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Reaction between Criegee intermediates and hydroxyacetonitrile: reaction mechanisms, kinetics, and atmospheric implications

Chaolu Xie et al.

Correspondence to: Bo Long (wwwltcommon@sina.com)

Table S1. Standard scale factors for vibrational frequencies of the methods used for optimization and zero-point energies in this study.

Methods	Scale Factor
CCSD(T)-F12a/cc-pVDZ-F12	0.983
DF-CCSD(T)-F12b/jun-cc-pVDZ	0.981
M11-L/MG3S	0.985
M06-CR/MG3S	0.980

Table S2. Specific Reaction Scale Factors Calculated by Using the MPW1K/6-311 + G(2df,2p) Method.

	CH_2OO	CH_3CHOO	$HOCH_2CN$	TS1	s-TS1
ZPE (Harm)	20.309	38.474	32.918	55.681	73.596
ZPE (Anh)	20.072	37.987	32.490	54.960	72.663
λ^{Anh}[a]	0.988	0.987	0.987	0.987	0.987
λ_H[b]	0.997	0.997	0.997	0.997	0.997
$\lambda^{ZPE}=\lambda^{Anh} * \lambda\_H$[c]	0.985	0.984	0.984	0.984	0.984

[a] λ^{Anh} equals the ratio of anharmonic zero-point vibrational energy to harmonic zero-point vibrational energy of the MPW1K/6-311G(2df,2p) method.

[b] λ_H is equal to 0.997 for DF-CCSD(T)-F12b/jun-cc-pVDZ

[c] λ^{ZPE} is the product of λ^{Anh} and the general parameter λ_H, which is based on previous studies[1].

Table S3. The activate enthalpies at 0 K for the CH_2OO + $HOCH_2CN$ reaction at different methods.

Method	$\Delta H_0^{\ddagger}$	MUD
	TS1	
W2X//CCSD(T)-F12a/cc-pVDZ-F12	–6.16	0.00
W2X//DF-CCSD(T)-F12B/jun-cc-pVDZ	–6.19	0.03

Table S4. The anharmonicity effect for the enthalpy of activation at 0 K for CH_2OO/syn-CH_3CHOO + $HOCH_2CN$.

Method	$\Delta H_0^{\ddagger}$		MUD
	TS1	s-TS1	
W3X-L//DF-CCSD(T)-F12B/jun-cc-pVDZ[a]	–5.61	–1.39	0.00
W3X-L//DF-CCSD(T)-F12B/jun-cc-pVDZ[b]	–5.62	–1.38	0.01

[a] The enthalpy of activation at 0 K calculated with harmonic zero-point vibration energy with standard scale factors.

[b] The enthalpy of activation at 0 K calculated with anharmonic zero-point vibration energies using the specific reaction scale factors.

Table S5. The rate constants (cm^3 $molecule^{-1}$ s^{-1}) of the reaction of CH_2OO + $HOCH_2CN$ for TS1 at various temperatures.

T/K	k_{HL}^{TST}	κ_{LL}^{SCT}	k_{LL}^{TST}	k_{LL}^{CVT}	Γ_{CVT}^{LL}	$F_{act}^{MS-T,LL}$	k	$k_{VRC-TST}$	k_{R1}
190	8.43E-10	3.75E+00	5.19E+02	5.02E+02	0.97	0.80	4.87E-09	3.40E-10	3.18E-10
200	3.91E-10	2.24E+00	1.38E+03	1.33E+03	0.97	0.80	6.75E-10	3.40E-10	3.18E-10
210	1.96E-10	1.68E+00	3.33E+03	3.21E+03	0.97	0.80	2.52E-10	3.28E-10	2.64E-10
220	1.04E-10	1.43E+00	7.39E+03	7.14E+03	0.97	0.80	1.15E-10	3.18E-10	1.95E-10
230	5.89E-11	1.31E+00	1.53E+04	1.48E+04	0.97	0.80	5.96E-11	3.08E-10	1.32E-10
240	3.50E-11	1.25E+00	2.98E+04	2.87E+04	0.96	0.80	3.36E-11	2.71E-10	8.28E-11
250	2.17E-11	1.21E+00	5.48E+04	5.28E+04	0.96	0.80	2.02E-11	2.41E-10	5.26E-11
260	1.40E-11	1.18E+00	9.62E+04	9.27E+04	0.96	0.80	1.27E-11	2.15E-10	3.39E-11
270	9.31E-12	1.16E+00	1.62E+05	1.56E+05	0.96	0.80	8.33E-12	1.93E-10	2.25E-11
280	6.40E-12	1.14E+00	2.62E+05	2.52E+05	0.96	0.80	5.65E-12	1.74E-10	1.52E-11
290	4.52E-12	1.13E+00	4.10E+05	3.93E+05	0.96	0.80	3.95E-12	1.58E-10	1.05E-11
298	3.49E-12	1.12E+00	5.73E+05	5.50E+05	0.96	0.80	3.02E-12	1.44E-10	7.49E-12
300	3.28E-12	1.12E+00	6.22E+05	5.96E+05	0.96	0.81	2.84E-12	1.34E-10	5.79E-12
310	2.43E-12	1.11E+00	9.17E+05	8.79E+05	0.96	0.81	2.08E-12	1.31E-10	5.44E-12
320	1.84E-12	1.10E+00	1.32E+06	1.26E+06	0.96	0.81	1.56E-12	1.20E-10	4.03E-12
330	1.41E-12	1.10E+00	1.86E+06	1.78E+06	0.96	0.81	2.39E-12	1.03E-10	2.34E-12
340	1.11E-12	1.09E+00	2.56E+06	2.45E+06	0.96	0.81	1.87E-12	9.52E-11	1.83E-12
350	8.80E-13	1.08E+00	3.47E+06	3.31E+06	0.95	0.81	1.48E-12	8.85E-11	1.45E-12

Table S6. The rate constants (cm^3 $molecule^{-1}$ s^{-1}) of the reaction of syn-CH_3CHOO + $HOCH_2CN$ for TS1 at various temperatures.

