Supporting Information for

**Exploring the Chemical Dynamics of Phenylethynyl Radical (C6H5CC; X2A1) Reactions with Allene (H2CCCH2; X1A1) and Methylacetylene (CH3CCH; X1A1)**

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**1. Precursor Synthesis and Characterization**

The synthesis of the (2-iodoethynyl)benzene precursor was performed analogously to a reported procedure[1](#_ENREF_1) with an increase in the concentration of the starting materials due to the large scale of precursor needed. Regarding the purification, badges performed with less than 10 g of phenylacetylene could be purified by either column chromatography or distillation whereas larger badges (20–50 g) decomposed before affording the desired product and, thus, had to be purified by column chromatography. A solution of phenylacetylene (26.0 mL, 24.2 g, 0.16 mol) in MeOH (300 mL) was cooled to 0 °C and KOH (32.5 g, 0.41 mol) was added. After 20 min of stirring at 0 °C, N-iodosuccinimide (63.1 g, 0.27 mol) was added to the mixture in portions and stirred at 0 °C for 15 min. The cold bath was replaced by a rt water bath and the mixture was stirred for 30 min. Then, Et2O (1 L) was added and the mixture was extracted with brine (5 x 150 mL), dried over MgSO4, filtered and evaporated to afford a brown oil/liquid. This liquid was purified by column chromatography (SiO2; hexane) to afford the product as a light-yellow oil (32.5 g, 60%). 1H NMR (200 MHz, CDCl3): δ = 7.44 (dd, 2H), 7.34 (m, 3H) ppm. 13C NMR (50 MHz, CDCl3): δ = 132.43, 128.92, 128.36, 123.46, 94.26 and 6.48 ppm. GC-MS: m/z 228.1 [M+] 101.1 [M+–I]. The characteristic C≡C stretching vibration was found at 2172 cm−1 whereas for the starting material it is observed at 2110 cm−1. The provided characterization is in accordance with the literature.[1](#_ENREF_1) 1H and 13C NMR data were recorded with a Bruker DPX-200 NMR spectrometer referenced towards CDCl3 (7.26 ppm for 1H NMR and 77.16 ppm for 13C NMR). The GC-MS data were recorded with an Agilent 7820A GC spectrometer. IR data were recorded with a Bruker Equinox 55 FT-IR spectrometer.

**Table S1.** RRKM calculated rate constants (*k*(*E*), s−1) of the reaction of phenylethynyl (C6H5CC) with allene (H2CCCH2) as functions of the internal energy (*E,* kJ mol−1) of the intermediate states for unimolecular reaction steps at different collision energies (*E*C*,* kJ mol−1).

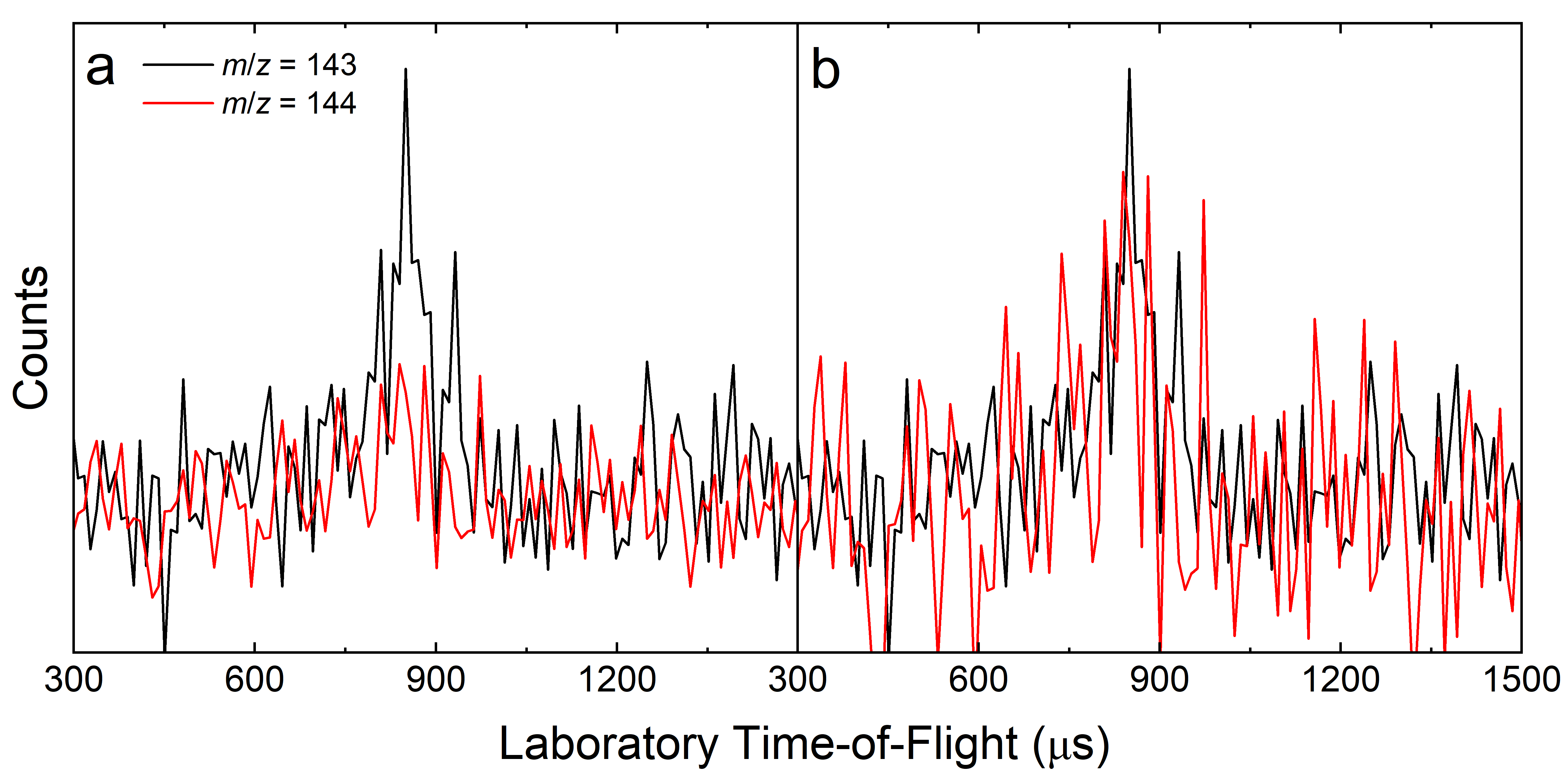
|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ***E*C** | 0 | | 10 | | 20 | | 30 | | 40 | |
| **Reaction step** | *k(E)* | *E* | *k(E)* | *E* | *k(E)* | *E* | *k(E)* | *E* | *k(E)* | *E* |
| ***i9 – p2*** | 2.70E+04 | 234 | 6.22E+04 | 244 | 1.33E+05 | 254 | 2.66E+05 | 264 | 5.03E+05 | 274 |
| ***i9 – p1*** | 1.12E+04 | 234 | 3.11E+04 | 244 | 7.76E+04 | 254 | 1.78E+05 | 264 | 3.80E+05 | 274 |
| ***i2 – p3*** | 4.05E+05 | 259 | 8.01E+05 | 269 | 1.50E+06 | 279 | 2.68E+06 | 289 | 4.61E+06 | 299 |
| ***i2 – p2*** | 5.55E+04 | 259 | 1.24E+05 | 269 | 2.59E+05 | 279 | 5.10E+05 | 289 | 9.56E+05 | 299 |
| ***i1 – i11*** | 1.35E+02 | 260 | 3.11E+02 | 270 | 6.70E+02 | 280 | 1.36E+03 | 290 | 2.65E+03 | 300 |
| ***i11 – i1*** | 1.80E+01 | 268 | 4.19E+01 | 278 | 9.15E+01 | 288 | 1.89E+02 | 298 | 3.70E+02 | 308 |
| ***i7 – i8*** | 8.11E+06 | 343 | 1.13E+07 | 353 | 1.54E+07 | 363 | 2.07E+07 | 373 | 2.74E+07 | 383 |
| ***i8 – i7*** | 2.64E+12 | 214 | 2.80E+12 | 224 | 2.96E+12 | 234 | 3.12E+12 | 244 | 3.27E+12 | 254 |
| ***i1 – i6*** | 2.42E+03 | 260 | 5.68E+03 | 270 | 1.25E+04 | 280 | 2.58E+04 | 290 | 5.08E+04 | 300 |
| ***i6 – i1*** | 2.58E+01 | 303 | 6.59E+01 | 313 | 1.57E+02 | 323 | 3.52E+02 | 333 | 7.43E+02 | 343 |
| ***i9 – i8*** | 1.36E+08 | 234 | 1.87E+08 | 244 | 2.52E+08 | 254 | 3.32E+08 | 264 | 4.29E+08 | 274 |
| ***i8 – i9*** | 6.57E+09 | 214 | 8.54E+09 | 224 | 1.09E+10 | 234 | 1.37E+10 | 244 | 1.69E+10 | 254 |
| ***i9 – i11*** | 1.02E+00 | 234 | 3.77E+00 | 244 | 1.22E+01 | 254 | 3.56E+01 | 264 | 9.44E+01 | 274 |
| ***i11 – i9*** | 2.12E-02 | 268 | 8.43E-02 | 278 | 2.95E-01 | 288 | 9.20E-01 | 298 | 2.60E+00 | 308 |
| ***i9 – i10*** | 1.09E+01 | 234 | 4.05E+01 | 244 | 1.34E+02 | 254 | 4.03E+02 | 264 | 1.10E+03 | 274 |
| ***i10 – i9*** | 8.33E+00 | 224 | 3.02E+01 | 234 | 9.81E+01 | 244 | 2.87E+02 | 254 | 7.68E+02 | 264 |
| ***i4 – p4*** | 3.73E+06 | 247 | 7.28E+06 | 257 | 1.34E+07 | 267 | 2.37E+07 | 277 | 4.00E+07 | 287 |
| ***i4 – i7*** | 2.18E+04 | 247 | 4.34E+04 | 257 | 8.20E+04 | 267 | 1.48E+05 | 277 | 2.57E+05 | 287 |
| ***i7 – i4*** | 1.23E+00 | 343 | 2.95E+00 | 353 | 6.67E+00 | 363 | 1.42E+01 | 373 | 2.90E+01 | 383 |
| ***i10 – p1*** | 1.73E+03 | 224 | 4.98E+03 | 234 | 1.29E+04 | 244 | 3.03E+04 | 254 | 6.59E+04 | 264 |
| ***i10 – p6*** | 1.86E+08 | 224 | 2.92E+08 | 234 | 4.43E+08 | 244 | 6.52E+08 | 254 | 9.34E+08 | 264 |
| ***i1 – i2*** | 1.12E+12 | 260 | 1.21E+12 | 270 | 1.29E+12 | 280 | 1.37E+12 | 290 | 1.45E+12 | 300 |
| ***i2 – i1*** | 1.50E+12 | 259 | 1.60E+12 | 269 | 1.70E+12 | 279 | 1.80E+12 | 289 | 1.90E+12 | 299 |
| ***i4 – i6*** | 5.26E-06 | 247 | 1.30E-04 | 257 | 1.41E-03 | 267 | 9.71E-03 | 277 | 4.99E-02 | 287 |
| ***i6 – i4*** | 1.33E-08 | 303 | 3.70E-07 | 313 | 4.50E-06 | 323 | 3.46E-05 | 333 | 1.97E-04 | 343 |
| ***i9 – i5*** | 2.13E+03 | 234 | 4.89E+03 | 244 | 1.04E+04 | 254 | 2.10E+04 | 264 | 4.00E+04 | 274 |
| ***i5 – i9*** | 1.28E-02 | 370 | 3.79E-02 | 380 | 1.04E-01 | 390 | 2.63E-01 | 400 | 6.26E-01 | 410 |
| ***i11 – p5*** | 1.05E+07 | 268 | 1.85E+07 | 278 | 3.13E+07 | 288 | 5.09E+07 | 298 | 8.03E+07 | 308 |
| ***i11 – p2*** | 6.99E+03 | 268 | 1.65E+04 | 278 | 3.62E+04 | 288 | 7.46E+04 | 298 | 1.45E+05 | 308 |
| ***i6 – p3*** | 1.84E+04 | 303 | 3.66E+04 | 313 | 6.91E+04 | 323 | 1.25E+05 | 333 | 2.18E+05 | 343 |
| ***i6 – p4*** | 1.16E+06 | 303 | 2.16E+06 | 313 | 3.88E+06 | 323 | 6.68E+06 | 333 | 1.11E+07 | 343 |
| ***i2 – i5*** | 1.52E+03 | 259 | 3.49E+03 | 269 | 7.47E+03 | 279 | 1.51E+04 | 289 | 2.89E+04 | 299 |
| ***i5 – i2*** | 4.42E-02 | 370 | 1.23E-01 | 380 | 3.19E-01 | 390 | 7.69E-01 | 400 | 1.75E+00 | 410 |
| ***i2 – i3*** | 7.42E+07 | 259 | 1.05E+08 | 269 | 1.45E+08 | 279 | 1.96E+08 | 289 | 2.61E+08 | 299 |
| ***i3 – i2*** | 1.13E+11 | 187 | 1.30E+11 | 197 | 1.47E+11 | 207 | 1.66E+11 | 217 | 1.85E+11 | 227 |
| ***i4 – i3*** | 2.00E+08 | 247 | 2.75E+08 | 257 | 3.70E+08 | 267 | 4.88E+08 | 277 | 6.34E+08 | 287 |
| ***i3 – i4*** | 9.65E+10 | 187 | 1.11E+11 | 197 | 1.26E+11 | 207 | 1.41E+11 | 217 | 1.58E+11 | 227 |
| ***i5 – p2*** | 1.65E+00 | 370 | 4.50E+00 | 380 | 1.14E+01 | 390 | 2.69E+01 | 400 | 6.00E+01 | 410 |
| ***i11 – i5*** | 2.55E+00 | 268 | 7.18E+00 | 278 | 1.86E+01 | 288 | 4.51E+01 | 298 | 1.02E+02 | 308 |
| ***i5 – i11*** | 7.40E-04 | 370 | 2.49E-03 | 380 | 7.67E-03 | 390 | 2.19E-02 | 400 | 5.80E-02 | 410 |
| ***i10 – i5*** | 1.68E+04 | 224 | 3.26E+04 | 234 | 6.01E+04 | 244 | 1.06E+05 | 254 | 1.79E+05 | 264 |
| ***i5 – i10*** | 6.58E-02 | 370 | 1.69E-01 | 380 | 4.09E-01 | 390 | 9.30E-01 | 400 | 2.01E+00 | 410 |
| ***i6 – i5*** | 1.00E+03 | 303 | 2.04E+03 | 313 | 3.95E+03 | 323 | 7.32E+03 | 333 | 1.31E+04 | 343 |
| ***i5 – i6*** | 3.62E+00 | 370 | 8.20E+00 | 380 | 1.76E+01 | 390 | 3.61E+01 | 400 | 7.09E+01 | 410 |
| ***i10 – i12*** | 5.37E-01 | 224 | 1.85E+00 | 234 | 5.79E+00 | 244 | 1.67E+01 | 254 | 4.41E+01 | 264 |
| ***i12 – i10*** | 1.10E-01 | 249 | 3.99E-01 | 259 | 1.32E+00 | 269 | 4.01E+00 | 279 | 1.11E+01 | 289 |
| ***i12 – p5*** | 1.10E+08 | 249 | 1.76E+08 | 259 | 2.72E+08 | 269 | 4.08E+08 | 279 | 5.97E+08 | 289 |
| ***i12 – p1*** | 8.24E+02 | 249 | 2.28E+03 | 259 | 5.71E+03 | 269 | 1.32E+04 | 279 | 2.83E+04 | 289 |

**Table S2.** RRKM calculated rate constants (*k*(*E*), s−1) of the reaction of phenylethynyl (C6H5CC) with methylacetylene (H3CCCH) as functions of the internal energy (*E,* kJ mol−1) of the intermediate states for unimolecular reaction steps at different collision energies (*E*C*,* kJ mol−1).

