Electronic Supporting Information (ESI) for the paper

Combined crossed-beams and theoretical study of the $O(^3P, ^1D)$ + acrylonitrile (CH_2CHCN) reactions and implications for combustion and extraterrestrial environments

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Table T1: List of all the possible combination of products identified for the $O(^3P, ^1D)$ + CH_2CHCN reactions evaluated at the CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level of theory.

$O(^3P)$ + CH_2CHCN	—>	CH_2CHN + CO	- 179 kJ/mol
	—>	CH_2CN + HCO	- 126 kJ/mol
	—>	CH_2CO + HCN	- 119 kJ/mol
	—>	COCN + CH_3	- 69 kJ/mol
	—>	HCOCHCN + H	- 62 kJ/mol
	—>	CH_2O + HCCN	- 58 kJ/mol
	—>	$OCCH_2CN$ + H	- 56 kJ/mol
	—>	HCOCH + HCN	- 40 kJ/mol
	—>	CH_2COCN + H	- 36 kJ/mol
	—>	CH_2CH + NCO	- 1 kJ/mol
	—>	CH_3CO + CN	+ 4 kJ/mol
	—>	OCHCN + CH_2	+ 5 kJ/mol
	—>	CHCHCN + OH	+ 27 kJ/mol
$O(^1D)$ + CH_2CHCN	—>	CH_3CN + CO	- 653 kJ/mol
	—>	CH_2CNH + CO	-538 kJ/mol
	—>	OCCHCN + H_2	- 509 kJ/mol
	—>	HNCO + H_2CC	- 322 kJ/mol
	—>	CH_2CN + HCO	- 316 kJ/mol
	—>	COCN + CH_3	- 259 kJ/mol
	—>	HCOCHCN + H	- 252 kJ/mol
	—>	$OCCH_2CN$ + H	- 246 kJ/mol
	—>	CH_2COCN + H	- 226 kJ/mol
	—>	CH_2NC + HCO	- 218 kJ/mol
	—>	HCOCCN + H_2	- 209 kJ/mol
	—>	CH_2CH + OCN	- 192 kJ/mol
	—>	CH_2CNCO + H	- 180 kJ/mol
	—>	t-HCOCHNC+ H	- 164 kJ/mol
	—>	c-HCOCHNC+ H	- 159 kJ/mol
	—>	$OCCH_2NC$ + H	- 152 kJ/mol
	—>	*c*-CH_2(O)CCN + H	- 90 kJ/mol
	—>	*c*-CH(OCH)CN + H	- 60 kJ/mol
	—>	*c*-CH_2CCC(O)N + H	+ 109 kJ/mol