T/K	k_{HL}^{TST}	κ_{LL}^{SCT}	k_{LL}^{TST}	k_{LL}^{CVT}	Γ_{CVT}^{LL}	$F_{act}^{MS-T,LL}$	k_{R2}
190	4.86E-15	1.30E+01	1.37E-02	1.32E-02	0.97	0.96	1.17E-13
200	4.00E-15	4.07E+00	6.08E-02	5.89E-02	0.97	0.95	3.00E-14
210	3.37E-15	2.09E+00	2.35E-01	2.27E-01	0.97	0.95	1.29E-14
220	2.89E-15	1.55E+00	7.99E-01	7.73E-01	0.97	0.94	8.16E-15
230	2.51E-15	1.37E+00	2.44E+00	2.36E+00	0.97	0.94	6.25E-15
240	2.22E-15	1.30E+00	6.79E+00	6.56E+00	0.97	0.93	5.19E-15
250	1.98E-15	1.26E+00	1.74E+01	1.68E+01	0.97	0.93	4.46E-15
260	1.79E-15	1.23E+00	4.14E+01	3.99E+01	0.97	0.92	3.92E-15
270	1.64E-15	1.20E+00	9.22E+01	8.89E+01	0.96	0.92	3.50E-15
280	1.51E-15	1.19E+00	1.94E+02	1.87E+02	0.96	0.92	3.16E-15
290	1.40E-15	1.17E+00	3.87E+02	3.73E+02	0.96	0.91	2.88E-15
298	1.32E-15	1.16E+00	6.51E+02	6.27E+02	0.96	0.91	2.69E-15
300	1.30E-15	1.16E+00	7.38E+02	7.10E+02	0.96	0.91	2.65E-15
310	1.23E-15	1.15E+00	1.35E+03	1.30E+03	0.96	0.91	2.45E-15
320	1.16E-15	1.14E+00	2.37E+03	2.28E+03	0.96	0.90	2.29E-15
330	1.10E-15	1.13E+00	4.03E+03	3.87E+03	0.96	0.90	2.15E-15
340	1.05E-15	1.12E+00	6.64E+03	6.36E+03	0.96	0.90	2.03E-15
350	1.01E-15	1.11E+00	1.06E+04	1.02E+04	0.96	0.90	1.93E-15

Table S7. The fitting parameters for k_1 and k_2.

	A	n	E	T_0
k_1	2.00×10^{-14}	–4.83	–2.09	–160.57
k_2	1.40×10^{-16}	–1.35	–2.05	–186.43

Table S8. Absolute energies (Hartree) and the Cartesian coordinates (Å) of the optimized geometries calculated. a) by DF-CCSD(T)-F12b/jun-cc-pVDZ.

species	Absolute energies	Cartesian coordinates			
CH_2OO	-189.7223443	C	1.0660225138	-0.1999266640	0.0000039153
		H	1.9735296996	0.4018633779	0.0000279758
		H	1.0066341191	-1.2906143732	-0.0000015535
		O	-0.0192402934	0.4711326975	0.0000083562
		O	-1.1781680390	-0.2053890381	-0.0000066938
syn-CH_3CHOO	-304.4407151	C	-0.4644616478	0.7116447360	-0.0000556775
		H	-0.7818597042	1.7570667258	-0.0001872212
		O	0.8067596690	0.5843008506	0.0001035434
		O	1.2899193668	-0.6867898603	0.0002313318
		C	-1.3442487789	-0.4720035924	-0.0000114694
		H	-2.3992992602	-0.1759645337	0.0002505132
		H	-1.1018975213	-1.0937048951	-0.8778195050
		H	-1.1014581234	-1.0939044309	0.8775224846
$HOCH_2CN$	-494.1654463	C	0.5748079743	0.5917020524	0.0367895892
		H	0.7341681180	1.2837052366	-0.7994754596
		H	0.7123091470	1.1507100773	0.9771008250
		O	1.5080110303	-0.4531576742	-0.1131643637
		H	1.3715321079	-1.0821570629	0.6063938509
		C	-0.8288088344	0.1111375296	-0.0089473061
		N	-1.9296115431	-0.2845911588	-0.0166761357
TS1	-494.1638441	C	-2.0640125275	0.2482236948	0.0571834237
		O	-1.4827939658	-0.8279841232	-0.3351482622
		O	-0.4081143982	-1.1211701931	0.4993793449
		H	-2.0593440951	0.4873396326	1.1212205584
		H	-2.8448232953	0.6042643037	-0.6184474669
		C	0.4294268204	0.9017284839	0.0643542300
		N	-0.5339857199	1.5437793362	-0.2014154782
		C	1.8236442514	0.4270275502	0.2866389955
		H	1.9397144143	0.2686072733	1.3729826177

		H	2.5083211463	1.2264475018	-0.0305200483
		O	2.1048246793	-0.7183834996	-0.4674031285
		H	1.3443706900	-1.3106179608	-0.3156257863
s-TS1	-494.1666033	C	-1.7265285313	-0.0748297826	-0.4754874577
		O	-0.9463294576	-1.1052082538	-0.5888980002
		O	-0.0027346708	-1.1420322973	0.4342750897
		H	-2.3313470245	0.0459124229	-1.3812451565
		C	0.6623579921	0.8447892882	-0.1622307741
		N	-0.2870095908	1.3290014397	-0.6924063183
		C	2.0392188651	0.6294279808	0.3636592217
		H	1.9721697407	0.6610843788	1.4656802744
		H	2.6687803948	1.4639837731	0.0235036902
		O	2.5935291791	-0.5650871032	-0.1138612681
		H	1.8824174873	-1.2261256491	-0.0178090420
		C	-2.2618822986	0.4109657429	0.8315822450
		H	-1.5009226248	0.3583920790	1.6152874786
		H	-2.6337086617	1.4363679980	0.7147713534
		H	-3.1054607986	-0.2484270176	1.0982936639

b) by M11-L/MG3S

species	Absolute energies	Cartesian coordinates			
CH_2OO	-189.582948	C	1.04396400	-0.19587800	-0.00000500
		H	1.95364200	0.40499900	0.00004000
		H	1.00382900	-1.28953000	-0.00000300
		O	-0.00960500	0.45046600	-0.00000500
		O	-1.14305200	-0.19299100	0.00000500
syn-CH_3CHOO	-228.923119	C	-0.45795600	0.69941500	0.00000300
		H	-0.77763900	1.74508800	0.00000500
		O	0.77868700	0.56789500	-0.00000500
		O	1.22441600	-0.67690400	-0.00000800
		C	-1.32707800	-0.45293100	0.00000900
		H	-2.38226000	-0.17728900	0.00001500