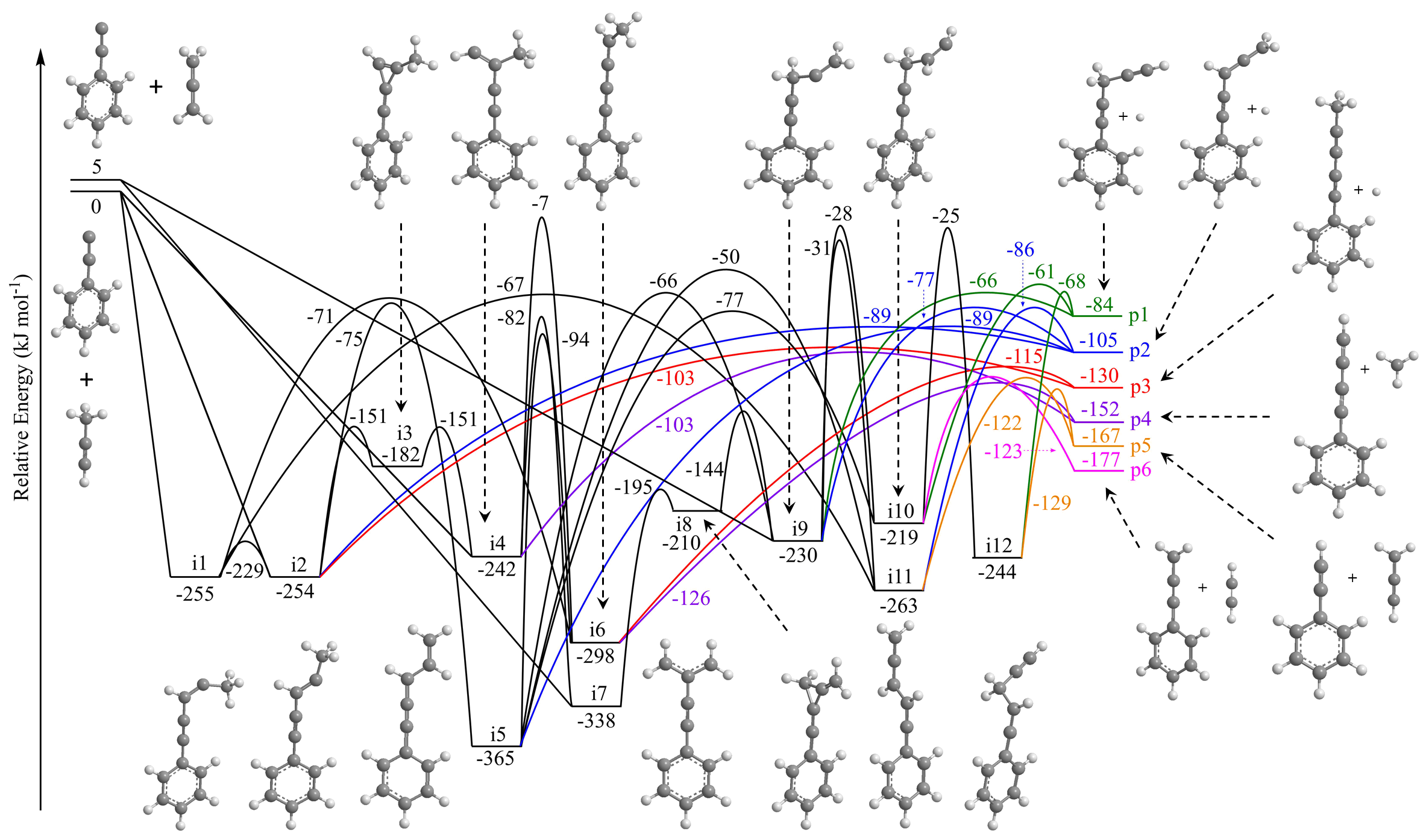
|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ***E*C** | 0 | | 10 | | 20 | | 30 | | 40 | |
| **Reaction step** | *k(E)* | *E* | *k(E)* | *E* | *k(E)* | *E* | *k(E)* | *E* | *k(E)* | *E* |
| ***i9 – p2*** | 1.64E+04 | 230 | 3.95E+04 | 240 | 8.77E+04 | 250 | 1.81E+05 | 260 | 3.53E+05 | 270 |
| ***i9 – p1*** | 6.16E+03 | 230 | 1.81E+04 | 240 | 4.76E+04 | 250 | 1.14E+05 | 260 | 2.51E+05 | 270 |
| ***i2 – p3*** | 2.81E+05 | 254 | 5.73E+05 | 264 | 1.10E+06 | 274 | 2.02E+06 | 284 | 3.53E+06 | 294 |
| ***i2 – p2*** | 3.60E+04 | 254 | 8.36E+04 | 264 | 1.80E+05 | 274 | 3.66E+05 | 284 | 7.01E+05 | 294 |
| ***i1 – i11*** | 8.69E+01 | 255 | 2.07E+02 | 265 | 4.59E+02 | 275 | 9.61E+02 | 285 | 1.91E+03 | 295 |
| ***i11 – i1*** | 1.15E+01 | 263 | 2.77E+01 | 273 | 6.23E+01 | 283 | 1.32E+02 | 293 | 2.65E+02 | 303 |
| ***i7 – i8*** | 6.83E+06 | 338 | 9.58E+06 | 348 | 1.32E+07 | 358 | 1.79E+07 | 368 | 2.39E+07 | 378 |
| ***i8 – i7*** | 2.56E+12 | 210 | 2.72E+12 | 220 | 2.88E+12 | 230 | 3.04E+12 | 240 | 3.19E+12 | 250 |
| ***i1 – i6*** | 1.53E+03 | 255 | 3.73E+03 | 265 | 8.46E+03 | 275 | 1.80E+04 | 285 | 3.64E+04 | 295 |
| ***i6 – i1*** | 1.56E+01 | 298 | 4.16E+01 | 308 | 1.02E+02 | 318 | 2.36E+02 | 328 | 5.14E+02 | 338 |
| ***i9 – i8*** | 1.10E+08 | 230 | 1.53E+08 | 240 | 2.08E+08 | 250 | 2.77E+08 | 260 | 3.63E+08 | 270 |
| ***i8 – i9*** | 5.71E+09 | 210 | 7.51E+09 | 220 | 9.67E+09 | 230 | 1.22E+10 | 240 | 1.52E+10 | 250 |
| ***i9 – i11*** | 4.82E-01 | 230 | 1.91E+00 | 240 | 6.60E+00 | 250 | 2.02E+01 | 260 | 5.62E+01 | 270 |
| ***i11 – i9*** | 1.00E-02 | 263 | 4.28E-02 | 273 | 1.60E-01 | 283 | 5.27E-01 | 293 | 1.56E+00 | 303 |
| ***i9 – i10*** | 5.14E+00 | 230 | 2.03E+01 | 240 | 7.15E+01 | 250 | 2.26E+02 | 260 | 6.45E+02 | 270 |
| ***i10 – i9*** | 4.18E+00 | 219 | 1.61E+01 | 229 | 5.50E+01 | 239 | 1.70E+02 | 249 | 4.74E+02 | 259 |
| ***i4 – p4*** | 2.61E+06 | 242 | 5.24E+06 | 252 | 9.94E+06 | 262 | 1.79E+07 | 272 | 3.09E+07 | 282 |
| ***i4 – i7*** | 1.51E+04 | 242 | 3.09E+04 | 252 | 6.00E+04 | 262 | 1.11E+05 | 272 | 1.96E+05 | 282 |
| ***i7 – i4*** | 7.76E-01 | 338 | 1.92E+00 | 348 | 4.46E+00 | 358 | 9.79E+00 | 368 | 2.04E+01 | 378 |
| ***i10 – p1*** | 9.67E+02 | 219 | 2.98E+03 | 229 | 8.09E+03 | 239 | 1.99E+04 | 249 | 4.50E+04 | 259 |
| ***i10 – p6*** | 1.46E+08 | 219 | 2.34E+08 | 229 | 3.61E+08 | 239 | 5.38E+08 | 249 | 7.82E+08 | 259 |
| ***i1 – i2*** | 1.08E+12 | 255 | 1.16E+12 | 265 | 1.25E+12 | 275 | 1.33E+12 | 285 | 1.41E+12 | 295 |
| ***i2 – i1*** | 1.45E+12 | 254 | 1.55E+12 | 264 | 1.65E+12 | 274 | 1.75E+12 | 284 | 1.85E+12 | 294 |
| ***i4 – i6*** | 5.40E-07 | 242 | 2.99E-05 | 252 | 4.56E-04 | 262 | 3.85E-03 | 272 | 2.26E-02 | 282 |
| ***i6 – i4*** | 1.29E-09 | 298 | 8.04E-08 | 308 | 1.38E-06 | 318 | 1.30E-05 | 328 | 8.47E-05 | 338 |
| ***i9 – i5*** | 1.30E+03 | 230 | 3.11E+03 | 240 | 6.90E+03 | 250 | 1.43E+04 | 260 | 2.80E+04 | 270 |
| ***i5 – i9*** | 7.17E-03 | 365 | 2.22E-02 | 375 | 6.31E-02 | 385 | 1.66E-01 | 395 | 4.08E-01 | 405 |
| ***i11 – p5*** | 7.79E+06 | 263 | 1.40E+07 | 273 | 2.41E+07 | 283 | 4.00E+07 | 293 | 6.41E+07 | 303 |
| ***i11 – p2*** | 4.41E+03 | 263 | 1.08E+04 | 273 | 2.46E+04 | 283 | 5.23E+04 | 293 | 1.05E+05 | 303 |
| ***i6 – p3*** | 1.28E+04 | 298 | 2.61E+04 | 308 | 5.05E+04 | 318 | 9.34E+04 | 328 | 1.66E+05 | 338 |
| ***i6 – p4*** | 8.29E+05 | 298 | 1.59E+06 | 308 | 2.91E+06 | 318 | 5.11E+06 | 328 | 8.64E+06 | 338 |
| ***i2 – i5*** | 1.06E+03 | 254 | 2.51E+03 | 264 | 5.53E+03 | 274 | 1.14E+04 | 284 | 2.24E+04 | 294 |
| ***i5 – i2*** | 2.77E-02 | 365 | 8.03E-02 | 375 | 2.15E-01 | 385 | 5.33E-01 | 395 | 1.25E+00 | 405 |
| ***i2 – i3*** | 6.18E+07 | 254 | 8.85E+07 | 264 | 1.24E+08 | 274 | 1.69E+08 | 284 | 2.27E+08 | 294 |
| ***i3 – i2*** | 1.05E+11 | 182 | 1.22E+11 | 192 | 1.38E+11 | 202 | 1.56E+11 | 212 | 1.75E+11 | 222 |
| ***i4 – i3*** | 1.69E+08 | 242 | 2.35E+08 | 252 | 3.20E+08 | 262 | 4.26E+08 | 272 | 5.57E+08 | 282 |
| ***i3 – i4*** | 8.98E+10 | 182 | 1.04E+11 | 192 | 1.18E+11 | 202 | 1.33E+11 | 212 | 1.49E+11 | 222 |
| ***i5 – p2*** | 1.04E+00 | 365 | 2.96E+00 | 375 | 7.74E+00 | 385 | 1.88E+01 | 395 | 4.31E+01 | 405 |
| ***i11 – i5*** | 1.47E+00 | 263 | 4.31E+00 | 273 | 1.16E+01 | 283 | 2.92E+01 | 293 | 6.83E+01 | 303 |
| ***i5 – i11*** | 3.89E-04 | 365 | 1.37E-03 | 375 | 4.40E-03 | 385 | 1.30E-02 | 395 | 3.58E-02 | 405 |
| ***i10 – i5*** | 1.27E+04 | 219 | 2.53E+04 | 229 | 4.77E+04 | 239 | 8.56E+04 | 249 | 1.47E+05 | 259 |
| ***i5 – i10*** | 4.31E-02 | 365 | 1.14E-01 | 375 | 2.83E-01 | 385 | 6.62E-01 | 395 | 1.46E+00 | 405 |
| ***i6 – i5*** | 6.90E+02 | 298 | 1.44E+03 | 308 | 2.85E+03 | 318 | 5.39E+03 | 328 | 9.82E+03 | 338 |
| ***i5 – i6*** | 2.36E+00 | 365 | 5.48E+00 | 375 | 1.21E+01 | 385 | 2.53E+01 | 395 | 5.08E+01 | 405 |
| ***i10 – i12*** | 2.79E-01 | 219 | 1.00E+00 | 229 | 3.30E+00 | 239 | 9.91E+00 | 249 | 2.73E+01 | 259 |
| ***i12 – i10*** | 5.29E-02 | 244 | 2.02E-01 | 254 | 7.05E-01 | 264 | 2.23E+00 | 274 | 6.48E+00 | 284 |
| ***i12 – p5*** | 8.17E+07 | 244 | 1.34E+08 | 254 | 2.10E+08 | 264 | 3.21E+08 | 274 | 4.76E+08 | 284 |
| ***i12 – p1*** | 4.52E+02 | 244 | 1.33E+03 | 254 | 3.50E+03 | 264 | 8.40E+03 | 274 | 1.87E+04 | 284 |

**Table S3.** Statistical branching ratios (%) for all products of the reaction of phenylethynyl (C6H5CC) with allene (H2CCCH2) and with methylacetylene (H3CCCH) at different collision energies (*E*C*,* kJ mol−1).