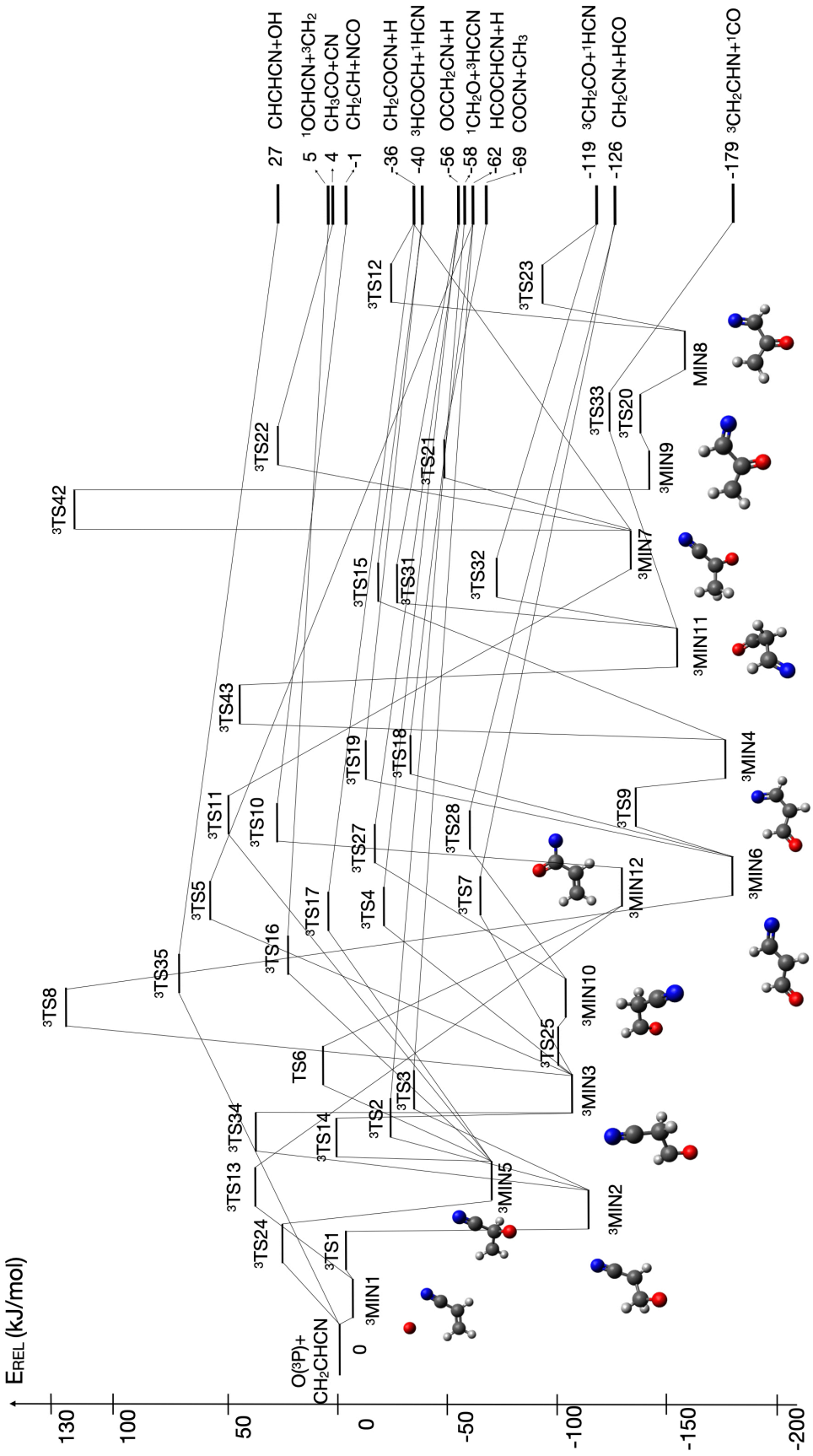

Fig. S1: Schematic representation of the global PES for the reaction O(^{3}P) + CH_2CHCN, with the energies evaluated at the CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level of theory.