		H	-1.07736300	-1.08731500	-0.86393500
		H	-1.07735300	-1.08731400	0.86395000
$HOCH_2CN$	-207.974692	C	0.56954900	0.56777600	0.03786900
		H	0.72625500	1.27280100	-0.79089000
		H	0.69877900	1.15137100	0.96905800
		O	1.48592000	-0.44083200	-0.10689600
		H	1.36232900	-1.07361800	0.59455200
		C	-0.81095100	0.10951000	-0.00694700
		N	-1.88947300	-0.26965900	-0.01472500
TS1	-397.573137	C	-1.99146100	0.22842500	0.05587600
		O	-1.43813300	-0.82082100	-0.34539800
		O	-0.41726900	-1.15666000	0.48612300
		H	-1.99130500	0.45102500	1.12677900
		H	-2.78195000	0.60463000	-0.60114700
		C	0.44951900	0.95032700	0.04507700
		N	-0.53277600	1.50990200	-0.20642600
		C	1.78738000	0.42297700	0.27355600
		H	1.89129900	0.30410000	1.37172500
		H	2.50999300	1.19971000	-0.02864000
		O	2.02857900	-0.70785100	-0.43603800
		H	1.24335200	-1.25650200	-0.30828800
s-TS1	-436.904346	C	-1.65984200	-0.06166400	-0.47021900
		O	-0.91854900	-1.08681800	-0.58840800
		O	-0.02797900	-1.15497300	0.43622300
		H	-2.27660300	0.07179600	-1.37011600
		C	0.65572500	0.87473800	-0.17548000
		N	-0.30255300	1.28181700	-0.69079800
		C	1.98843600	0.61827400	0.35192100
		H	1.90959200	0.70526700	1.45587400
		H	2.64736600	1.43810200	0.01877300
		O	2.49719800	-0.56522000	-0.07587100
		H	1.76206100	-1.18908100	-0.01558300
		C	-2.19670400	0.39664400	0.81898900

		H	-1.44117700	0.34224100	1.60229400
		H	-2.58369000	1.41349000	0.72876600
		H	-3.03073100	-0.26639800	1.08875000
C1	-397.580912	C	-2.13958100	0.39176000	0.02600500
		O	-1.59168800	-0.63604700	-0.36049800
		O	-0.77546500	-1.23522400	0.51396800
		H	-1.98224400	0.74301700	1.04982500
		H	-2.78358500	0.88115000	-0.70832500
		C	0.86810300	1.09139500	0.05540500
		N	0.03906900	1.86070600	-0.12848500
		C	1.91182900	0.09136800	0.26813800
		H	1.95196300	-0.09730100	1.35956000
		H	2.87424900	0.55342000	-0.00226000
		O	1.73760900	-1.02671500	-0.48258300
		H	0.86037700	-1.36848200	-0.26378600
M1	-397.658355	C	1.60098700	0.88117600	-0.08036800
		O	1.91810300	-0.47073600	0.13603600
		O	0.69530000	-1.15102000	-0.10426300
		H	1.91286700	1.21376900	-1.09443800
		H	2.16169200	1.46010700	0.67175800
		C	-0.20400100	-0.19566200	0.00254300
		N	0.19914100	0.98871600	0.06695300
		C	-1.62599000	-0.59134600	0.02277200
		H	-1.79704500	-1.20418000	0.92930800
		H	-1.81805300	-1.26376800	-0.83331400
		O	-2.43898600	0.50125500	-0.01537200
		H	-1.87476200	1.27205400	0.05712300
s-C1	-436.921909	C	-1.89493000	0.04915500	-0.54601200
		O	-1.04436900	-0.83067700	-0.72618000
		O	-0.50804900	-1.33992400	0.39888700
		H	-2.29093700	0.44812700	-1.48572700
		C	1.22340600	1.14640900	-0.04998300
		N	0.41787100	1.87627400	-0.40944500

		C	2.22037200	0.17850400	0.40667100
		H	2.13852500	0.13945700	1.51222000
		H	3.21474500	0.59906300	0.18892400
		O	2.11287900	-1.03025100	-0.19931200
		H	1.21798000	-1.35839800	-0.02294000
		C	-2.30711400	0.46260300	0.77256600
		H	-1.42064200	0.81724100	1.31602300
		H	-3.07958200	1.23072500	0.73860500
		H	-2.63929100	-0.42334700	1.33239500
TS1a	-397.558594	O	-0.04713900	0.67667200	-0.66876500
		H	-0.97395400	0.91967100	-0.10664900
		C	-0.85875200	-1.07996700	-0.00414200
		O	-2.00668000	-0.64331100	-0.18770600
		O	-2.08660200	0.57565200	0.50035300
		H	-0.34030800	-0.88203900	0.94120200
		H	-0.53365400	-1.88630900	-0.67377600
		C	1.04590500	1.06475700	0.04563500
		H	1.52805800	1.94684300	-0.41420600
		H	0.80690600	1.35658800	1.08859700
		C	2.03042400	-0.00685400	0.11014400
		N	2.76155100	-0.88492600	0.15770700
TS1b	-397.560592	O	0.08190600	-0.82754500	0.76137900
		H	1.07796300	-0.92573800	0.27688800
		C	0.88984900	1.03325500	0.55612900
		O	1.41395400	0.76063600	-0.54039800
		O	2.11968100	-0.43597800	-0.35980900
		H	1.38853800	0.74955700	1.48777400
		H	0.09387700	1.79035100	0.53079100
		C	-0.86789400	-1.06052000	-0.19597400
		H	-0.44605000	-1.10052600	-1.21914200
		H	-1.36292900	-2.03413500	-0.02803400
		C	-1.88414300	-0.02124100	-0.17950900
		N	-2.64322900	0.83351700	-0.14593300

M1a	-397.636701	O	0.27480300	-1.18825800	-0.60498100
		H	0.13653100	1.70642600	-0.42168800
		C	1.33504300	-0.67241600	0.10474600
		O	1.09634900	0.54470400	0.65359400
		O	1.07174000	1.48123600	-0.39845400
		H	2.18403800	-0.65921400	-0.59487800
		H	1.56655500	-1.30241500	0.98819000
		C	-0.88986800	-1.20668600	0.12028900
		H	-1.55751100	-1.95736600	-0.32599000
		H	-0.72725300	-1.49135200	1.17754700
		C	-1.56565800	0.08287100	0.08855100
		N	-2.06037100	1.11140700	0.01343400
TS1c	-397.528360	O	0.86265900	1.63599000	0.42027800
		C	-1.01714900	-0.20757000	1.04974800
		O	-1.69206400	-0.74962700	0.13709200
		O	-1.81588400	0.14300800	-0.87704200
		H	-0.64909000	-0.90273700	1.81175700
		H	-1.04875000	0.87543000	1.20164300
		C	0.67738500	0.61084400	-0.48439600
		H	-0.70605200	0.43778300	-0.82782700
		H	0.83798100	0.93389600	-1.53246400
		C	1.46261600	-0.55858400	-0.24513200
		N	2.04122100	-1.52965500	-0.03973200
		H	1.70256100	2.06011500	0.26107200
M1c	-397.642991	O	0.41418000	1.55793500	0.11397100
		C	-0.42506000	-0.62359700	0.57530500
		O	-1.70074300	-0.10223000	0.58456500
		O	-2.21055400	-0.25881400	-0.72182100
		H	-0.40811800	-1.67562400	0.24488500
		H	-0.10163300	-0.56937900	1.62628000
		C	0.47828500	0.24589500	-0.28176900
		H	0.17445600	0.11681200	-1.34182500
		C	1.84655100	-0.22758000	-0.17722800

