Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

The unimolecular dissociation of magnesium chloride squarate ($ClMgC_4O_4^-$) and reductive cyclooligomerisation of CO on magnesium – Supporting Information

Joakim S. Jestilä[1], Zsuzsanna Iker[2], Mauritz J. O. Ryding[1] and Einar Uggerud[1*]

[1] Department of Chemistry and Hylleraas Centre for Quantum Molecular Sciences, University of Oslo, PO Box 1033, Blindern, Oslo N-0135, Norway

[2] Budapest University of Technology and Economics, Department of Organic Chemistry and Technology, Műegyetem rkp. 3., H1111, Budapest, Hungary

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SI-A. Energy-resolved cross-sections and pressure extrapolation

All appearance curves were acquired by measuring 150, 250 or 300 scans on each collision energy increment. For the linear extrapolation, the threshold energies were estimated by fitting asymmetric double sigmoidal functions to the curves, and subsequently extrapolating the linear portion (assumed to be the inflection point) of the fitted function to baseline. In addition, we utilized the L-CID software of Chen and coworkers[1] to further refine the results. The following parameters were used for all dissociation reactions:

Temperature	298 K
TS (0 = loose)(1 = tight)	0
FWHM of ion beam kin. E	2
Corr. for Elab to reach detector	0
Free rotors	0
Degrees of freedom	3N − 6

The analysis was conducted three times on each curve to estimate the numerical error of the procedure.

The measurements were done at four different plus one background collision gas (Ar) pressures, in order to extrapolate the threshold energies to vacuum. To account for the decreasing signal-to-noise ratio with pressure, the threshold energies are weighted by their relative signal intensities in the linear extrapolation procedure, giving lower priority to more uncertain measurements. For calibration, the same analysis was done on two reference systems with known reaction energetics, the decarboxylation of benzoate, $C_6H_5CO_2^- \rightarrow C_6H_5^- + CO_2$, and the dissociation of the Cs^+(15-crown-5) complex, Cs^+(15-crown-5) → Cs^+ + (15-crown-5).

Linear extrapolation example: threshold energy of $ClMgC_3O_3^-$ (*m/z* 143)

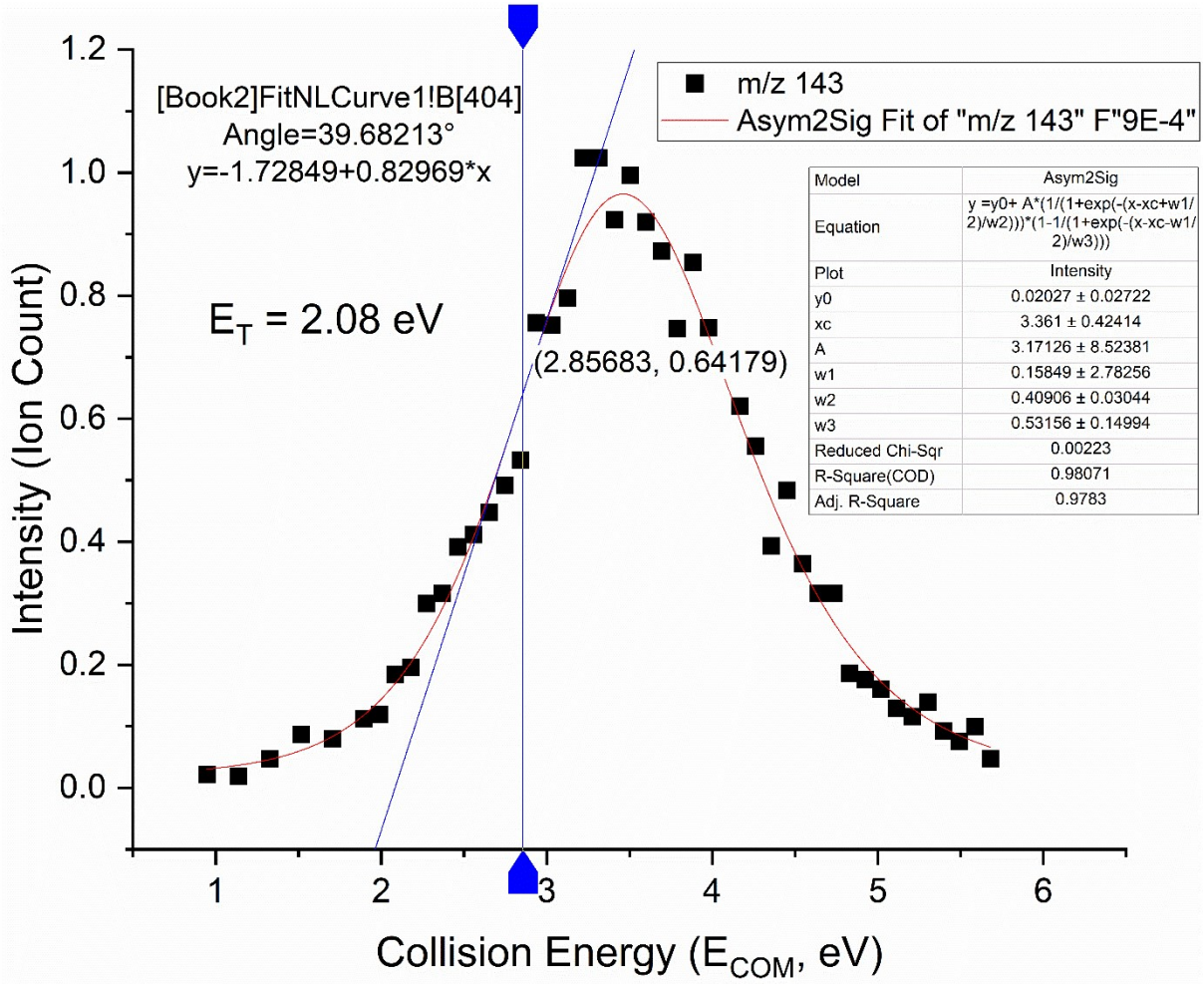

Figure S1. Appearance curve of $ClMgC_3O_3^-$ (*m/z* 143) taken at 9.45×10^{-4} mbar Ar pressure with fitted asymmetric double sigmoidal function. Threshold energy is determined by following the tangent line of the inflection point (2.86, 0.64) to the abscissa.

Threshold energies for dissociation of $ClMgC_4O_4^-$ (*m/z* 171)

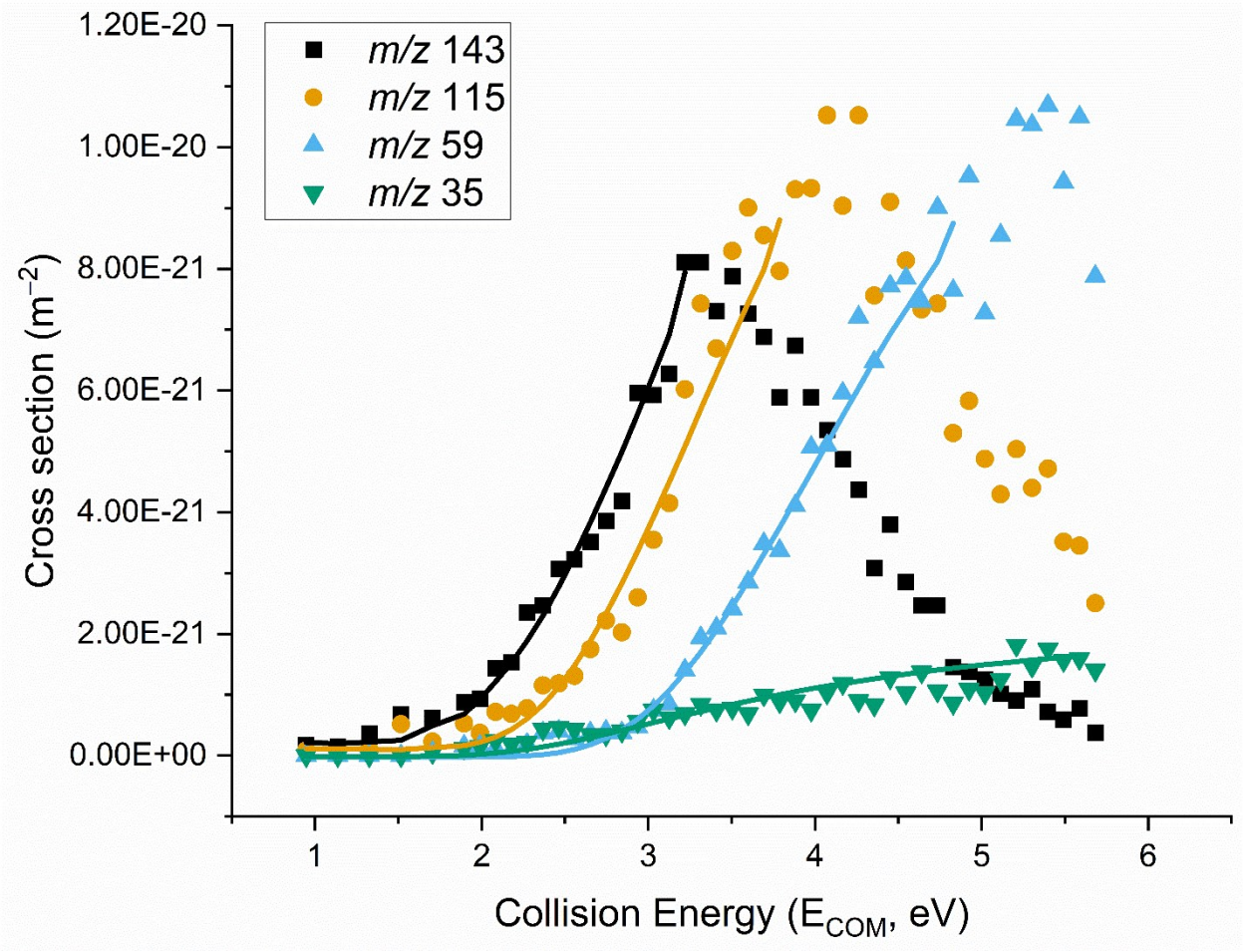

Figure S2. Energy-resolved CID cross sections and L-CID fits for the dissociation of $ClMgC_4O_4^-$ (*m/z* 171) at 9.45×10^{-4} mbar Ar pressure.

Table S1. L-CID output and results of linear extrapolation (9.45×10^{-4} mbar Ar pressure).

	***m/z* 143**	***m/z* 115**	***m/z* 59**	***m/z* 35**
E_{0_Linear} (eV)	2.08	2.32	3.12	1.76
E_{0_LCID} (eV)	1.61 ± 0.02	2.00 ± 0.02	2.39 ± 0.01	1.77 ± 0.11
ν_{eff} (cm^{-1})	1003 ± 5	744 ± 39	807 ± 71	813 ± 192
a' (cm^{-1})	5733 ± 574	5747 ± 423	5853 ± 12	5713 ± 241

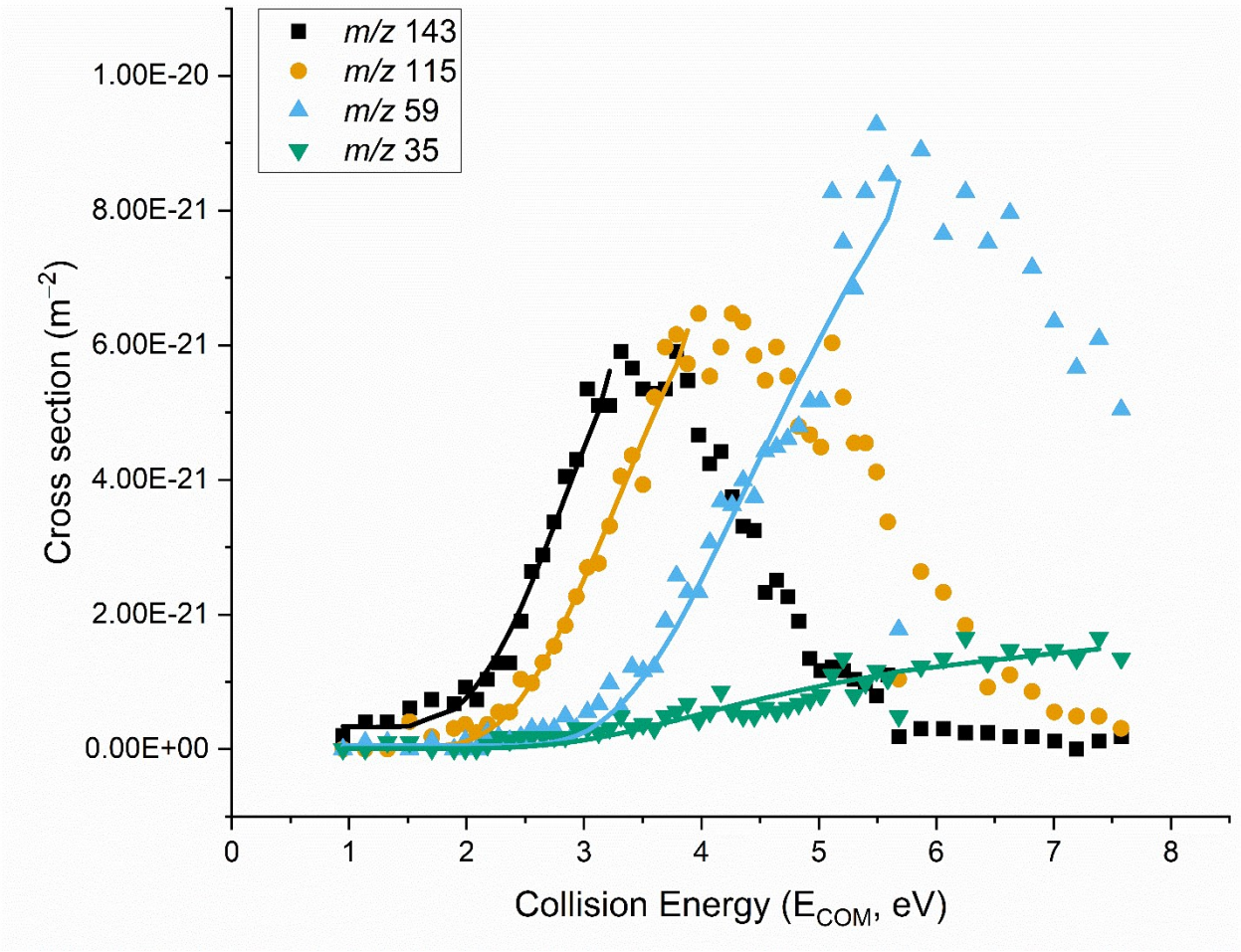

Figure S3. Energy-resolved CID cross sections and L-CID fits for the dissociation of $ClMgC_4O_4^-$ (*m/z* 171) at 6.66×10^{-4} mbar Ar pressure.

Table S2. L-CID output and results of linear extrapolation (6.66×10^{-4} mbar Ar pressure).

	***m/z* 143**	***m/z* 115**	***m/z* 59**	***m/z* 35**
$E_{0\ Linear}$ (eV)	2.15	2.52	3.15	2.63
$E_{0\ LCID}$ (eV)	1.78 ± 0.05	1.97 ± 0.01	2.59 ± 0.01	2.09 ± 0.01
ν_{eff} (cm^{-1})	771 ± 126	811 ± 74	799 ± 54	1004 ± 3
a' (cm^{-1})	5733 ± 272	5580 ± 420	5800 ± 193	5987 ± 194

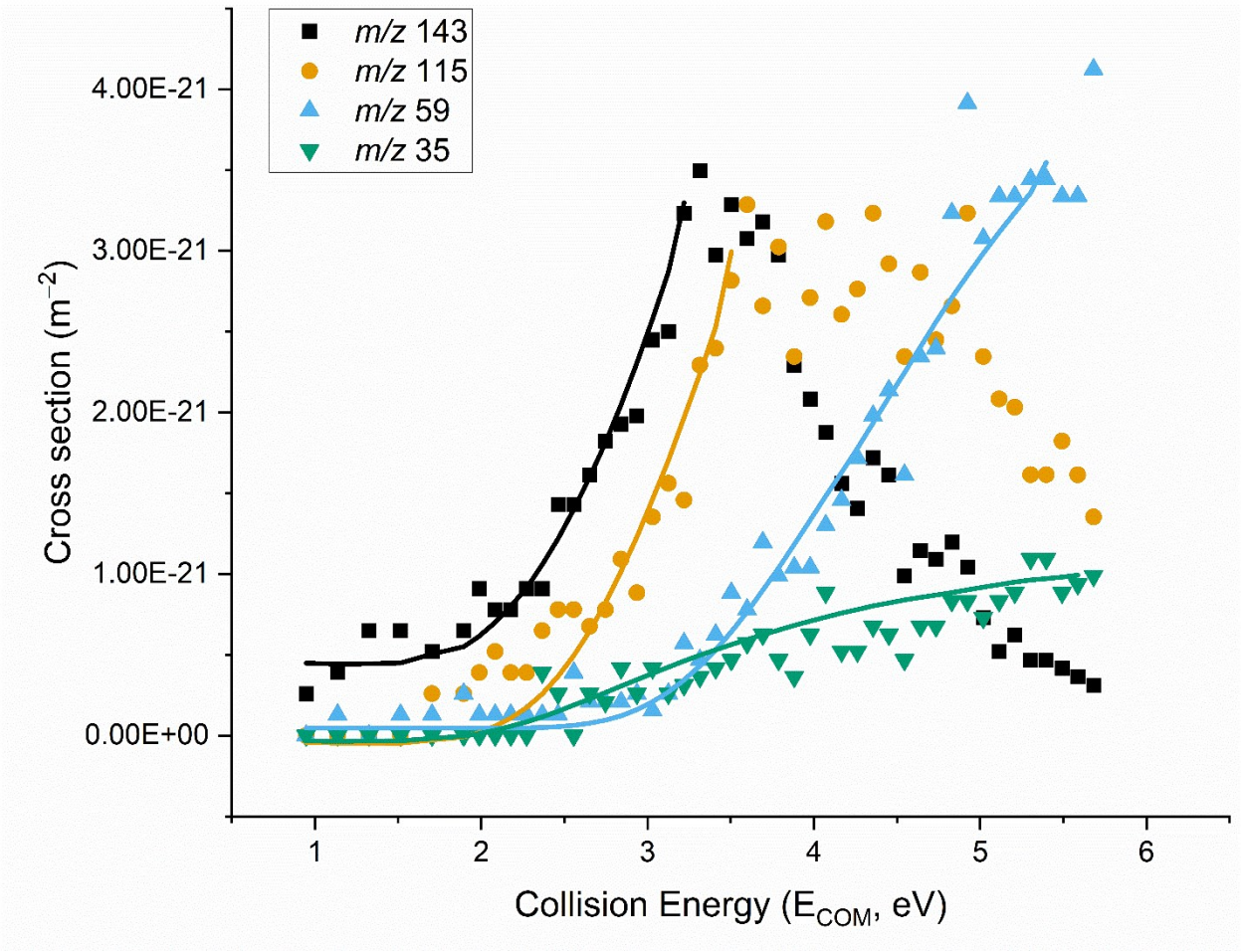

Figure S4. Energy-resolved CID cross sections and L-CID fits for the dissociation of $ClMgC_4O_4^-$ (*m/z* 171) at 4.73×10^{-4} mbar Ar pressure.