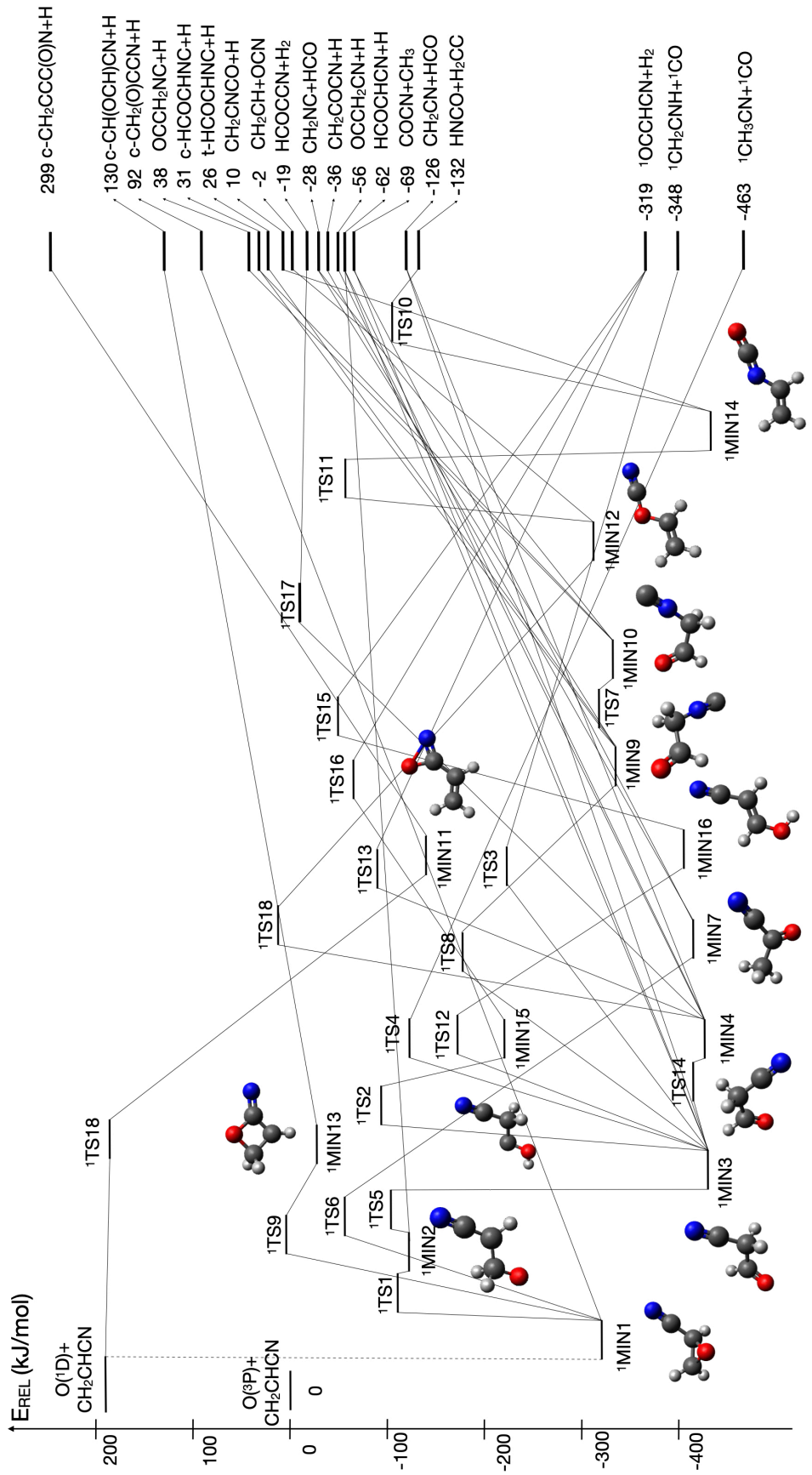

Fig. S2: Schematic representation of the global PES for the reaction O(¹D) + CH_2CHCN, with the energies evaluated at the CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level of theory.

