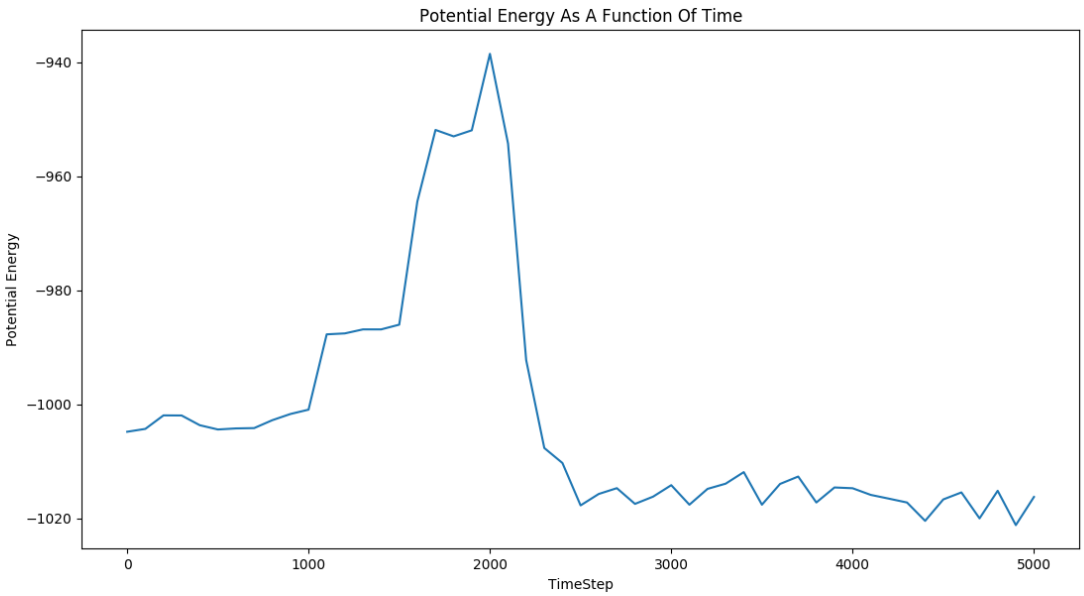
גרף של לחץ כתלות בזמן



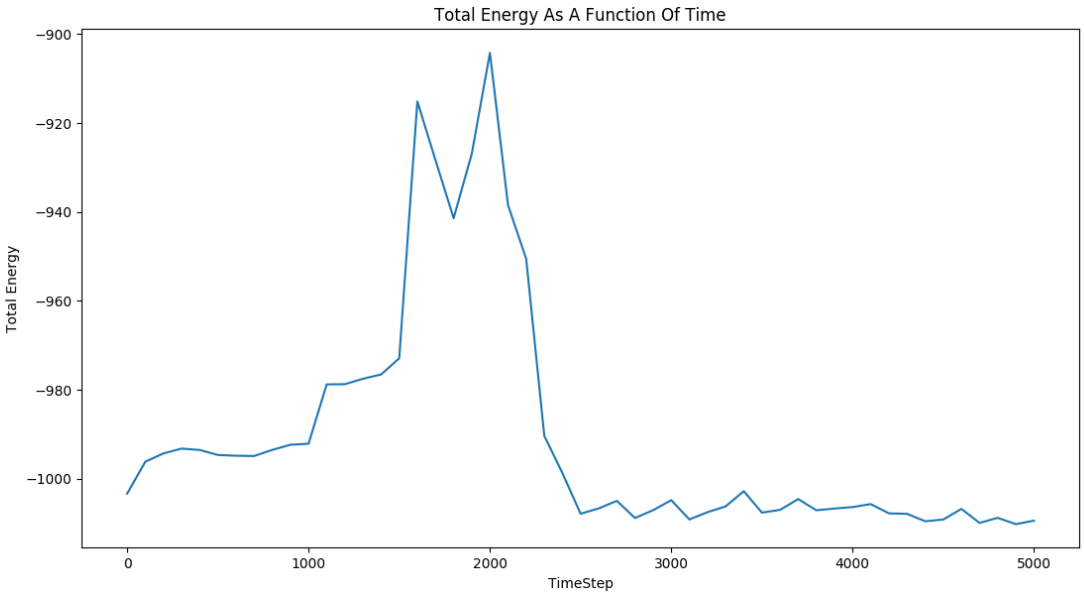
גרף של האנרגיה שהפוטנציאל הוסיף כתלות בזמן



