Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information for the article:
The Effect of Molecular Dynamics Sampling on the Calculated Observable Gas-Phase Structures

Unique terms for Benzene at 300K obtained using different methods at BLYP/TZVP level of theory. For the abbreviations used see the article's text.

Table S1. ElDiff

At1	At2	re	l	re-ra	kappa	#of eqv. terms
C1	H12	1.0899	0.0752	-0.0161	11.2	6
C3	C7	1.4020	0.0460	-0.0068	1.4	6
C3	H9	2.1637	0.0980	-0.0133	2.9	12
C6	C7	2.4284	0.0550	-0.0094	0.6	6
H4	H8	2.4919	0.1588	-0.0123	-15.8	6
C2	C7	2.8040	0.0613	-0.0101	0.1	3
C2	H11	3.4160	0.0940	-0.0161	6.3	12
C3	H8	3.8940	0.0933	-0.0169	9.0	6
H5	H11	4.3162	0.1287	-0.0202	2.0	6
H11	H12	4.9839	0.1170	-0.0222	17.8	3

Table S2. PIMD

At1	At2	re	l	re-ra	kappa	#of eqv. terms
C1	H12	1.0899	0.0770	-0.0131	12.8	6
C3	C7	1.4020	0.0464	-0.0040	1.5	6
C3	H9	2.1637	0.0993	-0.0084	4.4	12
C6	C7	2.4284	0.0553	-0.0047	0.4	6
H4	H8	2.4919	0.1604	-0.0064	-10.1	6
C2	C7	2.8040	0.0605	-0.0047	-1.2	3
C2	H11	3.4160	0.0953	-0.0086	7.0	12
C3	H8	3.8940	0.0939	-0.0084	8.4	6
H5	H11	4.3162	0.1301	-0.0103	3.7	6
H11	H12	4.9839	0.1188	-0.0105	16.2	3

Table S3. NH

At1	At2	re	l	re-ra	kappa	#of eqv. terms
C1	H12	1.0899	0.0217	0.0004	0.2	6
C3	C7	1.4020	0.0242	-0.0003	0.4	6
C3	H9	2.1637	0.0473	0.0027	-0.6	12
C6	C7	2.4284	0.0430	0.0013	0.1	6
H4	H8	2.4919	0.0883	0.0048	-4.8	6
C2	C7	2.8040	0.0585	0.0023	-1.0	3
C2	H11	3.4160	0.0488	0.0052	0.3	12
C3	H8	3.8940	0.0620	0.0067	-0.6	6
H5	H11	4.3162	0.0609	0.0093	-1.2	6
H11	H12	4.9839	0.0658	0.0117	-0.2	3

Table S4. NH+QA

At1	At2	re	l	re-ra	kappa	#of eqv. terms
C1	H12	1.0899	0.0759	-0.0065	8.4	6
C3	C7	1.4020	0.0467	-0.0054	2.1	6
C3	H9	2.1637	0.1083	0.0105	-5.5	12
C6	C7	2.4284	0.0599	0.0019	0.1	6
H4	H8	2.4919	0.1690	0.0181	-22.2	6
C2	C7	2.8040	0.0663	0.0029	-0.7	3
C2	H11	3.4160	0.1117	0.0065	2.9	12
C3	H8	3.8940	0.1245	0.0109	-2.9	6
H5	H11	4.3162	0.1422	0.0167	-9.8	6
H11	H12	4.9839	0.1503	0.0147	2.2	3

Table S5. GLE

At1	At2	re	l	re-ra	kappa	#of eqv. terms
C1	H12	1.0899	0.0300	-0.0019	0.8	6
C3	C7	1.4020	0.0283	-0.0074	0.8	6
C3	H9	2.1637	0.0544	-0.0048	0.2	12
C6	C7	2.4284	0.0404	-0.0103	0.4	6
H4	H8	2.4919	0.0990	-0.0035	-2.0	6
C2	C7	2.8040	0.0496	-0.0109	-0.0	3
C2	H11	3.4160	0.0531	-0.0067	0.8	12
C3	H8	3.8940	0.0571	-0.0065	0.6	6
H5	H11	4.3162	0.0700	-0.0028	-0.1	6
H11	H12	4.9839	0.0640	-0.0010	0.3	3

Table S6. GLE+QA

At1	At2	re	l	re-ra	kappa	#of eqv. terms
C1	H12	1.0899	0.0754	-0.0121	11.4	6
C3	C7	1.4020	0.0471	-0.0102	1.7	6
C3	H9	2.1637	0.1044	-0.0014	0.5	12
C6	C7	2.4284	0.0575	-0.0095	-0.1	6
H4	H8	2.4919	0.1641	0.0045	-5.5	6
C2	C7	2.8040	0.0641	-0.0099	-0.6	3
C2	H11	3.4160	0.1030	-0.0063	3.1	12
C3	H8	3.8940	0.1067	-0.0054	1.7	6
H5	H11	4.3162	0.1382	0.0006	-0.4	6
H11	H12	4.9839	0.1314	0.0010	1.6	3

Table S7. Q-GLE

At1	At2	re	l	re-ra	kappa	#of eqv. terms
C1	H12	1.0899	0.0682	-0.0108	18.9	6
C3	C7	1.4020	0.0500	-0.0046	5.3	6
C3	H9	2.1637	0.0991	-0.0054	14.1	12
C6	C7	2.4284	0.0556	-0.0061	1.9	6
H4	H8	2.4919	0.1677	-0.0018	-2.8	6
C2	C7	2.8040	0.0629	-0.0061	1.8	3
C2	H11	3.4160	0.0909	-0.0061	15.2	12
C3	H8	3.8940	0.0892	-0.0060	17.5	6
H5	H11	4.3162	0.1260	-0.0044	16.1	6
H11	H12	4.9839	0.1098	-0.0036	36.9	3