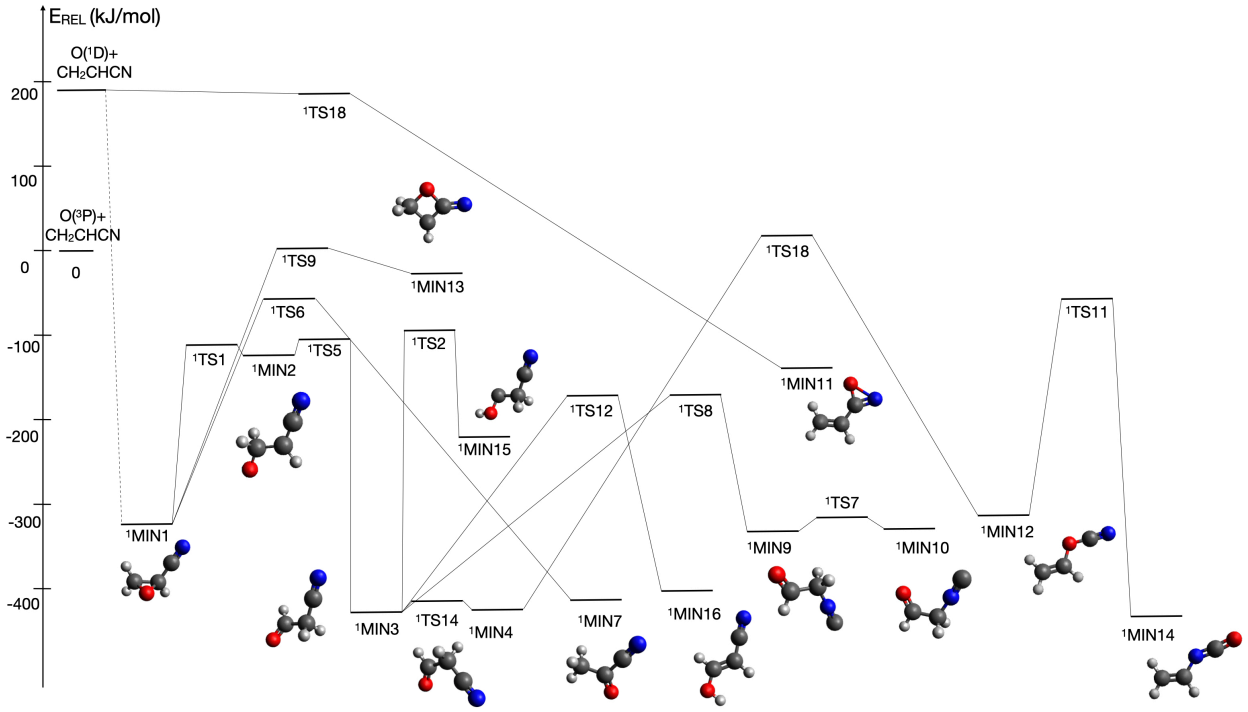

Fig. S3: Schematic representation of the isomerisation process identified in the singlet PES for the reaction O(1D) + CH_2CHCN.

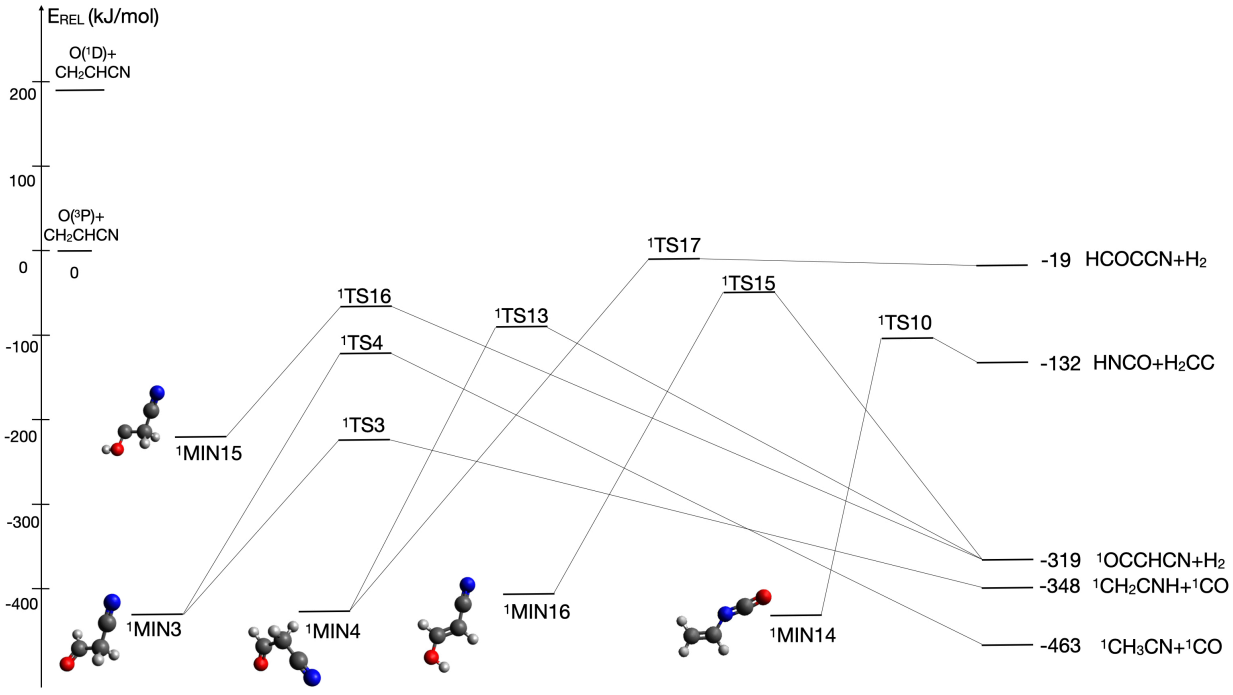

Fig. S4: Schematic representation of the singlet PES reporting the product channels with exit barrier for the reaction O(1D) + CH_2CHCN.