גרף אנרגיה פוטנציאלית כתלות בזמן



גרף סך האנרגיה כתלות בזמן

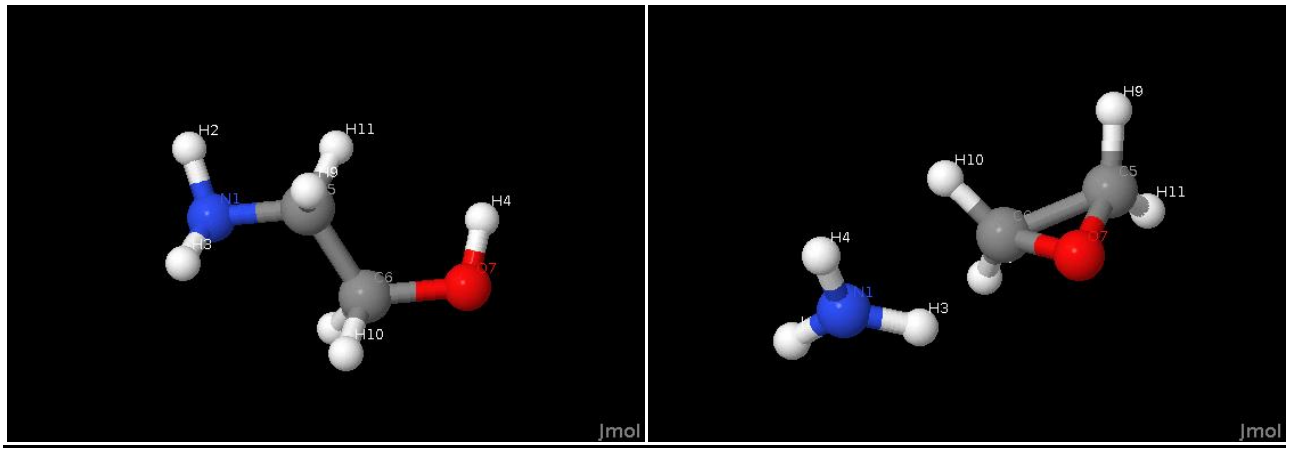


קובץ SPECIES.OUT

```
# Timestep    No_Moles    No_Specs    H3N    C2H4O
100    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
200    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
300    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
400    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
500    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
600    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
700    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
800    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
900    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
1000    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
1100    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
1200    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
1300    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
1400    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
1500    2    2    1    1
# Timestep    No_Moles    No_Specs    H3N    C2H4O
1600    2    2    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
1700    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
1800    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
1900    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
2000    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
2100    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
2200    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
2300    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
2400    1    1    1
```

```
# Timestep    No_Moles    No_Specs    C2H7ON
2500    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
2600    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
2700    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
2800    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
2900    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
3000    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
3100    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
3200    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
3300    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
3400    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
3500    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
3600    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
3700    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
3800    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
3900    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
4000    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
4100    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
4200    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
4300    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
4400    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
4500    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
4600    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
4700    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
4800    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
4900    1    1    1
# Timestep    No_Moles    No_Specs    C2H7ON
5000    1    1    1
```