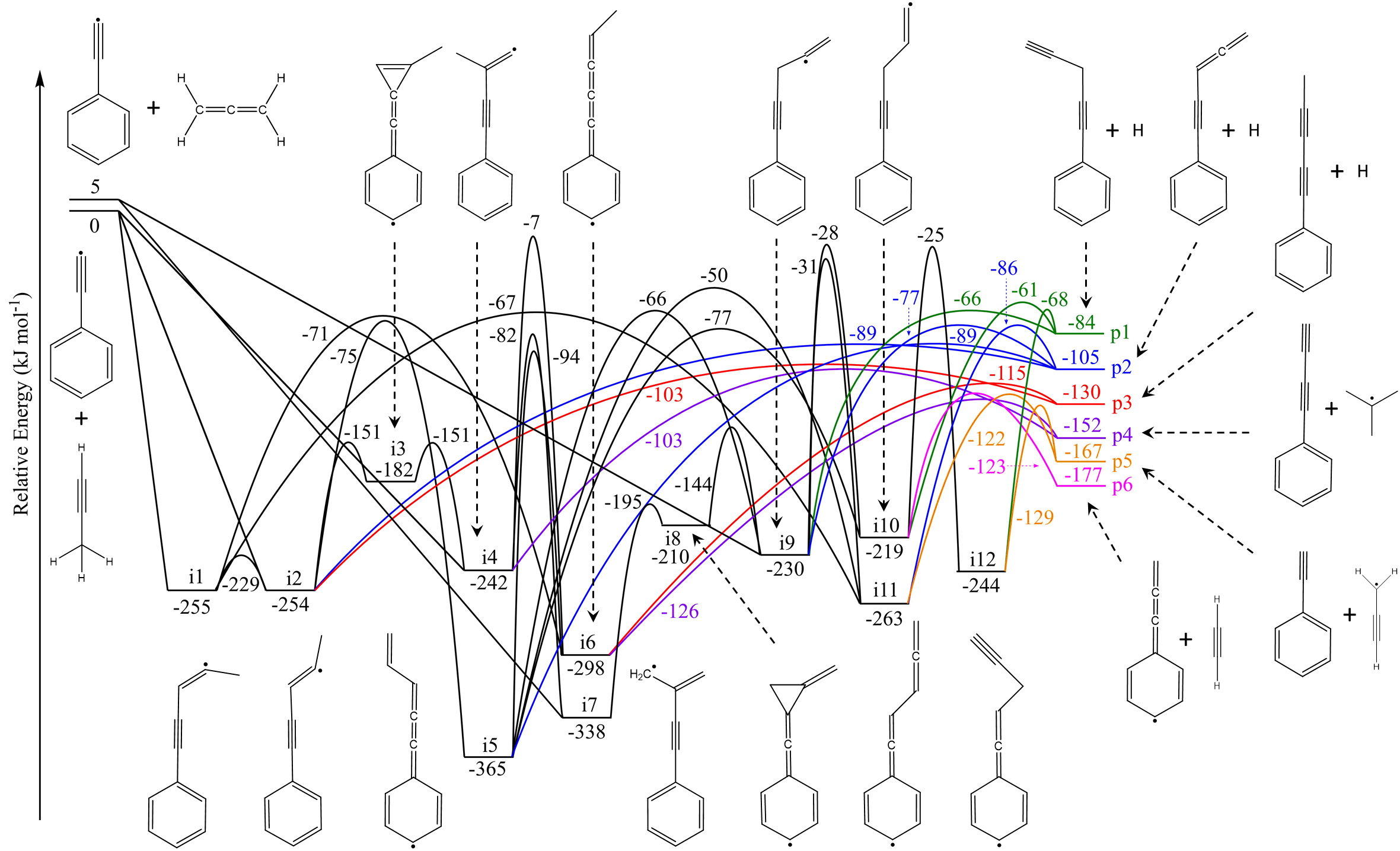
|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Phenylethynyl + Allene | | | | | | | | | | |
|  | Initial intermediate ***i7*** | | | | | Initial intermediate ***i9*** | | | | |
| *EC* | **0** | **10** | **20** | **30** | **40** | **0** | **10** | **20** | **30** | **40** |
| ***p1*** | 23.1 | 27.2 | 31.0 | 34.5 | 37.6 | 23.1 | 27.2 | 31.0 | 34.5 | 37.6 |
| ***p2*** | 57.4 | 56.5 | 55.1 | 53.5 | 51.9 | 57.4 | 56.5 | 55.1 | 53.5 | 51.9 |
| ***p3*** | 4.2 | 3.4 | 2.8 | 2.4 | 2.0 | 4.2 | 3.4 | 2.8 | 2.4 | 2.0 |
| ***p4*** | 15.2 | 12.8 | 11.0 | 9.5 | 8.4 | 15.2 | 12.8 | 11.0 | 9.5 | 8.3 |
| ***p5*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p6*** | 0.1 | 0.1 | 0.1 | 0.1 | 0.2 | 0.1 | 0.1 | 0.1 | 0.1 | 0.2 |
| Phenylethynyl + Methylacetylene | | | | | | | | | | |
|  | Initial intermediates ***i1/i2*** | | | | | Initial intermediate ***i4*** | | | | |
| *EC* | **0** | **10** | **20** | **30** | **40** | **0** | **10** | **20** | **30** | **40** |
| ***p1*** | 0.1 | 0.1 | 0.1 | 0.1 | 0.2 | 0.1 | 0.1 | 0.1 | 0.2 | 0.2 |
| ***p2*** | 3.5 | 3.9 | 4.4 | 4.8 | 5.3 | 3.4 | 3.8 | 4.2 | 4.5 | 4.8 |
| ***p3*** | 25.3 | 25.1 | 25.0 | 25.0 | 25.0 | 24.6 | 24.1 | 23.6 | 23.1 | 22.7 |
| ***p4*** | 71.1 | 70.9 | 70.5 | 70.1 | 69.5 | 71.9 | 72.0 | 72.1 | 72.2 | 72.3 |
| ***p5*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p6*** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |



**Figure S1.** Time-of-flight (TOF) spectra for the reaction of phenylethynyl (C6H5CC) with allene-*d4* (D2CCCD2) taken at *m*/*z* = 143 (black) and 144 (red). Absolute counts are shown in (**a**) while the two spectra are scaled in (**b**).



**Figure S2.** Calculated potential energy surface for the reaction of phenylethynyl (C6H5CC) with allene (H2CCCH2) and with methylacetylene (H3CCCH) at the G3(MP2,CC)// ωB97X-D/6-311G(d,p) level. Energies are in units of kJ mol−1 and colored pathways denote exit channels to the products. Carbon atoms are gray and hydrogen atoms are white.



**Figure S3.** Calculated potential energy surface as shown in Figure S2 with two-dimensional structures.

Chart

Description automatically generated

**Figure S3**. 1H NMR spectrum of (2-iodoethynyl)benzene.

Chart

Description automatically generated

**Figure S4**. 13C NMR spectrum of (2-iodoethynyl)benzene.

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm−1) for all intermediates, transition states, reactants, and products involved in the C8H5 + C3H4 reactions at the ωB97X-D/6-311G(d,p) level.