Table S3. L-CID output and results of linear extrapolation (4.73×10^{-4} mbar Ar pressure).

	***m/z* 143**	***m/z* 115**	***m/z* 59**	***m/z* 35**
E_{0_Linear} (eV)	2.10	2.45	3.43	2.08
E_{0_LCID} (eV)	1.74 ± 0.01	1.90 ± 0.05	2.50 ± 0.03	1.75 ± 0.08
ν_{eff} (cm^{-1})	1004 ± 4	1002 ± 3	770 ± 32	889 ± 101
a' (cm^{-1})	5593 ± 110	5627 ± 549	5827 ± 361	5513 ± 280

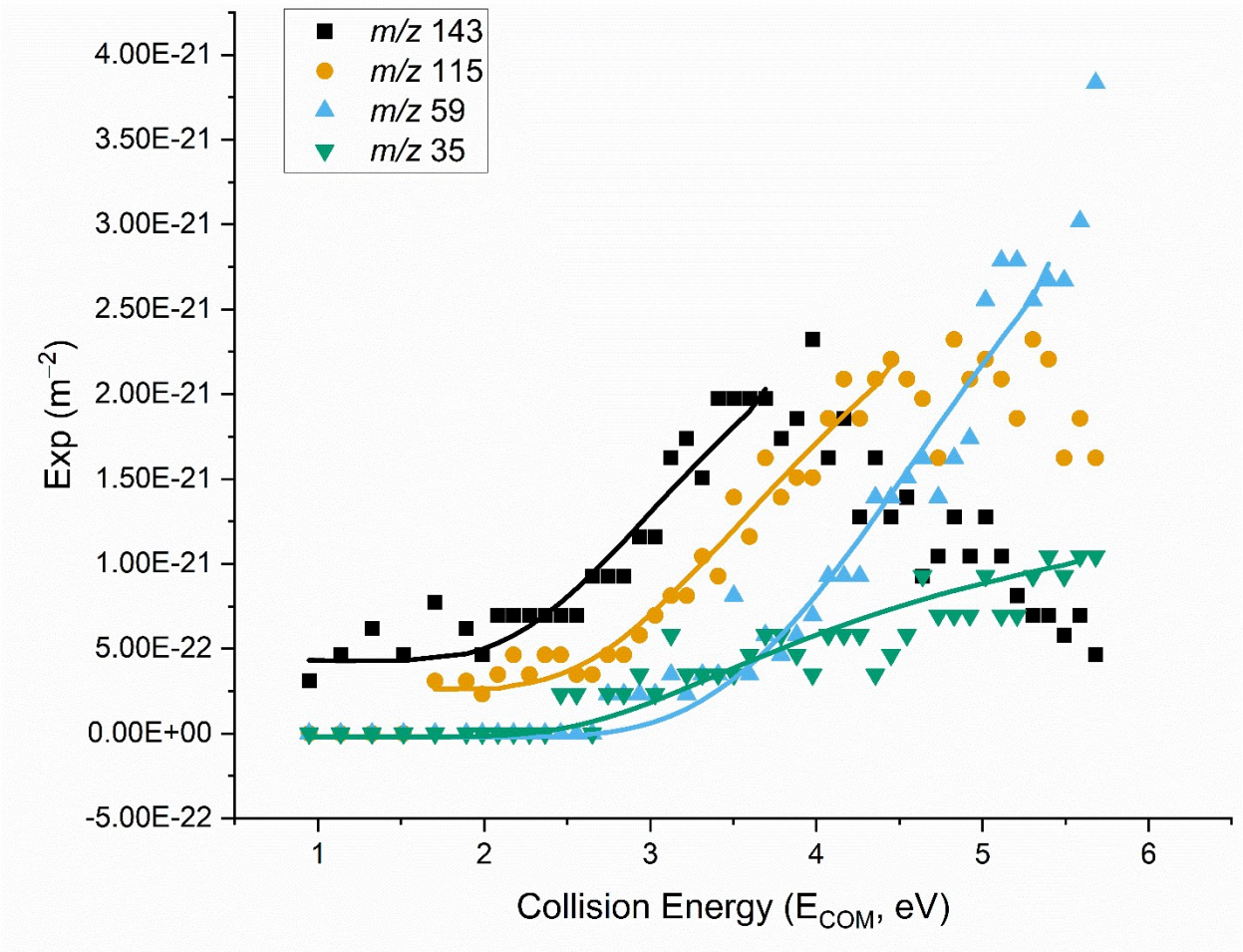

Figure S5. Energy-resolved CID cross sections and L-CID fits for the dissociation of $ClMgC_4O_4^-$ (*m/z* 171) at 2.76×10^{-4} mbar Ar pressure.

Table S4. L-CID output and results of linear extrapolation (2.76×10^{-4} mbar Ar pressure).

	***m/z* 143**	***m/z* 115**	***m/z* 59**	***m/z* 35**
E_{0_Linear} (eV)	2.17	2.40	3.90	2.86
E_{0_LCID} (eV)	1.77 ± 0.04	2.16 ± 0.02	2.54 ± 0.06	2.02 ± 0.04
ν_{eff} (cm^{-1})	938 ± 118	715 ± 125	986 ± 20	735 ± 76
a' (cm^{-1})	5880 ± 505	5660 ± 314	5573 ± 560	5720 ± 191

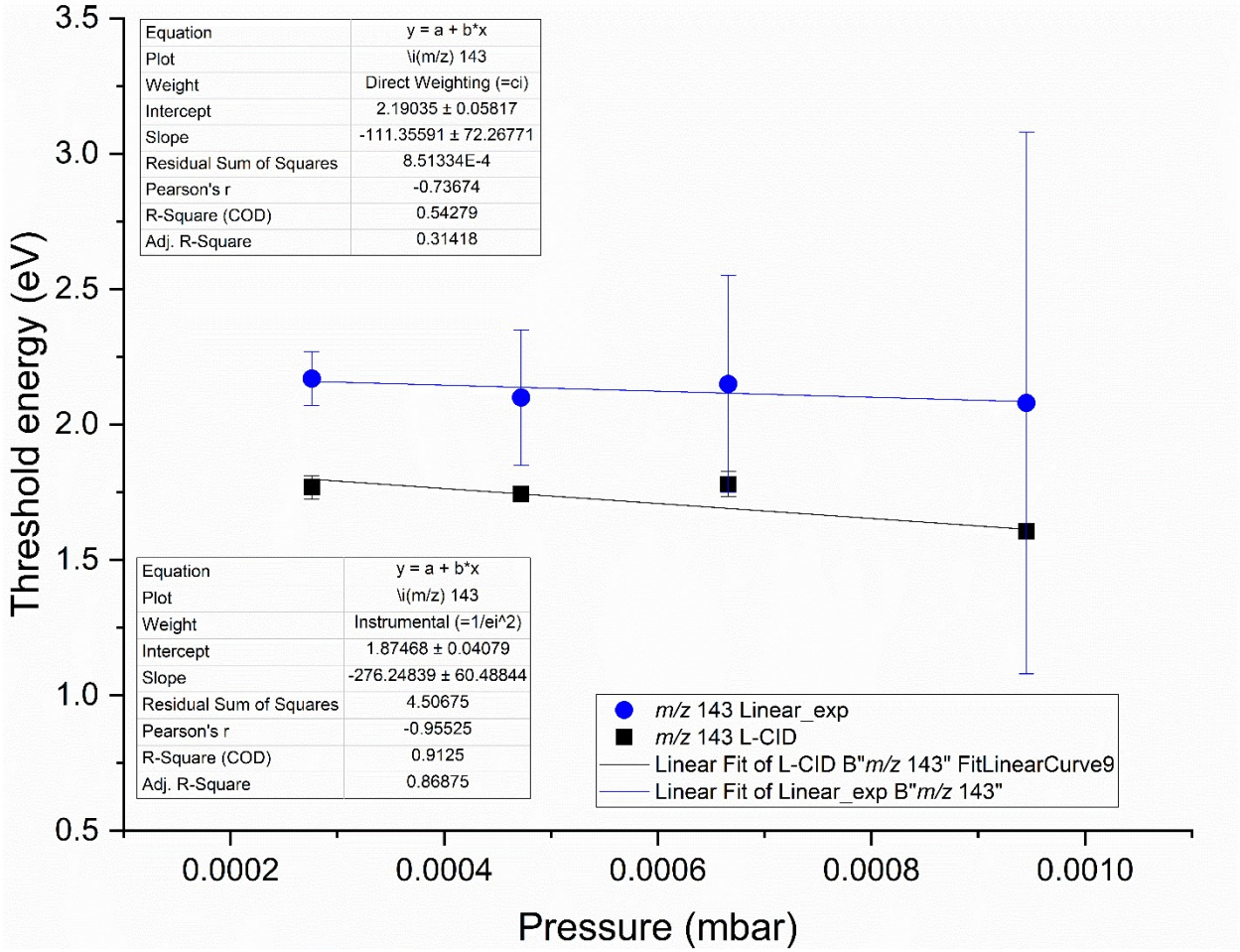

Figure S6. Pressure extrapolation of $ClMgC_3O_3^-$ (*m/z* 143) threshold energies (linear and L-CID) to zero pressure. The fitting of the linearly extrapolated energies uses direct weighing ($w_i = c_i$) as represented by error bars corresponding to the highest signal intensity in each experiment, while the error bars on the L-CID energies are used in instrumental weighing ($w_i = 1/e_i^2$).

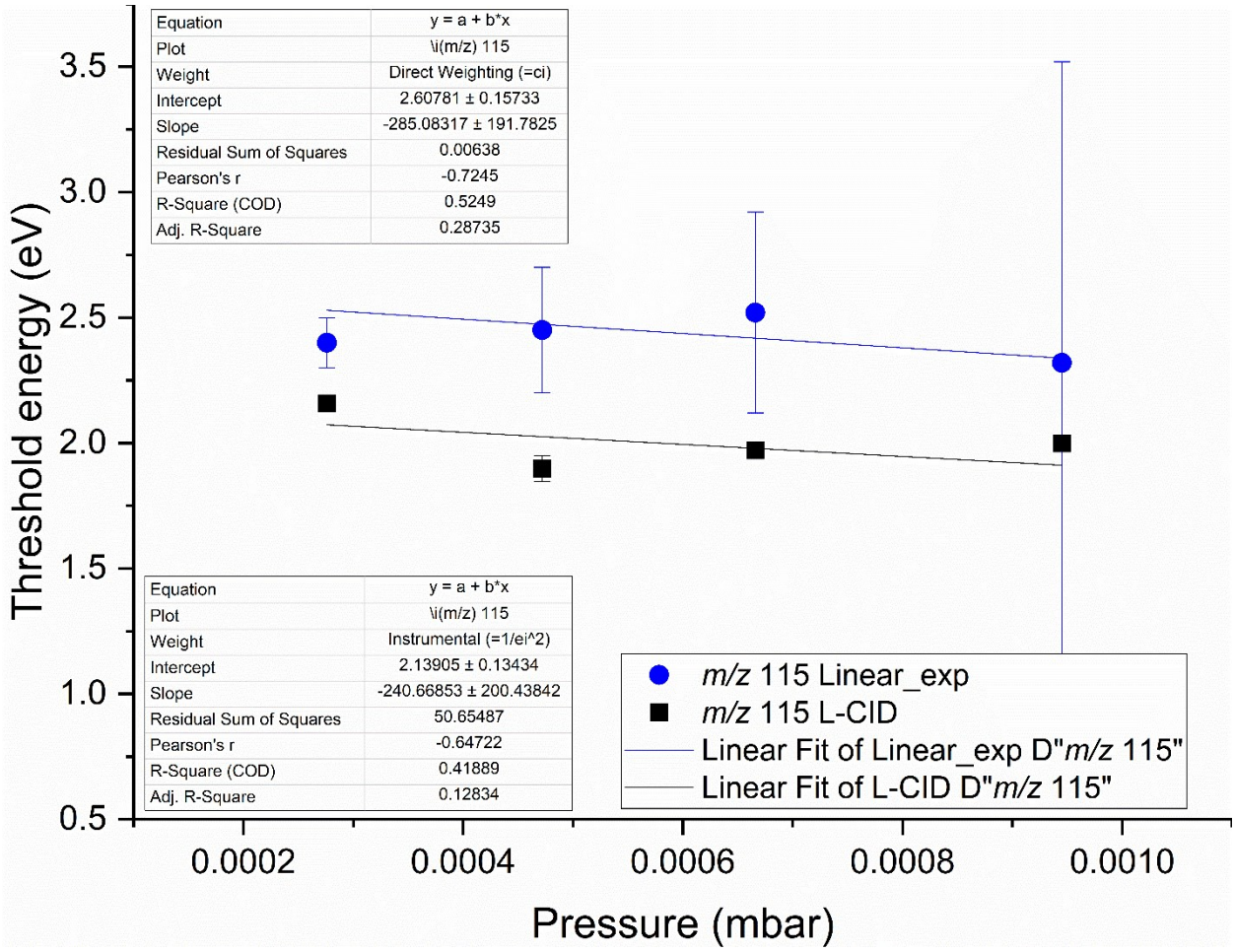

Figure S7. Pressure extrapolation of $ClMgC_2O_2^-$ (*m/z* 115) threshold energies (linear and L-CID) to zero pressure. The fitting of the linearly extrapolated energies uses direct weighing ($w_i = c_i$) as represented by error bars corresponding to the highest signal intensity in each experiment, while the error bars on the L-CID energies are used in instrumental weighing ($w_i = 1/e_i^2$).

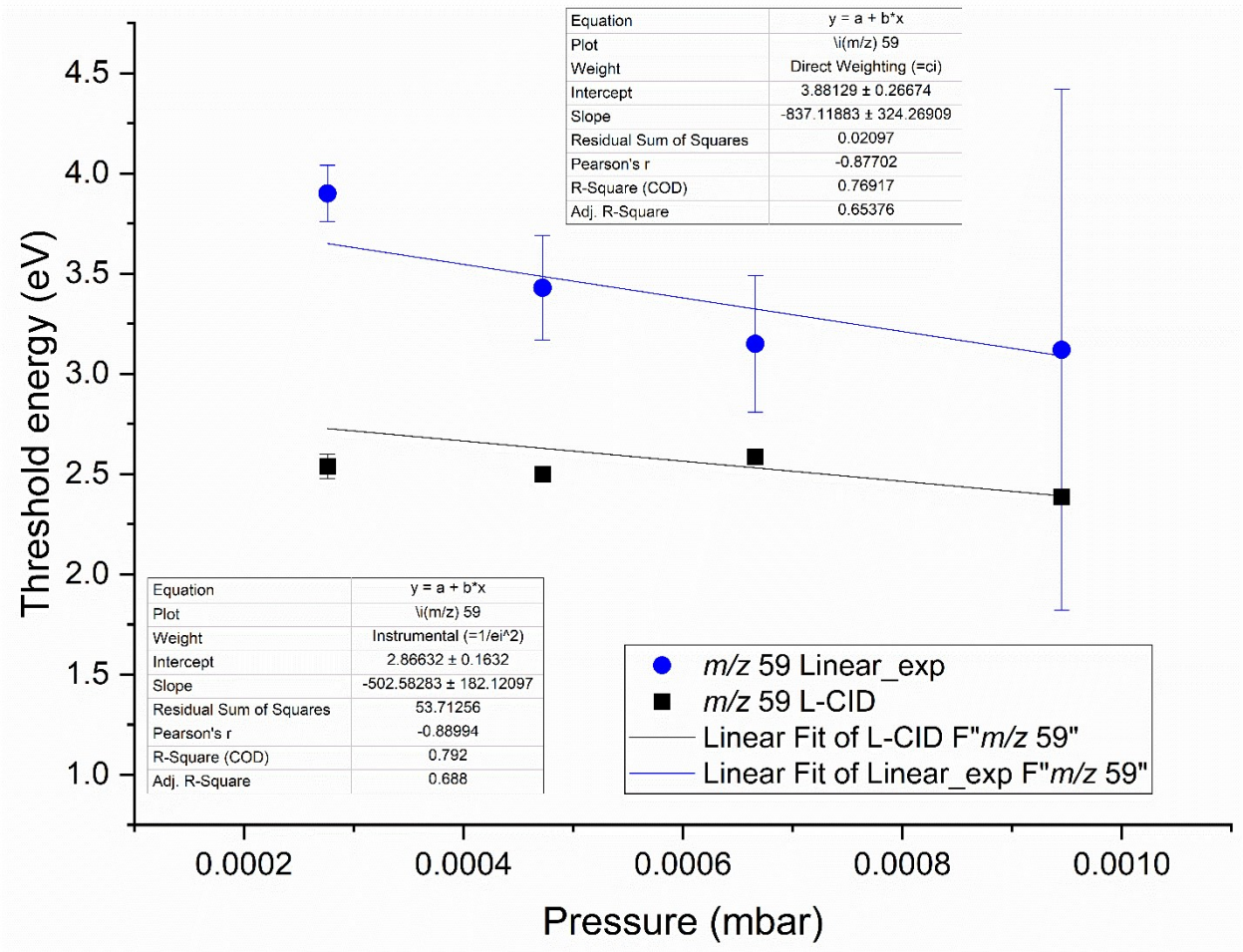

Figure S8. Pressure extrapolation of $ClMg^-$ (*m/z* 59) threshold energies (linear and L-CID) to zero pressure. The fitting of the linearly extrapolated energies uses direct weighing ($w_i = c_i$) as represented by error bars corresponding to the highest signal intensity in each experiment, while the error bars on the L-CID energies are used in instrumental weighing ($w_i = 1/e_i^2$).