ציור קבצי DUMP הראשון והאחרון בmolviewer

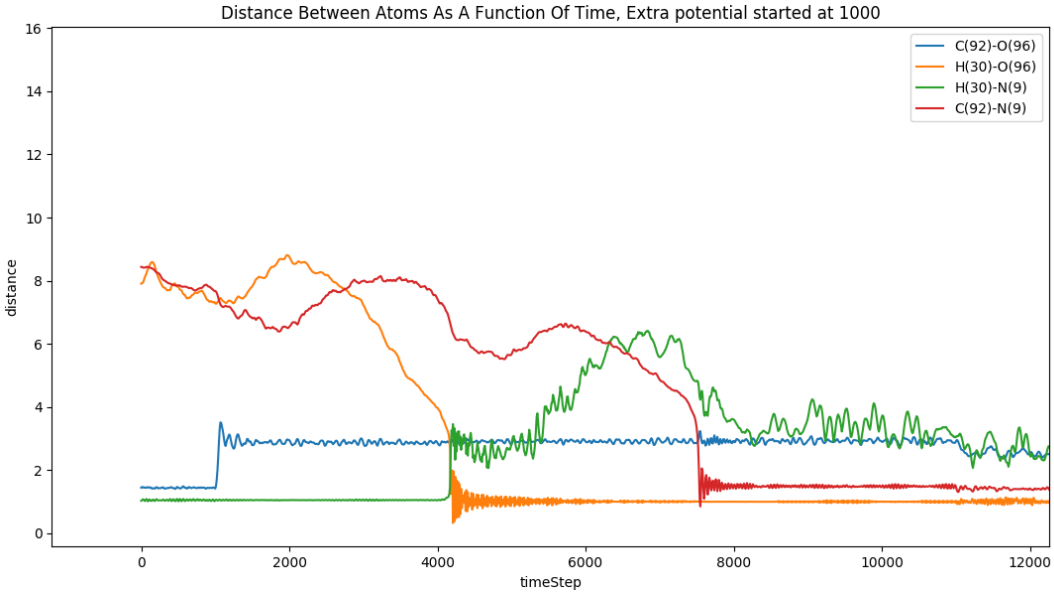


ריצה 2- המולקולות הגדולות (סה"כ 117 אטומים)

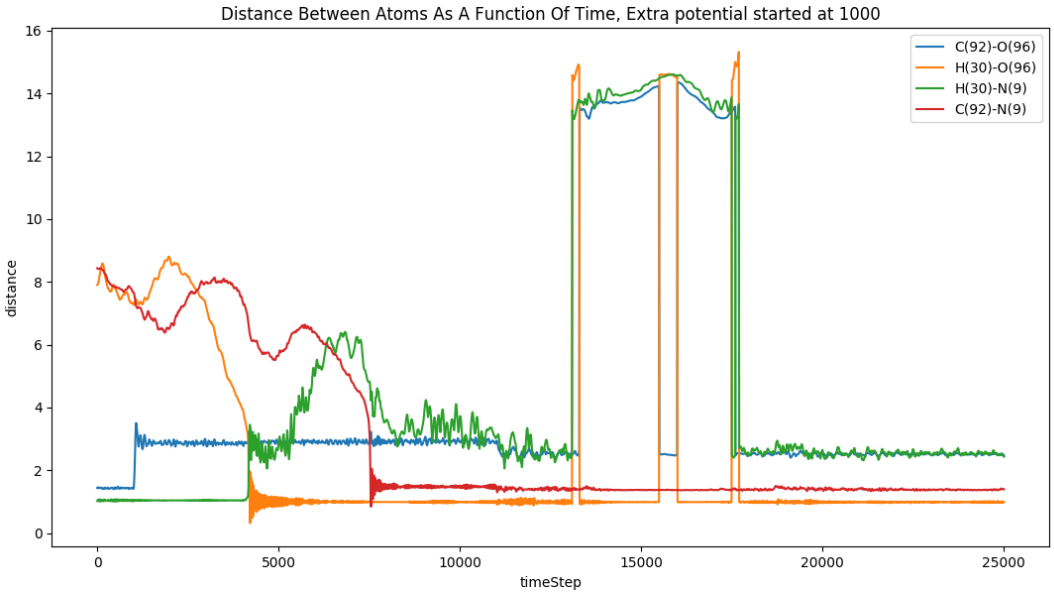
ריצה של 25,000 צעדי זמן, הפעלת הפוטנציאל בכל פעם למשך 10,000 צעדי זמן על רביעייה חשודה עם הפרמטרים:

TYPE1	TYPE2	F1	F2	R12
C	O	70	0.5	3.0
O	H	140	1.0	1.0
C	N	140	1.0	1.5

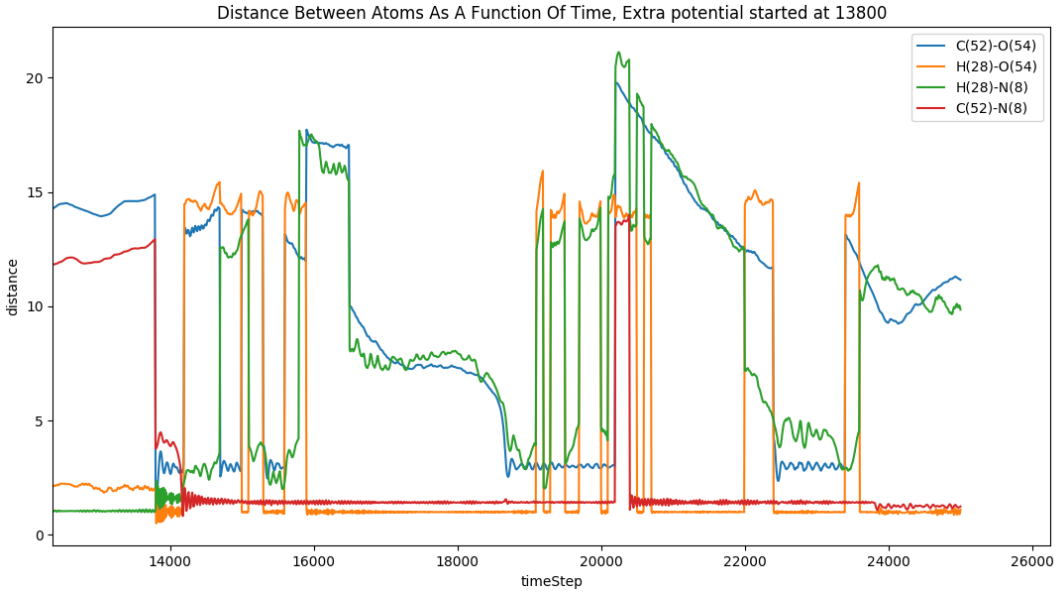
בצעד זמן 1000 נמצאה רביעייה אחת חשודה שהגיעה לריאקציה



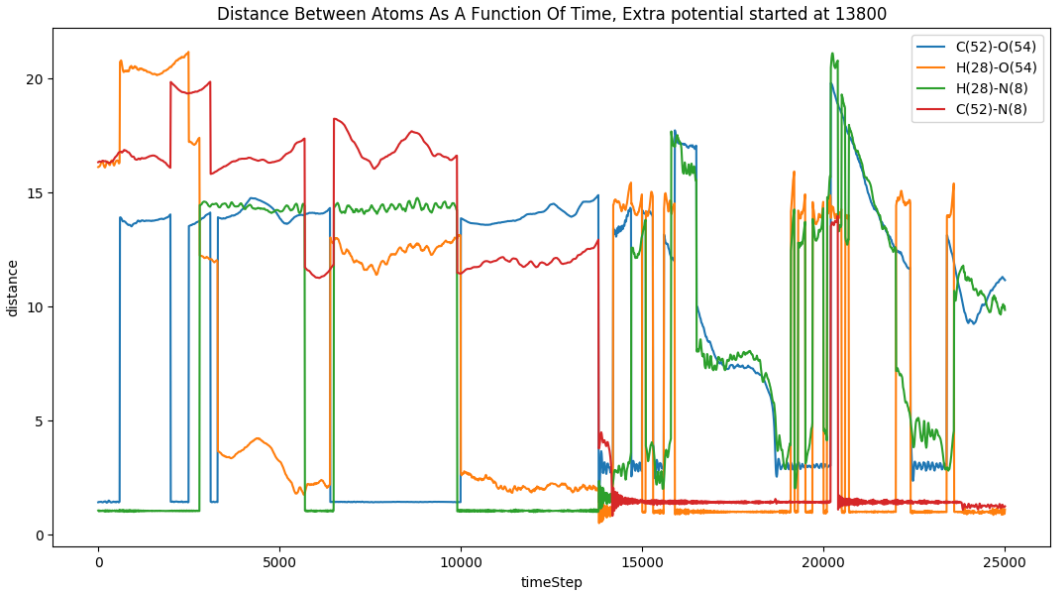
גרף המרחקים לכל אורך הריצה (הפוטנציאל נוסף בין צעדי זמן 1000-11,000)