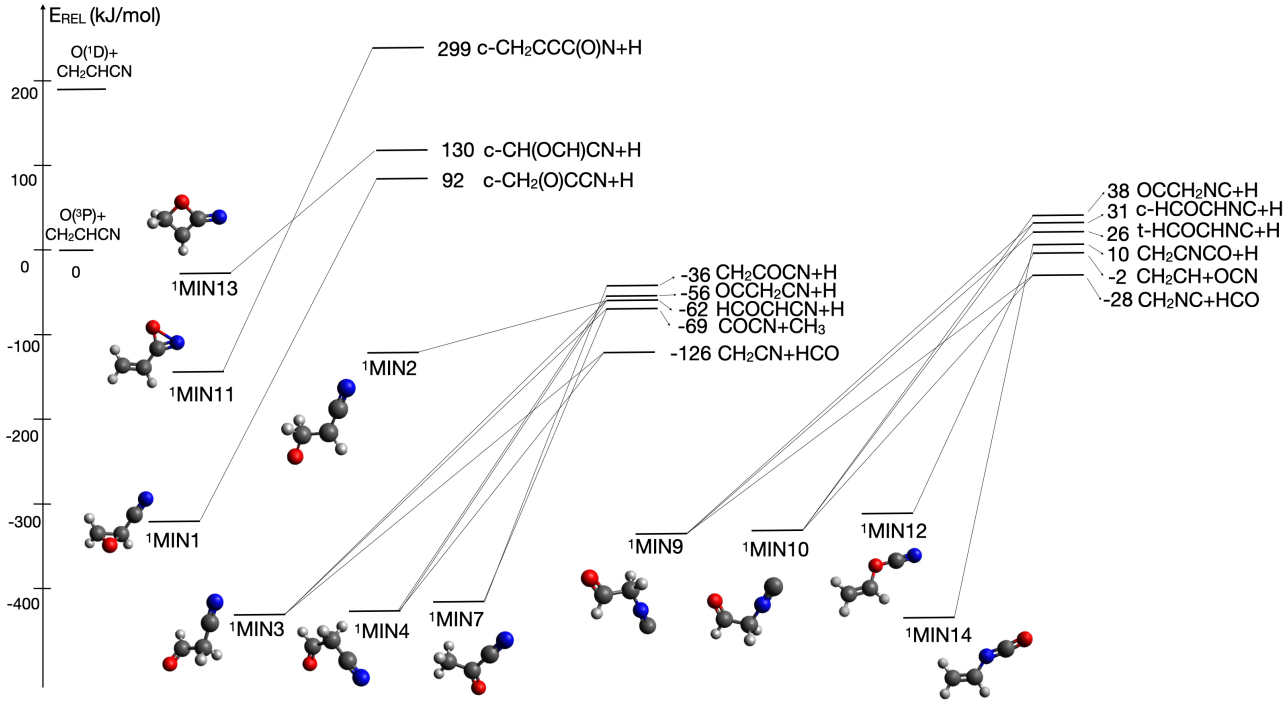

Fig. S5: Schematic representation of the singlet PES reporting the product channels without exit barrier for the reaction O(¹D) + CH_2CHCN.

