Electronic Supplementary Material (ESI) for New Journal of Chemistry.

- Supporting Information -

for

Variation of trough-space magnetic response properties upon formation of Cation-π interactions. A survey of $[Ag(\eta\text{-}CH_2CH_2)_3]^+$ via DFT calculations.

Content:

- **Table S1**. Calculated ^1H and ^{13}C NMR parameters, including the population π_1 and π_2 orbitals of ethylene, and Ag-C and CC Widberg bond order.
- **Figure S1**. Position of (3,-1) critical points and selected points in the space.

	Cent-Ag (Å)	δC* (ppm)	δH* (ppm)	Pop. π_1 (a.u.)	Pop. π_2 (a.u.)	Ag-C WBO	CC WBO
Free CH_2CH_2		124.9	6.4	2.00	0.00		2.00
$[Ag(C_2H_2)_3]^+$ Eq. structure	2.280	114.8	6.0	1.84	0.11	0.34	1.79
	2.400	115.3	6.3	1.86	0.08	0.15	1.83
	2.600	118.0	6.6	1.88	0.04	0.13	1.88
	2.800	124.6	6.8	1.89	0.02	0.11	1.91
	3.000	128.2	6.9	1.91	0.01	0.09	1.93
	3.200	129.8	6.9	1.91	0.01	0.09	1.95
	3.400	130.6	6.9	1.91	0.00	0.08	1.95
	3.600	131.2	6.9	1.91	0.00	0.08	1.96
	3.800	131.6	6.9	1.92	0.00	0.08	1.96
	4.000	131.8	6.9	1.91	0.00	0.08	1.96
	4.200	132.2	6.9	1.91	0.00	0.08	1.95

*Calculated chemical shift for C and H, which were referenced to TMS, at the QZ4P/GIAO/ZORA/BP86 level.

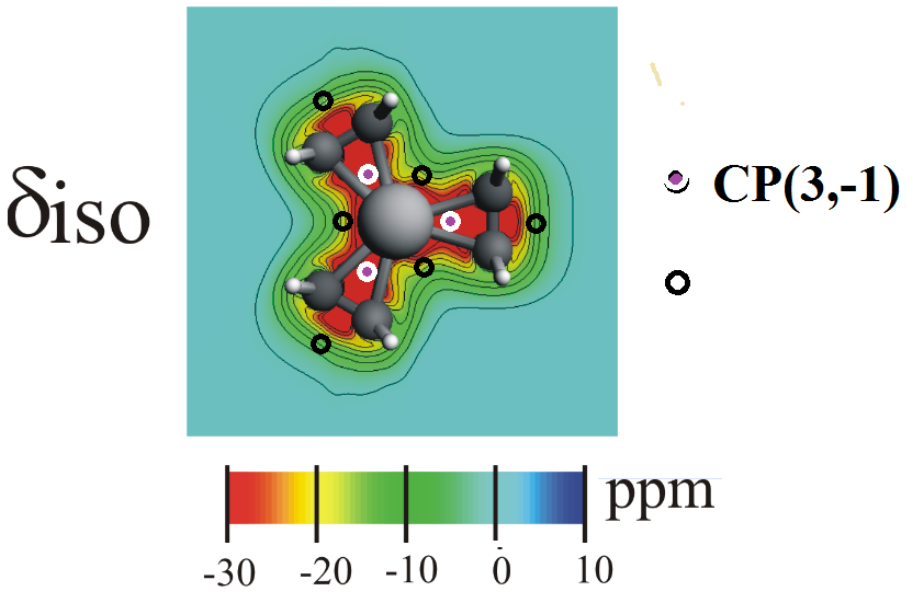

Figure S1. Position of (3,-1) critical points and selected points in the space, given for comparison.