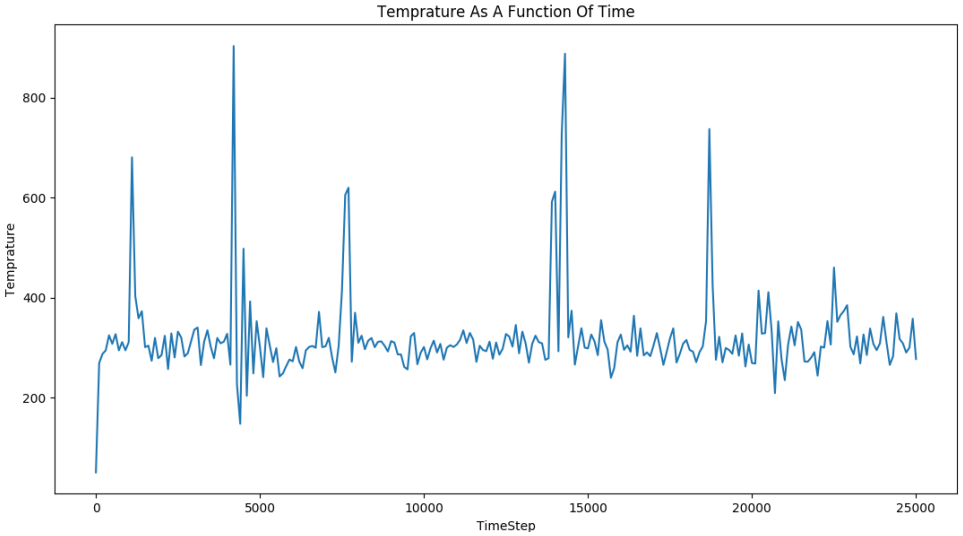
בצעד זמן 13,800 נמצאה רביעייה אחרת חשודה שגם הגיעה לריאקציה



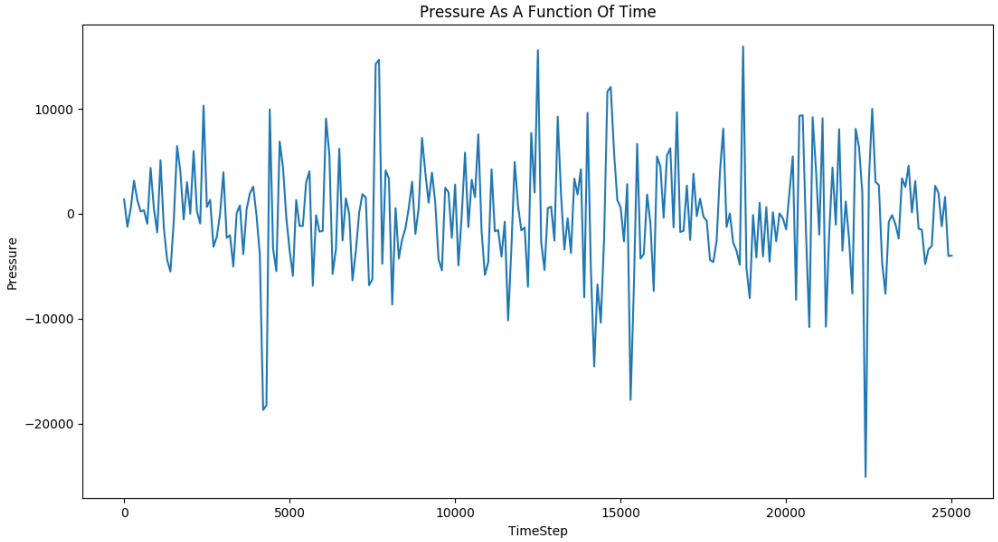
גרף המרחקים לכל אורך הריצה (הפוטנציאל נוסף בין צעדי זמן 13,800-23,800)



