ESI

Carbon monoxide formation from trimethylamine-boranecarboxylate: DFT studies of S_Ni and chelotropic mechanisms

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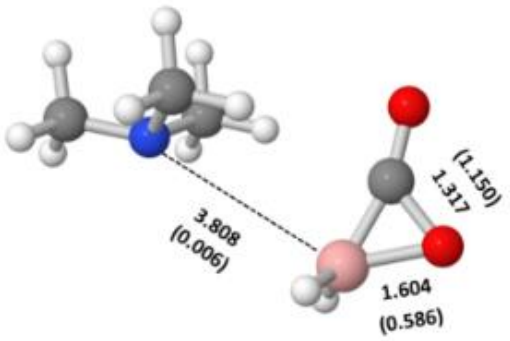
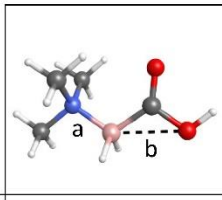
ELECTRONIC SUPPORTING INFORMATION

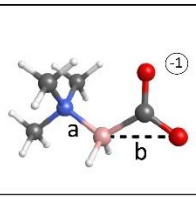


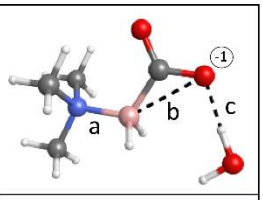
	$TMA..BH_2COO^-$ (vdW)	
	PCM/M06-2X/6-311++G(2d,p)	
E_{elect} (a.u.)	-389.174907	
ZPE	0.154664	
Internal energy	-389.009016	
Enthalpy	-389.008072	
Gibbs free energy	-389.059841	
	PCM/CCSD(T)/6-311++G(2d,p)	
E_{elect} (a.u.)	-388.420672	
Internal energy	-388.254782	
Enthalpy	-388.253838	
Gibbs free energy	-388.305607	

Figure S1. Van der Waals complex of trimethylamine with carboxyborane anion (C_s). Distance in Å; Wiberg bond order in parentheses.

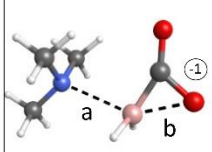
Figure S2. Comparing M06-2X optimized geometries for four basis sets.

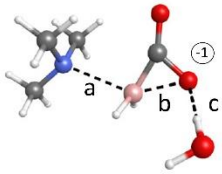


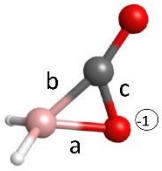


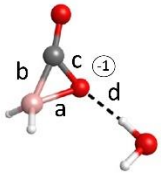


	Trimethylamine carboxyborane		Trimethylamine boranecarboxylate		Water-trimethylamine boranecarboxylate		
Basis set	a	b	a	b	a	b	c
6-311++G(2d,p) (gas)	1.623	2.465	1.674	2.444	1.658	2.462	1.666
6-311++G(2d,p)	1.607	2.460	1.630	2.455	1.623	2.467	1.600
jun-cc-pVTZ	1.608	2.459	1.631	2.454	1.624	2.466	1.602
jul-cc-pVTZ	1.608	2.459	1.631	2.454	1.624	2.466	1.608
aug-cc-pVTZ	1.608	2.459	1.631	2.454	1.624	2.465	1.603

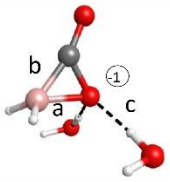


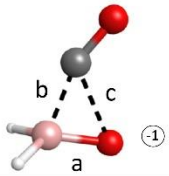


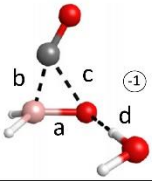


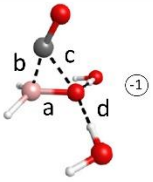


	Trimethylamine boranecarboxylate S_Ni transition state		Water-trimethylamine boranecarboxylate S_Ni transition state			Carboxyborane anion			Water-carboxyborane anion			
Basis set	a	b	a	b	c	a	b	c	a	b	c	d
6-311++G(2d,p) (gas)	2.436	2.006	2.453	1.963	1.829	1.583	1.546	1.322	1.588	1.544	1.336	1.914
6-311++G(2d,p)	2.574	1.864	2.607	1.846	1.793	1.600	1.543	1.316	1.609	1.542	1.331	1.844
jun-cc-pVTZ	2.550	1.857	2.599	1.836	1.784	1.595	1.543	1.318	1.606	1.541	1.330	1.837
jul-cc-pVTZ	2.551	1.855	2.600	1.835	1.785	1.595	1.543	1.318	1.606	1.541	1.330	1.837
aug-cc-pVTZ	2.551	1.855	2.600	1.834	1.784	1.595	1.543	1.318	1.606	1.541	1.330	1.836









	Two-water-carboxyborane anion			Carboxyborane anion CO-loss transition state			Water-carboxyborane anion CO-loss transition state				Two-water-carboxyborane anion CO-loss transition state			
Basis set	a	b	c	a	b	c	a	b	c	d	a	b	c	d
6-311++G(2d,p) gas	1.592	1.541	1.945	1.362	1.783	1.919	1.393	1.682	1.944	1.604	1.421	1.635	1.908	1.682
6-311++G(2d,p)	1.618	1.540	1.855	1.401	1.654	1.938	1.438	1.603	1.878	1.542	1.463	1.580	1.826	1.623
jun-cc-pVTZ	1.616	1.539	1.857	1.398	1.662	1.958	1.436	1.606	1.892	1.542	1.462	1.580	1.834	1.618
jul-cc-pVTZ	1.615	1.539	1.856	1.398	1.662	1.958	1.435	1.606	1.893	1.541	1.462	1.580	1.834	1.618
aug-cc-pVTZ	1.615	1.539	1.855	1.398	1.662	1.958	1.435	1.606	1.892	1.540	1.462	1.580	1.834	1.617