Threshold energies for dissociation of $ClMgC_3O_3^-$ (*m/z* 143)

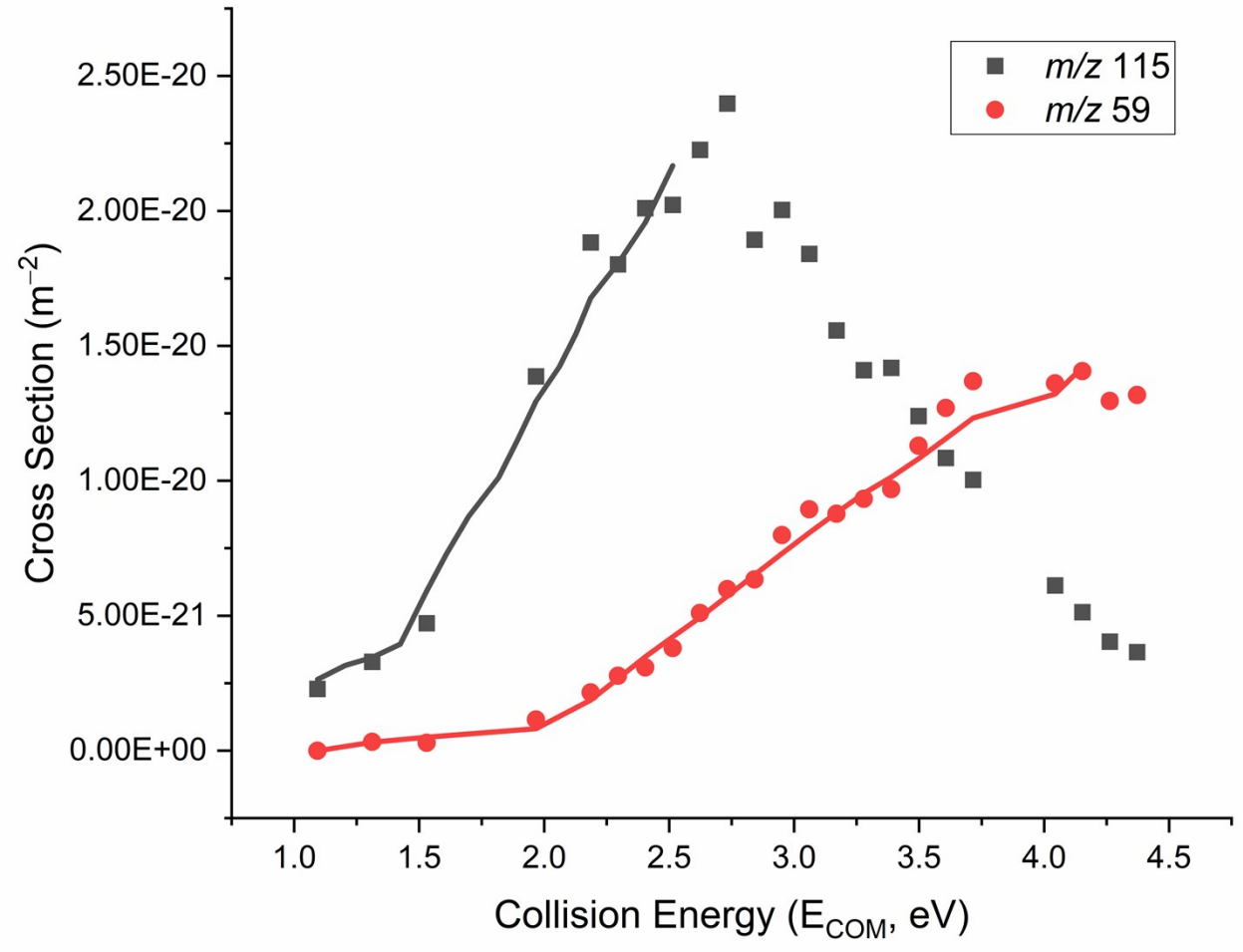

Figure S9. Energy-resolved CID cross sections and L-CID fits for the dissociation of $ClMgC_3O_3^-$ (*m/z* 143) at 4.63×10^{-4} mbar Ar pressure. Extra arbitrary points were added for the *m/z* 115 curve between 1.5 and 2.0 eV to enable L-CID fitting.

Table S5. L-CID output and results of linear extrapolation (4.63×10^{-4} mbar Ar pressure).

	***m/z* 115**	***m/z* 59**
$E_{0\ Linear}$ (eV)	1.32	2.16
$E_{0\ LCID}$ (eV)	1.14 ± 0.01	1.67 ± 0.01
ν_{eff} (cm^{-1})	671 ± 22	715 ± 58
a' (cm^{-1})	5620 ± 322	5593 ± 269

Threshold energies for the reference system, $C_6H_5^-$ (*m/z* 121) → $C_6H_5^-$ (*m/z* 77) + CO_2

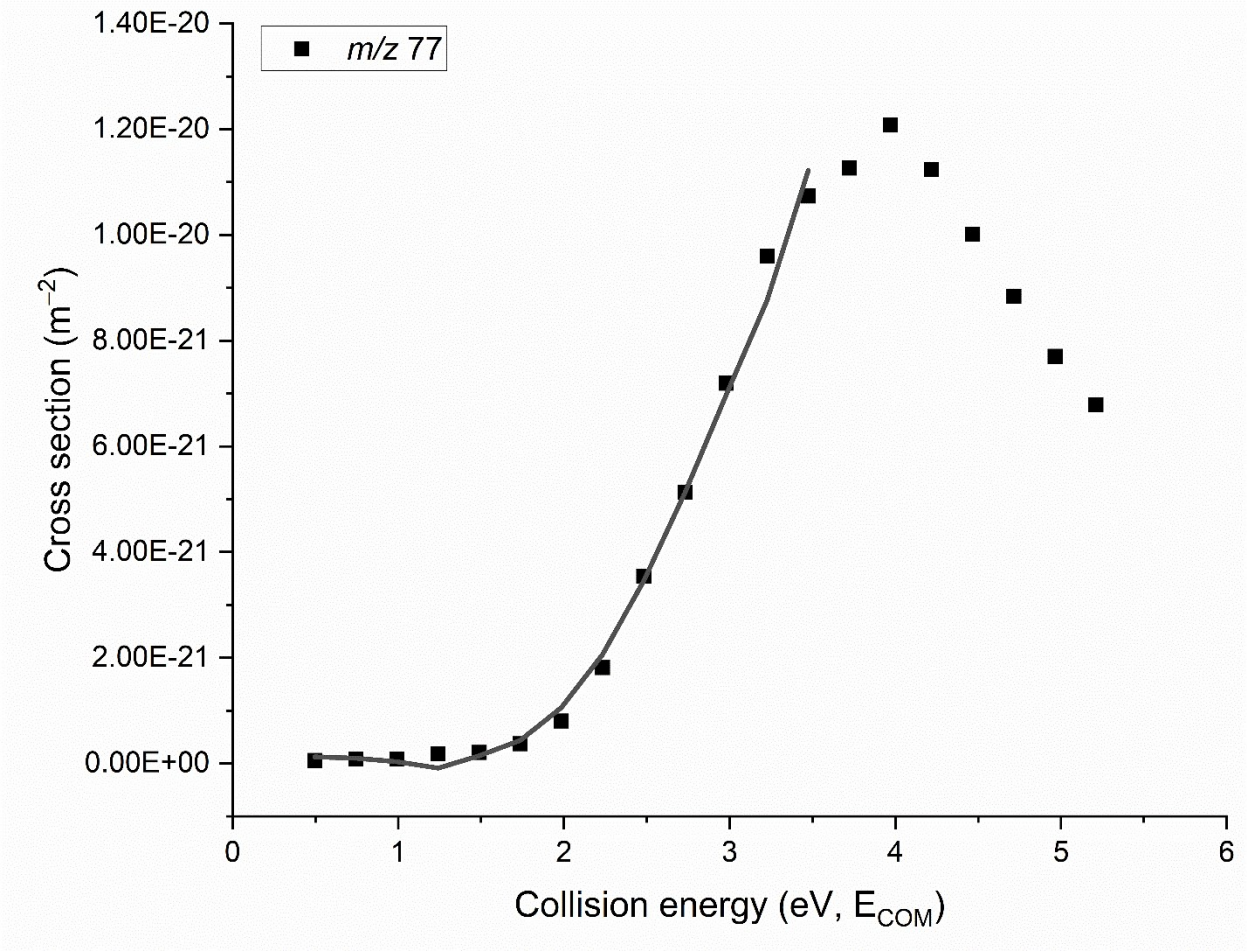

Figure S10. Energy-resolved CID cross sections and L-CID fits for the dissociation of benzoate (*m/z* 121) at 5.35 × 10^{-4} mbar Ar pressure.

Table S6. L-CID output and results of linear extrapolation (5.35 × 10^{-4} mbar Ar pressure).

	***m/z* 77**
E_{0_Linear} (eV)	2.17
E_{0_LCID} (eV)	1.73 ± 0.01
ν_{eff} (cm^{-1})	776 ± 39
a' (cm^{-1})	5833 ± 133

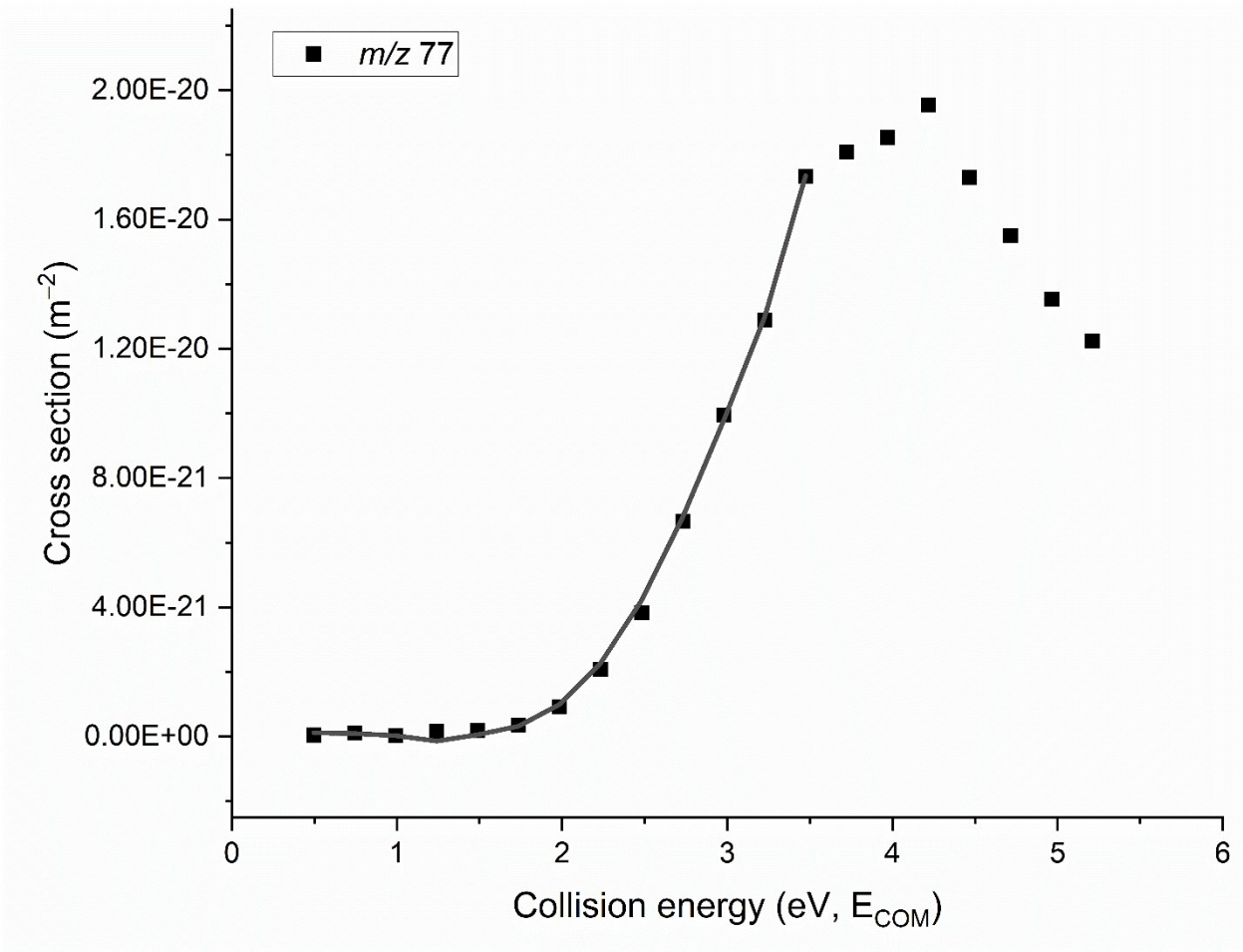

Figure S11. Energy-resolved CID cross sections and L-CID fits for the dissociation of benzoate (*m/z* 121) at 4.00×10^{-4} mbar Ar pressure.

Table S7. L-CID output and results of linear extrapolation (4.00×10^{-4} mbar Ar pressure).

	***m/z* 77**
E_{0_Linear} (eV)	2.32
E_{0_LCID} (eV)	1.86 ± 0.03
ν_{eff} (cm^{-1})	786 ± 132
a' (cm^{-1})	5900 ± 265

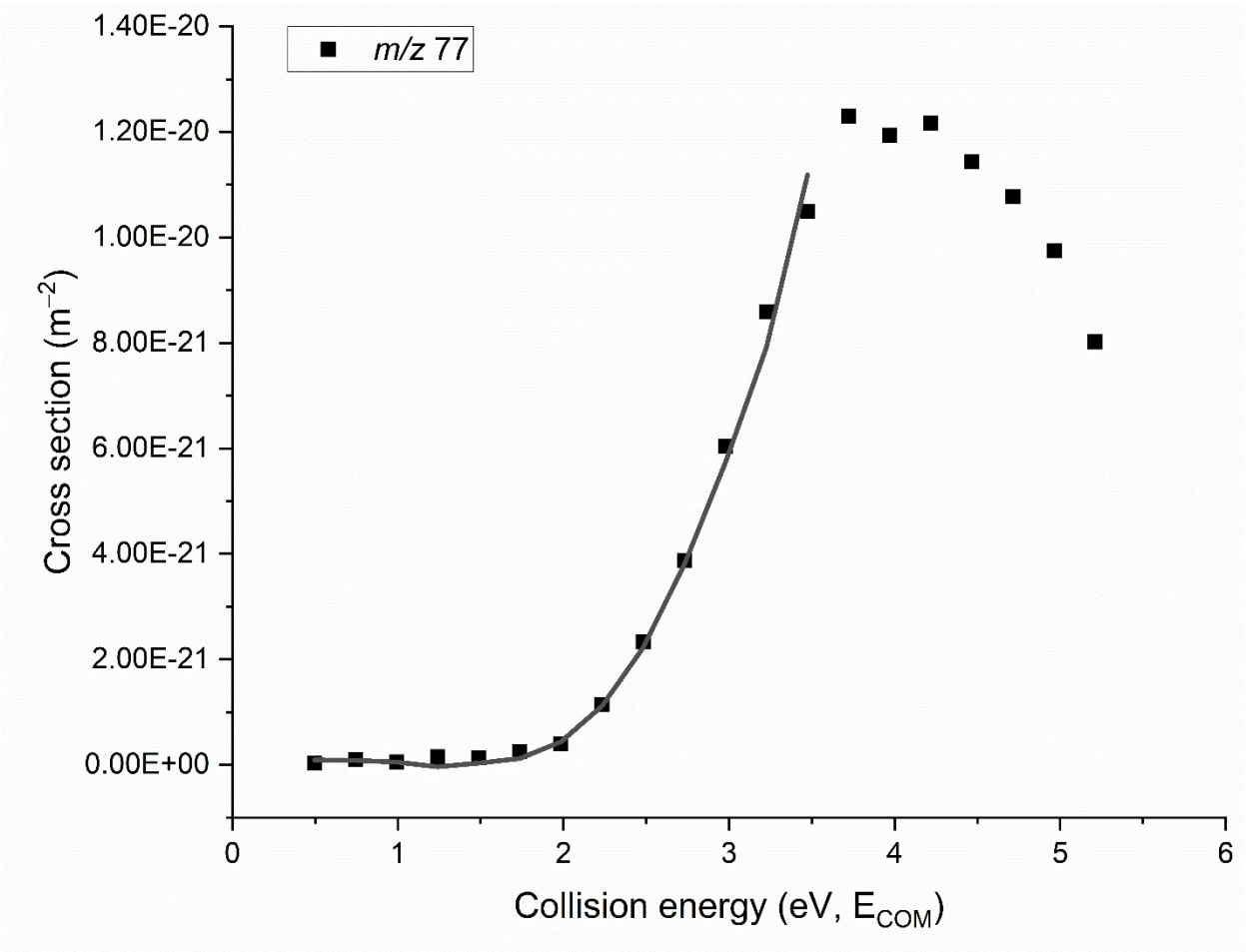

Figure S12. Energy-resolved CID cross sections and L-CID fits for the dissociation of benzoate (*m/z* 121) at 3.02×10^{-4} mbar Ar pressure.

Table S8. L-CID output and results of linear extrapolation (3.02×10^{-4} mbar Ar pressure).

