Electronic supplementary information

In situ analysis and real-time monitoring of the decomposition of the 2nd Grubbs catalyst in CH_3CN by droplet spray ionization tandem mass spectrometry

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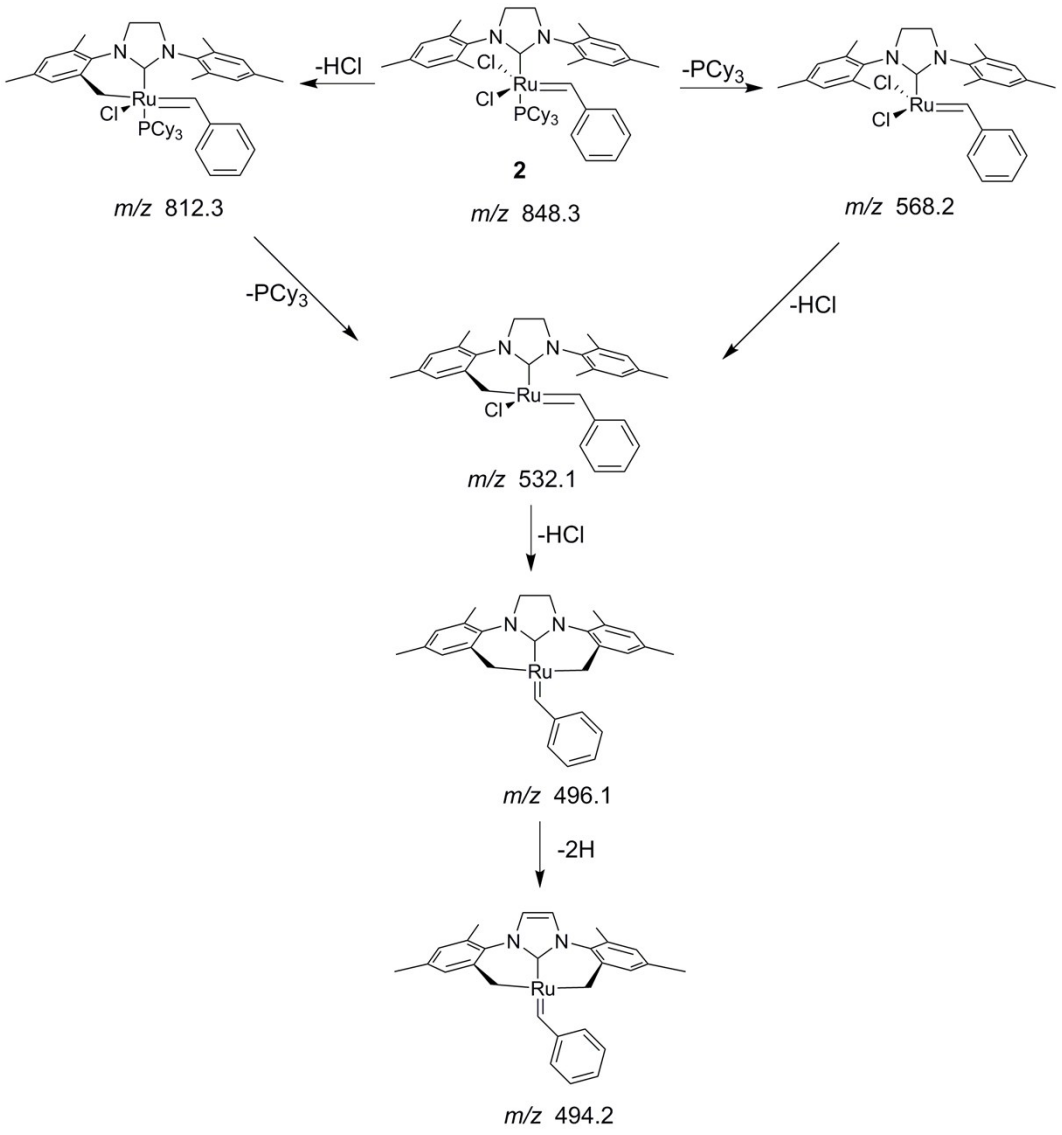

Fig. S1 Proposed fragment mechanism of **2** at *m/z* 848.

