

Reaction mechanisms of C(3PJ) and C+ (2PJ) with benzene in the interstellar medium from quantum mechanical molecular dynamics simulations

(Mohammad Ebrahim Izadi, Kristof M. Bal, Ali Maghari and Erik C. Neyts)

Table S1. Mechanisms and products observed over first 30 simulations, the ones reported in the manuscript and 30 new simulations with the same settings except the initial random velocities/positions of benzene. It should be noted that all orientations are also included, and they are shown using different colors so that the red represent face collisions, blue edge in-plane and black edge out-of-plane.

Extra 30 simulation			Original simulations		
ID	Mechanism	Product	ID	Mechanism	Product
1	Insertion between C-C bond	C ₇ H ₆	1	Insertion between C-C bond	C ₇ H ₆
2	Insertion between C-C bond	C ₇ H ₆	2	Insertion between C-C bond	C ₇ H ₆
3	Insertion between C-C bond	C ₇ H ₆	3	Insertion between C-C bond	C ₇ H ₆
4	Insertion between C-C bond	C ₇ H ₆	4	Insertion between C-C bond	C ₇ H ₆
5	C eject a CH out of the ring	C ₆ H ₅ -C-H	5	Insertion between C-C bond	C ₇ H ₆
6	Insertion between C-C bond	C ₇ H ₆	6	Insertion between C-C bond	C ₇ H ₆
7	Insertion between C-C bond	C ₇ H ₆	7	C eject a CH out of the ring	C ₆ H ₅ -C-H
8	Insertion between C-C bond	C ₇ H ₆	8	Insertion between C-C bond	C ₇ H ₆
9	Insertion between C-C bond	C ₇ H ₆	9	Insertion between C-C bond	C ₇ H ₆
10	Insertion between C-C bond	C ₇ H ₆	10	Insertion between C-C bond	C ₇ H ₆
11	Insertion between C-H bond	C ₆ H ₅ -C-H	11	Insertion between C-H bond	C ₆ H ₅ -C-H
12	Insertion between C-H bond	C ₆ H ₅ -C-H	12	Insertion between C-C bond	C ₇ H ₆
13	Insertion between C-C bond	C ₇ H ₆	13	C eject a CH out of the ring	C ₆ H ₅ -C-H
14	Insertion between C-H bond	C ₆ H ₅ -C-H	14	Insertion between C-H bond	C ₆ H ₅ -C-H
15	C eject a CH out of the ring	C ₆ H ₅ -C-H	15	Insertion between C-H bond	C ₆ H ₅ -C-H
16	Insertion between C-H bond	C ₆ H ₅ -C-H	16	Insertion between C-H bond	C ₆ H ₅ -C-H
17	Insertion between C-H bond	C ₆ H ₅ -C-H	17	Insertion between C-H bond	C ₆ H ₅ -C-H
18	Insertion between C-H bond	C ₆ H ₅ -C-H	18	Insertion between C-H bond	C ₆ H ₅ -C-H
19	Insertion between C-H bond	C ₆ H ₅ -C-H	19	Insertion between C-H bond	C ₆ H ₅ -C-H
20	Insertion between C-H bond	C ₆ H ₅ -C-H	20	Insertion between C-H bond	C ₆ H ₅ -C-H
21	Insertion between C-H bond	C ₆ H ₅ -C-H	21	C eject a CH out of the plane	C ₇ H ₆
22	Insertion between C-C bond	C ₇ H ₆	22	Insertion between C-C bond	C ₇ H ₆
23	C eject a CH out of the plane	C ₇ H ₆	23	Insertion between C-C bond	C ₇ H ₆
24	Insertion between C-H bond	C ₆ H ₅ -C-H	24	Insertion between C-H bond	C ₆ H ₅ -C-H
25	Insertion between C-C bond	C ₇ H ₆	25	Insertion between C-H bond	C ₆ H ₅ -C-H
26	Insertion between C-H bond	C ₆ H ₅ -C-H	26	Insertion between C-H bond	C ₆ H ₅ -C-H
27	Insertion between C-H bond	C ₆ H ₅ -C-H	27	Insertion between C-H bond	C ₆ H ₅ -C-H
28	Insertion between C-H bond	C ₆ H ₅ -C-H	28	Insertion between C-H bond	C ₆ H ₅ -C-H
29	Insertion between C-C bond	C ₇ H ₆	29	Insertion between C-H bond	C ₆ H ₅ -C-H
30	Insertion between C-H bond	C ₆ H ₅ -C-H	30	Insertion between C-C bond	C ₇ H ₆