***Reactants***

***C8H5***



**Cartesian coordinates**

C 0.045775 1.219540 0.013382

C 1.426126 1.212650 -0.006714

C 2.115813 -0.000010 -0.017253

C 1.426105 -1.212662 -0.006715

C 0.045755 -1.219531 0.013384

C -0.671544 0.000009 0.023596

C -2.068345 0.000016 0.040729

C -3.340546 -0.000008 -0.055969

H -0.510694 2.148691 0.019942

H 1.973361 2.147570 -0.015716

H 3.199878 -0.000024 -0.035097

H 1.973339 -2.147581 -0.015717

H -0.510719 -2.148680 0.019947

**Frequencies**

109.1212 143.9347 246.8164

390.7115 476.4153 484.9854

507.4479 629.6306 687.8436

783.4529 788.1472 862.7349

967.3232 1013.8868 1014.0002

1029.0644 1049.7885 1112.7315

1182.8967 1188.0328 1227.9584

1322.9787 1353.0819 1478.2436

1508.7173 1612.2257 1638.8824

1988.9682 3202.8066 3213.5662

3220.9948 3230.0795 3233.7590

***Methylacetylene***



**Cartesian coordinates**

C -0.219275 -0.000871 -0.000237

C -1.417960 0.000091 0.000010

C 1.238342 0.000094 0.000115

H -2.481089 0.001227 0.000307

H 1.624994 0.232644 -0.994855

H 1.626340 -0.976957 0.297065

H 1.623113 0.747205 0.698157

**Frequencies**

346.1945 348.5118 683.1649

683.3323 952.2647 1057.0201

1061.1503 1416.9837 1481.6045

1486.1575 2257.5004 3056.2365

3129.3053 3132.9810 3484.4471

***Allene***



**Cartesian coordinates**

C 1.300828 0.000065 -0.000100

C -0.000003 -0.000043 0.000099

C -1.300848 0.000162 0.000179

H 1.860165 -0.617755 -0.694468

H 1.860571 0.617258 0.694514

H -1.860086 0.694522 -0.617768

H -1.860516 -0.695130 0.616650

**Frequencies**

374.2550 374.2736 885.8717

886.0208 892.1538 1020.4348

1020.4726 1117.3684 1422.7168

1485.3699 2081.8102 3152.6728

3154.9596 3237.1291 3237.1866

***Intermediates***

***i1***



**Cartesian coordinates**

C -1.866871 1.217741 0.066268

C -3.217169 0.902718 0.085219

C -3.628453 -0.424034 0.022609

C -2.680721 -1.437726 -0.059520

C -1.328644 -1.130446 -0.078946

C -0.906321 0.202815 -0.016463

C 0.486027 0.522043 -0.038216

C 1.661342 0.792252 -0.059621

C 3.996015 0.181557 -0.010107

C 3.055302 1.104415 -0.088160

C 4.104198 -1.274978 0.120975

H -1.542000 2.250209 0.116031

H -3.952763 1.696376 0.148994

H -4.684887 -0.666345 0.037652

H -2.996206 -2.473662 -0.109949

H -0.586672 -1.917403 -0.143696

H 3.325519 2.154157 -0.181575

H 4.606100 -1.710659 -0.747498

H 3.104741 -1.723616 0.204467

H 4.677939 -1.547197 1.011348

**Frequencies**

20.5526 58.6745 86.0164

118.0515 128.4693 233.9918

310.5158 360.9435 381.0915

413.9244 450.7137 537.4562

556.4986 625.8414 644.7342

711.0825 745.2729 780.9028

809.8854 866.5720 911.7574

943.3511 1000.3561 1017.8434

1021.1900 1024.8066 1045.1794

1061.0372 1068.8140 1112.9055

1188.7191 1208.7490 1285.1840

1317.7799 1321.8541 1356.2133

1399.0735 1461.5067 1470.9684

1488.5923 1542.4382 1647.0311

1678.8879 1737.0315 2346.5316

3008.2324 3091.2696 3116.3588

3152.5443 3191.0583 3200.9220

3209.9129 3218.1493 3223.4995

***i2***



**Cartesian coordinates**

C 1.943497 -1.203388 0.014566

C 3.318386 -1.023825 0.021706

C 3.857948 0.257508 0.010333

C 3.013957 1.362368 -0.007683

C 1.637941 1.190784 -0.014676

C 1.086991 -0.096144 -0.003797

C -0.329897 -0.277415 -0.013114

C -1.526790 -0.419822 -0.022468

C -2.934965 -0.631843 -0.040264

H 1.518024 -2.199816 0.023594

H 3.972729 -1.888097 0.035958

H 4.933175 0.395159 0.015777

H 3.430606 2.363139 -0.016933

H 0.975356 2.047981 -0.028946

H -3.267917 -1.672355 -0.118223

C -3.842866 0.321866 0.026918

C -5.304135 0.442392 0.028889

H -5.659420 0.904774 0.954167

H -5.775186 -0.546730 -0.062802

H -5.647754 1.061058 -0.805057

**Frequencies**

31.9807 59.7647 76.6186

148.0435 154.4828 191.0489

284.8947 295.6726 363.4684

413.4081 433.8967 523.5969

555.1421 584.1764 643.7912

710.3673 747.7393 779.4855

796.5435 866.8113 920.7189

943.2506 1001.4078 1017.0283

1023.9584 1045.0231 1047.2666

1065.1884 1073.3376 1112.2766

1188.9262 1206.2322 1266.5415

1316.5845 1325.6720 1355.4267

1403.7355 1457.0294 1477.6827

1488.9912 1541.0459 1647.0062

1678.7228 1755.0991 2355.0228

3000.8700 3063.4442 3088.8445

3115.0075 3191.7889 3201.4334

3211.6677 3220.6157 3225.4730

***i3***



**Cartesian coordinates**

C 1.526427 -1.216317 -0.051405

C 2.891238 -1.205832 0.153445

C 3.586810 0.000119 0.258574

C 2.891052 1.205964 0.153457

C 1.526239 1.216236 -0.051387

C 0.793599 -0.000097 -0.159111

C -0.571672 -0.000175 -0.362211

C -1.846751 -0.000065 -0.496020

H 0.988988 -2.153881 -0.133909

H 3.426201 -2.146026 0.233997

H 4.658518 0.000202 0.419956

H 3.425867 2.146242 0.234015

H 0.988651 2.153716 -0.133882

C -3.209995 0.000017 0.039030

C -3.088140 0.000099 -1.264395

C -4.036881 -0.000007 1.258442

H -3.554819 0.000235 -2.236482

H -3.801013 0.879547 1.863109

H -3.802220 -0.880511 1.862202

H -5.101724 0.000828 1.020470

**Frequencies**

38.1395 41.1010 57.5982

103.6750 168.2127 246.7127

261.6050 371.6465 416.7166

435.6177 472.4259 493.8407

496.0675 631.2155 679.6607

694.7710 719.7154 759.1626

764.7686 839.1064 910.3111

911.2774 984.7165 988.2985

1000.2295 1003.5586 1041.7085

1048.0781 1053.0723 1106.7622

1145.4102 1175.5430 1197.1733

1300.0843 1317.5915 1347.8369

1407.2294 1472.1032 1474.5932

1478.5049 1505.9901 1592.8436

1619.4679 1791.3992 1988.1866

3051.0278 3122.1431 3144.6560

3187.1551 3193.3643 3208.9722

3213.6255 3221.1225 3278.1397

***i4***



**Cartesian coordinates**

C 1.527460 -1.197082 -0.066832

C 2.913083 -1.249419 -0.066024

C 3.657918 -0.077346 0.001435

C 3.010243 1.150836 0.068990

C 1.624694 1.211360 0.068083

C 0.868202 0.035722 0.000052

C -0.559704 0.090535 -0.003229

C -1.764807 0.135848 -0.008673

C -3.198463 0.157744 -0.014908

C -3.834873 1.307471 -0.131218

C -3.909563 -1.169763 0.115998

H 0.943048 -2.107925 -0.119819

H 3.413854 -2.209252 -0.119672

H 4.741026 -0.121600 0.001742

H 3.586490 2.067446 0.122351

H 1.115659 2.166286 0.121138

H -3.564692 2.348709 -0.236111

H -3.608044 -1.839493 -0.693532

H -4.990406 -1.031699 0.080007

H -3.642081 -1.647903 1.061858

**Frequencies**

21.7254 62.4932 68.4786

149.9013 171.1113 216.8517

281.2870 375.7872 413.1299

453.5372 482.7813 519.4341

564.1217 585.6346 642.7695

698.0218 710.9193 710.9905

781.4076 828.3125 867.1153

909.2449 945.6057 1001.4021

1018.7996 1023.7609 1037.2860

1057.1279 1062.5678 1112.3537

1178.4095 1188.0368 1212.2778

1318.6382 1328.2735 1356.9085

1412.6475 1480.0955 1487.8833

1488.6311 1543.2989 1646.5775

1667.7859 1681.9136 2346.4793

3056.9169 3128.3822 3156.9245

3193.8456 3202.1910 3212.3174

3219.7659 3225.5886 3262.1045

***i5***



**Cartesian coordinates**

C -1.896015 -1.216595 -0.000016

C -3.270371 -1.042727 -0.000014

C -3.816173 0.237003 0.000002

C -2.977749 1.347338 0.000015

C -1.601980 1.184047 0.000011

C -1.041934 -0.102784 -0.000004

C 0.366035 -0.276891 -0.000002

C 1.575126 -0.428890 0.000010

C 2.946396 -0.607958 0.000027

C 3.875160 0.461098 -0.000033

C 5.220362 0.292661 0.000001

H -1.465431 -2.210762 -0.000029

H -3.921080 -1.909763 -0.000025

H -4.892006 0.369192 0.000005

H -3.400319 2.345571 0.000029

H -0.944337 2.045137 0.000023

H 3.325618 -1.626455 0.000096

H 3.466303 1.468001 -0.000112

H 5.895082 1.139489 -0.000047

H 5.663030 -0.698220 0.000082

**Frequencies**

30.7495 55.6762 59.9992

142.6306 165.3310 285.9414

321.7522 409.7708 412.4060

440.0543 529.9652 542.0810

595.5511 597.8958 642.5782

706.0432 758.4969 768.2109

776.4393 863.2020 877.4851

939.8836 946.3990 1000.4697

1006.2164 1016.6905 1020.0918

1055.7005 1082.1061 1112.9420

1187.7332 1188.5878 1205.8293

1281.6824 1301.8553 1315.8315

1354.9155 1387.0728 1465.3605

1487.3596 1541.7654 1560.8710

1638.8649 1667.5470 2172.3185

3160.4151 3172.9310 3183.8370

3192.7671 3202.0582 3211.9128

3221.7102 3226.4493 3259.3604

***i6***



**Cartesian coordinates**

C -1.801597 -1.212323 -0.013201

C -3.180585 -1.204232 0.104476

C -3.876344 0.000184 0.164374

C -3.180352 1.204456 0.104304

C -1.801363 1.212257 -0.013378

C -1.086670 -0.000107 -0.073078

C 0.314242 -0.000217 -0.188207

C 1.548805 -0.000221 -0.282785

C 4.157909 -0.000075 -0.465574

C 2.854414 -0.000178 -0.386936

C 5.094014 0.000245 0.714206

H -1.257878 -2.148200 -0.059994

H -3.718385 -2.144344 0.150803

H -4.956040 0.000294 0.258663

H -3.717962 2.144682 0.150509

H -1.257455 2.148018 -0.060297

H 4.622547 -0.000182 -1.453187

H 5.742538 -0.880923 0.686019

H 4.545603 0.000272 1.656509

H 5.742201 0.881656 0.685776

**Frequencies**

38.6312 45.9070 88.7615

96.8998 116.9881 221.4186

244.9759 338.6318 404.6867

411.4858 475.7924 483.6153

519.3581 570.9122 637.9239

695.4548 704.4176 724.8039

774.1558 855.2508 877.4750

934.9643 996.0218 1010.8892

1015.7718 1040.0572 1051.4500

1059.8388 1098.7364 1112.0776

1184.5588 1207.3999 1265.8438

1311.8084 1355.7783 1384.6957

1405.7216 1481.9200 1485.9817

1490.3463 1527.3906 1624.4442

1646.4175 1907.4788 2054.1240

3040.9401 3102.7663 3111.3226

3152.6080 3194.4934 3203.0751

3213.6132 3221.0572 3226.2850

***i7***



**Cartesian coordinates**

C 1.586899 1.205971 0.046927

C 2.973717 1.202017 0.047041

C 3.670537 -0.000001 0.000002

C 2.973716 -1.202018 -0.047039

C 1.586898 -1.205971 -0.046929

C 0.878418 0.000001 -0.000002

C -0.551111 0.000001 -0.000003

C -1.755644 0.000000 -0.000003

C -3.862130 1.215052 -0.083798

C -3.193214 0.000000 0.000000

C -3.862129 -1.215053 0.083802

H 1.039857 2.140485 0.083861

H 3.512540 2.141867 0.084364

H 4.754579 -0.000001 0.000004

H 3.512538 -2.141868 -0.084360

H 1.039855 -2.140483 -0.083864

H -3.322237 2.149957 -0.150099

H -4.945320 1.241920 -0.084851

H -3.322234 -2.149958 0.150099

H -4.945318 -1.241921 0.084862

**Frequencies**

15.8263 56.0266 66.6903

177.9849 205.8122 297.3887

378.1348 413.2230 470.9354

500.3772 524.6132 531.9952

546.5506 601.8323 625.9806

643.0375 698.0043 710.7544

761.9773 781.1118 789.9572

866.3098 912.6641 945.3882

981.6417 1000.5831 1018.0771

1022.7152 1042.9662 1062.0190

1111.7196 1187.4483 1211.6021

1252.9520 1288.8184 1318.7223

1356.7087 1411.5763 1475.5573

1487.2479 1527.1680 1548.9876

1646.3827 1679.1422 2359.9001

3168.5147 3174.4619 3195.1878

3203.5742 3213.8008 3220.6425

3226.7153 3278.5467 3280.1039

***i8***



**Cartesian coordinates**

C -1.497681 1.219995 -0.008560

C -2.872733 1.206733 0.100850

C -3.572928 0.000234 0.157152

C -2.873052 -1.206463 0.101164

C -1.498000 -1.220125 -0.008239

C -0.767170 -0.000170 -0.066185

C 0.604910 -0.000299 -0.166740

C 1.876756 -0.000252 -0.312635

C 3.212976 0.000038 0.201214

C 3.061643 -0.000171 -1.273140

C 4.017493 0.000319 1.246442

H -0.955832 2.157182 -0.051379

H -3.412103 2.146425 0.144008

H -4.652829 0.000389 0.245518

H -3.412679 -2.145999 0.144552

H -0.956410 -2.157472 -0.050826

H 3.261801 -0.919478 -1.817766

H 3.261447 0.919056 -1.818030

H 3.618590 0.000325 2.254331

H 5.094742 0.000536 1.121654

**Frequencies**

31.0185 58.1739 82.8647

174.9840 235.8392 260.4182

362.0532 364.0447 411.8284

457.5039 487.2522 540.1295

631.7287 668.8393 675.0716

689.2627 737.7980 757.7078

834.1880 897.4042 904.7317

917.7164 945.9584 960.0238

987.6087 1002.2174 1003.3324

1035.4549 1047.4941 1048.0417

1110.7024 1133.8119 1178.0116

1197.2857 1294.9681 1303.6357

1350.6928 1432.3372 1464.2404

1471.4423 1504.4960 1593.4801

1619.3877 1809.0019 1975.0650

3109.3931 3158.1577 3192.6874

3199.4326 3199.8194 3213.0089

3218.8448 3224.9283 3251.4445

***i9***



**Cartesian coordinates**

C 1.916371 -1.196651 0.072543

C 3.273294 -0.912238 0.116639

C 3.715226 0.404321 0.053040

C 2.792628 1.438487 -0.055547

C 1.434554 1.161300 -0.101110

C 0.982429 -0.161204 -0.037228

C -0.420290 -0.444821 -0.083535

C -1.600490 -0.667489 -0.124324

C -3.038677 -0.931866 -0.175570

C -3.852398 0.142054 0.441145

C -4.751451 1.010006 0.061168

H 1.566997 -2.221104 0.123722

H 3.989605 -1.721482 0.201296

H 4.776312 0.623097 0.089159

H 3.132662 2.466627 -0.105752

H 0.710377 1.962836 -0.184707

H -3.248240 -1.885062 0.323021

H -3.349872 -1.056067 -1.224989

H -5.213654 1.704091 0.757234

H -5.071358 1.075671 -0.982314

**Frequencies**

22.0444 42.0554 75.5169

98.8458 169.1591 259.9868

308.1030 358.1712 399.5048

413.9447 434.6829 545.6109

555.3945 606.1041 642.9403

712.2996 742.1912 782.2437

867.7284 871.3510 900.9986

925.4954 946.2860 1001.2710