		N	2.89992700	-0.66261500	-0.09802300
		H	-0.51430000	1.75943800	0.22091800
		H	-2.87160900	-0.93636800	-0.57565800
TS1d	-397.536941	C	-0.53311500	-1.05365500	-0.02574900
		O	-1.66026300	-0.67964500	0.43243000
		O	-2.22438200	0.20432700	-0.32938000
		H	-0.40383300	-1.06923200	-1.11240500
		H	-0.01822300	-1.78474100	0.60397500
		C	0.37927400	0.73456600	0.08713600
		N	-0.41193700	1.56995400	-0.13310600
		C	1.78711600	0.37852200	0.38647700
		H	1.84882000	0.12376700	1.45490100
		H	2.40107300	1.28272800	0.23403500
		O	2.24253900	-0.70657200	-0.31747000
		H	2.39293000	-0.44367900	-1.22059300
M1d	-397.612791	C	-0.53808700	1.10345100	0.21586600
		O	-1.80802000	0.75484500	-0.13411400
		O	-1.79049200	-0.75425600	-0.19824400
		H	-0.48899300	1.56888800	1.22538900
		H	-0.10747700	1.81941900	-0.51021500
		C	0.20909100	-0.18769500	0.20667600
		N	-0.58334600	-1.13753200	-0.02541600
		C	1.65332000	-0.36382800	0.44479700
		H	1.87761900	-1.44404800	0.46887300
		H	1.91325500	0.03741200	1.43711600
		O	2.42924800	0.33833700	-0.45830400
		H	2.29719100	-0.04193000	-1.32199100
M1-TSa		C	1.59874400	-0.80163300	0.21135400
		O	2.17785300	0.25481500	-0.29244800
		O	0.47095900	1.36646100	0.00178700
		H	1.83915100	-1.01981800	1.28758300
		H	2.06075900	-1.66742000	-0.33834300
	-397.620334	C	-0.21767500	0.36457200	0.01228500

		N	0.21423600	-0.87567900	0.01422800
		C	-1.73045400	0.47753200	0.20295100
		H	-2.09768100	1.36049800	-0.33708200
		H	-1.88173400	0.65827800	1.28601900
		O	-2.34105900	-0.62983800	-0.27444600
		H	-1.78585900	-1.37611400	-0.03645800
M2		C	-1.84243000	0.06492800	0.28664100
		O	-3.03377200	-0.28361700	-0.02467300
		O	0.44479400	1.35464700	-0.17040500
		H	-1.68231500	0.13336000	1.40021000
		H	-1.70744300	1.17348500	0.07451800
		C	0.40915100	0.16219900	-0.15164400
		N	-0.74820000	-0.56649700	-0.29889300
		C	1.61580200	-0.71787100	-0.05523500
		H	1.66489000	-1.26463700	-1.01969100
		H	1.40709200	-1.49745000	0.70598400
		O	2.71377200	0.04145600	0.21119300
	-397.630850	H	3.46168400	-0.53470900	0.32373200
M2-TSb		C	-1.69361300	-0.43743300	0.54170500
		O	-2.39261300	-0.32619300	-0.59056300
		O	-0.07646800	1.68141600	0.07601300
		H	-1.88788300	-1.34787100	1.14710900
		H	-1.80160400	0.47493500	1.16926000
		C	0.38407600	0.58601300	0.00935100
		N	-0.40719200	-0.54564000	-0.06134500
		C	1.84035800	0.25952600	-0.13463700
		H	2.16329600	0.62183300	-1.13094600
		H	2.39481200	0.86158100	0.59747400
		O	2.12034700	-1.06176900	0.09506500
	-397.618143	H	1.58667300	-1.58727200	-0.49611600
M3		C	1.96791900	0.12039200	0.54288900
	-397.670563	O	1.60791500	-0.93755300	-0.23465600

		O	-0.77911300	1.52737300	-0.03189300
		H	2.98781400	0.50586200	0.42726600
		H	1.57556600	0.12428500	1.57079500
		C	-0.26984000	0.46406700	-0.15119800
		N	1.08719100	0.38489900	-0.51744200
		C	-1.04237300	-0.80447100	-0.03466100
		H	-0.88210200	-1.39493600	-0.95691500
		H	-0.58820700	-1.41447900	0.77026900
		O	-2.35415700	-0.54109900	0.19856000
		H	-2.43479300	0.41528000	0.21240100
M3-TSc		C	-1.80700400	0.05423800	0.24759300
		O	-3.00896000	-0.16889400	0.02479600
		O	0.45463500	1.25410700	-0.21912300
		H	-1.56908900	0.37952800	1.31708000
		H	-1.47518500	1.14744300	-0.01770200
		C	0.39297000	0.04786200	-0.16791000
		N	-0.75609300	-0.64940900	-0.28279800
		C	1.64458400	-0.75785500	-0.03059800
		H	1.50728400	-1.54808400	0.72733900
		H	1.74974400	-1.29847500	-0.99594300
		O	2.71107000	0.02395700	0.26570400
	-397.637893	H	2.44262900	0.92662200	0.08328800
M3-TSc1		O	-2.44361300	0.27367600	-0.29321000
		O	0.48639300	1.45615800	0.00130400
		C	0.22613700	0.32589100	-0.21077800
		N	-0.61362400	-0.60082100	-0.37032400
		C	-1.97958200	-0.45487700	0.59414400
		H	-1.63081400	-0.01556900	1.56132600
		H	-2.31193000	-1.51349700	0.69820200
		C	1.56844400	-0.67673100	-0.40099800
		H	1.40327400	-1.75145000	-0.29003100
	-397.622344	H	1.78663500	-0.42404300	-1.45739200