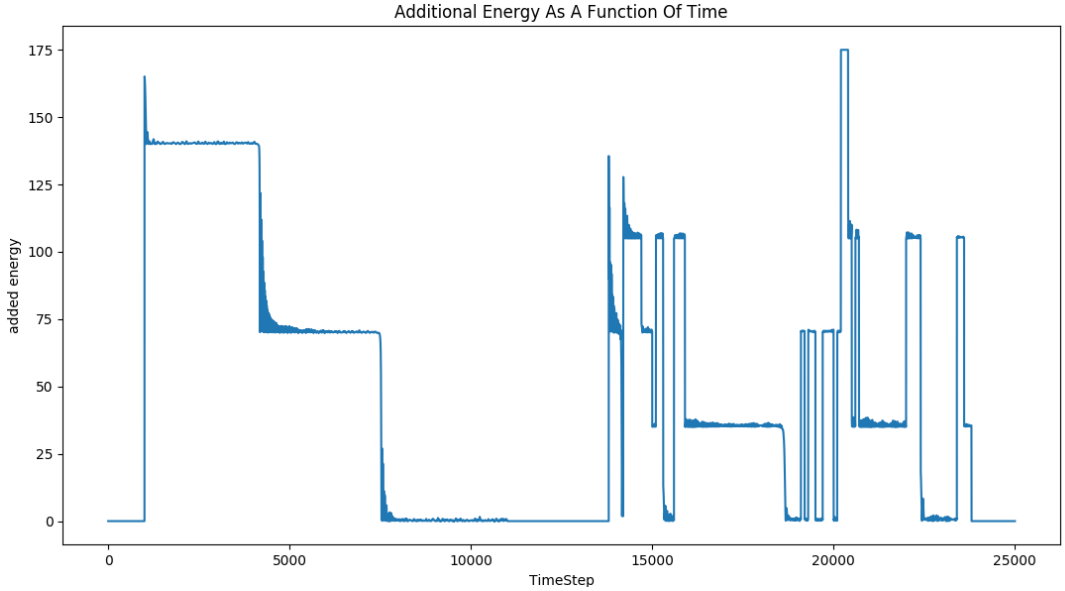
גרף טמפרטורה כתלות בזמן



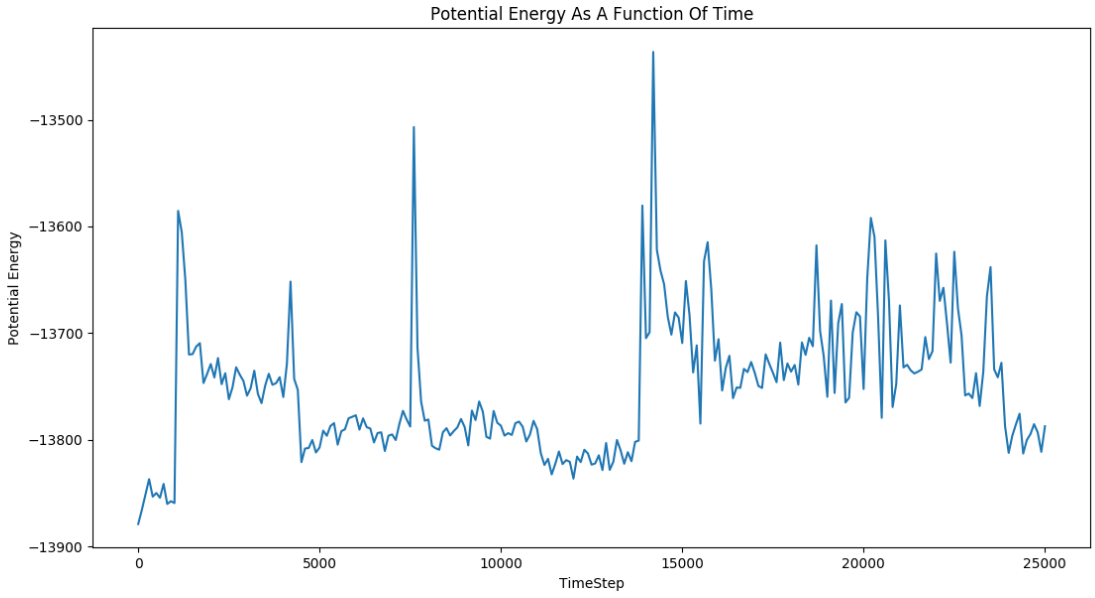
גרף של לחץ כתלות בזמן



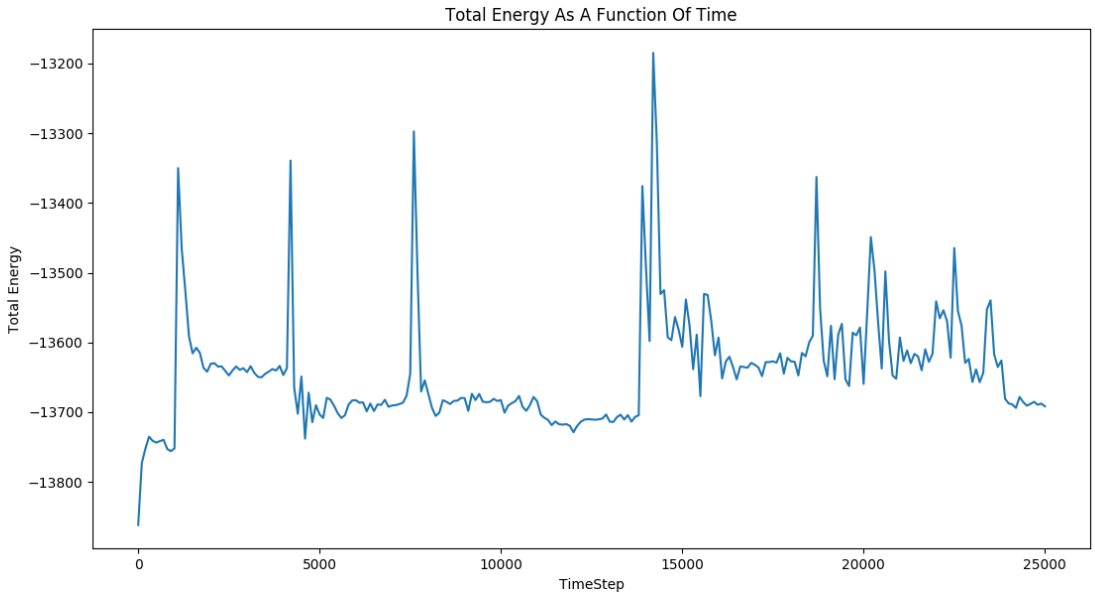
גרף של האנרגיה שהפוטנציאל הוסיף כתלות בזמן