1007.8859 1018.5980 1024.2334

1055.0556 1064.3031 1111.3262

1188.7974 1207.0222 1220.7231

1283.7245 1316.8106 1333.1355

1355.2038 1413.5742 1452.8987

1488.0070 1541.4943 1648.1465

1680.1384 1763.2156 2386.0095

2988.8551 3066.3774 3073.1366

3186.3459 3192.4445 3201.2446

3211.4112 3218.6062 3224.2903

***i10***



**Cartesian coordinates**

C 1.754546 -1.195290 0.113432

C 3.121786 -1.056095 0.300438

C 3.712814 0.200427 0.235421

C 2.929492 1.320747 -0.017846

C 1.561553 1.188605 -0.205303

C 0.959465 -0.072591 -0.141576

C -0.452385 -0.213440 -0.333809

C -1.637753 -0.331775 -0.499453

C -3.081012 -0.475275 -0.671145

C -3.846767 -0.133913 0.602662

C -4.784237 0.770351 0.677751

H 1.288908 -2.172319 0.163737

H 3.728171 -1.932697 0.498042

H 4.781403 0.307313 0.382577

H 3.386527 2.302312 -0.069648

H 0.946650 2.058838 -0.401715

H -3.305954 -1.510707 -0.950579

H -3.422565 0.159940 -1.492908

H -3.560921 -0.704325 1.485857

H -5.267233 1.481133 0.021196

**Frequencies**

6.1724 53.2133 79.5552

106.6822 165.3351 303.0153

322.3224 351.7360 414.6719

421.4374 502.0102 548.2856

569.8212 642.0793 678.9391

716.3134 744.3362 788.5389

826.4770 862.6284 867.0886

946.4170 952.8848 1000.8200

1004.9219 1022.9500 1026.6297

1036.9391 1063.8338 1112.6047

1189.7605 1208.7334 1215.5677

1274.8104 1290.0201 1317.6307

1338.5649 1356.4033 1463.7471

1489.3574 1543.1820 1648.2166

1680.5453 1691.9805 2380.2837

3048.1113 3100.4450 3134.0289

3193.0557 3202.2712 3212.1402

3219.9046 3225.2378 3252.7345

***i11***



**Cartesian coordinates**

C 1.695516 1.222131 -0.086880

C 3.058472 1.207906 0.119060

C 3.753215 0.000431 0.224799

C 3.059038 -1.207331 0.119340

C 1.696135 -1.222161 -0.086569

C 0.967217 -0.000259 -0.195648

C -0.387493 -0.000494 -0.395419

C -1.677120 -0.000722 -0.585616

C -3.966395 0.000063 0.283143

C -2.676276 -0.000372 0.498071

C -5.246899 0.000613 0.057208

H 1.157957 2.159184 -0.169189

H 3.594148 2.147202 0.200298

H 4.824453 0.000717 0.387550

H 3.595033 -2.146432 0.200740

H 1.158992 -2.159465 -0.168692

H -2.308077 0.000047 1.520217

H -5.800008 -0.928739 -0.038235

H -2.075906 -0.001723 -1.602162

H -5.799059 0.930377 -0.039466

**Frequencies**

18.6480 36.6877 104.7945

156.1217 185.5417 187.6805

340.9825 341.7247 410.8852

469.1215 494.2605 532.0186

580.9634 593.1928 629.7887

688.9884 761.0925 795.1152

831.7858 849.0917 896.0317

907.8826 909.6704 987.4334

989.8843 1005.7508 1019.1038

1038.4811 1045.7004 1110.0051

1133.5291 1167.0110 1176.4957

1214.5926 1263.0657 1301.4224

1349.6575 1389.9093 1468.7482

1482.1239 1501.6521 1587.8705

1614.6482 1895.7713 2071.8308

3103.3084 3142.7649 3177.3472

3192.9566 3199.1970 3213.5649

3218.6648 3224.9295 3225.1946

***i12***



**Cartesian coordinates**

C -1.804639 -1.207999 0.003432

C -3.127240 -0.906611 0.249077

C -3.566701 0.419507 0.267212

C -2.655268 1.452436 0.034306

C -1.327384 1.178993 -0.213707

C -0.858942 -0.168081 -0.235771

C 0.458884 -0.448065 -0.489635

C 1.720645 -0.691365 -0.660625

C 2.738042 -0.772288 0.470053

C 3.816616 0.200023 0.301444

C 4.692557 1.002765 0.141317

H -1.464967 -2.236813 -0.012190

H -3.833094 -1.709761 0.429389

H -4.608778 0.644663 0.459887

H -2.993591 2.482587 0.048088

H -0.619702 1.979173 -0.394492

H 2.123582 -0.844986 -1.663369

H 3.169415 -1.779044 0.495712

H 2.239753 -0.609088 1.428606

H 5.467968 1.717385 0.005743

**Frequencies**

22.2220 44.1733 74.0020

132.9458 185.8542 244.7528

344.3546 364.4510 410.6418

468.2702 498.8388 540.7598

550.3158 633.1193 687.8849

706.1736 715.4441 751.0485

759.3165 813.3357 830.5268

905.4687 939.1431 964.1518

984.0921 989.8908 1002.0263

1029.3173 1044.0360 1110.5942

1157.3696 1178.2758 1208.1202

1225.4937 1303.0284 1307.1316

1348.5568 1368.9347 1468.5153

1471.7807 1495.4498 1591.3770

1614.4843 1920.5525 2252.3828

3056.2008 3099.4444 3113.7916

3190.5790 3197.0685 3210.3846

3216.3414 3222.5481 3485.3129

***Transition states***

***i9 – p2***

**Cartesian coordinates**

C -1.908614 -1.191460 -0.089600

C -3.270724 -0.931876 -0.095529

C -3.735009 0.376071 -0.013031

C -2.829344 1.427161 0.075280

C -1.465741 1.175925 0.081427

C -0.991346 -0.138280 -0.000839

C 0.413552 -0.399024 0.007512

C 1.599156 -0.606439 0.020247

C 3.002715 -0.881821 0.021801

C 3.915117 0.076048 -0.119240

C 4.828396 0.994345 -0.124113

H -1.541450 -2.208865 -0.153520

H -3.974062 -1.753894 -0.163649

H -4.800524 0.575214 -0.017310

H -3.187494 2.448191 0.141120

H -0.754832 1.990605 0.150234

H 3.307023 -1.910814 -0.152380

H 3.154717 -1.333641 1.853163

H 5.171062 1.452559 -1.047238

H 5.276610 1.336745 0.806094

**Frequencies**

-917.4723 26.8895 47.6026

84.2680 135.9517 209.1841

252.2584 328.7978 358.3735

373.2181 413.3896 442.9981

481.1165 543.5969 549.6081

609.3710 632.8057 643.8005

710.8056 760.0490 780.3710

868.5764 899.4346 944.9632

956.0667 982.3768 994.3922

1002.4793 1018.5715 1023.4059

1059.8276 1108.4831 1111.4600

1189.2408 1206.2160 1282.5496

1316.6119 1354.9035 1366.8557

1460.8764 1487.7641 1541.5630

1646.9372 1678.6475 2009.0563

2365.2743 3126.2013 3164.4318

3194.1532 3203.1473 3208.6515

3212.9749 3220.4482 3225.9085

***i9 – p1***

**Cartesian coordinates**

C -1.930684 -1.196688 -0.071716

C -3.283213 -0.890584 -0.104902

C -3.702832 0.433589 -0.049032

C -2.762959 1.453901 0.040653

C -1.409059 1.155525 0.074438

C -0.980180 -0.174880 0.018590

C 0.418378 -0.479930 0.053730

C 1.595250 -0.717986 0.084150

C 3.029003 -1.010386 0.124196

C 3.861630 0.191718 0.097626

C 4.616593 1.124600 -0.034711

H -1.598804 -2.227227 -0.116190

H -4.013252 -1.688786 -0.174616

H -4.760569 0.669132 -0.075967

H -3.085734 2.487791 0.084922

H -0.671435 1.946047 0.143256

H 3.300069 -1.643916 -0.729390

H 3.261065 -1.587932 1.025813

H 5.699895 0.674162 -1.613794

H 5.157202 2.037453 0.057846

**Frequencies**

-747.8847 16.2105 51.8250

71.0573 88.3716 138.1942

235.2363 239.5011 323.0405

367.5373 395.4066 413.6091

444.3888 539.4065 555.6114

605.3536 643.8467 699.5281

712.0260 743.5876 781.7729

811.8756 867.9212 922.4427

936.9938 946.5204 1001.8861

1019.2746 1021.7762 1024.7884

1064.4823 1112.7810 1189.2465

1208.7179 1245.8551 1289.3512

1318.6528 1356.4048 1359.6274

1450.9121 1488.9656 1543.2500

1649.0541 1681.0086 2188.0742

2390.2343 3036.8345 3075.2187

3192.1602 3201.5941 3210.8078

3218.8901 3224.1523 3457.1955

***i2 – p3***

**Cartesian coordinates**

C -1.894481 -1.199522 0.011588

C -3.279213 -1.126831 0.014803

C -3.915605 0.109206 0.005456

C -3.161580 1.277343 -0.006846

C -1.776524 1.213819 -0.009894

C -1.129568 -0.027257 -0.000746

C 0.296209 -0.096420 -0.004819

C 1.501306 -0.147919 -0.008429

C 4.054368 0.108527 0.012113

C 2.878724 -0.214736 -0.015288

C 5.497721 0.251892 0.019594

H -1.392394 -2.159473 0.018641

H -3.863783 -2.039589 0.024425

H -4.998298 0.162766 0.007869

H -3.654815 2.242455 -0.014341

H -1.183503 2.120500 -0.019506

H 3.019619 -2.071027 -0.184119

H 5.843016 0.680658 0.963576

H 5.829038 0.901630 -0.794248

H 5.972973 -0.726528 -0.107492

**Frequencies**

-909.3028 35.3723 57.7765

67.0984 110.8614 149.4608

156.9670 277.0852 285.4684

332.7100 396.2346 412.3413

482.6347 512.5206 546.1420

572.9173 584.2069 642.4461

672.9299 710.2316 782.2650

845.5520 867.2942 948.3495

1002.3978 1019.8627 1023.9706

1042.3051 1055.3853 1060.8945

1113.0294 1137.5128 1188.8031

1211.9278 1319.0178 1343.5498

1357.6545 1418.7884 1474.2477

1479.3273 1488.2597 1544.5097

1646.5537 1679.5672 2223.0143

2379.4960 3038.4626 3109.8698

3126.4906 3193.8870 3202.9917

3211.7682 3222.6561 3227.3741

***i2 – p2***

**Cartesian coordinates**

C 1.959160 -1.198959 0.000591

C 3.322802 -0.947391 0.000864

C 3.793736 0.360768 0.000367

C 2.893291 1.420102 -0.000399

C 1.528069 1.176837 -0.000671

C 1.046737 -0.137542 -0.000183

C -0.358961 -0.391950 -0.000488

C -1.546444 -0.595337 -0.000759

C -3.873729 0.045724 0.000134

C -2.942601 -0.874376 -0.001162

C -4.872823 0.894046 0.001371

H 1.587466 -2.216658 0.000982

H 4.021285 -1.776294 0.001468

H 4.860254 0.554283 0.000575

H 3.256161 2.441526 -0.000794

H 0.822097 1.998670 -0.001273

H -3.246442 -1.920018 -0.002655

H -6.533695 -0.245981 -0.000315

H -5.231275 1.327837 -0.926731

H -5.231268 1.325103 0.930750

**Frequencies**

-689.5498 22.5744 48.2074

85.3278 131.5218 175.6017

255.6387 279.7593 352.1639

367.4631 405.9602 414.3967

422.4994 544.8128 555.5986

623.4673 643.8126 692.6658

714.5254 758.2076 785.7166

869.9520 900.3443 934.5146

950.8103 981.4256 1003.8532

1017.5847 1024.0925 1024.1343

1061.4469 1112.5523 1118.7077

1189.2742 1209.4344 1288.0442

1319.2935 1356.4533 1372.6433

1469.5480 1488.5812 1544.3384

1647.5466 1680.4523 2024.8995

2361.3066 3137.3645 3140.6447

3188.8424 3197.4583 3207.7718

3214.7982 3220.4648 3225.4648

***i1 – i11***

**Cartesian coordinates**

C 1.573289 -1.212312 -0.038017

C 2.949133 -1.205685 0.112448

C 3.641400 0.000008 0.188143

C 2.949130 1.205695 0.112396

C 1.573286 1.212312 -0.038071

C 0.861385 -0.000003 -0.114328

C -0.537713 -0.000011 -0.271715

C -1.786310 -0.000014 -0.215907

C -4.098275 -0.000007 -0.261668

C -3.031926 -0.000052 -1.035643

C -4.040223 0.000052 1.127398

H 1.027830 -2.146421 -0.097843

H 3.487535 -2.144543 0.171608

H 4.718876 0.000012 0.305607

H 3.487531 2.144557 0.171516

H 1.027826 2.146418 -0.097939

H -2.977726 -0.000105 -2.115976

H -4.289662 0.914271 1.665309

H -2.511592 0.000040 0.942123

H -4.289664 -0.914125 1.665381

**Frequencies**

-2223.1903 47.1183 59.4539

80.8943 201.6975 217.7650

315.0989 337.2880 394.2870

413.3474 516.6704 517.5798

565.8576 636.8506 667.2004

676.7047 705.4269 780.8768

827.2572 860.3101 864.0961

945.4649 948.2098 1003.1184

1003.6712 1014.4417 1018.6197

1022.3469 1057.8040 1101.4456

1105.0868 1112.7297 1187.7652

1202.9496 1244.6282 1282.9749

1316.2079 1354.6527 1470.8612

1483.8852 1523.4552 1533.2703

1630.3634 1656.5901 1735.6269

2050.1709 3104.0259 3180.4766

3190.1447 3198.8708 3209.0031

3216.4579 3221.5559 3233.4499

***i7 – i8***

**Cartesian coordinates**

C 1.520186 -1.212398 0.068856

C 2.903177 -1.203901 0.024595

C 3.602858 -0.000004 0.001973

C 2.903187 1.203899 0.024515

C 1.520196 1.212409 0.068774

C 0.801112 0.000009 0.089767

C -0.601697 0.000015 0.139612

C -1.839113 0.000007 0.029221

C -3.248994 0.000001 0.083679

C -3.042726 -0.000087 -1.363201

C -4.215216 0.000062 0.988680

H 0.975283 -2.148655 0.087301

H 3.442663 -2.144180 0.007263

H 4.685997 -0.000010 -0.032112

H 3.442681 2.144173 0.007125

H 0.975301 2.148672 0.087161

H -3.049671 0.933191 -1.912223

H -3.049642 -0.933437 -1.912103

H -3.985955 0.000135 2.047137

H -5.254478 0.000041 0.681628

**Frequencies**

-664.6794 50.4206 54.5332

70.4485 186.2794 228.0607

280.8288 302.9319 350.6726

412.2697 457.4451 508.6794

535.7559 616.7028 640.1096

703.9995 704.6498 741.7038

761.0624 770.4324 855.8471

927.6165 934.1152 936.2755

959.4033 996.0669 1013.4116

1014.0388 1025.0921 1056.7898

1112.5293 1171.8175 1184.7700

1205.2864 1312.1269 1312.3983

1354.6215 1419.1605 1456.2670

1482.0901 1525.3010 1623.7789

1647.3600 1781.3986 2061.4842

3152.1320 3163.2985 3187.6856

3195.2190 3207.3159 3213.5497

3219.5920 3261.8223 3266.1141

***i1 – i6***

**Cartesian coordinates**

C 1.804139 -1.208300 0.005922

C 3.184378 -1.202871 -0.121985

C 3.879165 0.000131 -0.186214

C 3.184274 1.203052 -0.121605

C 1.804033 1.208321 0.006301

C 1.096377 -0.000031 0.071494

C -0.320378 -0.000123 0.203338

C -1.532040 -0.000203 0.280411

C -4.153826 -0.000266 0.336174

C -2.880286 -0.000425 0.554143

C -5.206437 0.000503 -0.712298

H 1.259602 -2.143582 0.056105

H 3.721282 -2.143284 -0.171941

H 4.958408 0.000194 -0.286240

H 3.721097 2.143527 -0.171269

H 1.259417 2.143541 0.056772

H -3.644405 -0.001205 1.563047

H -5.842788 -0.882136 -0.617451

H -4.745810 0.001555 -1.707342

H -5.843201 0.882660 -0.615768

**Frequencies**

-2181.8281 28.5883 52.4793

65.3579 100.9567 132.5854

211.0117 250.3775 267.6215

352.6243 399.6159 413.2537

485.7005 497.8151 549.7508

571.3613 643.2712 669.0747

712.6381 781.6361 839.7466

867.0333 945.1339 1001.6954

1021.0860 1021.9389 1025.3476

1031.2476 1055.1614 1073.4513

1112.6710 1188.1572 1209.4862

1313.3459 1316.7091 1356.5937