	***m/z* 77**
E_{0_Linear} (eV)	2.37
E_{0_LCID} (eV)	1.88 ± 0.02
ν_{eff} (cm^{-1})	864 ± 67
a' (cm^{-1})	5800 ±72

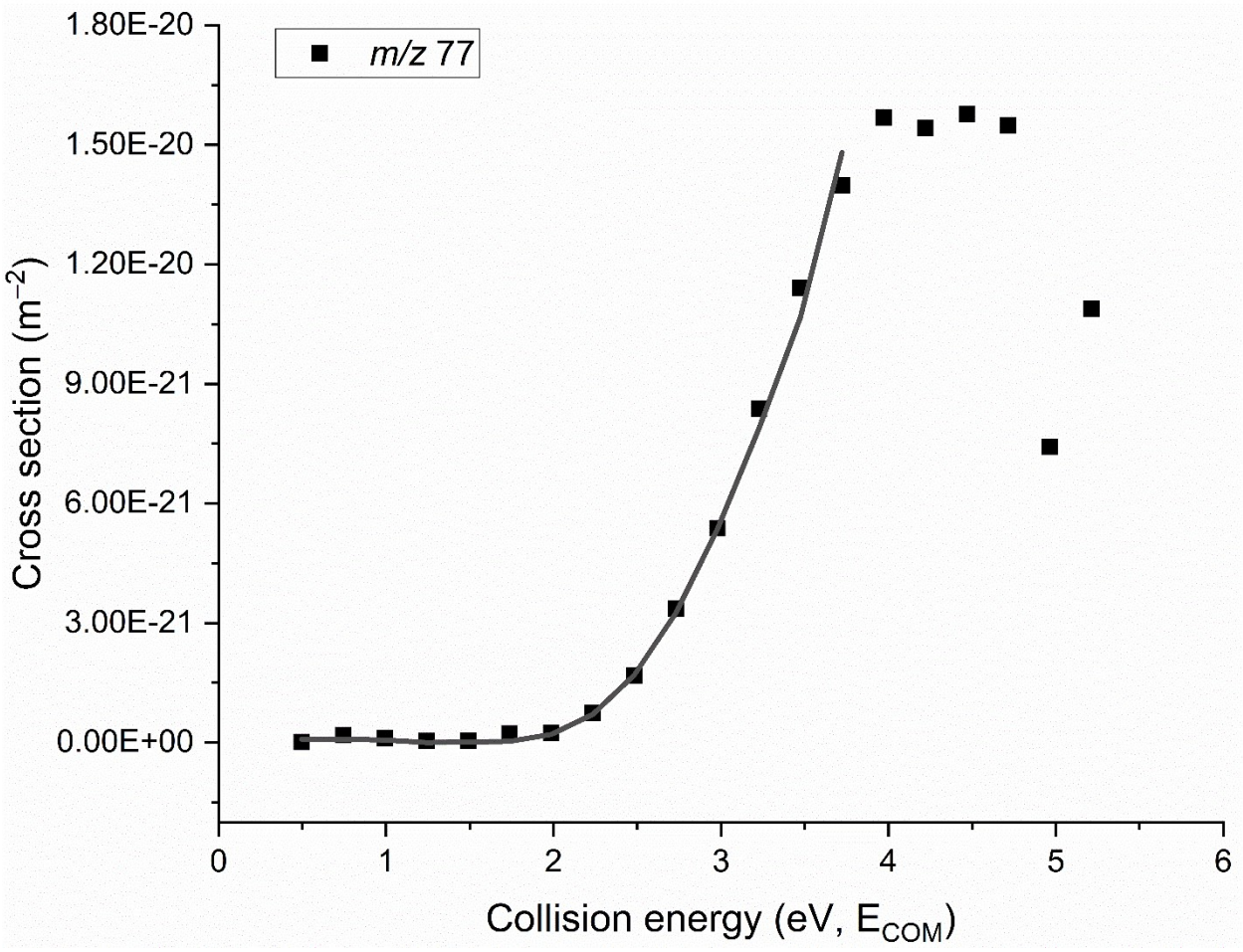

Figure S13. Energy-resolved CID cross sections and L-CID fits for the dissociation of benzoate (*m/z* 121) at 1.97×10^{-4} mbar Ar pressure.

Table S9. L-CID output and results of linear extrapolation (1.97×10^{-4} mbar Ar pressure).

	***m/z* 77**
E_{0_Linear} (eV)	2.57
E_{0_LCID} (eV)	1.99 ± 0.01
ν_{eff} (cm^{-1})	833 ± 29
a' (cm^{-1})	5687 ± 273

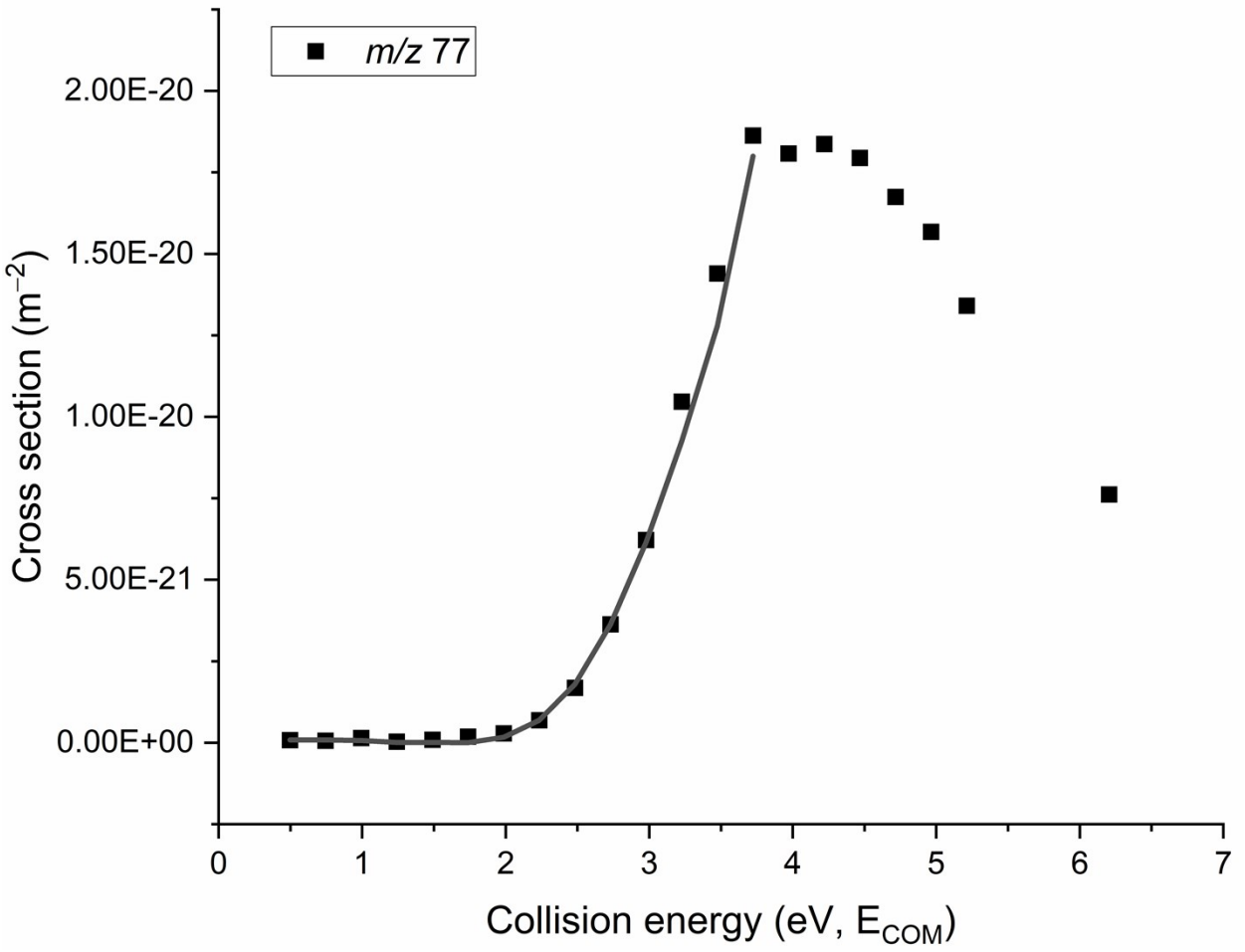

Figure S14. Energy-resolved CID cross sections and L-CID fits for the dissociation of benzoate (*m/z* 121) at 1.04×10^{-4} mbar Ar pressure.

Table S10. L-CID output and results of linear extrapolation (1.04×10^{-4} mbar Ar pressure).

	***m/z* 77**
E_{0_Linear} (eV)	2.65
E_{0_LCID} (eV)	2.03 ± 0.01
ν_{eff} (cm^{-1})	896 ± 13
a' (cm^{-1})	5847 ± 253

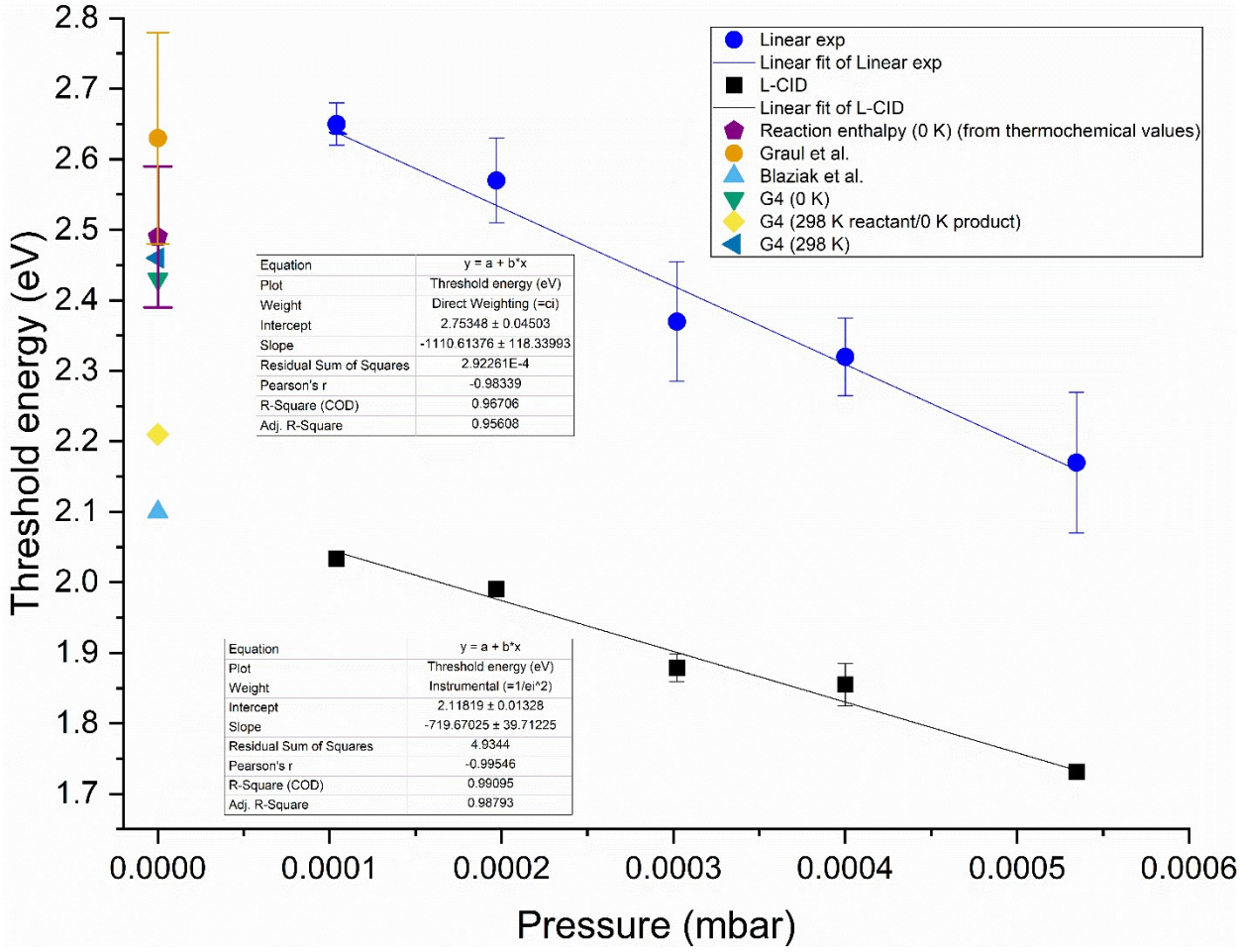

Figure S15. Pressure extrapolation of $C_6H_5^-$ (*m*/z 77) threshold energies (Linear and L-CID) to zero pressure. The fitting of the linearly extrapolated energies uses direct weighing ($w_i = c_i$) as represented by error bars corresponding to the highest signal intensity in each experiment, while the error bars on the L-CID energies are used in instrumental weighing ($w_i = 1/e_i^2$).

Table S11. Experimental and calculated reaction enthalpies ($\Delta_rH°$) and threshold energies (E_T) for $C_6H_5CO_2^- \rightarrow C_6H_5^- + CO_2$ in eV (kJ/mol in parentheses). Our estimates in **bold** (experimental and computational G4 (0 K)).

Experimental		
$\Delta_rH°$ (298 K)	E_T (linear extrapolation)	E_T (L-CID)
2.49 ± 0.1 (240 ± 10)	**2.75 ± 0.05 (265 ± 4)**	**2.12 ± 0.01 (205 ± 1)**
	2.63 ± 0.15 (254 ± 14)[2]	
	2.10 (203)[3]	
Computational		
$\Delta_rH°$ (298 K)	$\Delta_rH°$ (298 K reactant /0 K product)	E_T (0 K)
2.46 (237)	**2.21 (213)**	**2.43 (234)**
2.27 (219)[3]		2.37 (229)[3]

Calculation of reaction enthalpy for $C_6H_5CO_2^- \rightarrow C_6H_5^- + CO_2$ at 0 K

$\Delta_{f,gas}H°_{0K}(C_6H_5CO_2^-) = -381.8 \pm 10$ kJ/mol

$\Delta_{f,gas}H°_{0K}(C_6H_5^-) = 244.9 \pm 0.5$ kJ/mol[4]

$\Delta_{f,gas}H°_{0K}(CO_2) = -393.11 \pm 0.02$ kJ/mol

$\Delta_{decarb,gas}H°_{0K}$ = (244.9 kJ/mol + (−393.1 kJ/mol)) – (−381.8 kJ/mol)

$\Delta_{decarb,gas}H°_{0K}$ = **233.7 ± 10.0 kJ/mol**

Thermochemical parameters used in the calculation of the enthalpy of formation for benzoate:

PA = $-\Delta_{rxn}H°$ = 1423 ± 9 kJ/mol[5] for $C_6H_5CO_2^- + H^+ \rightarrow C_6H_5CO_2H$

$\Delta_fH°_{0K}(H^+)$ = 1528.03 kJ/mol

$\Delta_{Sub}H°(C_6H_5CO_2H)$ = 90 ± 4 kJ/mol (NIST database, average of 13 values)

$\Delta_{f,solid}H°_{0K}(C_6H_5CO_2H)$ = −366.8 ± 0.5 kJ/mol (NIST database)

$\Delta_{f,gas}H°_{0K}(C_6H_5CO_2H)$ = −366.8 kJ/mol + $\Delta_{Sub}H°(C_6H_5CO_2H)$ = −276.8 ± 4 kJ/mol

$\Delta_{f,gas}H°_{0K}(C_6H_5CO_2^-) = \Delta_{f,gas}H°_{0K}(C_6H_5CO_2H) - \Delta_fH°_{0K}(H^+) + PA$

Calculation of reaction enthalpy for $C_6H_5CO_2^- \rightarrow C_6H_5^- + CO_2$ at 298 K

$\Delta_{f,gas}H°_{,\ 298K}(C_6H_5CO_2^-) = -401.9 \pm 10$ kJ/mol

$\Delta_{f,gas}H°_{,\ 298K}(C_6H_5^-) = 232.0 \pm 0.5$ kJ/mol[4]

$\Delta_{f,gas}H°_{,\ 298K}(CO_2) = -393.50 \pm 0.02$ kJ/mol

$\Delta_{decarb,gas}H°_{,\ 298K} = (232.0\text{ kJ/mol} + (-393.5\text{ kJ/mol})) - (-401.9\text{ kJ/mol})$

$\Delta_{decarb,gas}H°_{,\ 298K} =$ **240.4 ± 10.0 kJ/mol**

Thermochemical parameters used in the calculation of the enthalpy of formation for benzoate:

PA = $-\Delta_{rxn}H°$ = 1423 ± 9 kJ/mol[5] for $C_6H_5CO_2^- + H^+ \rightarrow C_6H_5CO_2H$

$\Delta_fH°_{,\ 298K}(H^+) = 1530.05$ kJ/mol

$\Delta_{Sub}H°(C_6H_5CO_2H) = 90 \pm 4$ kJ/mol (NIST database, average of 13 values)

$\Delta_{f,solid}H°_{,\ 298K}(C_6H_5CO_2H) = -384.8 \pm 0.5$ kJ/mol (NIST database)

$\Delta_{f,gas}H°_{,\ 298K}(C_6H_5CO_2H) = -384.8\text{ kJ/mol} + \Delta_{Sub}H°(C_6H_5CO_2H) = -294.8 \pm 4$ kJ/mol

$\Delta_{f,gas}H°_{,\ 298K}(C_6H_5CO_2^-) = \Delta_{f,gas}H°_{,\ 298K}(C_6H_5CO_2H) - \Delta_fH°_{,\ 298K}(H^+) + PA$

Threshold energies for the reference system, Cs^+(15-crown-5) (*m/z* 353) → Cs^+ (*m/z* 133) + 15-crown-5