גרף אנרגיה פוטנציאלית כתלות בזמן



גרף סך האנרגיה כתלות בזמן



קובץ SPECIES.OUT

Initial state

# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
100	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
200	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
300	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
400	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
500	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
600	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
700	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
800	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
900	3	2 1	2	

Start operate the potential on the #1 fourset

# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
1000	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
1100	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
1200	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
1300	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
1400	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
1500	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
1600	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
1700	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
1800	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
1900	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
2000	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
2100	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
2200	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4
2300	3	2 1	2	
# Timestep	No_Moles	No_Specs	C11H18N2	C19H20O4

2400 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
2500 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
2600 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
2700 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
2800 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
2900 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
3000 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
3100 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
3200 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
3300 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
3400 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
3500 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
3600 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
3700 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
3800 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
3900 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
4000 3 2 1 2
Timestep No_Moles No_Specs C11H18N2 C19H20O4
4100 3 2 1 2
Timestep No_Moles No_Specs C11H17N2 H C19H20O4
4200 4 3 1 1 2
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
4300 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
4400 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
4500 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
4600 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
4700 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
4800 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
4900 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
5000 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
5100 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
5200 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
5300 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
5400 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
5500 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
5600 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
5700 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
5800 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
5900 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
6000 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
6100 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
6200 3 3 1 1 1
Timestep No_Moles No_Specs C11H17N2 C19H21O4 C19H20O4
6300 3 3 1 1 1

```
# Timestep    No_Moles    No_Specs    C11H17N2    C19H21O4    C19H20O4
6400    3    3 1    1    1
# Timestep    No_Moles    No_Specs    C11H17N2    C19H21O4    C19H20O4
6500    3    3 1    1    1
# Timestep    No_Moles    No_Specs    C11H17N2    C19H21O4    C19H20O4
6600    3    3 1    1    1
# Timestep    No_Moles    No_Specs    C11H17N2    C19H21O4    C19H20O4
6700    3    3 1    1    1
# Timestep    No_Moles    No_Specs    C11H17N2    C19H21O4    C19H20O4
6800    3    3 1    1    1
# Timestep    No_Moles    No_Specs    C11H17N2    C19H21O4    C19H20O4
6900    3    3 1    1    1
# Timestep    No_Moles    No_Specs    C11H17N2    C19H21O4    C19H20O4
7000    3    3 1    1    1
# Timestep    No_Moles    No_Specs    C11H17N2    C19H21O4    C19H20O4
7100    3    3 1    1    1
# Timestep    No_Moles    No_Specs    C11H17N2    C19H21O4    C19H20O4
7200    3    3 1    1    1
# Timestep    No_Moles    No_Specs    C11H17N2    C19H21O4    C19H20O4
7300    3    3 1    1    1
# Timestep    No_Moles    No_Specs    C11H17N2    C19H21O4    C19H20O4
7400    3    3 1    1    1
# Timestep    No_Moles    No_Specs    C11H17N2    C19H21O4    C19H20O4
7500    3    3 1    1    1

The reaction happens
# Timestep    No_Moles    No_Specs    C11H17N    C19H20O4N    C19H20O4    H
7600    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
7700    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
7800    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
7900    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
8000    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
8100    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
8200    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
8300    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
8400    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
8500    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
8600    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
8700    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
8800    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
8900    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
9000    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
9100    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
9200    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
9300    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
9400    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
9500    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
9600    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
9700    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
9800    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
9900    4    4 1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
10000    4    4    1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
10100    4    4    1    1    1    1
# Timestep    No_Moles    No_Specs    C11H16N    C19H21O4N    C19H20O4    H
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10200	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
10300	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
10400	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
10500	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
10600	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
10700	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
10800	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
10900	4	4	1	1	1	1	

end of extra potential on the #1 fourset

# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
11000	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
11100	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
11200	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
11300	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
11400	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
11500	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
11600	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
11700	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
11800	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
11900	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
12000	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
12100	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
12200	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