1389.3401 1469.0178 1477.8808

1486.9154 1539.3779 1642.7080

1673.8575 1968.0383 2269.9420

2387.2351 3022.0361 3110.0044

3130.0497 3188.2509 3196.9307

3207.5168 3214.7274 3220.1890

***i8 – i9***

**Cartesian coordinates**

C -1.514941 -1.210118 0.106237

C -2.863715 -1.203072 -0.207620

C -3.545294 0.000050 -0.365889

C -2.863724 1.203130 -0.207292

C -1.514950 1.210090 0.106568

C -0.816810 -0.000034 0.267801

C 0.557719 -0.000077 0.590516

C 1.777944 -0.000099 0.735578

C 3.273960 0.000066 -0.364658

C 3.200064 -0.000224 1.089343

C 3.939974 0.000267 -1.488329

H -0.983416 -2.146256 0.228915

H -3.388699 -2.143669 -0.330738

H -4.600954 0.000079 -0.611104

H -3.388709 2.143762 -0.330146

H -0.983427 2.146193 0.229512

H 3.547382 0.902638 1.597462

H 3.547295 -0.903325 1.597099

H 3.436972 0.000468 -2.451219

H 5.032186 0.000237 -1.503303

**Frequencies**

-682.3928 35.9979 51.8581

93.5088 154.1448 156.3072

265.3577 286.6048 363.4456

407.1236 413.4358 510.3382

517.9624 551.4116 640.9749

708.0890 710.2620 773.7841

860.1168 901.3538 922.4600

932.5143 939.1022 997.5189

998.7716 1015.4155 1017.1793

1031.4137 1060.3903 1112.5042

1135.7418 1186.1124 1201.6271

1209.4610 1311.6925 1314.1068

1355.5234 1430.0692 1449.4080

1484.6793 1531.4459 1631.6208

1657.3771 1792.0617 2132.2734

3051.8126 3075.0528 3117.7747

3180.2285 3186.7476 3194.4942

3206.4691 3212.7899 3218.8703

***i9 – i11***

**Cartesian coordinates**

C -1.915443 -1.196689 0.058573

C -3.270646 -0.912805 0.037541

C -3.715829 0.404995 -0.006422

C -2.789463 1.443217 -0.030828

C -1.431186 1.174082 -0.014633

C -0.971878 -0.154427 0.029351

C 0.411453 -0.433299 0.051203

C 1.610323 -0.674056 -0.080764

C 3.030468 -0.916701 -0.051216

C 3.964493 0.033844 0.233779

C 4.788163 1.017874 0.017419

H -1.569449 -2.222720 0.097770

H -3.986806 -1.726506 0.058011

H -4.777592 0.621399 -0.020151

H -3.129224 2.472221 -0.064124

H -0.709831 1.982283 -0.034077

H 2.283091 -0.783899 -1.247793

H 3.327139 -1.961317 -0.089676

H 4.941985 1.423493 -0.984476

H 5.357957 1.478832 0.820487

**Frequencies**

-1920.7034 42.9513 47.5135

81.0381 126.0104 216.8519

242.0408 307.8458 352.0003

412.5413 419.5903 510.5105

543.1810 559.5891 629.9522

641.0079 708.5958 715.2190

753.1107 773.2001 859.6402

918.2231 931.6344 956.0333

993.8509 997.3058 1009.6131

1015.7517 1017.1841 1056.9394

1099.4758 1112.9746 1186.5640

1207.1254 1301.4155 1314.4312

1356.1879 1367.5915 1457.0023

1484.9177 1531.2742 1607.2646

1631.8933 1666.3496 1912.6153

2179.5837 3079.9651 3165.7478

3170.5114 3187.6687 3195.0192

3206.9607 3212.7617 3219.4007

***i9 – i10***

**Cartesian coordinates**

C -1.894672 -1.192517 -0.123355

C -3.253697 -0.925081 -0.197672

C -3.717053 0.381214 -0.090813

C -2.813886 1.422219 0.091598

C -1.453663 1.161829 0.167846

C -0.979981 -0.150209 0.060796

C 0.423938 -0.420597 0.138516

C 1.603205 -0.642492 0.204738

C 3.037281 -0.906920 0.287115

C 3.870237 0.159639 -0.361407

C 4.813179 1.021460 -0.193889

H -1.528867 -2.208978 -0.206939

H -3.954131 -1.740048 -0.340218

H -4.779593 0.587519 -0.149657

H -3.170444 2.442495 0.175177

H -0.745431 1.969354 0.310029

H 3.258189 -1.868082 -0.187706

H 3.340524 -0.989614 1.339825

H 4.251986 0.890455 -1.348120

H 5.518435 1.465625 0.506765

**Frequencies**

-2108.5527 7.8376 37.0519

77.5536 90.5746 165.6452

231.1406 262.8435 337.5420

357.4406 406.4152 414.8211

500.4291 553.9903 568.9864

642.3671 650.1868 715.4673

745.1486 786.2434 827.8078

871.0174 903.5735 937.6845

951.1341 1003.9131 1011.7405

1023.4877 1024.5684 1064.0545

1111.6680 1188.6064 1208.9079

1217.8865 1281.9742 1318.6774

1327.8673 1355.6957 1455.6048

1488.2765 1542.7230 1648.7873

1681.0546 1875.6236 2383.9460

2440.7925 3013.0827 3080.1600

3120.0504 3187.8020 3196.8649

3206.8045 3214.2766 3219.8149

***i4 – p4***

**Cartesian coordinates**

C -1.443836 1.142503 0.000012

C -2.822817 1.287326 0.000010

C -3.643897 0.165263 -0.000001

C -3.081017 -1.106097 -0.000011

C -1.702907 -1.259490 -0.000010

C -0.870225 -0.134373 0.000002

C 0.549448 -0.286143 0.000004

C 1.747776 -0.423899 0.000005

C 3.128097 -0.548182 0.000006

C 4.167297 -1.204028 0.000014

C 3.590213 1.644236 -0.000021

H -0.798591 2.012898 0.000021

H -3.258640 2.279715 0.000018

H -4.721586 0.281510 -0.000003

H -3.718636 -1.982572 -0.000021

H -1.257699 -2.247110 -0.000018

H 5.185100 -1.517063 0.000017

H 3.094124 1.917577 -0.923830

H 4.673016 1.674752 -0.000024

H 3.094128 1.917599 0.923784

**Frequencies**

-605.2552 11.5381 56.6844

73.1724 97.7950 143.1082

201.0713 248.2612 365.1806

385.3750 414.0095 424.6704

477.8417 504.4992 550.4921

562.3710 568.8506 580.8465

642.9322 682.6263 708.2390

714.1968 787.3522 871.1903

897.0402 953.9580 978.6770

1005.4877 1024.4666 1025.9854

1063.4258 1112.9531 1189.7066

1210.0226 1299.2615 1319.6676

1356.8090 1419.2791 1423.3337

1488.5005 1541.6115 1647.7871

1679.1863 2001.5670 2360.6580

3096.2310 3189.5556 3198.6665

3208.0185 3215.7825 3221.1531

3265.0428 3265.5492 3453.5765

***i4 – i7***

**Cartesian coordinates**

C -1.606843 1.204962 -0.000090

C -2.993164 1.233180 -0.000205

C -3.717478 0.046303 -0.000121

C -3.049476 -1.173125 0.000087

C -1.663350 -1.209687 0.000205

C -0.927401 -0.018929 0.000114

C 0.500265 -0.053272 0.000179

C 1.705803 -0.091886 0.000165

C 3.120473 -0.105812 0.000034

C 4.018555 -1.084425 -0.000439

C 4.077987 1.056115 0.000193

H -1.037065 2.126474 -0.000144

H -3.510805 2.185515 -0.000357

H -4.801125 0.071718 -0.000223

H -3.611064 -2.100215 0.000136

H -1.137018 -2.156643 0.000346

H 4.008900 -2.171299 -0.000911

H 4.173954 1.628547 -0.921618

H 4.947438 -0.032531 -0.000297

H 4.174562 1.627888 0.922334

**Frequencies**

-2203.4688 22.0670 61.3625

70.5124 177.2740 196.8588

320.4878 367.3529 414.1151

462.7533 479.8975 502.2329

569.8668 579.4511 603.1084

643.9494 714.0500 726.8499

752.2775 786.8941 870.2610

904.6833 952.4537 970.1459

997.3039 1004.4135 1024.6219

1024.7649 1053.9983 1062.1614

1112.7026 1114.8911 1189.2419

1196.4306 1211.2627 1319.8592

1331.1019 1356.3308 1425.7867

1488.6288 1541.1932 1647.8490

1673.2550 1693.5308 1909.5724

2351.9153 3087.5542 3175.2161

3189.3326 3191.7621 3198.5662

3208.1131 3215.8357 3221.1051

***i10 – p1***

**Cartesian coordinates**

C -1.449600 1.140613 -0.252572

C -2.809149 1.389761 -0.137646

C -3.688977 0.353481 0.153643

C -3.203474 -0.937004 0.330920

C -1.844977 -1.193569 0.218596

C -0.954552 -0.155650 -0.074900

C 0.448840 -0.412887 -0.192955

C 1.628507 -0.614942 -0.294343

C 3.062659 -0.869875 -0.422427

C 3.902387 0.228915 0.091794

C 4.704339 0.872253 0.728935

H -0.758731 1.943600 -0.479962

H -3.183506 2.397501 -0.276568

H -4.751055 0.551268 0.242382

H -3.885905 -1.747916 0.558352

H -1.461658 -2.197536 0.356828

H 3.309883 -1.048968 -1.473519

H 3.324298 -1.779879 0.127329

H 3.257262 1.528489 -1.156809

H 5.373390 1.546871 1.207695

**Frequencies**

-799.1961 9.6084 50.1261

80.4317 111.6457 159.5522

251.1485 332.2560 364.5403

401.5106 411.8295 414.3977

495.4590 539.9982 555.6770

599.5996 642.7852 662.9925

714.0960 715.2369 745.2249

786.0467 871.1207 932.8881

937.3593 951.7159 1004.1893

1021.7584 1023.9174 1024.8127

1064.6314 1112.0789 1188.7165

1209.2707 1244.8925 1290.1644

1319.3354 1355.9097 1356.3957

1461.9256 1488.5260 1542.9584

1649.1831 1681.1969 2157.8488

2388.8808 3052.7459 3092.1799

3188.0466 3197.2066 3206.9922

3214.6037 3220.0240 3475.0155

***i10 – p6***

**Cartesian coordinates**

C 1.702535 -1.201534 0.024021

C 3.053718 -1.142682 0.327156

C 3.705232 0.084493 0.391434

C 2.996861 1.256954 0.150260

C 1.645366 1.207485 -0.153188

C 0.980004 -0.024967 -0.220507

C -0.407917 -0.080096 -0.529865

C -1.585316 -0.123722 -0.824225

C -2.965180 -0.176398 -1.040055

C -3.857680 -0.132152 0.888812

C -4.994329 0.329313 0.940577

H 1.191248 -2.155391 -0.028421

H 3.602126 -2.058922 0.513890

H 4.762016 0.127001 0.628659

H 3.500876 2.215431 0.199216

H 1.089257 2.118074 -0.341372

H -3.389002 -1.128680 -1.339611

H -3.437311 0.698728 -1.470406

H -3.020601 -0.563109 1.402070

H -5.938372 0.766703 0.709453

**Frequencies**

-726.7527 25.5515 34.6171

51.5243 95.6689 126.8817

256.3877 297.0050 306.9050

414.3534 420.7683 464.3495

511.5085 542.1874 551.3096

590.5809 641.9397 702.6585

712.0249 734.1064 781.5493

782.9170 827.6455 867.4210

938.7292 947.0262 1002.5204

1021.3958 1021.7477 1037.5396

1066.4465 1072.1047 1112.2240

1188.1566 1208.4307 1317.6558

1329.8770 1355.5391 1462.4673

1487.1935 1541.6042 1642.1070

1672.4637 1853.0867 2226.0252

3148.1013 3188.0909 3196.8782

3207.1128 3214.4227 3220.0285

3237.9009 3333.6698 3454.0779

***i1 – i2***

**Cartesian coordinates**

C -1.976718 -1.192727 0.058843

C -3.332361 -0.901395 0.084254

C -3.766952 0.418378 0.033694

C -2.836913 1.448884 -0.042478

C -1.479858 1.165228 -0.067848

C -1.033829 -0.160970 -0.017646

C 0.364676 -0.452304 -0.044854

C 1.548608 -0.679517 -0.069034

C 2.951944 -0.970498 -0.101881

H -1.633689 -2.219787 0.099086

H -4.054066 -1.708149 0.143558

H -4.827411 0.642217 0.053890

H -3.170625 2.479591 -0.083244

H -0.750781 1.964496 -0.127099

H 3.207277 -2.029244 -0.223839

C 3.887467 -0.063082 0.003838

C 4.935005 0.930350 0.111831

H 4.668631 1.856402 -0.412912

H 5.888946 0.578387 -0.304932

H 5.105289 1.182007 1.163178

**Frequencies**

-274.3866 26.8231 57.0113

91.6697 105.1958 165.4290

253.2449 298.7281 360.2125

409.4053 414.0087 498.7024

553.9845 580.0321 642.9791

711.0477 729.0353 780.6338

798.8620 866.4032 874.6019

943.1507 984.3381 1000.1767

1016.7123 1023.0968 1029.5733

1041.9743 1064.6794 1111.3534

1188.2528 1206.9702 1287.6745

1316.1250 1323.5161 1355.1953

1406.9552 1458.0537 1474.8654

1487.6731 1541.1858 1646.3186

1678.8494 1833.0424 2348.8947

2993.0683 3041.5145 3048.2608

3100.4989 3191.3199 3200.7905

3210.7610 3218.8282 3224.0112

***i4 – i6***

**Cartesian coordinates**

C 1.552349 -1.180951 -0.054020

C 2.933156 -1.279512 -0.026667

C 3.722810 -0.134883 0.029957

C 3.115651 1.117210 0.059919

C 1.736095 1.231695 0.034440

C 0.929397 0.080257 -0.023330

C -0.475694 0.189519 -0.050845

C -1.698398 0.294681 -0.054903

C -3.033495 0.398479 -0.151454

C -4.260614 0.832021 0.130061

H 0.939239 -2.073256 -0.098693

H 3.398617 -2.258474 -0.050109

H 4.803081 -0.217919 0.050734

H 3.724055 2.013523 0.104396

H 1.264345 2.206658 0.059246

H -4.961493 1.039337 -0.688512

C -3.990374 -1.001551 0.136379

H -3.516772 -1.603045 -0.641961

H -5.064664 -1.040775 -0.052392

H -3.771693 -1.347838 1.140070

**Frequencies**

-435.4001 52.0191 58.4668

66.5085 127.8973 176.6401

231.8169 259.5221 356.5747

378.2749 412.0515 469.7127

518.2276 582.1478 611.1792

641.8041 693.0273 707.8858

771.9393 856.3494 861.8384

881.3647 918.4216 927.7068

972.5062 995.6738 1010.5002

1013.8397 1018.5906 1058.5564

1112.9220 1185.6933 1206.1753

1289.6734 1313.2189 1316.1832

1355.8697 1443.4421 1469.5784

1484.0366 1527.4076 1629.3433

1656.1306 1789.2307 2145.1553

3034.8349 3067.7253 3141.3799

3186.8004 3194.0568 3206.3217

3212.3755 3218.9694 3219.2821

***i5 – i9***

**Cartesian coordinates**

C -1.925068 -1.199963 0.055221

C -3.292082 -0.971253 0.090271

C -3.786761 0.327743 0.052257

C -2.905656 1.401113 -0.018968

C -1.536992 1.181645 -0.050363

C -1.031325 -0.123994 -0.014709

C 0.376184 -0.353302 -0.049217

C 1.569304 -0.537269 -0.073345

C 2.966674 -0.776585 -0.111888

C 3.926854 0.288553 -0.204186

C 5.080741 0.676096 0.302476

H -1.535606 -2.210674 0.081936

H -3.975127 -1.811149 0.145789

H -4.856075 0.503141 0.078189

H -3.286663 2.415517 -0.048240

H -0.846305 2.014741 -0.102534

H 3.408919 -0.335071 -1.264585

H 3.316739 -1.771840 0.164318

H 5.752185 1.339107 -0.231981

H 5.370691 0.379515 1.311818

**Frequencies**

-1989.3701 30.6000 50.9735

86.5090 131.4059 194.8547

279.5605 286.6433 367.9159

412.6729 414.2815 506.7558

547.9830 570.8874 642.5115

659.4943 713.7956 744.9228

783.6939 832.0746 869.0260

891.5026 948.3639 949.3788

1003.1065 1022.7496 1023.3441

1029.3058 1061.4475 1099.8268

1112.6948 1129.6298 1188.7872

1209.1542 1259.2941 1318.8404

1355.4363 1356.5573 1442.4128

1488.2674 1543.4459 1645.7337

1678.0547 1725.0717 2169.8099

2319.5301 3090.1503 3109.8195