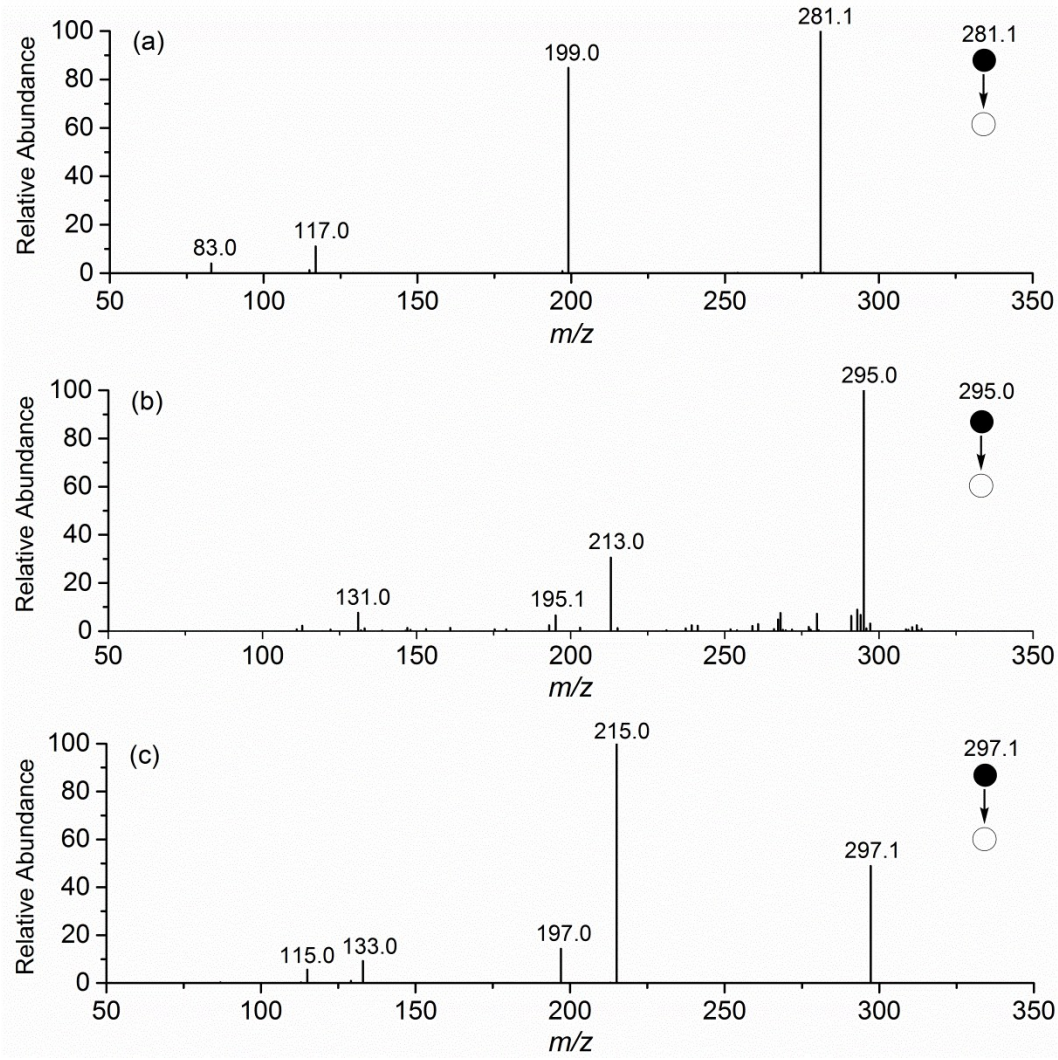

Fig. S2 DSI-MS/MS spectra for CID of ions: (a) $[Cy_3P+H]^+$ at *m/z* 281; (b) $[Cy_3PCH_3]^+$ at *m/z* 295; (c) the hydride of $[Cy_3PCH_3]^+$ at *m/z* 297.