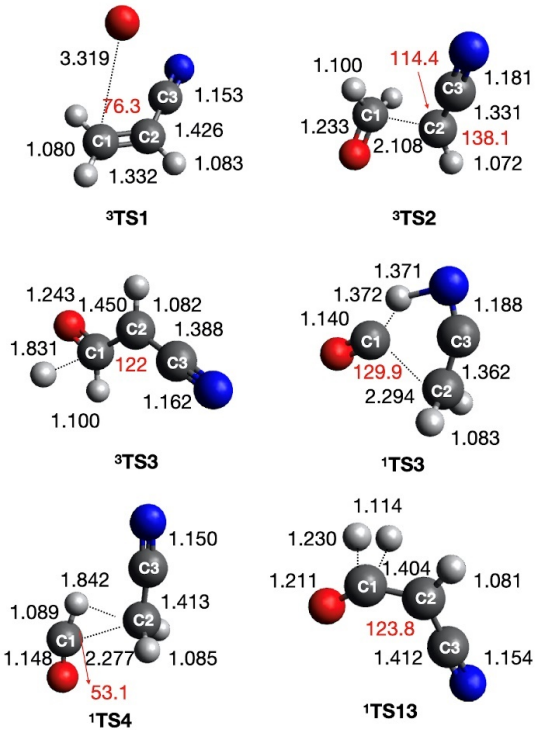

Fig. S6: B3LYP optimized geometries of the most important transition states identified along the triplet/ singlet PESs for the O(³P,¹D) + acrylonitrile reactions. The angles (°) are indicated in red, while the bond lengths (Å) are indicated in black.

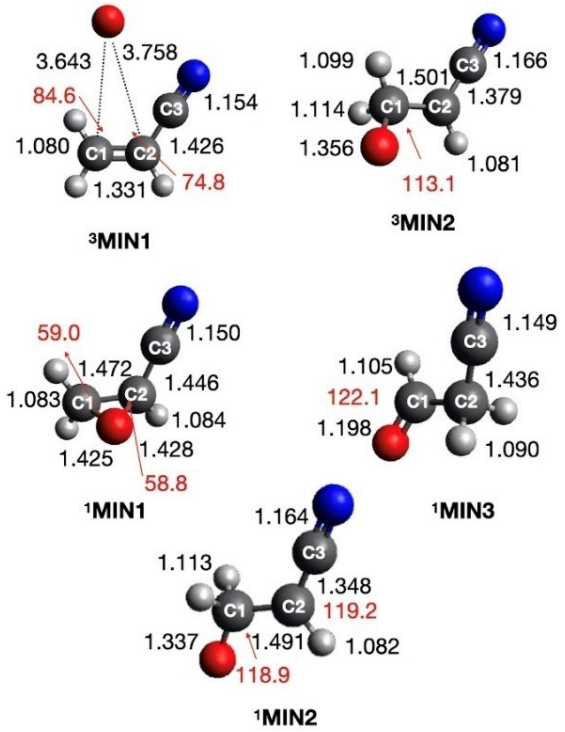

Fig. S7: B3LYP optimized geometries of the most important minima identified along the triplet/singlet PESs for the O(^{3}P,^{1}D) + acrylonitrile reactions. The angles (°) are indicated in red, while the bond lengths (Å) are indicated in black.

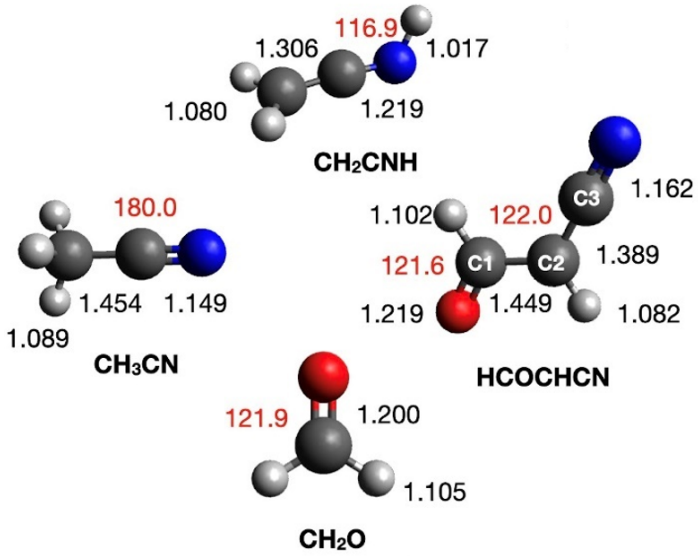

Fig. S8: B3LYP optimized geometries of the most important products identified on the triplet/singlet PESs for the O(^{3}P,^{1}D) + acrylonitrile reactions. The angles (°) are indicated in red, while the bond lengths (Å) are indicated in black.