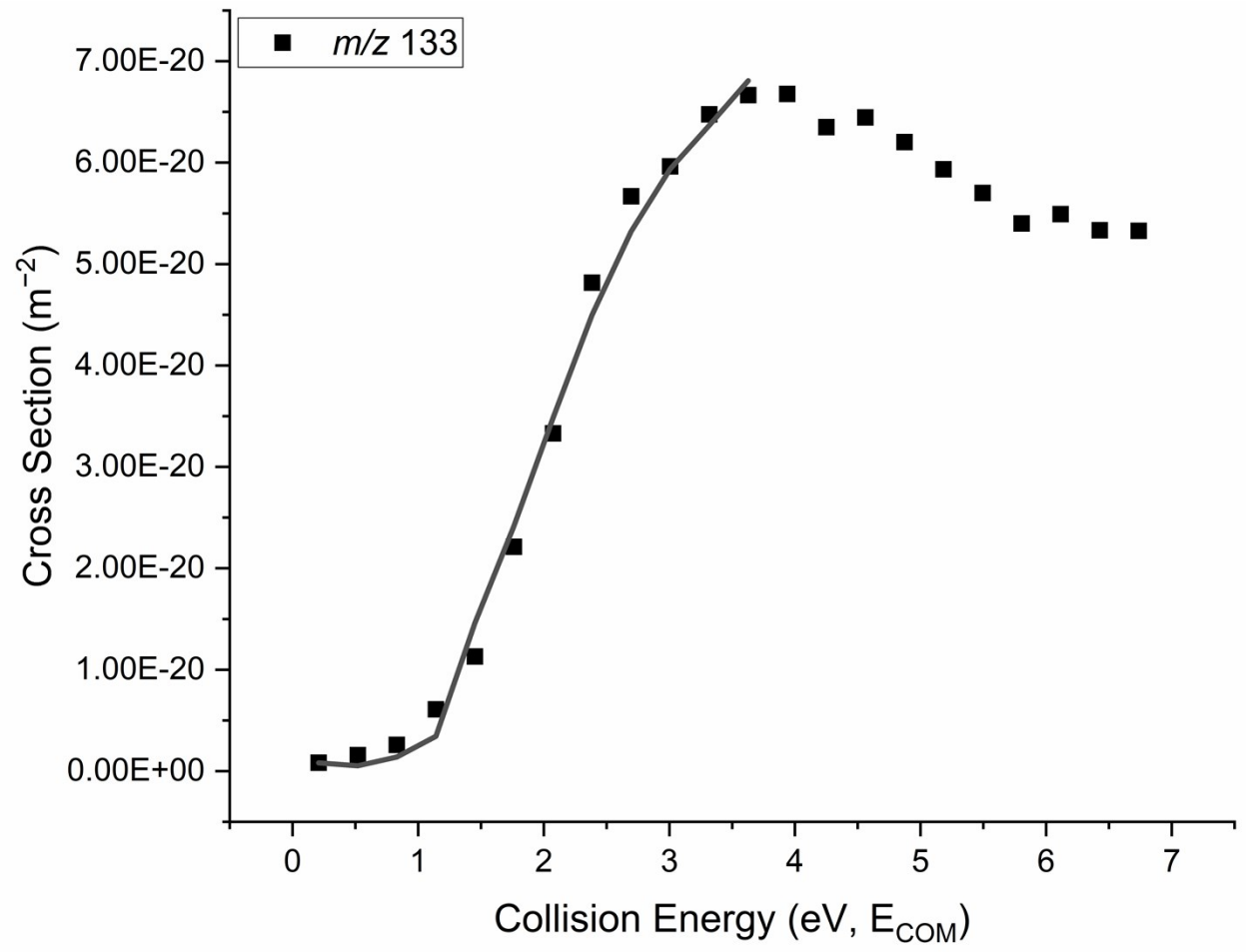

Figure S16. Energy-resolved CID cross sections and L-CID fit for the dissociation of Cs^+(15-crown-5) (*m/z* 353) at 4.95×10^{-4} mbar Xe pressure.

Table S12. L-CID output and results of linear extrapolation (4.95×10^{-4} mbar Xe pressure).

	***m/z* 77**
E_{0_Linear} (eV)	1.26
E_{0_LCID} (eV)	1.19
ν_{eff} (cm^{-1})	962
a' (cm^{-1})	5760

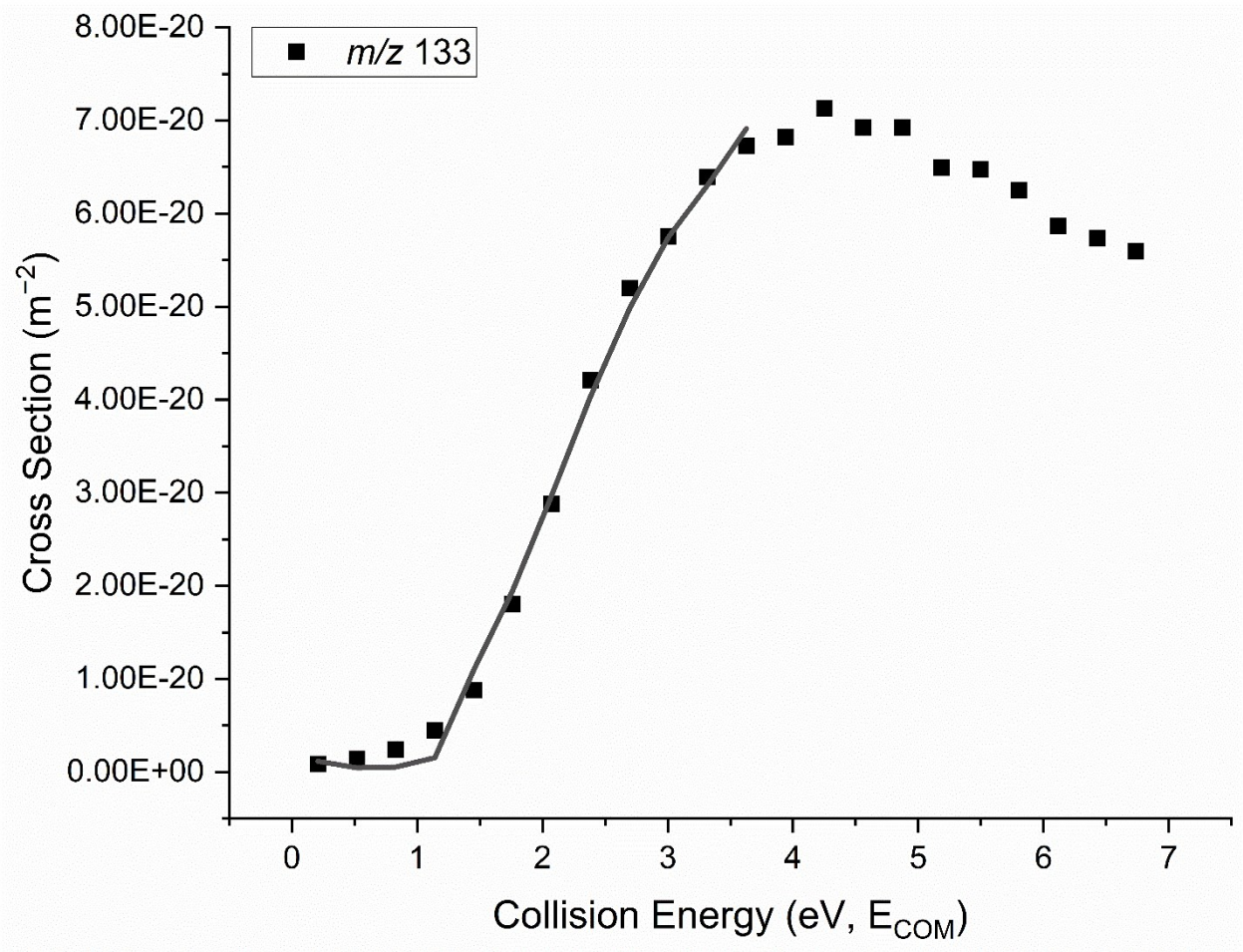

Figure S17. Energy-resolved CID cross sections and L-CID fit for the dissociation of Cs^+(15-crown-5) (*m/z* 353) at 4.00×10^{-4} mbar Xe pressure.

Table S13. L-CID output and results of linear extrapolation (4.00×10^{-4} mbar Xe pressure).

	***m/z* 77**
E_{0_Linear} (eV)	1.34
E_{0_LCID} (eV)	1.32 ± 0.01
ν_{eff} (cm^{-1})	769 ± 51
a' (cm^{-1})	6170 ± 41

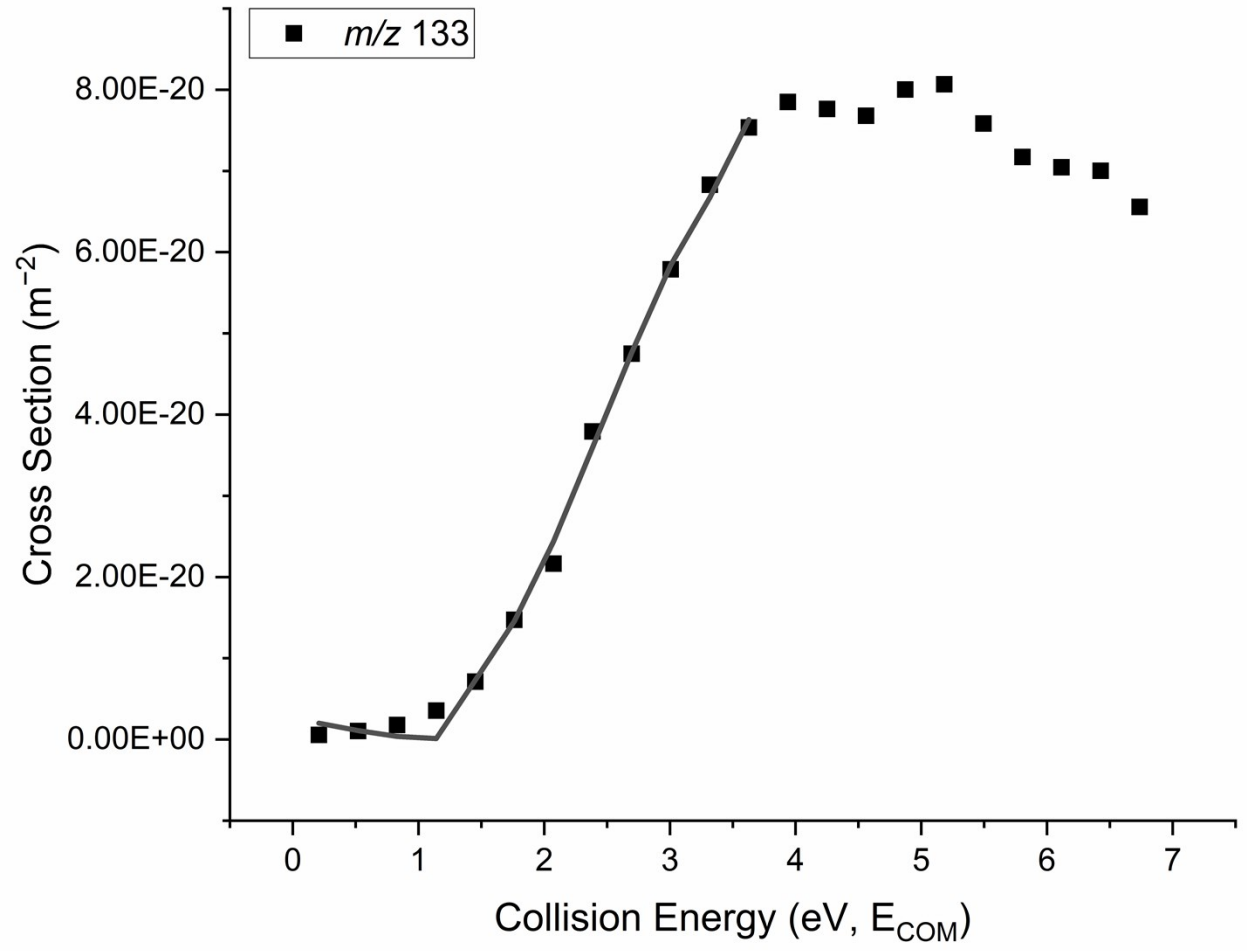

Figure S18. Energy-resolved CID cross sections and L-CID fit for the dissociation of Cs^+(15-crown-5) (*m/z* 353) at 3.00×10^{-4} mbar Xe pressure.

Table S14. L-CID output and results of linear extrapolation (3.00×10^{-4} mbar Xe pressure).

	***m/z* 77**
E_{0_Linear} (eV)	1.54
E_{0_LCID} (eV)	1.40 ± 0.02
ν_{eff} (cm^{-1})	806 ± 44
a' (cm^{-1})	6030 ± 282

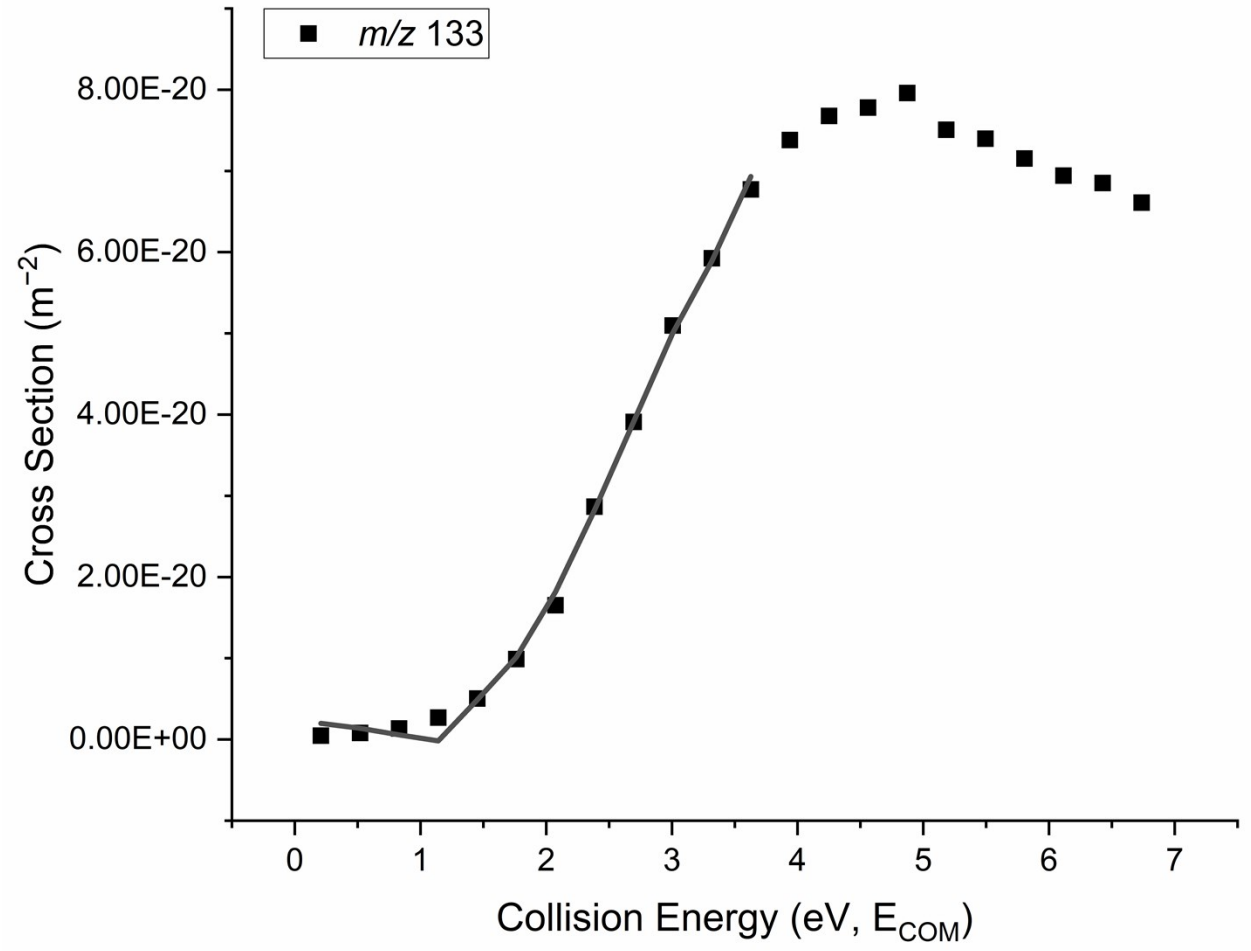

Figure S19. Energy-resolved CID cross sections and L-CID fit for the dissociation of Cs^+(15-crown-5) (*m/z* 353) at 2.00×10^{-4} mbar Xe pressure.

Table S15. L-CID output and results of linear extrapolation (2.00×10^{-4} mbar Xe pressure).

	***m/z* 77**
E_{0_Linear} (eV)	1.70
E_{0_LCID} (eV)	1.45 ± 0.02
ν_{eff} (cm^{-1})	614 ± 69
a' (cm^{-1})	5680 ± 220

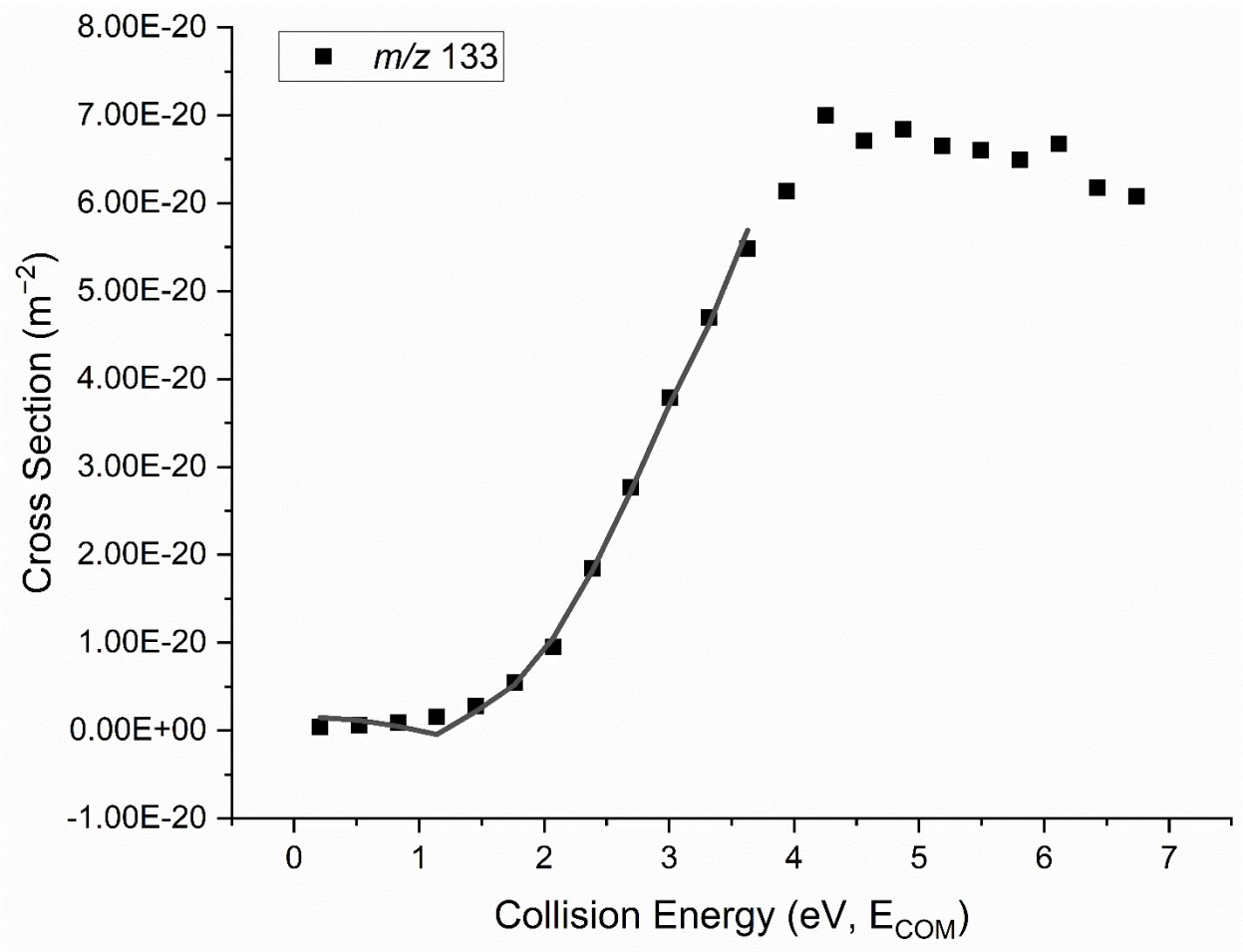

Figure S20. Energy-resolved CID cross sections and L-CID fit for the dissociation of Cs^+(15-crown-5) (*m/z* 353) at 1.00×10^{-4} mbar Xe pressure.