		O	2.42794700	-0.22840300	0.50502600
		H	2.39239700	0.73315900	0.48099500
$HOCH_2NCO$		O	-2.43127800	0.01193300	0.00001700
		C	-1.28483900	-0.06612900	-0.00000400
		N	-0.11885300	-0.29075700	-0.00003000
		C	1.04254100	0.49469500	-0.00000600
		H	1.05440400	1.15264900	-0.89581500
		H	1.05437400	1.15265300	0.89580000
	-283.229093	O	2.09100300	-0.38200400	0.00001300
		H	2.89918200	0.11915900	0.00004500
HCHO		O	-0.66285600	0.00000000	0.00000000
		C	0.51031700	0.00000000	0.00000100
		H	1.12047300	0.94465000	-0.00000200
	-114.509429	H	1.12046700	-0.94465400	-0.00000200
M4		C	-1.51206200	-0.84713400	0.08684200
		O	-1.94958700	0.25041700	-0.08893800
		O	1.93489600	-0.82233900	-0.17160400
		H	-2.18141200	-1.69385500	0.36701000
		H	1.87290400	-1.72340200	-0.49997500
		C	0.72543900	-0.43067500	0.08808900
		N	-0.22843200	-1.25786200	-0.07805200
		C	0.65254100	0.99265600	0.56972300
		H	0.00050400	1.02059000	1.46289500
		H	1.65967700	1.30426100	0.87540100
		O	0.23196100	1.82417800	-0.43190800
	-397.772024	H	-0.68632100	1.59031000	-0.58728500
M4-TSd		C	1.48976700	-0.88905600	0.03840400
		O	1.98976100	0.15940700	-0.24453200
		O	-1.86584700	-1.05228800	-0.00019400
		H	2.09776500	-1.80614800	0.21045900
		H	-0.91178500	-1.89275400	0.19786000
	-397.725877	C	-0.85858100	-0.32386800	-0.03178300

		N	0.17432600	-1.13726200	0.17567500
		C	-0.90030600	1.13944000	-0.28504200
		H	-0.82535300	1.24249500	-1.39110000
		H	-1.91027800	1.48269500	-0.02372300
		O	0.00879800	1.87132100	0.40504300
		H	0.88238900	1.54792700	0.16477100
M5		C	1.98396400	0.25187100	-0.00000600
		O	3.03230500	-0.29094800	-0.00000400
		O	-0.59299600	1.32864600	-0.00000700
		H	1.82488500	1.35262500	-0.00001300
		H	0.87695000	-1.44034800	0.00000800
		C	-0.42599300	0.14879800	0.00000000
		N	0.80164100	-0.43445600	0.00000100
		C	-1.59604100	-0.79009500	0.00000800
		H	-1.51266600	-1.45505700	-0.88349400
		H	-1.51266300	-1.45504500	0.88352000
		O	-2.75872400	-0.09476400	0.00000600
	-397.796439	H	-2.50425600	0.83210200	0.00000000
M5-TS		C	2.03879500	0.37262200	-0.07806900
		O	3.09425500	-0.02315300	-0.17446600
		O	-0.26347700	1.08670000	0.19305100
		H	0.94823800	1.09874500	0.05199900
		H	0.51625400	-1.89688400	0.06333300
		C	-0.40173300	-0.16767800	0.12667800
		N	0.64723100	-0.90791800	0.22901800
		C	-1.79931800	-0.66097900	-0.09017800
		H	-1.80205100	-1.26979400	-1.01599300
		H	-2.04506600	-1.36258400	0.72909000
		O	-2.70300700	0.35590600	-0.15544100
	-397.723540	H	-2.19661800	1.16652600	-0.08729600
M5-TS1		C	-1.68183000	-0.18831100	-0.07625400
	-397.688543	O	-2.65810100	-0.46575800	-0.62984900

		O	0.70976500	1.53784600	-0.27483500
		H	-0.46251800	-0.11884300	-0.89013100
		H	-1.46579300	0.37689900	1.82666000
		C	0.37354700	0.42830200	-0.04887400
		N	-1.01657000	0.15076700	0.94638000
		C	1.31857900	-0.67340900	0.38242700
		H	1.52224000	-0.47013000	1.45523600
		H	0.83714300	-1.65683700	0.31637600
		O	2.43394900	-0.67400000	-0.39698300
		H	2.73824500	0.22934300	-0.46325300
M6		O	-0.48342400	1.24965000	0.09193500
		H	-1.36810800	1.59664100	-0.02855100
		H	-1.61522400	-1.60870700	-0.19982400
		C	-0.58348800	-0.06615500	0.02036600
		N	-1.70217400	-0.59903700	-0.14699100
		C	0.75898400	-0.69506900	0.22834300
		H	0.84958600	-0.90328300	1.31607800
		H	0.77634000	-1.67205900	-0.27294500
		O	1.80584600	0.04881200	-0.24891400
	-284.435924	H	1.64026500	0.96032400	-0.02224100
CO		C	0.00000000	0.00000000	-0.63728200
	-113.320427	O	0.00000000	0.00000000	0.47796200
M61		O	1.32626200	-0.58699900	0.00000000
		H	1.40176800	1.43398700	-0.00000400
		C	0.81096100	0.47900000	-0.00000100
		C	-0.66758300	0.62435100	0.00000100
		H	-0.94118000	1.24470700	0.87848400
		H	-0.94118600	1.24471400	-0.87847400
		O	-1.29855200	-0.57636500	-0.00000200
	-229.063992	H	-0.60133900	-1.23660700	0.00000600
HNCO		C	0.00000000	-0.05199700	0.00000000
	-168.703925	O	-0.57429100	-1.04202600	0.00000000

		H	1.43967600	1.22564000	0.00000000
		N	0.45066500	1.06036400	0.00000000
M6-TS		O	-0.55596100	1.20116600	0.00000100
		H	-1.79114500	0.81094500	0.00000500
		H	-1.95250300	-1.48384000	0.00002000
		C	-0.49215700	-0.06155500	-0.00000200
		N	-1.69708100	-0.50891100	-0.00000300
		C	0.82415800	-0.73820700	0.00000100
		H	0.86689400	-1.40566300	0.88113800
		H	0.86689500	-1.40566700	-0.88113500
		O	1.85939400	0.15125600	-0.00000100
	-284.384222	H	1.46995700	1.02580000	0.00000900
Glycolamide	-284.461076	O	-0.36269200	1.31712300	-0.00000600
		H	-2.51578200	0.07698700	0.00001500
		H	-1.76981700	-1.47652000	0.00000900
		C	-0.49798800	0.12683500	-0.00000300
		N	-1.68275400	-0.47995100	0.00000700
		C	0.72006400	-0.76204500	-0.00001100
		H	0.67625400	-1.42820400	0.88456900
		H	0.67626700	-1.42816600	-0.88462000
		O	1.84458200	-0.00201100	0.00001200
		H	1.52478600	0.90593200	0.00001700
s-C1	-436.921909	C	-1.89493000	0.04915500	-0.54601200
		O	-1.04436900	-0.83067700	-0.72618000
		O	-0.50804900	-1.33992400	0.39888700
		H	-2.29093700	0.44812700	-1.48572700
		C	1.22340600	1.14640900	-0.04998300
		N	0.41787100	1.87627400	-0.40944500
		C	2.22037200	0.17850400	0.40667100
		H	2.13852500	0.13945700	1.51222000
		H	3.21474500	0.59906300	0.18892400
		O	2.11287900	-1.03025100	-0.19931200