12300	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
12400	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
12500	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
12600	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
12700	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
12800	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
12900	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
13000	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
13100	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
13200	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
13300	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
13400	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
13500	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
13600	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
13700	4	4	1	1	1	1	

Start operate the potential on the #2 fourset

# Timestep	No_Moles	No_Specs	C11H16N		C19H21O4N	C19H20O4	H
13800	4	4	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H16ON		C19H21O4N	C19H20O3	H
13900	4	4	1	1	1	1	

# Timestep	No_Moles	No_Specs	C11H15N	C19H21O4N	C19H21O4	H
14000	4	4	1	1	1	

Reaction happens??

# Timestep	No_Moles	No_Specs	C30H36O4N	C19H21O4N	H	
14100	3	3	1	1	1	
# Timestep	No_Moles	No_Specs	C11H14	C19H22O4N	C19H21O4N	H
14200	4	4	1	1	1	
# Timestep	No_Moles	No_Specs	C30H36O4N	C19H21O4N	H	
14300	3	3	1	1	1	
# Timestep	No_Moles	No_Specs	C30H36O4N	C19H21O4N	H	
14400	3	3	1	1	1	
# Timestep	No_Moles	No_Specs	C30H36O4N	C19H21O4N	H	
14500	3	3	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	C19H21O4N	H	
14600	4	3	1	2	1	
# Timestep	No_Moles	No_Specs	C11H15	C19H21O4N	H	
14700	4	3	1	2	1	
# Timestep	No_Moles	No_Specs	C11H15	C19H21O4N	H	
14800	4	3	1	2	1	
# Timestep	No_Moles	No_Specs	C11H15	C19H21O4N	H	
14900	4	3	1	2	1	
# Timestep	No_Moles	No_Specs	C11H15	C19H21O4N	H	
15000	4	3	1	2	1	

The distances between the pairs as wanted

# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
15100	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
15200	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
15300	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
15400	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
15500	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
15600	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
15700	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
15800	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
15900	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
16000	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
16100	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
16200	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
16300	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
16400	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
16500	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
16600	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
16700	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
16800	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
16900	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
17000	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
17100	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
17200	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
17300	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
17400	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
17500	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
17600	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H

17700 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
17800 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
17900 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
18000 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
18100 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
18200 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
18300 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
18400 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
18500 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
18600 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 C38H41O8N2 H
18700 4 3 1 1 2
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
18800 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
18900 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
19000 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
19100 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
19200 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
19300 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
19400 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 C19H21O4N H
19500 4 3 1 2 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
19600 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
19700 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
19800 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
19900 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
20000 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
20100 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
20200 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
20300 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
20400 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
20500 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
20600 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
20700 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
20800 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
20900 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
21000 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
21100 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
21200 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
21300 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
21400 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
21500 5 5 1 1 1 1 1
Timestep No_Moles No_Specs C11H15 CH2N C19H21O4N C18H19O4 H
21600 5 5 1 1 1 1 1

# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
21700	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CHN	C19H21O4N	C18H19O4	H
21800	6	5	1	1	1	2	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
21900	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
22000	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
22100	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
22200	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
22300	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
22400	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
22500	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
22600	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	HO	C18H18O3	H
22700	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
22800	5	5	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C18H19O4	H
22900	5	5	1	1	1	1	

The distances between the pairs as wanted

# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	
23000	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
23100	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
23200	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
23300	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
23400	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
23500	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
23600	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
23700	6	6	1	1	1	1	1	

End of the potential on the #2 foursets

# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	
23800	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
23900	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
24000	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
24100	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
24200	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
24300	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
24400	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
24500	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
24600	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H20O4N	C2H4O	C16H15O3	H2
24700	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
24800	6	6	1	1	1	1	1	
# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
24900	6	6	1	1	1	1	1	

Final state

# Timestep	No_Moles	No_Specs	C11H15	CH2N	C19H21O4N	C2H4O	C16H15O3	H
25000	6	6	1	1	1	1	1	