Table S16. L-CID output and results of linear extrapolation (1.00×10^{-4} mbar Xe pressure).

	***m/z* 77**
E_{0_Linear} (eV)	1.94
E_{0_LCID} (eV)	1.51 ± 0.01
ν_{eff} (cm^{-1})	655 ± 43
a' (cm^{-1})	5540 ± 140

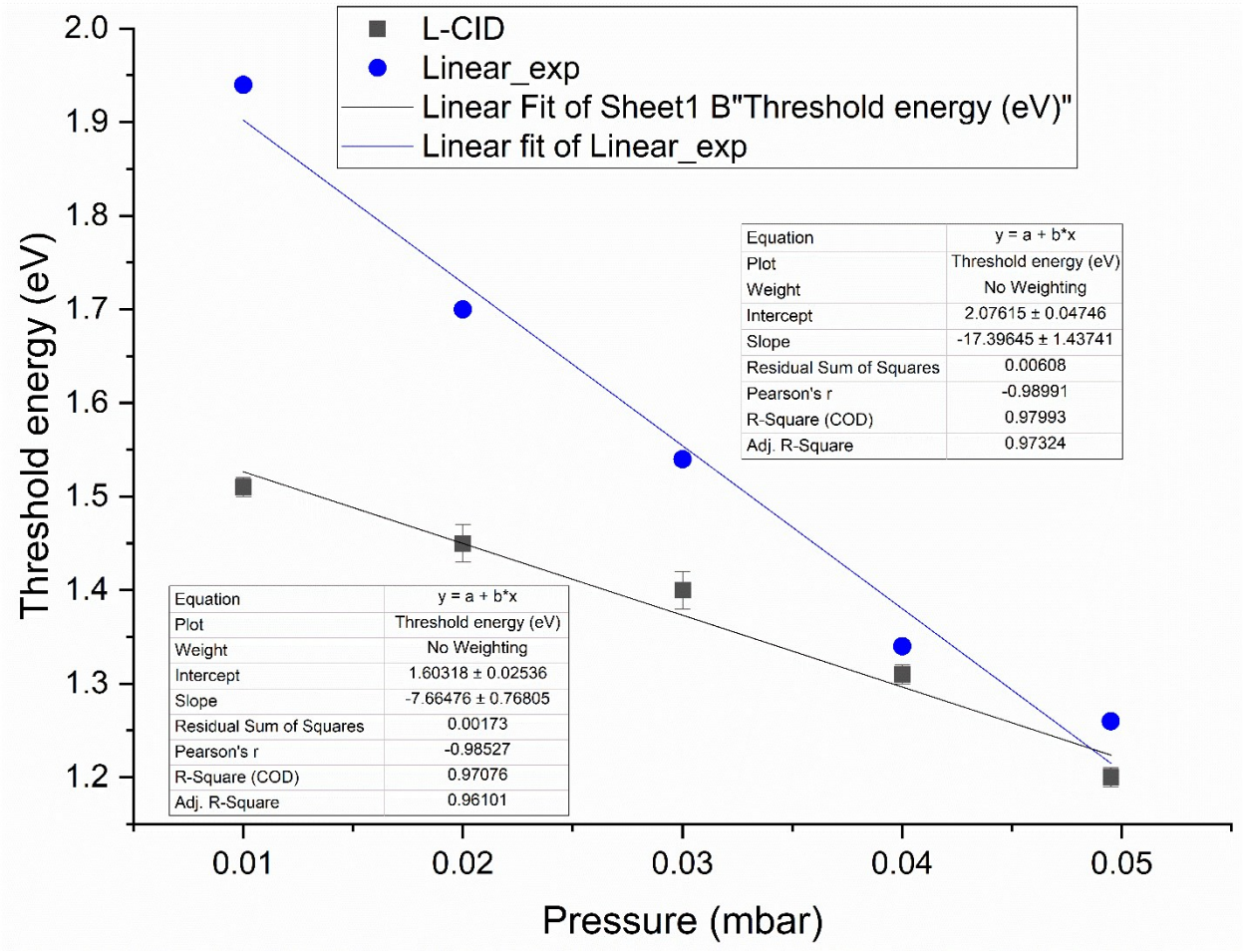

Figure S21. Pressure extrapolation of Cs^+ (*m/z* 133) threshold energies (Linear and L-CID) to zero pressure. The L-CID energies are instrumentally weighed ($w_i = 1/e_i^2$).

Table S17. Threshold energies of Cs^+ (*m/z* 133) extrapolated to vacuum and corresponding literature values.

	***m/z* 77**
$\mathbf{E_{0\_Linear}}$ **(eV)**	2.08 ± 0.05
$\mathbf{E_{0\_LCID}}$ **(eV)**	1.60 ± 0.03
$\mathbf{E_{0\_LCID\_CHEN}}$ **(eV)**[1]	1.43 ± 0.05
$\mathbf{E_{0\_CRUNCH\_CHEN}}$ **(eV)**[1]	1.45
$\mathbf{E_{0\_CRUNCH\_ARMENTROUT}}$ **(eV)**[6]	1.04 ± 0.06
$\mathbf{E_{0\_TCID\_ARMENTROUT}}$ **(eV)**[7]	1.65 ± 0.10

SI-B. Metastable fragmentation

We calculated peak corresponding to metastable fragmentation in the first field-free region of the TOF as described by Harvey and coworkers[8] and done in a previous study by us.[9] The following expression provides the apparent mass of the metastable ion,

$$M^* = M_p\left[\frac{1+\left(\frac{M_f}{M_p}\right)r}{(1+r)}\right]^2$$

where r is an instrumental parameter describing the relative traversal times of an ion through the field-free and the ion mirror (reflectron) regions. This is calibrated by assigning a metastable peak, M^*, to a specific precursor-fragment ion (M_p-M_f) transition. For our instrument, r = 0.82, calibrated through the spontaneous metastable fragmentation of water clusters, providing known precursor-fragment transitions. The results of this analysis are shown in Figures S22 – S23 and Table S18.

Table S18. Precursor (M_p), fragment (M_f) and calculated metastable (M^*) peak positions with r = 0.82

M_p	M_f	M^*
170.92	142.93	*146.63*
	114.94	*124.20*
	98.94	*112.21*
	58.96	*84.92*
	34.98	*70.37*
142.93	114.94	*118.82*
	98.94	*106.04*
	58.96	*77.28*
	34.98	*62.21*
114.94	58.96	*70.03*
	34.98	*54.18*
58.96	34.98	*39.33*

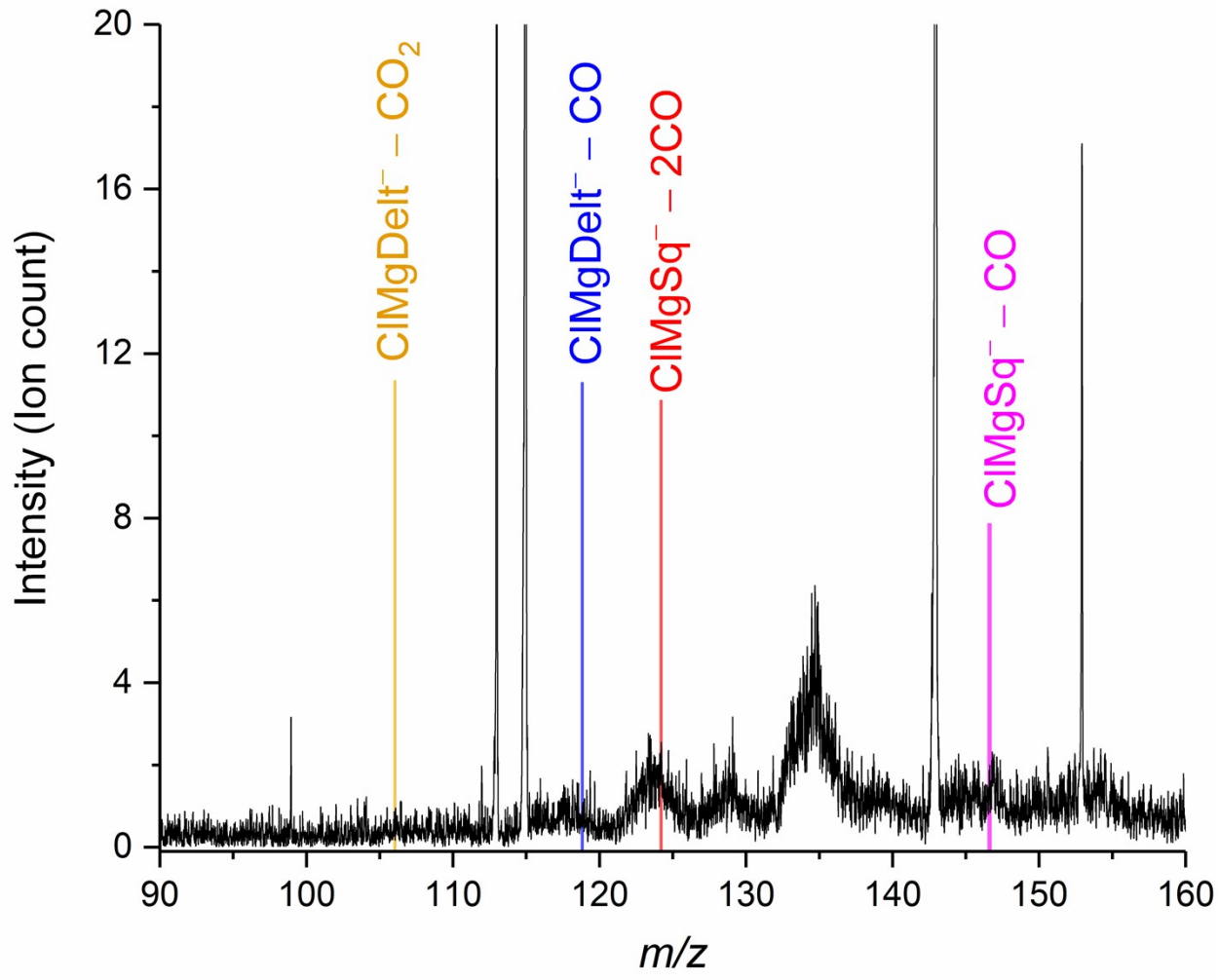

Figure S22. Metastable peaks between *m/z* 90 and 160 from the MSMS of *m/z* 171 ($ClMgSq^-$, $ClMgC_4O_4^-$), combined and averaged three times over collision energies between 90 – 550 kJ/mol in the center of mass frame. The instrumental r-value used in the calculation of the metastable peaks is 0.82.

The strongest metastable signals in Figure S22 correspond to the following dissociation reactions

$$ClMgC_4O_4^- \ (m/z\ 171) \rightarrow ClMgC_3O_3^- \ (m/z\ 143) + CO \qquad \text{(SI-1)}$$

$$ClMgC_4O_4^- \ (m/z\ 171) \rightarrow ClMgC_2O_2^- \ (m/z\ 115) + 2CO. \qquad \text{(SI-2)}$$

In addition, we have indicated the calculated metastable positions for

$$ClMgC_3O_3^- \ (m/z\ 143) \rightarrow ClMgC_2O_2^- \ (m/z\ 115) + CO \quad \text{(SI-3)}$$

$$ClMgC_3O_3^- \ (m/z\ 143) \rightarrow ClMgC_2O^- \ (m/z\ 99) + CO_2. \quad \text{(SI-4)}$$

The signal corresponding to SI-3 can be discerned from the noise-level, while the SI-4 metastable signal is too weak. We speculate that the origin of the two broad peaks at *m/z* 130 and 135 is from metastable fragmentation in the ion-mirror region, but have not made specific assignments.

The analysis was repeated for the MSMS of *m/z* 143 ($ClMgC_3O_3^-$) shown in Figure S23, further strengthening the assignments made above. Unsurprisingly, we do not observe the transitions corresponding to SI-1 and SI-2 here, but we do observe those corresponding to SI-3 and SI-4. The latter has a relatively high metastable signal compared to the focused fragment at *m/z* 99, which could be connected to the high stability of the neutral fragment CO_2.

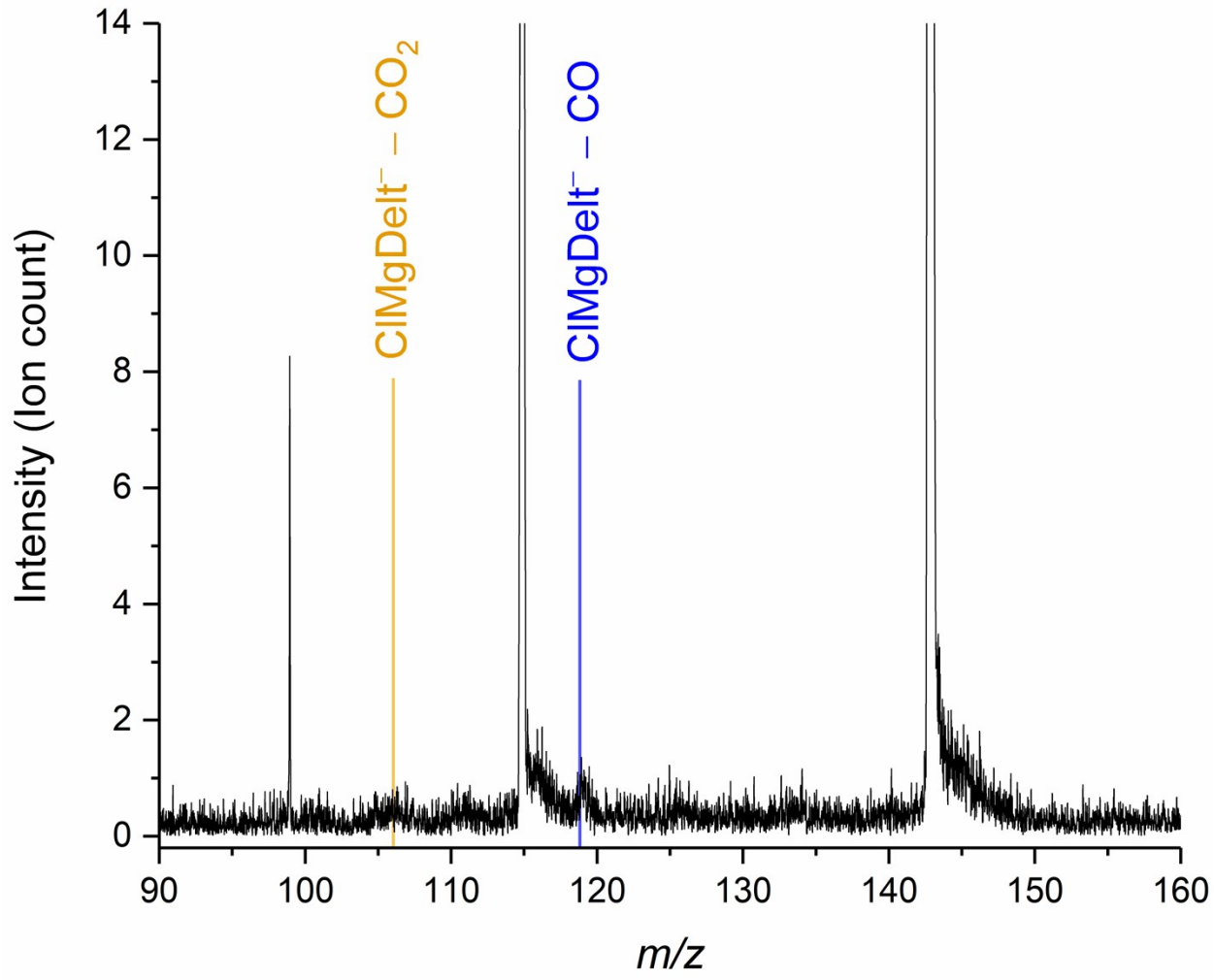

Figure S23. Metastable peaks between *m/z* 90 and 160 from the MSMS of *m/z* 143 ($ClMgDelt^-$, $ClMgC_3O_3^-$), combined and averaged three times over collision energies between 130 – 420 kJ/mol in the center of mass frame. The instrumental r-value used in the calculation of the metastable peaks is 0.82.

