

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

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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 |