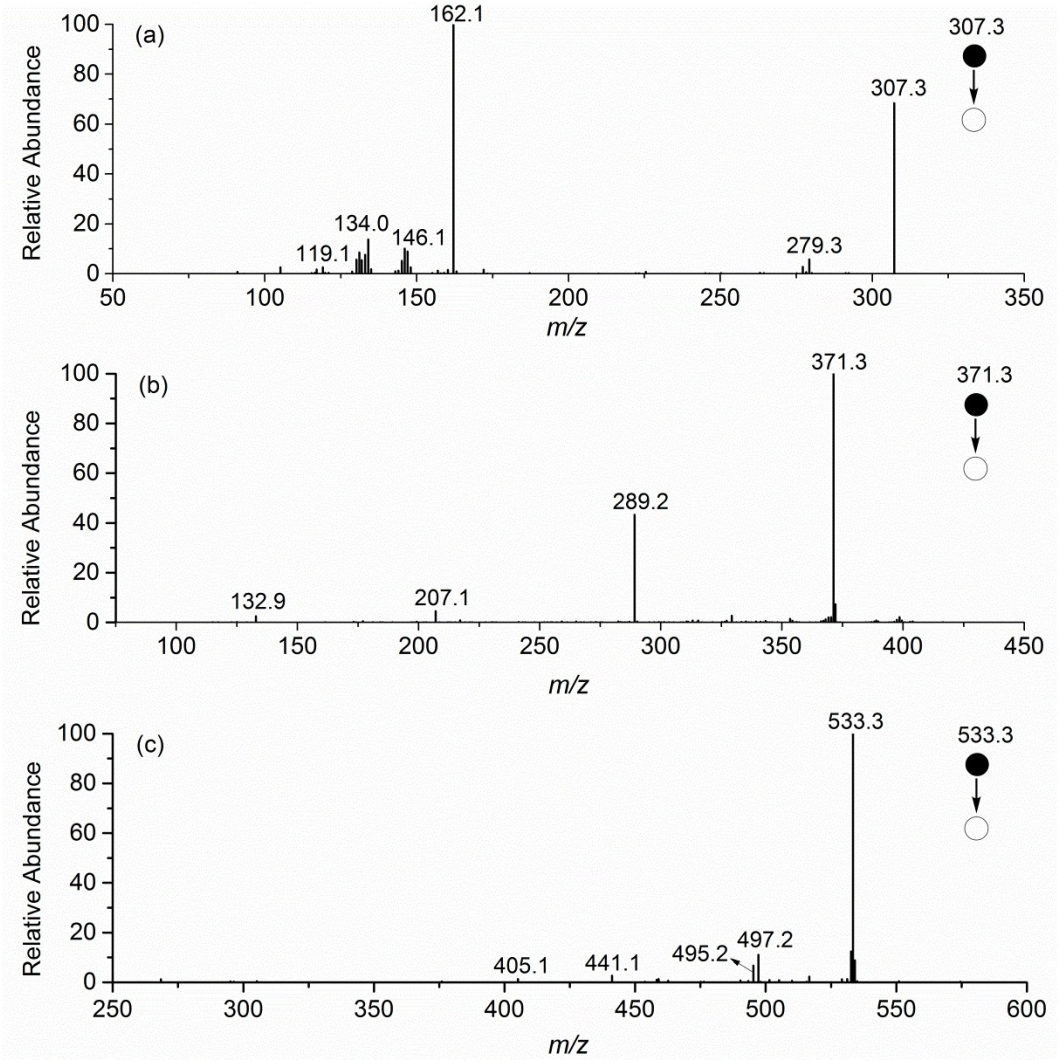

Fig. S3 DSI-MS/MS spectra for CID of ions: (a) $[H_2IMes+H]^+$ at *m/z* 307; (b) $[Cy_3PCH_2Ph]^+$ at *m/z* 371; (c) $[(H_2IMes)ClRu=CHPh]^+$ at *m/z* 533.

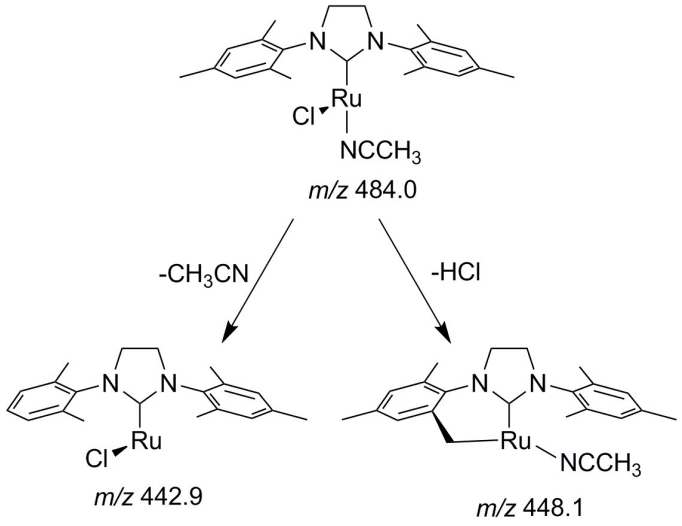

Fig. S4 Proposed fragmentation mechanism of the ions of **12** at *m/z* 484.

