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Theoretical Study of the Gas-Phase Reaction between Formyl Cation and Aromatics

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Table S1. Zero Point Energies (ZPE), Enthalpy Changes ($H^0_{298} - H^0_0$), and Absolute Entropies (S^0_{298}). Calculated using MP2(full)/6-31G**, vibrational frequencies (scaled by 0.93)

Species	ZPE /(kcal mol^{-1})	$H^0_{298} - H^0_0$ /(kcal mol^{-1})	S^0_{298} /(cal mol^{-1} K^{-1})
1	86.06134	6.72931	90.78660
2	87.80534	5.98761	84.98712
3	87.31928	6.17586	87.08520
4	87.41027	6.12503	87.04056
toluene	75.69525	4.04738	69.43659
cumene	110.17996	6.03906	84.43749
p-cresol	78.13617	5.33249	78.93375
formyl cation	8.10615	2.41086	24.43389
m-formyl-*p*OH-toluene+	90.64024	6.67409	90.60804
p-formyl-cumene+	121.91025	7.70633	99.44490
*p*H-toluene+	82.17659	4.89011	75.97728
*p*H-cumene+	116.69757	6.44945	88.21236
*m*H-*p*OH-toluene+	85.44117	5.44921	79.80330
H_2	6.12488	2.07389	28.90905
H_3+	12.57128	2.36944	34.63506
CO	2.82531	2.07389	43.96947
COH+	7.56073	2.68821	37.41948
*o*H-*p*OH-toluene+	84.48525	5.60671	80.74167
*p*H-*p*OH-toluene+	84.67032	5.50882	80.18274
pOH_2-toluene+	91.67964	5.66946	81.3843

Table S2. Absolute Energies (-a.u.)

Species	MP2(full)/6-31G**//	/6-31++G**// MP2(full)/6-31G**			
	MP2(full)6-31G**	MP2(fc)	MP3(fc)	MP4SDQ(fc)	MP4SDTQ(fc)
1	384.02062	383.99763	384.02166	384.04331	384.10964
2	384.05511	384.027445	384.067798	384.084942	384.146419
3	384.04839	384.020385	384.061886	384.078198	384.139124
4	384.05454	384.026760	384.070074	384.086882	384.146041
toluene	270.72799	270.707750	270.746972	270.753216	270.800027
formyl cation	113.27109	113.266074	113.254276	113.287976	113.287976
*p*H-toluene+	271.03720	271.009871	271.059450	271.067225	271.110328
H_2	1.15766	1.157772	1.163277	1.164687	1.164687
H_3+	1.32428	1.325313	1.331356	1.332828	1.332828
CO	113.02818	113.02913	113.02470	113.03737	113.05161
COH+	113.20062	113.195509	113.201272	113.212009	113.223796

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Table S3. Absolute Energies (-a.u.)

Species	MP2(full)/6-31G**// MP2(full)6-31G**	/6-31G**// MP2(full)/6-31G**			
		MP2(fc)	MP3(fc)	MP4SDQ(fc)	MP4SDTQ(fc)
cumene	349.10659	349.060164	349.119223	349.128543	349.184505
p-cresol	345.76736	345.7285593	345.766037	345.7751123	345.826045
p-formyl-cumene+	462.43591	462.381728	462.444729	462.464384	462.532383
*p*H-cumene+	349.41839	349.372012	349.440460	349.451449	349.504388
*m*H-*p*OH-toluene+	346.08947	346.050681	346.096216	346.107612	346.156362
*o*H-*p*OH-toluene+	346.07492	346.036130	346.080935	346.091522	346.141408
*p*H-*p*OH-toluene+	346.05445	346.015906	346.063479	346.074217	346.122067
CO	113.02818	113.021213	113.017893	113.029870	113.043356
formyl cation	113.27109	113.26371	113.25215	113.26850	113.28526
m-formyl-*p*OH-toluene+	459.110361	459.0637228	459.1024277	459.1228471	459.1875355
pOH_2-toluene+	346.0732028	346.0344193	346.0758495	346.0844625	346.1344596