		H	1.21798000	-1.35839800	-0.02294000
		C	-2.30711400	0.46260300	0.77256600
		H	-1.42064200	0.81724100	1.31602300
		H	-3.07958200	1.23072500	0.73860500
		H	-2.63929100	-0.42334700	1.33239500
s-C1b	-436.920311	O	-1.54491500	-1.16679300	0.70403800
		H	-0.67821300	-1.37229700	0.31861000
		C	1.70957400	0.54917700	-0.26440900
		O	1.30681800	-0.35402500	-1.00837900
		O	0.92563600	-1.48911000	-0.38751800
		H	1.99717500	1.45141700	-0.81427000
		C	-2.16406200	-0.27855600	-0.11537900
		H	-2.28399300	-0.63138100	-1.15876100
		H	-3.18037500	-0.09064100	0.26389100
		C	-1.46440400	1.00436200	-0.17294500
		N	-0.84516200	1.96701000	-0.19615200
		C	1.78636000	0.39368700	1.16825900
		H	2.20399200	1.27659300	1.65211600
		H	0.78293200	0.17595400	1.56200200
		H	2.36949200	-0.51131500	1.39118600
s-TS1a	-436.892104	O	-0.11759200	-0.92701500	-0.42283600
		H	0.92000500	-1.11032900	0.17403200
		C	1.07335200	0.85146900	-0.50542000
		O	2.04074800	0.06563000	-0.62589400
		O	2.04022100	-0.82561100	0.45823800
		H	0.84025100	1.35250600	-1.45798100
		C	-1.20932400	-1.05897100	0.35163600
		H	-1.65686400	-2.07236300	0.27314300
		H	-1.02383000	-0.91431000	1.44078500
		C	-2.24942400	-0.10051100	-0.01709500
		N	-3.02501500	0.68732100	-0.31231200
		C	0.56054900	1.41237500	0.73349900
		H	1.08098400	2.37440600	0.86944000

		H	-0.50237500	1.65129600	0.63960900
		H	0.75900100	0.77734200	1.59537800
s-TS1b	-436.895085	O	0.14551800	-0.56804800	-0.96181100
		H	-0.80175200	-1.10308700	-0.39126700
		C	-0.84981000	0.82340000	0.35303400
		O	-1.07976600	-0.13126600	1.13751100
		O	-1.64410800	-1.18851800	0.41912300
		H	-0.13375200	1.53704600	0.79316100
		C	1.30267000	-1.01683900	-0.42462700
		H	1.16280800	-1.72240400	0.42271800
		H	1.91636100	-1.56685400	-1.16596100
		C	2.10922300	0.09101300	0.08300800
		N	2.66274900	1.00931200	0.48408000
		C	-1.65776000	1.23225800	-0.78357100
		H	-2.29137500	2.06313800	-0.43563400
		H	-1.01059400	1.62492900	-1.57066300
		H	-2.28003700	0.42571400	-1.16656400
s-P1a	-436.965145	O	0.21004000	-1.10516500	-0.43050900
		H	-0.54923500	1.70626700	-0.39784700
		C	1.06848700	-0.37189600	0.37145000
		O	0.50178100	0.79389300	0.81732600
		O	0.40390200	1.68667800	-0.26880000
		H	1.21893500	-0.90654900	1.33707900
		C	-1.01204100	-1.32026600	0.14880100
		H	-1.46404400	-2.20558600	-0.32141900
		H	-0.93657400	-1.52288900	1.23439900
		C	-1.91421800	-0.19329700	-0.04414100
		N	-2.58753600	0.71048000	-0.23995900
		C	2.34441900	-0.20665000	-0.37847600
		H	3.05100900	0.38113000	0.21255200
		H	2.78556800	-1.18411900	-0.59027200
		H	2.16143000	0.30779300	-1.32471700
s-TS1c	-436.860618	O	1.09091400	1.70026700	-0.10936900

		C	-1.02877500	-0.54852000	0.75139600
		O	-1.45102200	-1.05219900	-0.33653800
		O	-1.54898500	-0.06615100	-1.28172700
		H	-0.63992900	-1.33302600	1.41444900
		C	0.97732100	0.45927700	-0.70073500
		H	-0.52985400	0.27172600	-1.15824500
		H	1.23020200	0.48044200	-1.77475000
		C	1.69077500	-0.57599200	-0.04995500
		N	2.23709200	-1.42250500	0.50978400
		H	1.97213800	1.81229700	0.24123400
		C	-1.33906200	0.77868500	1.23610400
		H	-1.68707800	0.70657500	2.27433600
		H	-0.44882100	1.42824000	1.23978400
		H	-2.08511600	1.25524200	0.59491300
s-P1c	-436.969120	O	-0.39733500	-0.89313400	1.37448400
		C	0.42831300	0.55215500	-0.35034500
		O	1.71348700	0.26502400	0.09697800
		O	2.17142900	-0.85584200	-0.62128100
		H	0.42491500	0.67054700	-1.45069800
		C	-0.46804600	-0.63052200	0.02871800
		H	2.81652100	-0.44908700	-1.20065500
		H	-0.14889400	-1.50072000	-0.58048000
		C	-1.84383500	-0.34960600	-0.33785400
		N	-2.90396200	-0.10354300	-0.68627300
		H	0.53420100	-0.92259200	1.58866800
		C	0.04561600	1.82099600	0.34130700
		H	0.74857700	2.62257000	0.09719900
		H	-0.95575700	2.13283500	0.02964200
		H	0.03524000	1.68472600	1.42783100
s-TS1d	-436.866322	C	-0.56271800	0.78014400	-0.36270300
		O	-1.30245000	-0.02661800	-1.04592400
		O	-2.01025600	-0.79782000	-0.27413000
		H	0.07458700	1.36856400	-1.03579800