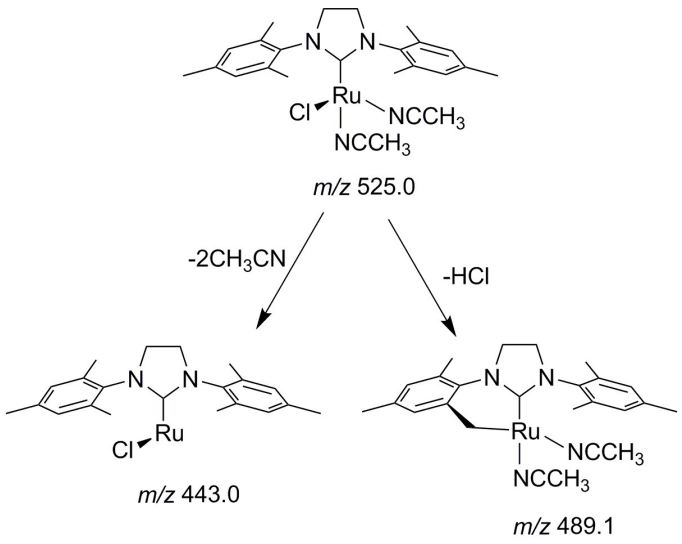

Fig. S5 Proposed fragmentation mechanism of the ions of **8** at *m/z* 525.

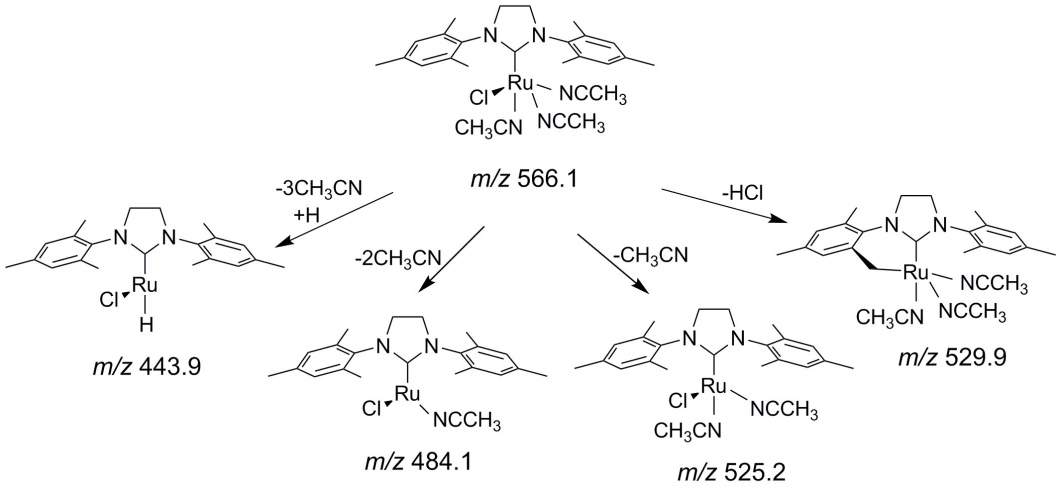

Fig. S6 Proposed fragmentation mechanism of the ions of **10** at *m/z* 566.