SI-C. G4 (0 K) $ClMgC_4O_4^-$ singlet potential energy surface

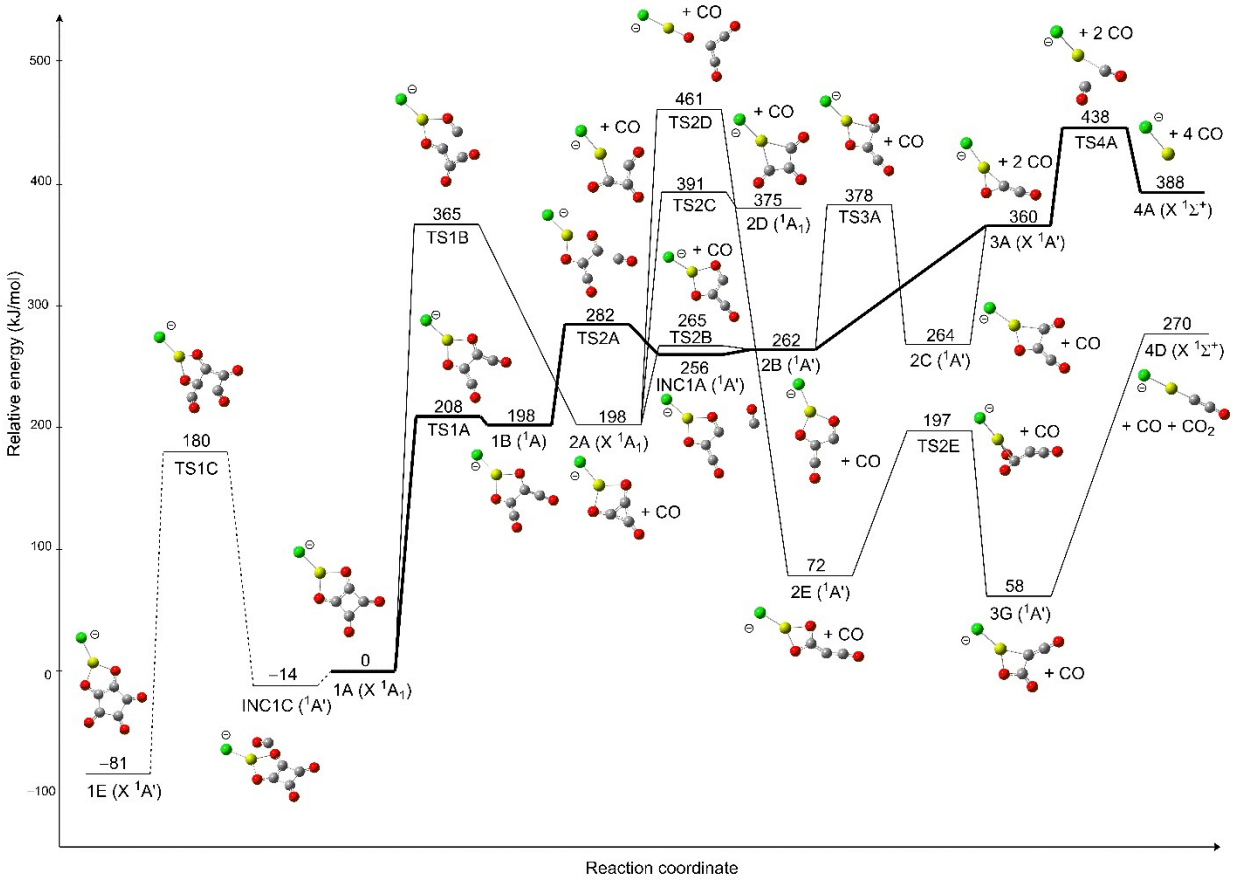

Figure S24. G4 (0 K) singlet PES for the dissociation of $ClMgC_4O_4^-$ and the formation of magnesium chloride croconate (1E) denoted by dashed lines.

SI-D. G4 (0 K) $ClMgC_4O_4^-$ triplet potential energy surface

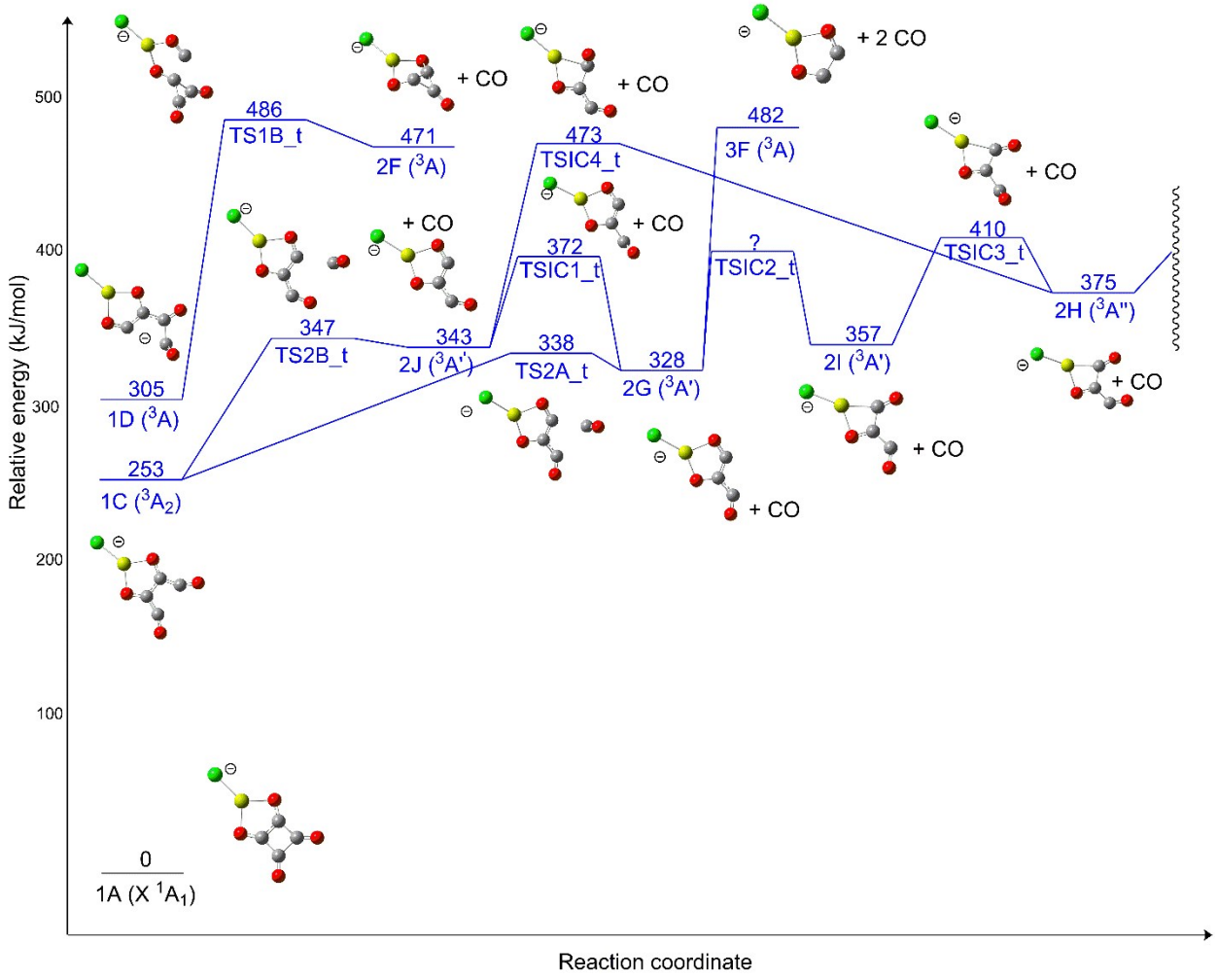

Figure S25. Part one of the G4 (0 K) triplet PES for the dissociation of $ClMgC_4O_4^-$.

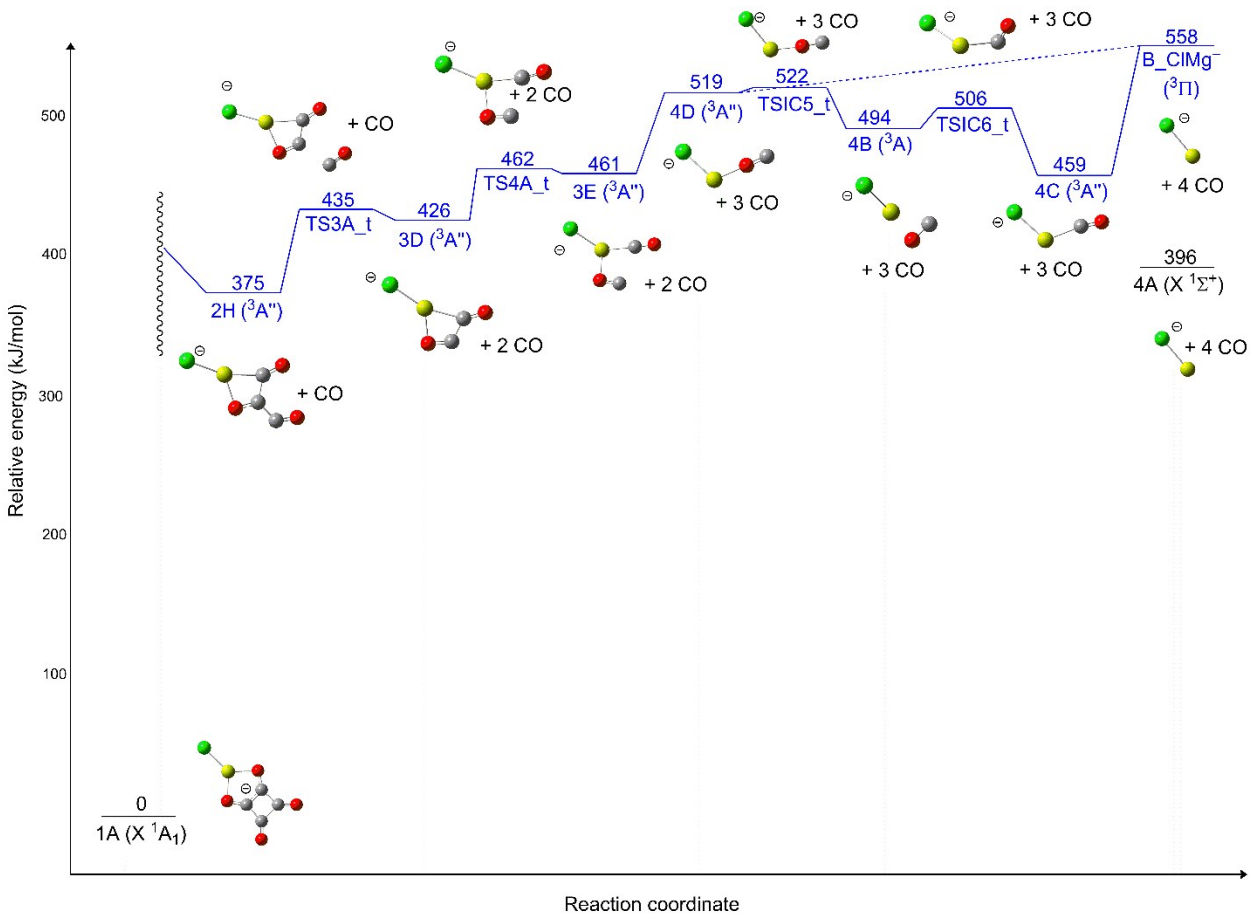

Figure S26. Part two of the G4 (0 K) triplet PES for the dissociation of $ClMgC_4O_4^-$.

SI-E. Optimized geometries and G4 (0 K) energies

Singlet PES

CO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.804635	0.161929	-0.002120
2	6	0	-2.935546	0.161929	-0.002120

G4 (0 K)= -113.289425

CO_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	8	0	0.000000	0.000000	1.162879
3	8	0	0.000000	0.000000	-1.162879

G4(0 K)= -188.535267

1A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.783019	-8.295918	-1.296009
2	8	0	-7.330509	-9.952772	0.284349
3	8	0	-8.456376	-10.920653	-2.175016
4	8	0	-6.068524	-9.401037	-4.104092
5	6	0	-6.838649	-9.698325	-0.897928
6	6	0	-6.351271	-9.510336	-2.929011
7	6	0	-5.738550	-8.983595	-1.590572
8	6	0	-7.389469	-10.171852	-2.101150
9	12	0	-8.853585	-11.054676	-0.262593
10	17	0	-10.474229	-12.097750	0.889818

G4 (0 K)= -1113.416747

1B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.003923	0.711277	0.186470
2	8	0	-0.139274	1.202480	0.734488
3	6	0	0.991049	-0.729326	-0.185634
4	8	0	-0.160389	-1.199774	-0.734609
5	6	0	2.040310	-1.454272	0.177438
6	8	0	3.001620	-2.078268	0.477469
7	6	0	2.066428	1.417123	-0.175721
8	8	0	3.039118	2.023626	-0.474945
9	17	0	-3.707298	0.033529	-0.001545
10	12	0	-1.450045	0.013113	-0.000603

G4 (0 K)= -1113.341335

1E

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.693907	-0.000003	-0.000093
2	6	0	1.794751	-1.236290	0.000028
3	6	0	0.428350	-0.706764	0.000195
4	6	0	0.428353	0.706768	0.000195
5	6	0	1.794756	1.236288	0.000028
6	8	0	-0.693721	-1.370214	0.000339
7	8	0	-0.693715	1.370223	0.000339
8	8	0	2.166652	2.397731	-0.000030
9	8	0	3.905448	-0.000005	-0.000252
10	8	0	2.166642	-2.397734	-0.000030
11	12	0	-2.065339	0.000007	0.000504
12	17	0	-4.301745	0.000012	0.000780

G4(0 K)= -1226.737095

2A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-7.307236	-9.814109	0.375905
2	8	0	-8.417444	-11.028977	-2.295036
3	8	0	-5.336506	-8.807006	-2.743825
4	6	0	-6.905820	-9.700130	-0.882982
5	6	0	-6.218714	-9.370922	-2.120629
6	6	0	-7.389254	-10.229138	-2.046029
7	12	0	-8.748155	-10.987764	-0.333823
8	17	0	-10.382134	-12.032219	0.820427

G4 (0 K)= -1000.051874

2B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.087202	-2.096198	-1.147287
2	8	0	-0.133796	-3.188411	-1.571651
3	6	0	0.030008	-0.981105	0.849319
4	8	0	0.084475	0.219481	1.388718
5	6	0	-0.032824	-0.862927	-0.628488
6	8	0	-0.035946	0.286273	-1.352680
7	12	0	0.058333	1.587789	0.023051
8	17	0	0.116095	3.852434	0.030786

G4 (0 K)= -1000.027669

2C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.441987	-1.080218	-0.043508
2	8	0	-3.619215	-1.210990	-0.066585
3	6	0	-1.004280	0.853341	-0.005017
4	8	0	-1.847041	1.721778	-0.015947
5	6	0	-1.192819	-0.670812	-0.017448
6	8	0	-0.023669	-1.372206	0.000640
7	12	0	1.104686	0.168002	0.030981
8	17	0	3.344444	0.569630	0.075774

G4 (0 K)= -1000.026735

2D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.008018	-1.706959	0.467325
2	8	0	1.964633	-2.248125	0.960887
3	6	0	0.390636	-1.699291	-0.889593
4	8	0	0.747048	-2.295448	-1.905015
5	6	0	-0.769887	-0.783134	-0.699098
6	8	0	-1.650019	-0.369899	-1.410563
7	12	0	-0.431577	-0.324009	1.452899
8	17	0	-1.088777	0.775264	3.325270

G4 (0 K)= -999.984644

2E

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.275208	-0.929512	-0.000000
2	8	0	0.054246	1.283056	0.000000
3	8	0	4.562267	-0.411792	0.000000
4	6	0	0.885179	0.250263	-0.000000
5	6	0	3.410921	-0.081830	0.000000
6	6	0	2.249981	0.406085	-0.000000
7	12	0	-1.395554	0.021261	0.000000
8	17	0	-3.627271	-0.190368	0.000000

G4(0 K)= -1000.099991

3A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-5.748239	-8.991157	-0.396043
2	8	0	-8.504720	-10.809861	-2.070600
3	6	0	-6.705304	-9.630948	-0.752703
4	6	0	-7.757309	-10.341187	-0.956318
5	12	0	-9.377958	-11.462076	-0.548228
6	17	0	-11.063400	-12.645908	0.365531

G4 (0 K)= -886.700913

3G

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-7.224149	-9.501035	-0.081727
2	8	0	-7.521886	-10.932590	-1.802547
3	8	0	-4.357863	-7.366628	-1.808303
4	6	0	-6.942748	-9.895331	-1.199628
5	6	0	-5.107854	-8.274807	-1.905750
6	6	0	-5.890311	-9.278520	-2.095715
7	12	0	-6.483734	-10.781989	-3.405546
8	17	0	-6.289816	-11.828558	-5.392886

G4(0 K)= -1000.105378

4A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	12	0	-0.058895	1.442929	0.442729
2	17	0	0.992001	2.812604	-1.238758

G4 (0 K)= -660.111153

4D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	-3.824627
2	6	0	0.000000	0.000000	-1.348044
3	6	0	0.000000	0.000000	-2.619200
4	12	0	0.000000	0.000000	0.552145
5	17	0	0.000000	0.000000	2.810278

G4 (0 K)= -811.489181

INC1A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.039063	-1.752948	0.000000
2	8	0	-3.070401	-2.305372	0.000000
3	6	0	-1.123976	0.354720	0.000000
4	8	0	-0.000835	1.022966	0.000000
5	6	0	-0.869757	-1.096390	0.000000
6	8	0	0.349796	-1.692173	0.000000
7	12	0	1.513427	-0.192652	0.000000
8	17	0	3.757123	0.059620	0.000000
9	6	0	-3.005861	2.370830	0.000000
10	8	0	-2.254491	3.231392	0.000000