		C	0.54024300	-0.62615700	0.42372000
		N	-0.14389100	-1.53869900	0.71338600
		C	1.93199800	-0.10431000	0.45553300
		H	2.57584200	-0.90448600	0.85972100
		H	1.96971500	0.73026800	1.17226300
		O	2.36933700	0.38114400	-0.74833200
		H	2.44519100	-0.34569400	-1.35995800
		C	-1.06300400	1.40393400	0.87777100
		H	-1.55811400	0.67046800	1.51475400
		H	-0.24695800	1.88621100	1.42427000
		H	-1.78518800	2.19024000	0.61220200
s-P1d	-436.937545	C	0.56688200	0.70026600	0.42436900
		O	1.72187600	-0.00507000	0.65937900
		O	1.55157900	-1.29733500	-0.07632900
		H	0.15152700	1.03137300	1.39806100
		C	-0.32885000	-0.33231400	-0.19144600
		N	0.32639400	-1.37622300	-0.45000300
		C	-1.76001300	-0.17333300	-0.51226700
		H	-2.10165800	-1.07274200	-1.05308300
		H	-1.89763200	0.67745800	-1.19778800
		O	-2.52219000	0.11817000	0.60385000
		H	-2.48621900	-0.63121500	1.19142600
		C	0.77807800	1.88968400	-0.47981700
		H	1.14710100	1.57321900	-1.46280300
		H	-0.15600300	2.44680400	-0.62064200
		H	1.51142300	2.57672500	-0.04538500

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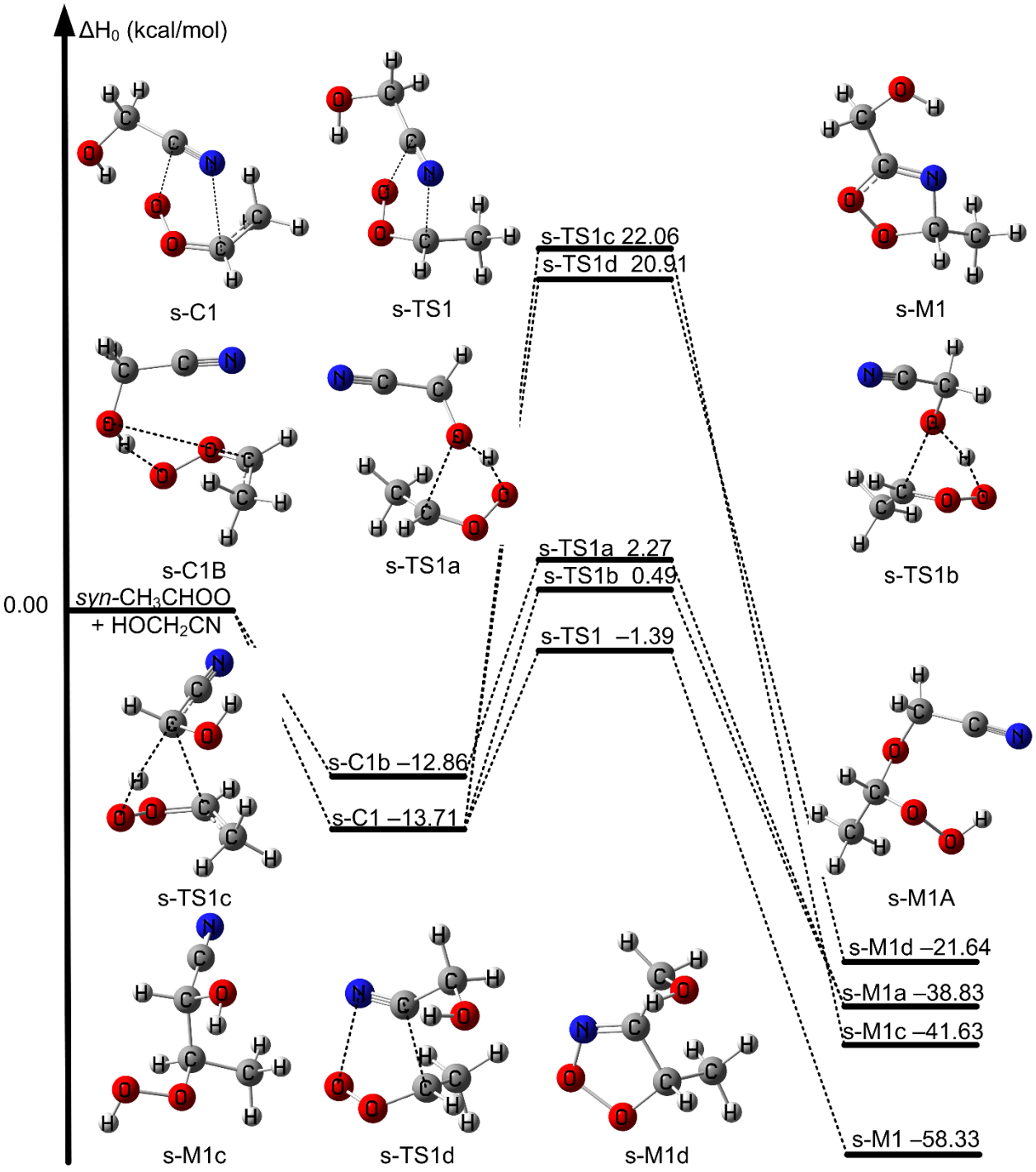

Figure S1. The relative enthalpies at 0 K for the reaction of syn-CH_3CHOO + $HOCH_2CN$. Values are given for all species as calculated by M11-L/MG3S.