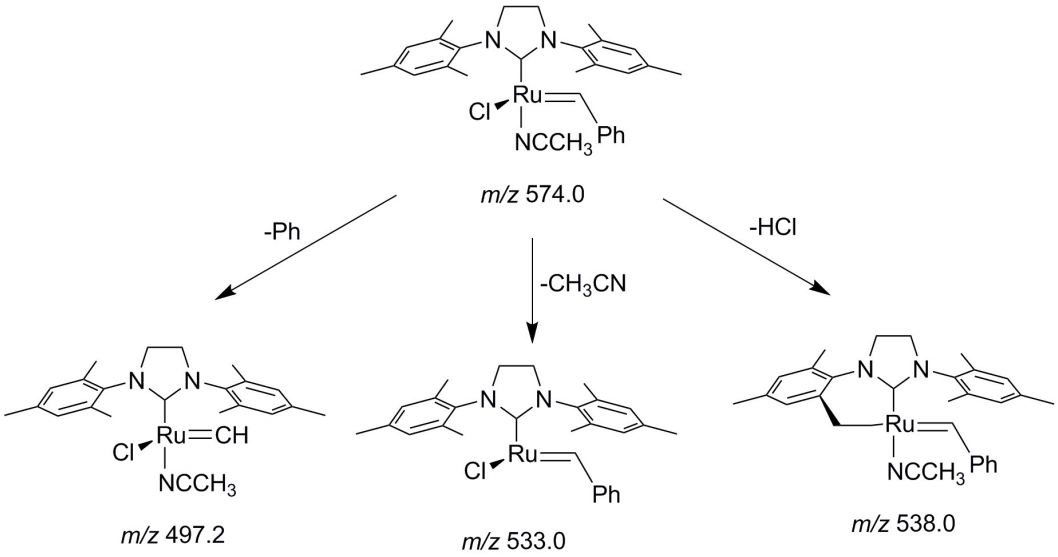

Fig. S7 Proposed fragmentation mechanism of the ions of **6** at *m/z* 574.

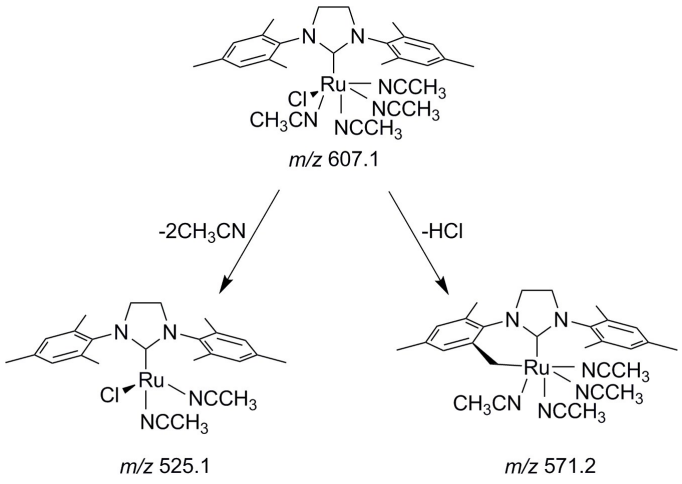

Fig. S8 Proposed fragmentation mechanism of the ions of **9** at *m/z* 607.

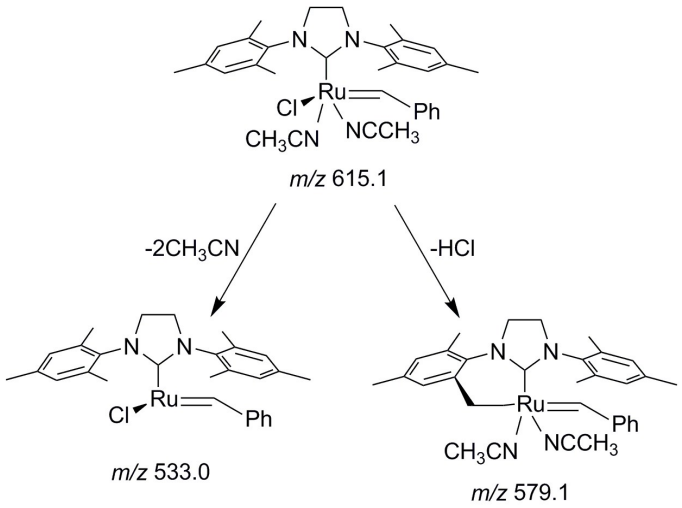

Fig. S9 Proposed fragmentation mechanism of the ions of **5** at *m/z* 615.

Table S1 The *m/z* error of compounds.

Compound	Theoretical *m/z*	Measured *m/z*	Error (ppm)
2	848.3300	848.3293	-0.83
3	813.3612	813.3600	-1.48
4	533.1292	533.1270	-4.13
5	615.1823	615.1821	-0.33
6	574.1558	574.1539	-3.31
7	854.3877	854.3855	-2.57
8	525.1354	525.1349	-0.95
9	607.1884	607.1895	+1.81
10	566.1619	566.1624	+0.88
11	846.3939	846.3937	-0.24
12	484.1088	484.1084	-0.83

References

1 H. Y. Wang, W. L. Yim, Y. L. Guo and J. O. Metzger, *Organometallics*, 2012, **31**, 1627-1634.

2 H. Y. Wang and J. O. Metzger, *Organometallics*, 2008, **27**, 2761-2766.