Table T2: Relative energies (kJ/mol, 0K) of all the possible stationary points, including minima and transition states, identified in both the singlet and triplet PES for the reaction $O(^3P) + CH_2CHCN$, evaluated at the CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level of theory.

$O(^3P) + CH_2CHCN$	0 kJ/mol	^{3}TS31	-27 kJ/mol
^{3}MIN1	-5 kJ/mol	^{3}TS32	-72 kJ/mol
^{3}MIN2	-115 kJ/mol	^{3}TS33	-122 kJ/mol
^{3}MIN3	-108 kJ/mol	^{3}TS34	+37 kJ/mol
^{3}MIN4	-176 kJ/mol	^{3}TS35	+72 kJ/mol
^{3}MIN5	-71 kJ/mol	^{3}TS42	+117 kJ/mol
^{3}MIN6	-179 kJ/mol	^{3}TS43	+43 kJ/mol
^{3}MIN7	-133 kJ/mol	$O(^1D) + CH_2CHCN$	+190 kJ/mol
^{3}MIN8	-157 kJ/mol	^{1}MIN1	-322 kJ/mol
^{3}MIN9	-140 kJ/mol	^{1}MIN2	-119 kJ/mol
^{3}MIN10	-105 kJ/mol	^{1}MIN3	-427 kJ/mol
^{3}MIN11	-154 kJ/mol	^{1}MIN4	-424 kJ/mol
^{3}MIN12	-128 kJ/mol	^{1}MIN7	-420 kJ/mol
^{3}TS1	+ 8 kJ/mol	^{1}MIN9	-334 kJ/mol
^{3}TS2	-25 kJ/mol	^{1}MIN10	-330 kJ/mol
^{3}TS3	-34 kJ/mol	^{1}MIN12	-313 kJ/mol
^{3}TS4	-23 kJ/mol	^{1}MIN13	-25 kJ/mol
^{3}TS5	+56 kJ/mol	^{1}MIN14	-430 kJ/mol
^{3}TS6	+5 kJ/mol	^{1}MIN15	-220 kJ/mol
^{3}TS7	-65 kJ/mol	^{1}MIN16	-409 kJ/mol
^{3}TS8	+126 kJ/mol	^{1}TS1	-108 kJ/mol
^{3}TS9	-134 kJ/mol	^{1}TS2	-96 kJ/mol
^{3}TS10	+29 kJ/mol	^{1}TS3	-222 kJ/mol
^{3}TS11	+51 kJ/mol	^{1}TS4	-124 kJ/mol

^{3}TS12	-25 kJ/mol	^{1}TS5	-103 kJ/mol
^{3}TS13	+37 kJ/mol	^{1}TS6	-58 kJ/mol
^{3}TS14	+1 kJ/mol	^{1}TS7	-318 kJ/mol
^{3}TS15	-19 kJ/mol	^{1}TS8	-179 kJ/mol
^{3}TS16	+22 kJ/mol	^{1}TS9	+13 kJ/mol
^{3}TS17	+4 kJ/mol	^{1}TS10	-102 kJ/mol
^{3}TS18	0 kJ/mol	^{1}TS11	-58 kJ/mol
^{3}TS19	-14 kJ/mol	^{1}TS12	-175 kJ/mol
^{3}TS20	-138 kJ/mol	^{1}TS13	-102 kJ/mol
^{3}TS21	-46 kJ/mol	^{1}TS14	-418 kJ/mol
^{3}TS22	+27 kJ/mol	^{1}TS15	-50 kJ/mol
^{3}TS23	-94 kJ/mol	^{1}TS16	-62 kJ/mol
^{3}TS24	+23 kJ/mol	^{1}TS17	-9 kJ/mol
^{3}TS25	-101 kJ/mol	^{1}TS18	+14 kJ/mol
^{3}TS27	-19 kJ/mol	^{1}TS19	+180 kJ/mol
^{3}TS28	-60 kJ/mol		