G4 (0 K)= -1113.319085

INC1C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.781684	-8.341947	-1.266281
2	8	0	-7.219223	-10.076881	0.392033
3	8	0	-8.662150	-10.691434	-2.020560
4	8	0	-6.427647	-9.042975	-4.018351
5	6	0	-6.846144	-9.710357	-0.799908
6	6	0	-6.579598	-9.288414	-2.839984
7	6	0	-5.795466	-8.954447	-1.528905
8	6	0	-7.552965	-10.011397	-1.981722
9	12	0	-8.939332	-10.905055	-0.084305
10	17	0	-10.468507	-12.033074	1.117604
11	6	0	-9.380482	-7.546865	-0.675884
12	8	0	-9.799119	-8.481672	-0.187384

G4(0 K)= -1226.711648

TS1A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.918528	-0.711647	0.172406
2	8	0	0.191512	-1.227426	0.722632
3	6	0	-0.918528	0.711647	-0.172406
4	8	0	0.191512	1.227426	-0.722632
5	6	0	-2.134268	1.243605	0.068372
6	8	0	-3.024354	1.929843	0.458588
7	6	0	-2.134268	-1.243605	-0.068372
8	8	0	-3.024355	-1.929843	-0.458588
9	17	0	3.750389	-0.000000	0.000000
10	12	0	1.497567	0.000000	0.000000

G4 (0 K)= -1113.337434

TS1B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.873648	0.820230	0.033040
2	8	0	0.306965	1.395889	-0.312174
3	6	0	-1.004042	-0.579944	0.506023
4	8	0	0.162619	-1.144920	0.641760
5	6	0	-2.233900	-1.699263	-0.584696
6	8	0	-3.274258	-2.049206	-0.189318
7	6	0	-2.030646	1.490332	0.053490
8	8	0	-3.058452	2.051636	0.066601
9	17	0	3.815403	-0.150700	-0.122889
10	12	0	1.574716	0.028882	0.032251

G4 (0 K)= -1113.309172

TS1C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-5.257081	-8.241925	-1.072012
2	8	0	-7.730882	-9.979323	0.492177
3	8	0	-8.819981	-10.849503	-1.984113
4	8	0	-6.468729	-9.412863	-3.870122
5	6	0	-7.621255	-9.225336	-0.625370
6	6	0	-6.870467	-9.337812	-2.715150
7	6	0	-6.281618	-8.737941	-1.455627
8	6	0	-7.936393	-9.906775	-1.918085
9	12	0	-8.809845	-11.445957	-0.109691
10	17	0	-9.771092	-13.231632	0.847522
11	6	0	-8.341688	-7.907930	-0.582816
12	8	0	-8.543294	-6.807507	-0.900357

G4 (0 K)= -1226.637653

TS2A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.873648	0.820230	0.033040
2	8	0	0.306965	1.395889	-0.312174
3	6	0	-1.004042	-0.579944	0.506023
4	8	0	0.162619	-1.144920	0.641760
5	6	0	-2.233900	-1.699263	-0.584696
6	8	0	-3.274258	-2.049206	-0.189318
7	6	0	-2.030646	1.490332	0.053490
8	8	0	-3.058452	2.051636	0.066601
9	17	0	3.815403	-0.150700	-0.122889
10	12	0	1.574716	0.028882	0.032251

G4 (0 K)= -1113.309172

TS2B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.662766	0.041496	-0.000000
2	8	0	1.120090	-0.509361	-0.000000
3	8	0	0.267509	-3.944331	-0.000000
4	6	0	-1.288857	-1.232519	-0.000000
5	6	0	0.149130	-2.775941	-0.000000
6	6	0	0.123376	-1.421532	-0.000000
7	12	0	0.000081	1.043944	0.000000
8	17	0	0.488095	3.255902	0.000000

G4 (0 K)= -1000.026288

TS2C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.918337	-1.697051	0.296948
2	8	0	1.736251	-2.017179	1.152368
3	6	0	0.463034	-1.815909	-1.082277
4	8	0	0.807078	-2.407564	-2.111694
5	6	0	-0.584985	-0.907554	-0.663964
6	8	0	-1.599563	-0.243511	-0.913579
7	12	0	-0.464820	-0.321158	1.387283
8	17	0	-1.105296	0.758378	3.237101

G4 (0 K)= -999.978400

TS2D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-7.652162	-8.786852	0.164180
2	8	0	-6.093175	-9.916667	-3.099784
3	8	0	-3.657051	-7.859547	-1.030348
4	6	0	-6.734540	-8.826451	-0.583950
5	6	0	-4.720587	-8.358419	-1.185041
6	6	0	-5.829644	-8.972797	-1.522953
7	12	0	-6.180449	-10.778630	-4.652422
8	17	0	-6.255618	-11.868960	-6.642282

G4(0 K)= -999.951598

TS2E

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-7.767004	-9.618933	-0.370434
2	8	0	-7.547121	-11.235648	-1.895125
3	8	0	-4.611394	-7.496616	-2.385363
4	6	0	-7.113732	-10.089259	-1.343449
5	6	0	-5.432212	-8.346226	-2.213369
6	6	0	-6.267134	-9.301979	-2.177450
7	12	0	-8.770314	-9.926789	-2.575202
8	17	0	-10.614729	-9.338641	-3.671011

G4(0 K)= -1000.052407

TS3A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.817745	-0.351495	-0.076316
2	8	0	-4.006910	-0.263744	-0.193515
3	6	0	-0.759591	1.051380	0.619387
4	8	0	-0.254929	1.689367	-0.317307
5	6	0	-1.543156	-0.275250	0.125824
6	8	0	-0.505602	-1.161448	0.029494
7	12	0	1.060801	-0.083695	0.132853
8	17	0	3.293380	-0.212915	-0.091238

G4 (0 K)= -999.983457

TS4A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.678455	-0.669996	0.344752
2	8	0	-2.020541	-1.620063	-0.270132
3	6	0	-1.480292	1.030942	-0.247728
4	8	0	-2.276220	1.900752	-0.134529
5	12	0	0.528465	0.233852	0.591377
6	17	0	2.535925	-0.529811	-0.323272

G4 (0 K)= -886.670962

Triplet PES

1C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.690309	-8.210133	-0.934837
2	8	0	-7.321351	-9.953905	0.233366
3	8	0	-8.419643	-10.889733	-2.155867
4	8	0	-6.276506	-9.561693	-4.385462
5	6	0	-6.758157	-9.647025	-0.935294
6	6	0	-6.571784	-9.683590	-3.233129
7	6	0	-5.638270	-8.888164	-1.202353
8	6	0	-7.324545	-10.129631	-2.167419
9	12	0	-8.829089	-11.038599	-0.279018
10	17	0	-10.454526	-12.084441	0.877811

G4 (0 K)= -1113.321382

1D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.792470	1.051170	-1.168891
2	8	0	-0.767623	-1.271759	0.932522
3	8	0	-0.146561	0.681202	-0.910208
4	8	0	3.871031	-0.264941	1.371224
5	6	0	0.437083	-0.966881	0.656172
6	6	0	3.126554	-0.591482	0.505342
7	6	0	2.224376	0.286244	-0.398594
8	6	0	0.829248	0.000957	-0.255661
9	12	0	-1.764155	-0.027025	-0.242851
10	17	0	-3.981029	0.218016	-0.493406

G4(0 K)= -1113.301923

2F

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-7.125756	-9.989199	0.277979
2	8	0	-8.304066	-11.089367	-2.275301
3	8	0	-5.253233	-9.074159	-2.672029
4	6	0	-7.211776	-9.247295	-0.845665
5	6	0	-6.261640	-9.429918	-2.081551
6	6	0	-7.518000	-10.079869	-2.100838
7	12	0	-8.694164	-10.985289	-0.310954
8	17	0	-10.336671	-12.075148	0.782381

G4 (0 K)= -999.949647

2G

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.046732	2.992124	0.000000
2	8	0	0.921430	3.714334	0.000000
3	6	0	-1.459725	1.027910	0.000000
4	8	0	-1.732961	-0.218774	0.000000
5	6	0	-0.194193	1.577488	0.000000
6	8	0	0.868301	0.690340	0.000000
7	12	0	0.075571	-1.014019	0.000000
8	17	0	0.650653	-3.194063	-0.000000

G4 (0 K)= -1000.003886

2H

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.981514	-2.599149	0.002986
2	8	0	0.348433	-3.626070	0.001310
3	6	0	-0.986836	-0.856387	-0.002821
4	8	0	-1.910054	-1.644426	-0.005351
5	6	0	0.480391	-1.234628	0.001397
6	8	0	1.293510	-0.205705	0.003584
7	12	0	-0.139098	1.160134	-0.000654
8	17	0	0.029170	3.428535	-0.000449

G4 (0 K)= -999.986576

2I

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.680515	-0.588608	-0.354766
2	8	0	3.205776	-1.662488	-0.511926
3	6	0	0.777713	1.146565	-0.025813
4	8	0	1.510833	2.121765	0.030790
5	6	0	1.270379	-0.255929	-0.217308
6	8	0	0.318418	-1.163093	-0.250748
7	12	0	-1.157002	0.146235	0.000291
8	17	0	-3.404185	-0.182538	0.123538

G4(0 K)= -999.984404

2J

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.776745	0.941916	0.002245
2	8	0	0.474627	1.524030	0.063092
3	6	0	-0.822208	-0.432006	-0.078386
4	8	0	0.183743	-1.221353	-0.102357
5	6	0	-1.955034	1.745435	0.023304
6	8	0	-3.135079	1.485459	-0.017324
7	17	0	3.888388	-0.318784	0.030202
8	12	0	1.669146	0.076299	0.005039

G4 (0 K)= -999.998314

3D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.796148	0.496919	0.000000
2	8	0	2.683728	1.335070	0.000000
3	6	0	1.801627	-0.964478	0.000000
4	8	0	0.709609	-1.648786	0.000000
5	12	0	-0.345883	0.025279	0.000000
6	17	0	-2.620564	0.284813	0.000000

G4 (0 K)= -886.678168

3E

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.616855	0.918365	0.081700
2	8	0	2.615219	1.529092	0.116896
3	6	0	1.735521	-1.506220	0.083684
4	8	0	0.572700	-1.803202	0.040124
5	12	0	-0.238166	0.058270	-0.593803
6	17	0	-2.360258	0.295999	0.289639

G4(0 K)= -886.657801

3F

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.036274	1.369884	0.202394
2	8	0	-0.059349	-1.387360	0.239377
3	6	0	-0.098730	0.734296	-0.975664
4	6	0	0.106317	-0.704937	-0.856374
5	12	0	0.024782	0.031116	1.548961
6	17	0	-0.009293	-0.042998	3.812127

G4 (0 K)= -886.656641

4B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.043455	-0.452419	0.671385
2	8	0	1.901949	-0.351104	-0.536169
3	12	0	0.244817	0.865493	0.013939
4	17	0	-1.780178	-0.286909	0.004739

G4 (0 K)= -773.363545

4C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.723584	-0.220853	-0.041277
2	8	0	2.803600	-0.685306	-0.083932
3	12	0	-0.065144	0.925663	-0.012788
4	17	0	-2.051996	-0.244443	0.291893

G4 (0 K)= -773.376632

4D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.833757	-0.490514	-0.000000
2	8	0	-1.738934	0.059456	-0.000000
3	12	0	-0.000069	0.928775	-0.000000
4	17	0	1.818508	-0.510469	0.000000

G4 (0 K)= -773.354250

B_ClMg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	12	0	-2.684820	0.334925	-1.890217
2	17	0	-3.500909	0.575753	-4.060963

G4 (0 K)= -660.049294

TS1B_t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.102466	-1.146241	-1.417539
2	8	0	-0.764036	-1.134228	1.443897
3	8	0	0.067277	0.541162	-0.700023
4	8	0	3.089185	1.653078	0.784835
5	6	0	0.458032	-1.160975	1.471889
6	6	0	2.454301	0.820679	0.148970
7	6	0	2.459500	-0.336170	-0.761254
8	6	0	1.195147	0.108903	-0.144333
9	12	0	-1.554685	-0.009538	0.009288
10	17	0	-3.748177	0.263089	-0.334180

G4 (0 K)= -1113.233171

TS2A_t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.873927	0.655607	0.066305
2	8	0	-0.305519	1.347436	-0.087184
3	6	0	0.785474	-0.712986	0.207366
4	8	0	-0.282881	-1.399916	0.238473
5	6	0	3.059212	-1.362681	0.429044
6	8	0	3.525335	-1.805977	-0.523028
7	6	0	2.171351	1.226455	0.070072
8	8	0	2.622259	2.336228	-0.031321
9	17	0	-3.885078	-0.174092	-0.086613
10	12	0	-1.647250	0.024918	0.005015

G4 (0 K)= -1113.289940

TS2B_t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.784180	0.907044	-0.001520
2	8	0	0.444124	1.522975	0.078871
3	6	0	-0.780646	-0.469192	-0.017126
4	8	0	0.242450	-1.228954	0.000150
5	6	0	-2.854667	-1.531594	-0.485740
6	8	0	-3.348613	-1.967193	0.450402
7	6	0	-1.989115	1.666851	-0.078439
8	8	0	-3.154787	1.351225	-0.123845
9	17	0	3.917102	-0.204667	0.203433
10	12	0	1.693089	0.116440	0.097902

G4 (0 K)= -1113.286591

TS3A_t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.788027	-3.235941	-0.000059
2	8	0	0.215480	-3.806732	-0.000027
3	6	0	1.021711	-0.691766	0.000036
4	8	0	2.038362	-1.365702	0.000068
5	6	0	-0.383034	-1.065882	-0.000022
6	8	0	-1.330088	-0.202077	-0.000048
7	12	0	0.017050	1.263531	0.000020
8	17	0	-0.302014	3.517413	0.000033

G4 (0 K)= -999.964566

TS4A_t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.684955	0.782587	0.082088
2	8	0	2.682509	1.421510	0.045968
3	6	0	1.780411	-1.306105	-0.001684
4	8	0	0.640648	-1.729477	0.062753
5	12	0	-0.261580	0.099029	-0.329779
6	17	0	-2.502280	0.261273	0.140654

G4(0 K)= -886.657325

TSIC1_t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.205405	1.497044	0.139238
2	8	0	1.095898	0.449619	0.131940
3	6	0	-1.130001	1.226070	-0.002528
4	8	0	-1.650178	0.035149	-0.049760
5	6	0	0.766920	2.836499	-0.004365
6	8	0	1.185755	3.666959	0.750731
7	17	0	0.216865	-3.299942	-0.076697
8	12	0	-0.040214	-1.058850	-0.007342

G4 (0 K)= -999.986876

TSIC2_t

n.a.

TSIC3_t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.384292	-2.764351	-0.326621
2	8	0	-0.625537	-3.530665	0.552995
3	6	0	1.183124	-0.683285	-0.104562
4	8	0	2.252312	-1.295191	-0.211132
5	6	0	-0.145659	-1.262057	-0.111680
6	8	0	-1.196342	-0.485280	-0.018905
7	12	0	-0.019390	1.116006	0.042238
8	17	0	-0.574774	3.317668	0.177667

G4 (0 K)= -999.972844

TSIC4_t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.357861	1.595570	0.038195
2	8	0	1.168474	0.546899	0.054776
3	6	0	-1.062049	1.036214	-0.089134
4	8	0	-1.589879	0.636230	0.975022
5	6	0	0.807697	2.935591	-0.012458
6	8	0	0.179945	3.981449	-0.057415
7	17	0	-0.114464	-3.150928	0.106385
8	12	0	-0.132016	-0.907881	0.016335

G4 (0 K)= -999.948828

TSIC5_t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.608779	-0.632640	0.531596
2	8	0	1.665281	-0.233214	-0.179947
3	12	0	0.077808	0.884025	-0.100519
4	17	0	-1.941824	-0.243111	-0.097237

G4 (0 K)= -773.352323

TSIC6_t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.926881	-0.320302	0.536834
2	8	0	2.360246	-0.542559	-0.568996
3	12	0	0.082909	0.867471	0.160173
4	17	0	-1.959993	-0.229550	0.025882

G4 (0 K)= -773.358559

Magnesium monocarbonyls

$^{1}ClMgCO^{-}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.802740	0.662951	-0.000000
2	8	0	3.741089	0.017820	-0.000000
3	12	0	-0.405933	-1.068977	-0.000000
4	17	0	-2.163548	0.563681	-0.000000

G4 (0 K)= -773.400143

$^{3}ClMg(\eta^{2}\text{-}CO)^{-}$ (4B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.043455	-0.452419	0.671385
2	8	0	1.901949	-0.351104	-0.536169
3	12	0	0.244817	0.865493	0.013939
4	17	0	-1.780178	-0.286909	0.004739

G4 (0 K)= -773.363545

$^{3}ClMg(\eta^{1}\text{-}CO)^{-}$ (4C)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.723584	-0.220853	-0.041277
2	8	0	2.803600	-0.685306	-0.083932
3	12	0	-0.065144	0.925663	-0.012788
4	17	0	-2.051996	-0.244443	0.291893

G4 (0 K)= -773.376632

$^{3}ClMg(\eta^{1}\text{-}OC)^{-}$ (4D, triplet PES)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.833757	-0.490514	-0.000000
2	8	0	-1.738934	0.059456	-0.000000
3	12	0	-0.000069	0.928775	-0.000000
4	17	0	1.818508	-0.510469	0.000000

G4 (0 K)= -773.354250

$^{2}ClMgCO^{\bullet}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.909909	0.322045	-0.000000
2	8	0	3.048324	0.262074	-0.000000
3	12	0	-0.106281	-0.795499	-0.000000
4	17	0	-2.015083	0.330433	-0.000000

G4 (0 K)= -773.340061

$^{1}ClMgCO^{+}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000000	0.000000	2.166158
2	8	0	-0.000000	0.000000	3.282055
3	12	0	-0.000000	0.000000	-0.103750
4	17	0	-0.000000	0.000000	-2.229463

G4 (0 K)= -773.099110

$^{2}MgCO^{+}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000000	0.000000	-0.674818
2	8	0	-0.000000	0.000000	-1.787617
3	12	0	-0.000000	0.000000	1.529344

G4 (0 K)= -312.448896

$^{1}MgCO^{+}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.990471	-1.126181	0.005310
2	8	0	2.833852	-1.861895	0.018243
3	12	0	0.107680	0.516249	-0.023564

G4 (0 K)= -312.939271

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