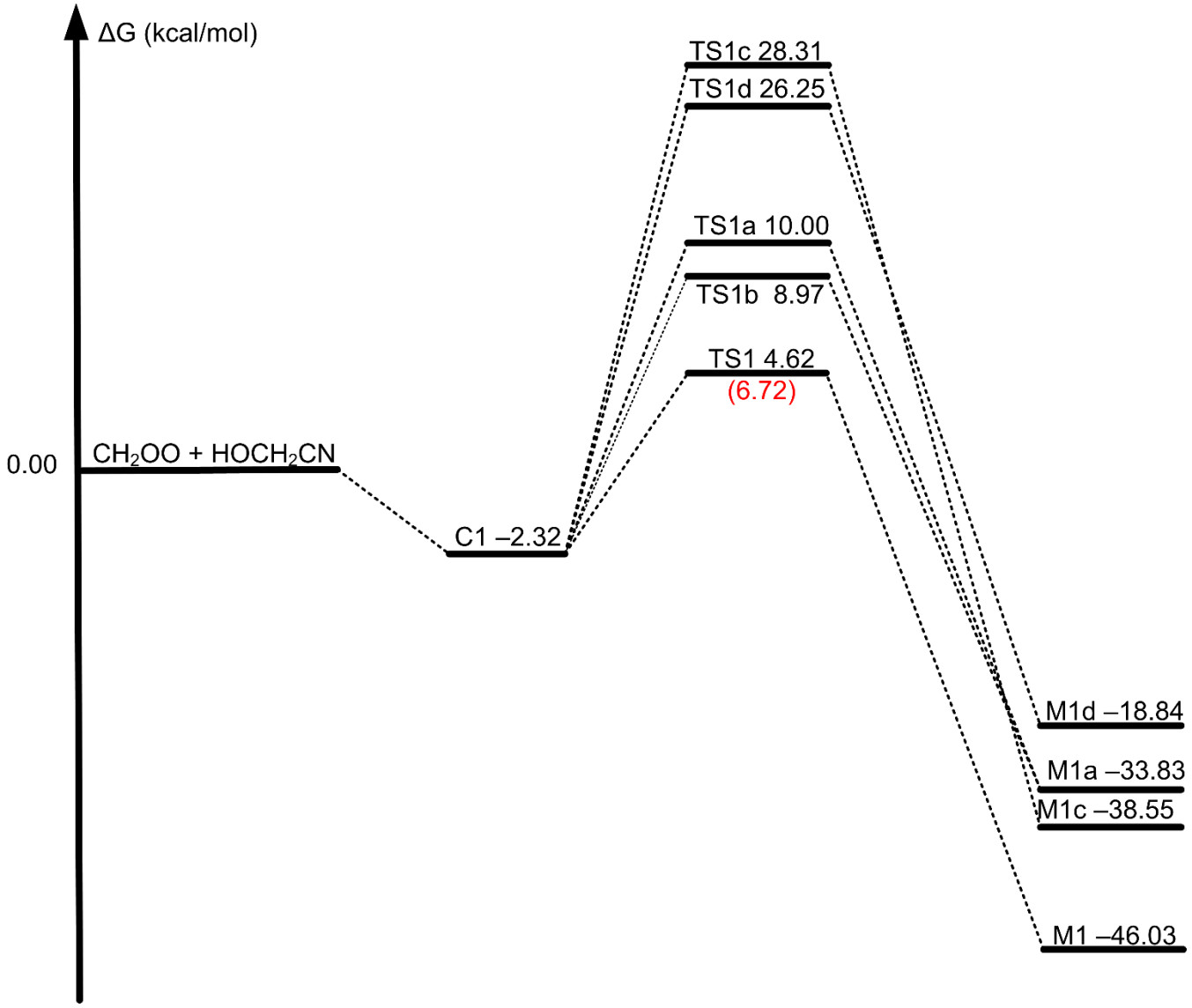

Figure S2. The relative Gibbs free energies at 298 K for the reaction of $CH_2OO + HOCH_2CN$. Values are given for all species as calculated by M11-L/MG3S. in small parentheses, values are given for the transition state TS1 calculated by W3X-L//DF-CCSD(T)-F12b/jun-cc-pVDZ.

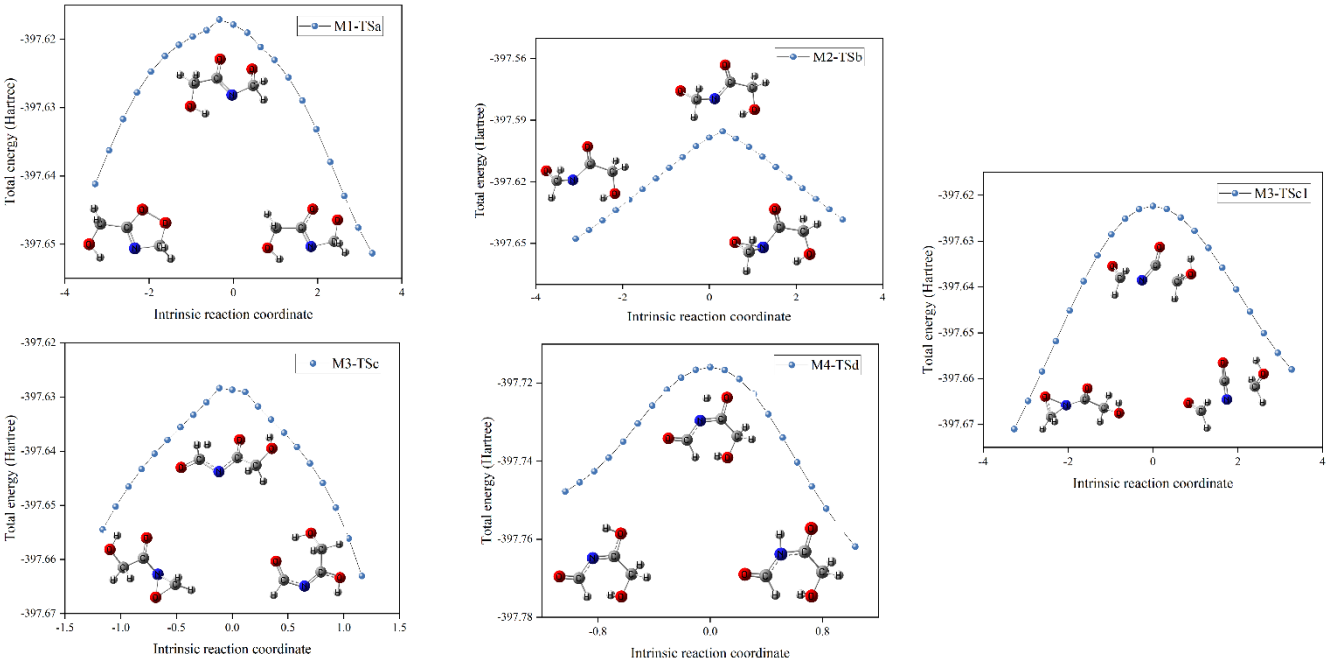

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Figure S3. The intrinsic reaction coordinate (IRC) for the reaction of CH_2OO + $HOCH_2CN$ calculated by M11-L/MG3S.

[1] Long, B., Xia, Y., Zhang, Y.-Q., and Truhlar, D. G.: Kinetics of Sulfur Trioxide Reaction with Water Vapor to Form Atmospheric Sulfuric Acid, Journal of the American Chemical Society, 145, 19866-19876, 10.1021/jacs.3c06032, 2023