3188.5858 3197.2431 3206.3231

3207.5322 3214.6525 3220.3219

***i11 – p5***

**Cartesian coordinates**

C 1.674344 -1.210402 0.192382

C 2.976543 -1.203094 -0.280759

C 3.630789 0.001792 -0.517431

C 2.974967 1.205275 -0.277989

C 1.672762 1.209789 0.195166

C 1.004465 -0.001021 0.435184

C -0.330917 -0.002390 0.912938

C -1.537988 -0.003123 1.111981

C -3.904508 0.000857 -0.586525

C -2.665023 -0.000271 -0.778126

C -5.189695 0.001859 -0.231407

H 1.159967 -2.145487 0.379021

H 3.484936 -2.142238 -0.466433

H 4.649699 0.002882 -0.886958

H 3.482127 2.145507 -0.461513

H 1.157152 2.143765 0.383940

H -2.413038 -0.004355 1.724574

H -1.892786 -0.000314 -1.519702

H -5.730255 0.932448 -0.101744

H -5.732237 -0.927841 -0.103653

**Frequencies**

-651.7144 8.9490 40.3977

41.1842 111.3223 168.0384

173.2083 311.2186 381.7158

384.9194 413.3621 464.6560

498.4611 543.2384 546.9998

640.2902 706.7695 710.5324

716.5527 724.3264 781.6038

784.6837 792.5046 829.7917

867.1773 947.1873 1003.6314

1020.8439 1023.0963 1032.7515

1058.6717 1112.7645 1157.3002

1188.4728 1204.7912 1234.9091

1318.5646 1355.8080 1467.2704

1486.3700 1531.0581 1639.0081

1666.2865 1900.6253 2079.1819

3151.1119 3189.5446 3198.4227

3208.4524 3215.8195 3221.1244

3242.4129 3365.0484 3402.4058

***i11 – p2***

**Cartesian coordinates**

C -1.717429 1.208435 -0.032296

C -3.092936 1.203905 0.140765

C -3.783781 0.000152 0.227548

C -3.093072 -1.203707 0.141158

C -1.717566 -1.208447 -0.031898

C -1.014655 -0.000061 -0.120671

C 0.399336 -0.000173 -0.296166

C 1.613641 -0.000221 -0.329328

C 4.033016 -0.000019 -0.021835

C 2.970952 -0.000476 -0.787645

C 5.107651 0.000410 0.705215

H -1.172908 2.142638 -0.098738

H -3.628481 2.143752 0.209482

H -4.859208 0.000235 0.363162

H -3.628721 -2.143472 0.210181

H -1.173148 -2.142733 -0.098032

H 1.990258 0.000690 1.660947

H 3.109880 -0.001101 -1.866578

H 5.565697 -0.929675 1.025783

H 5.565685 0.930872 1.024708

**Frequencies**

-693.7088 11.7570 58.5581

72.5969 101.4947 156.9068

274.6070 288.7581 345.8883

346.3382 413.8379 428.4074

461.6006 534.2884 566.3000

612.8166 636.9236 652.8434

712.8473 771.4898 785.8857

869.6565 889.6279 895.8787

952.1045 979.5906 1004.5922

1008.6897 1024.0123 1024.8106

1061.8046 1112.6666 1140.0295

1189.2960 1209.1507 1277.7992

1318.7637 1356.3310 1372.8725

1478.3834 1487.6531 1542.1557

1645.4350 1675.9173 2083.1958

2274.6818 3143.5102 3152.0372

3189.2654 3198.5754 3208.3577

3216.1240 3221.1683 3227.4364

***i6 – p3***

**Cartesian coordinates**

C 1.856097 -1.208729 -0.008190

C 3.242438 -1.203866 -0.005167

C 3.938321 -0.000003 -0.003627

C 3.242451 1.203867 -0.004961

C 1.856110 1.208745 -0.007980

C 1.149047 0.000012 -0.009817

C -0.276568 0.000019 -0.012560

C -1.485738 0.000023 -0.015111

C -4.061489 -0.000052 0.059159

C -2.849360 0.000030 -0.023033

C -5.501797 0.000174 -0.185088

H 1.307730 -2.143024 -0.008854

H 3.782406 -2.143631 -0.003715

H 5.022235 -0.000009 -0.001048

H 3.782428 2.143626 -0.003348

H 1.307753 2.143047 -0.008483

H -4.226991 -0.002032 2.074117

H -5.968499 -0.883910 0.254160

H -5.695581 0.001327 -1.260650

H -5.968554 0.883278 0.256066

**Frequencies**

-707.5136 37.0678 52.6330

54.1285 142.9519 146.6215

173.0080 296.1818 326.7254

337.3872 412.9692 417.1935

437.1122 493.3258 525.4455

573.6207 584.5919 644.4575

658.9445 713.1712 786.8386

841.8571 870.0453 953.4053

1005.0036 1024.4127 1025.5801

1044.2889 1060.3974 1061.0999

1113.2095 1135.8082 1189.6102

1210.5805 1319.6665 1351.6082

1357.0261 1417.4024 1478.3409

1481.6184 1488.0398 1543.2950

1646.7865 1677.9786 2251.5566

2348.0377 3051.5746 3129.8284

3131.9435 3190.3606 3199.9263

3209.1299 3217.1653 3222.0890

***i6 – p4***

**Cartesian coordinates**

C -1.780948 -1.208942 -0.021739

C -3.149604 -1.202823 0.198319

C -3.836638 0.001376 0.305893

C -3.148900 1.204624 0.192370

C -1.780240 1.208866 -0.027717

C -1.082048 -0.000521 -0.137067

C 0.324369 -0.001525 -0.362874

C 1.520080 -0.002438 -0.553145

C 4.079743 -0.003907 -0.836903

C 2.862383 -0.003531 -0.777434

C 5.049949 0.005870 1.347514

H -1.240273 -2.143857 -0.106640

H -3.682834 -2.142329 0.286209

H -4.906780 0.002115 0.477934

H -3.681586 2.144861 0.275633

H -1.239026 2.143040 -0.117219

H 5.058313 -0.005804 -1.258099

H 5.603100 -0.922698 1.277684

H 4.139467 0.007177 1.931340

H 5.600743 0.935210 1.269854

**Frequencies**

-443.0206 18.6053 36.0442

44.8013 72.5929 101.4350

225.6967 228.1727 365.7478

375.8399 412.8652 424.4724

463.4472 488.8626 489.6720

562.2044 586.7314 644.0597

667.0570 675.1382 708.9962

712.9384 785.2326 799.8216

869.6558 951.7784 987.8256

1004.7782 1023.8379 1025.2035

1063.5990 1113.6271 1189.9009

1210.2064 1309.7381 1318.9669

1357.4948 1411.7979 1420.5758

1488.1004 1540.4260 1645.5709

1676.1958 2086.5222 2303.3201

3103.1510 3190.3061 3199.2282

3209.0516 3216.4406 3221.6902

3272.8347 3282.9784 3441.6135

***i2 – i5***

**Cartesian coordinates**

C 1.923612 -1.205689 0.057565

C 3.293824 -1.001895 0.114196

C 3.813366 0.287538 0.079524

C 2.952910 1.376054 -0.012100

C 1.581369 1.180912 -0.068191

C 1.049350 -0.114759 -0.034024

C -0.360318 -0.318724 -0.092225

C -1.557261 -0.480771 -0.146469

C -2.950146 -0.698076 -0.177169

C -3.873396 0.287591 -0.238259

C -5.165558 0.466413 0.283714

H 1.515166 -2.208922 0.083154

H 3.960236 -1.854044 0.184972

H 4.885147 0.443527 0.123267

H 3.352783 2.383321 -0.040245

H 0.907262 2.026062 -0.140367

H -3.292833 -1.734050 -0.214693

H -4.147248 1.281862 0.549094

H -5.594669 -0.191690 1.043465

H -5.832354 1.182373 -0.188015

**Frequencies**

-1791.2439 34.4810 53.9851

86.1791 147.3993 174.5075

247.5352 323.6010 369.7862

414.6898 423.0386 510.9616

544.7915 563.9981 611.0216

644.0205 713.6339 758.0844

783.4907 796.4811 868.1726

919.5920 946.6072 988.7368

1001.9387 1020.8284 1023.6130

1053.8848 1067.1737 1112.0308

1126.1317 1175.3550 1188.0505

1208.8748 1277.5388 1318.0868

1355.2626 1356.1337 1476.1591

1487.8478 1539.7378 1587.2215

1645.0804 1679.2298 2229.0520

2306.7578 3061.4716 3099.3611

3187.2184 3196.1118 3196.4062

3206.7546 3214.1403 3219.5875

***i2 – i3***

**Cartesian coordinates**

C -1.560924 -1.209637 0.097517

C -2.905963 -1.203995 -0.230334

C -3.586073 -0.000559 -0.397362

C -2.906219 1.203332 -0.232519

C -1.561178 1.209870 0.095306

C -0.858852 0.000346 0.265727

C 0.508895 0.000804 0.603650

C 1.737357 0.001013 0.765530

C 3.296028 -0.000138 -0.151619

C 3.112129 0.001434 1.136948

C 4.176263 -0.001645 -1.325701

H -1.030120 -2.145144 0.228953

H -3.430466 -2.144553 -0.357096

H -4.639335 -0.000904 -0.653281

H -3.430933 2.143537 -0.360991

H -1.030576 2.145735 0.225022

H 3.654333 0.002519 2.076841

H 3.982353 0.878156 -1.944953

H 3.982286 -0.882984 -1.942738

H 5.233680 -0.001316 -1.034619

**Frequencies**

-679.0092 45.8815 50.7985

88.1999 122.1286 153.3255

224.5194 270.9990 374.6082

379.0548 415.8667 423.7518

518.1443 520.0761 639.1815

706.7820 718.6032 775.2077

788.8420 859.5181 881.4841

933.4336 997.5612 1000.3745

1014.0306 1016.7601 1034.9622

1045.1187 1059.0076 1110.1666

1159.4066 1184.5388 1204.2027

1310.6692 1343.2158 1352.6973

1397.9774 1467.7985 1472.8092

1482.4988 1528.7779 1626.3833

1650.4622 1827.5307 2055.5475

3018.1909 3099.1583 3117.7782

3171.7487 3184.5839 3192.4235

3204.9988 3211.4527 3217.4367

***i3 – i4***

**Cartesian coordinates**

C -1.558989 1.209962 0.037522

C -2.943409 1.203937 0.054588

C -3.642516 0.000000 0.063290

C -2.943397 -1.203932 0.054754

C -1.558977 -1.209946 0.037691

C -0.838786 0.000011 0.027291

C 0.571136 0.000015 0.014882

C 1.801146 -0.000010 -0.121353

C 3.229574 -0.000021 -0.090320

C 3.101795 -0.000190 -1.385954

C 4.232115 0.000135 1.009342

H -1.012071 2.145320 0.030357

H -3.483528 2.144068 0.060600

H -4.726332 -0.000004 0.076938

H -3.483507 -2.144067 0.060898

H -1.012049 -2.145300 0.030661

H 3.580638 -0.000311 -2.353773

H 4.096928 -0.882151 1.639828

H 4.096930 0.882608 1.639567

H 5.244835 0.000074 0.604535

**Frequencies**

-722.9327 50.6738 58.6041

67.7465 135.7700 180.3339

244.6581 275.6660 373.8390

414.7592 446.6317 454.6945

520.0755 530.1599 640.0133

664.8101 691.0645 706.9830

734.5903 776.3937 846.9447

860.5350 936.3747 998.4557

998.9195 1015.6568 1017.2753

1049.5015 1057.6061 1110.6317

1157.6980 1184.9082 1204.8956

1312.2515 1349.6206 1353.1430

1406.8458 1479.5289 1483.0818

1487.7390 1529.9748 1628.7090

1652.8078 1787.4037 2065.3843

3053.0567 3126.2278 3150.6191

3186.0206 3194.2548 3206.0432

3212.9681 3218.6151 3256.3367

***i5 – p2***

**Cartesian coordinates**

C -1.926298 -1.198641 -0.038036

C -3.287074 -0.932869 -0.033338

C -3.744231 0.379791 0.002639

C -2.833027 1.429588 0.033651

C -1.470560 1.172509 0.028239

C -1.002848 -0.146739 -0.007595

C 0.398986 -0.414130 -0.012374

C 1.586520 -0.626048 -0.017392

C 2.973988 -0.908896 -0.026075

C 3.912670 0.026333 0.031087

C 4.818524 0.931143 -0.200821

H -1.565002 -2.219710 -0.065037

H -3.994277 -1.753977 -0.057238

H -4.808697 0.584243 0.006746

H -3.185539 2.454211 0.062146

H -0.755829 1.986341 0.052345

H 3.278360 -1.952548 -0.018582

H 4.064865 -0.007176 2.092121

H 5.346378 1.442127 0.594582

H 5.059826 1.194243 -1.226980

**Frequencies**

-721.0973 25.1627 49.2824

76.8173 111.5851 145.5376

252.3135 340.4779 365.1202

376.4277 414.2592 416.8572

462.8120 542.9533 553.0114

623.5233 643.3646 654.7904

713.9022 762.1290 785.6282

869.5460 874.5931 913.7743

951.0508 990.1125 1004.0285

1008.9766 1023.8160 1024.2490

1061.3592 1112.5823 1119.1305

1189.2838 1209.2619 1292.3603

1319.4760 1356.4224 1380.3818

1471.0602 1488.3638 1544.3225

1646.7612 1679.2655 2007.1128

2337.7925 3143.5771 3159.1944

3189.1324 3197.8750 3208.0740

3215.2505 3220.7623 3237.1837

***i5 – i11***

**Cartesian coordinates**

C -1.734587 -1.219336 0.088494

C -3.097829 -1.124924 0.308945

C -3.730278 0.115223 0.284930

C -2.988140 1.266633 0.036747

C -1.624489 1.185327 -0.187407

C -0.972644 -0.062302 -0.161964

C 0.414327 -0.152388 -0.395062

C 1.660258 -0.164880 -0.359073

C 2.993784 -0.276555 -0.877279

C 3.779494 0.126960 0.129173

C 4.929756 0.217301 0.813171

H -1.237752 -2.181938 0.107667

H -3.673152 -2.023044 0.502651

H -4.797927 0.183966 0.458450

H -3.477889 2.233553 0.017681

H -1.042936 2.078277 -0.382989

H 3.286423 -0.581810 -1.877729

H 2.424619 0.346558 0.777122

H 5.234460 1.151628 1.270046

H 5.506246 -0.673541 1.043049

**Frequencies**

-2250.0929 39.7291 53.0899

100.2441 162.7262 191.5489

214.5718 307.5308 349.2599

413.4028 431.4110 468.4195

533.1833 535.1236 592.6753

638.0921 705.8174 751.4579

775.6977 777.5623 827.5740

861.4441 902.1309 940.5231

983.8292 1000.7470 1013.9523

1017.8665 1019.0825 1050.3865

1059.4878 1111.7772 1186.2971

1202.0791 1243.2016 1314.1188

1353.7484 1356.2670 1451.2551

1483.0455 1522.8838 1535.5284

1629.0039 1655.0121 1839.5133

2074.4173 3141.7454 3177.3944

3188.4122 3196.7145 3207.6347

3214.6813 3220.1290 3235.0993

***i5 – i10***

**Cartesian coordinates**

C -1.835619 -1.213339 -0.074797

C -3.203634 -0.997814 -0.140738

C -3.712584 0.295302 -0.090498

C -2.845184 1.375886 0.026188

C -1.475862 1.168835 0.092937

C -0.955079 -0.130494 0.043244

C 0.453250 -0.347141 0.111229

C 1.645941 -0.531712 0.180529

C 3.054110 -0.724364 0.198544

C 3.969922 0.444420 0.465916

C 4.527657 0.544997 -0.723406

H -1.434190 -2.218917 -0.113995

H -3.876238 -1.843002 -0.232015

H -4.782601 0.460561 -0.142410

H -3.237687 2.385582 0.065247

H -0.795636 2.007296 0.183253

H 3.394274 -1.692157 0.567486

H 4.090031 1.008155 1.384001

H 5.258166 1.170758 -1.227721

H 3.646374 -0.585729 -1.018726

**Frequencies**

-2222.2994 29.1469 56.8008

80.0054 145.1231 195.3601

308.3576 368.5721 414.3843

429.4283 494.8295 552.4394

575.1986 632.8415 643.4778

693.2855 713.4331 754.2633

784.3649 868.9577 888.4861

910.4602 941.2638 949.1038

992.6755 1003.1470 1022.6023

1024.0128 1058.6928 1084.0836

1112.3215 1161.9491 1188.5990

1208.7257 1211.8223 1274.9888

1318.7780 1355.9940 1364.5689

1488.0360 1542.7668 1645.6388

1657.3098 1677.3592 1846.5107

2300.6986 3122.6526 3173.0545

3188.3529 3197.3784 3207.4329

3214.9608 3215.9822 3220.3465

***i5 – i6***

**Cartesian coordinates**

C -1.772519 1.208228 -0.007234

C -3.158773 1.203419 -0.026415

C -3.855439 0.000005 -0.035976

C -3.158787 -1.203416 -0.026292

C -1.772532 -1.208240 -0.007108

C -1.063772 -0.000010 0.002695

C 0.361591 -0.000016 0.021445

C 1.572926 -0.000007 0.066245

C 4.077744 0.000254 0.662668

C 2.955995 -0.000038 -0.041126

C 5.067912 -0.000147 -0.463523

H -1.224730 2.142891 0.000258

H -3.698325 2.143508 -0.033976

H -4.939250 0.000011 -0.050994

H -3.698350 -2.143499 -0.033763

H -1.224754 -2.142909 0.000473

H 4.243504 0.000665 1.733917

H 5.612195 0.920218 -0.673939

H 3.791405 -0.000432 -1.141003

H 5.612236 -0.920644 -0.673250

**Frequencies**

-2288.0483 21.1772 56.1196

56.7317 161.3893 172.2241

321.0868 335.9445 370.7831

413.0876 455.7006 483.6954

558.2998 565.8698 608.6530

643.4773 713.1406 771.7362

784.2936 841.2763 869.0039

916.7649 950.1269 1003.5742

1011.8084 1023.5829 1024.5147

1051.8364 1053.5503 1063.2768

1109.8019 1112.7032 1188.8203

1209.2149 1228.8052 1313.8009

1318.0933 1356.4921 1431.9487

1487.4135 1538.9743 1645.3172

1675.1033 1770.2436 1856.9022

2278.3453 3085.2114 3183.9951

3189.2602 3198.5082 3205.6201

3208.2754 3216.0419 3221.1560

***i10 – i12***

**Cartesian coordinates**

C -1.646877 -1.210450 0.047399

C -3.012641 -1.204004 -0.181932

C -3.700996 0.000059 -0.297274

C -3.012579 1.204076 -0.181829

C -1.646815 1.210428 0.047499

C -0.942046 -0.000034 0.164041

C 0.451648 -0.000068 0.402802

C 1.685716 -0.000074 0.383351

C 3.057053 -0.000069 0.965787

C 3.830047 0.000007 -0.310212

C 4.869889 0.000113 -0.979300

H -1.107389 -2.145727 0.136960

H -3.545137 -2.143879 -0.272448

H -4.769892 0.000094 -0.476461

H -3.545025 2.143989 -0.272259

H -1.107275 2.145667 0.137143

H 3.255552 -0.886791 1.575974

H 3.255516 0.886594 1.576070

H 2.472709 -0.000054 -0.924307

H 5.496546 0.000204 -1.842646

**Frequencies**

-2255.4398 26.2760 54.9056

94.3029 169.8462 169.9903

293.9344 307.5772 339.3678

413.3893 447.3489 487.1479

493.9624 533.1988 567.4691

572.0553 641.3714 708.2654

721.8183 726.2731 778.0114

863.3625 879.9570 940.5909

967.2364 974.3179 1000.8460

1019.1630 1019.6656 1059.7771

1113.0441 1170.6337 1187.4943

1205.4204 1260.3081 1316.3118

1322.5590 1355.7081 1391.9692

1449.7877 1485.5473 1532.0873

1634.3367 1662.2626 2000.1138

2147.2424 3050.6757 3099.8438

3188.5586 3196.6806 3207.7803

3214.3500 3220.2229 3430.8105

***i12 – p5***

**Cartesian coordinates**

C 1.713555 -1.205724 0.152354

C 3.020407 -1.101584 -0.295232

C 3.603328 0.148572 -0.476975

C 2.870452 1.300077 -0.206905

C 1.562502 1.207961 0.240285

C 0.964956 -0.049252 0.423599

C -0.375548 -0.148643 0.872813

C -1.585442 -0.229701 1.049498

C -2.710466 -0.285728 -0.855924

C -4.025297 0.049238 -0.512108

C -5.136277 0.339466 -0.131538

H 1.255555 -2.176958 0.296581

H 3.588046 -2.001141 -0.504190

H 4.626033 0.225839 -0.827526

H 3.322331 2.275428 -0.346268

H 0.988643 2.102042 0.453126

H -2.455559 -0.289646 1.668767

H -2.492460 -1.324768 -1.071983

H -2.119110 0.448527 -1.388819

H -6.126500 0.592585 0.161111

**Frequencies**

-624.7930 13.5692 40.2075

52.3274 110.4412 173.2238

175.7372 347.9194 381.7141

414.1272 445.3525 486.7450

540.4370 548.4217 565.2823

584.7257 637.7340 683.1990

710.1806 716.7138 747.6940

780.8767 784.2719 874.0841

882.3034 944.6485 1009.3395

1018.4287 1023.6786 1038.0934

1059.4759 1064.1057 1113.8096

1188.2252 1205.3151 1233.4730

1317.5632 1357.4568 1455.0527

1486.8782 1532.1226 1637.1195

1665.2084 2032.6059 2137.6356

3159.7298 3190.6758 3197.7263

3209.5637 3215.4262 3222.4977

3254.5092 3383.0400 3480.0267

***i12 – p1***

**Cartesian coordinates**

C 1.854030 -1.194573 0.087119

C 3.213536 -0.926348 0.130052

C 3.671897 0.383490 0.041259

C 2.763955 1.428501 -0.090793

C 1.402778 1.169517 -0.135180

C 0.934268 -0.147227 -0.046457

C -0.465111 -0.415152 -0.089574

C -1.655757 -0.623998 -0.021365

C -3.068802 -0.916372 -0.308520

C -3.964601 0.203402 -0.013795

C -4.708938 1.112106 0.218047

H 1.490830 -2.212818 0.158080

H 3.918789 -1.742727 0.234740

H 4.735463 0.589714 0.075633

H 3.118199 2.450616 -0.158488

H 0.689665 1.978777 -0.236164

H -1.905982 -0.452502 1.971279

H -3.385695 -1.790950 0.267619

H -3.159862 -1.181705 -1.367335

H -5.364942 1.921519 0.429875

**Frequencies**

-689.6284 23.0838 48.2501

85.0566 116.4833 157.6844

256.2182 324.6405 330.9358

355.2944 413.9911 428.3914

448.5323 538.5524 565.9647

600.7306 642.3562 705.1301

713.1616 719.8800 750.6995

785.5135 869.9657 932.1685

939.4274 951.8726 1004.7306

1019.8476 1023.7054 1025.0856

1062.9538 1112.7375 1189.3266

1208.6441 1244.0041 1288.4819

1319.9997 1355.9825 1356.6337

1461.3324 1488.1188 1539.9990

1646.0137 1676.4197 2263.2885

2300.4897 3051.5598 3091.9426

3189.7547 3198.7967 3208.4905

3215.9988 3221.3020 3489.0484

***Products***

***p1 + H***



**Cartesian coordinates**

C -1.846119 -1.203156 0.000044

C -3.200494 -0.903304 0.000059

C -3.624419 0.420657 0.000019

C -2.686798 1.446975 -0.000036

C -1.331121 1.154768 -0.000050

C -0.897655 -0.175401 -0.000010

C 0.502793 -0.473583 -0.000027

C 1.681686 -0.703972 -0.000042

C 3.117619 -0.989096 -0.000066

C 3.945069 0.220378 0.000022

C 4.632033 1.201084 0.000092

H -1.510917 -2.233610 0.000076

H -3.928586 -1.706341 0.000101

H -4.683606 0.651293 0.000030

H -3.012864 2.480820 -0.000067

H -0.595175 1.949803 -0.000092

H 3.369327 -1.594703 -0.877641

H 3.369331 -1.594835 0.877416

H 5.236930 2.075474 0.000154

**Frequencies**

14.2435 53.3202 85.6235

137.1190 234.6947 318.7034

328.2668 369.6740 395.2488

413.5478 535.0242 554.6790

601.7671 643.8025 707.2440

710.8468 711.6921 743.4454

780.8974 868.0859 928.1277

937.4402 945.5021 1002.3849

1018.7452 1021.5633 1024.5850

1064.0633 1112.2338 1188.9183

1208.0908 1251.0000 1289.7829

1317.7485 1355.9784 1361.0885

1454.6591 1488.6556 1542.5842

1648.5143 1680.6454 2262.9352

2389.0902 3044.4988 3079.1697

3191.9361 3202.6127 3210.4018

3221.9017 3226.6643 3486.5474

***p2 + H***



**Cartesian coordinates**

C 1.877822 -1.199389 0.000342

C 3.237989 -0.929493 0.000500

C 3.691643 0.384803 0.000212

C 2.776967 1.431783 -0.000240

C 1.415336 1.170150 -0.000399

C 0.951031 -0.150547 -0.000109

C -0.451895 -0.419719 -0.000277

C -1.638870 -0.626826 -0.000421

C -3.034830 -0.906489 -0.000658

C -3.961183 0.021635 0.000092

C -4.887087 0.930526 0.000776

H 1.519401 -2.221960 0.000571

H 3.948154 -1.748486 0.000851

H 4.755663 0.591899 0.000345

H 3.126412 2.457994 -0.000471

H 0.697585 1.981706 -0.000748

H -3.338783 -1.950446 -0.001566

H -5.285039 1.324630 0.930709

H -5.284928 1.326066 -0.928595

**Frequencies**

26.7109 49.9205 88.8027

139.0759 237.9870 330.4301

336.0206 365.9591 399.4731

413.3260 543.8834 549.3694

623.8778 642.4346 643.4021

710.6141 761.4234 780.2720

867.5865 888.7163 902.2869

944.2093 991.4467 1002.1595

1013.2792 1018.3907 1023.1961

1060.5246 1111.1730 1129.3156

1188.8983 1206.4720 1287.0623

1315.9380 1354.8771 1375.5031

1479.8937 1487.5551 1542.5475

1646.0316 1678.5926 2076.6635

2361.4123 3138.3061 3156.0261

3193.7019 3203.5975 3212.7761

3220.0924 3222.0732 3226.8927

***p3 + H***



**Cartesian coordinates**

C -1.801631 -1.208022 0.000003

C -3.188224 -1.203515 -0.000008

C -3.884558 -0.000067 -0.000014

C -3.188311 1.203432 -0.000008

C -1.801719 1.208040 0.000004

C -1.094203 0.000035 0.000009

C 0.333053 0.000079 0.000017

C 1.540445 0.000086 0.000020

C 4.115565 -0.000003 0.000002

C 2.910496 0.000058 0.000015

C 5.569664 -0.000111 -0.000024

H -1.253360 -2.142418 0.000007

H -3.727872 -2.143544 -0.000013

H -4.968502 -0.000107 -0.000023

H -3.728028 2.143420 -0.000013

H -1.253517 2.142476 0.000007

H 5.955539 1.022011 0.026206

H 5.956141 -0.488236 -0.898267

H 5.956133 -0.533661 0.871999

**Frequencies**

16.9328 52.6986 55.3850

149.0832 155.7200 284.3378

327.4723 334.1129 395.9178

413.4043 505.5932 532.8185

611.5241 631.4390 647.5555

654.4455 714.2006 789.1215

841.8620 870.2112 952.9443

1004.4438 1024.6992 1024.7157

1052.7943 1053.1280 1060.6799

1112.7545 1139.9673 1189.1987

1210.4287 1319.0986 1349.9609

1356.7799 1419.1093 1480.0281

1480.3628 1488.0679 1543.9077

1647.5547 1679.5289 2299.9413

2418.5996 3047.0589 3122.1467

3122.5703 3189.4553 3198.9831

3208.4682 3216.4707 3221.4423

***p4 + methyl***



**Cartesian coordinates**

C 1.101948 -1.208695 0.000011

C 2.488454 -1.203815 0.000008

C 3.183998 -0.000052 -0.000007

C 2.488529 1.203755 -0.000018

C 1.102022 1.208726 -0.000015

C 0.396320 0.000039 -0.000001

C -1.030822 0.000064 0.000002

C -2.237708 0.000045 0.000005

C -3.608004 0.000006 0.000007

C -4.811060 -0.000041 0.000010

H 0.554126 -2.143332 0.000022

H 3.027906 -2.143845 0.000017

H 4.267994 -0.000084 -0.000009

H 3.028040 2.143752 -0.000029

H 0.554262 2.143399 -0.000024

H -5.874388 -0.000083 0.000012

**Frequencies**

63.7994 69.2295 195.6241

221.8239 367.7979 374.7847

411.6634 488.2825 518.1404

596.0311 601.8844 643.1885

676.5256 688.1483 706.6563

710.1392 784.1149 867.8304

950.2029 984.6685 1003.3430

1021.2971 1022.5669 1063.3330

1113.0519 1188.8240 1213.3784

1307.8266 1319.5175 1358.0635

1487.3873 1542.1019 1646.0589

1677.6539 2201.1368 2388.4930

3197.9903 3206.9418 3216.0666

3223.5376 3229.0018 3483.4703

***p5 + propargyl***



**Cartesian coordinates**

C -0.119235 1.207139 -0.000010

C -1.506283 1.203135 -0.000001

C -2.202504 -0.000024 0.000006

C -1.506242 -1.203162 0.000000

C -0.119194 -1.207118 -0.000010

C 0.586875 0.000022 -0.000008

C 2.019321 0.000039 0.000009

C 3.220060 -0.000020 0.000012

H 0.428457 2.141945 -0.000012

H -2.045318 2.143536 0.000006

H -3.286553 -0.000045 0.000040

H -2.045251 -2.143576 0.000007

H 0.428528 -2.141908 -0.000014

H 4.283350 -0.000015 -0.000019

**Frequencies**

137.3102 155.4248 366.7145

413.0878 474.7729 541.4990

555.6524 639.3903 663.7000

703.2868 711.5626 781.5994

782.0730 868.2462 948.3079

1002.3022 1019.5342 1023.1711

1060.8202 1112.1340 1187.9972

1211.5549 1234.3142 1319.7889

1357.2773 1487.8733 1539.4181

1648.1263 1679.1061 2244.4950

3196.3575 3205.2722 3214.7865

3222.1317 3227.8191 3483.1952

***p6 + acetylene***



**Cartesian coordinates**

C 0.671604 -1.210796 -0.000006

C 2.056210 -1.204514 0.000006

C 2.753575 0.000022 0.000011

C 2.056174 1.204539 0.000005

C 0.671569 1.210779 -0.000006

C -0.043767 -0.000019 -0.000012

C -1.455605 -0.000030 -0.000021

C -2.684676 -0.000009 -0.000010

C -4.040349 0.000013 0.000018

H 0.124573 -2.145982 -0.000010

H 2.596376 -2.144351 0.000011

H 3.837522 0.000040 0.000018

H 2.596315 2.144390 0.000010

H 0.124511 2.145950 -0.000010

H -4.593872 -0.931071 0.000029

H -4.593840 0.931116 0.000039

**Frequencies**

85.2764 89.3696 217.5537

258.1128 311.6489 413.1716

413.5641 437.2621 531.7243

536.4907 637.7591 703.4181

713.6937 735.7243 774.9341

860.1720 938.0475 999.1616

1014.1072 1015.1412 1035.0325

1049.8153 1075.0877 1112.0165

1185.6922 1209.8008 1315.0182

1355.3024 1361.1603 1476.4679

1483.8384 1542.1545 1630.3313

1654.7317 2079.6909 3161.3898

3196.2121 3204.3989 3214.9694

3221.7924 3227.5904 3258.5642

***Fragments***

***Methyl***



**Cartesian coordinates**

C -0.000084 0.000054 0.000034

H 0.330345 -1.029327 -0.000069

H -1.056667 0.228692 -0.000069

H 0.726826 0.800307 -0.000069

**Frequencies**

477.5911 1400.1589 1410.4961

3117.0568 3300.6263 3304.0767

***Acetylene***



**Cartesian coordinates**

C 0.000000 0.000000 -0.598212

C 0.000000 0.000000 0.598211

H 0.000000 0.000000 -1.662213

H 0.000000 0.000000 1.662218

**Frequencies**

675.1654 675.1654 768.9824

768.9824 2088.1359 3423.0212

3530.5719

***Propargyl***



**Cartesian coordinates**

C -0.117045 0.000056 -0.000045

C -1.335904 -0.000010 -0.000022

C 1.251979 -0.000012 0.000022

H -2.399234 -0.000053 0.000202

H 1.802428 -0.932378 0.000031

H 1.802624 0.932234 0.000031

**Frequencies**

355.7199 404.5134 494.3976

653.2122 674.3439 1036.2959

1088.1264 1459.5635 2025.8399

3166.2263 3267.3323 3471.5824

**Supporting References**

(1) Russo, M. V.; Lo Sterzo, C.; Franceschini, P.; Biagini, G.; Furlani, A. Synthesis of highly ethynylated mono and dinuclear Pt(II) tethers bearing the 4,4′-bis(ethynyl)biphenyl (debp) unit as central core. *J. Organomet. Chem.* **2001**, *619*, 49.