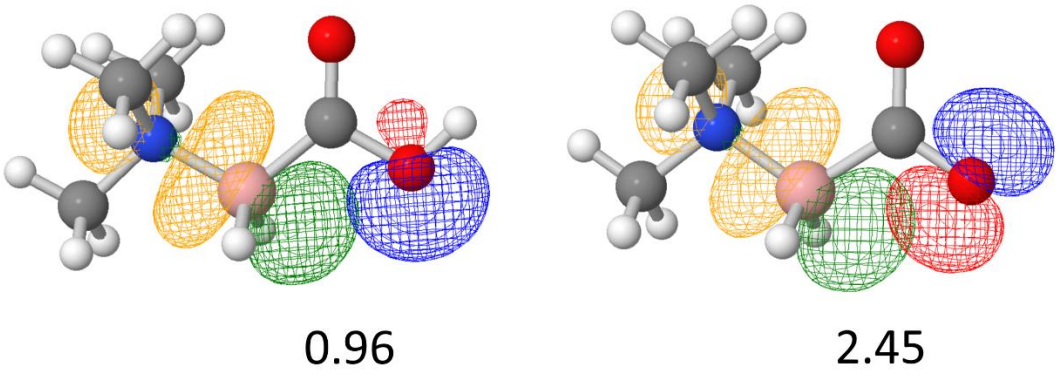


Figure S3. Secondary orbital donor-acceptor interactions in trimethylamine carboxyborane (l) and carboxyborane anion (r). Red/blue, donor; green/yellow, acceptor. E(2) interaction energy in kcal mol^{-1}. Orbital surfaces shown at the 0.065 e $Bohr^{-3}$ level.

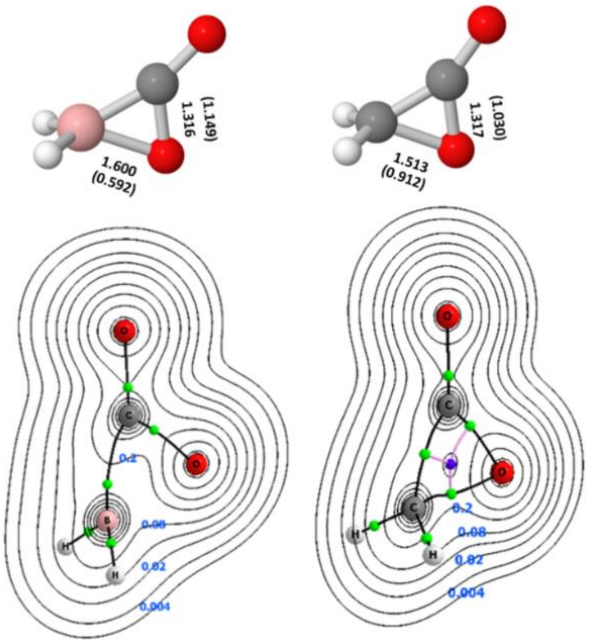
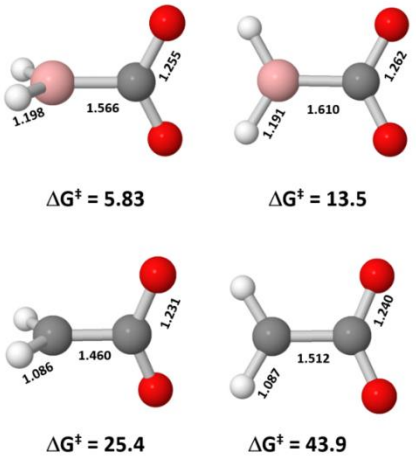


Figure S4. (upper) Optimized geometries of BH_2COO^- (l) and (*left*) and a-acetolactone (*right*). Distance, Å , Wiberg bond index in parantheses. (lower) Atoms-in-molecules analysis AIM analysis. Critical bond paths, black; bond critical points; green; ring critical paths, pink; and ring critical point, purple. Contours show electron density in the plane of the 3-membered ring (e $Bohr^{-3}$).



	BH_2COO^-		CH_2COO	
	perp	planar	perp	planar
	PCM/M06-2X/6-311++G(2d,p)			
E_{elect} (a.u.)	-214.7212004	-214.710396	-227.743893	-227.719837
ZPE	0.031304	0.031600	0.035865	0.035094
Internal Energy	-214.686031	-214.675103	-227.704407	-227.681022
Enthalpy	-214.685087	-214.674158	-227.703463	-227.680078
Gibbs Free Energy	-214.715265	-214.704022	-227.733127	-227.709948
	PCM/CCSD(T)/6-311++G(2,p)//PCM/M06-2X/6-311++G(2d,p)			
E_{elect} (a.u.)	-214.3269261	-214.315158	-227.3468663	-227.316433
Internal Energy	-214.2917567	-214.279865	-227.3073803	-227.277618
Enthalpy	-214.2908127	-214.278920	-227.3064363	-227.276674
Gibbs Free Energy	-214.3209907	-214.308784	-227.3361003	-227.306544

Figure S5. Transition states for internal rotation and inversion. Top, BH_2COO^- ; bottom, CH_2COO; left, COO invert; right, COO twist. PCM/CCSD(T)/6-311++G(2d,p)//PCM/M06-2X/6-311++G(2d,p). Bond distances in Å; Free energies in kcal mol^{-1} at 298.15 K.

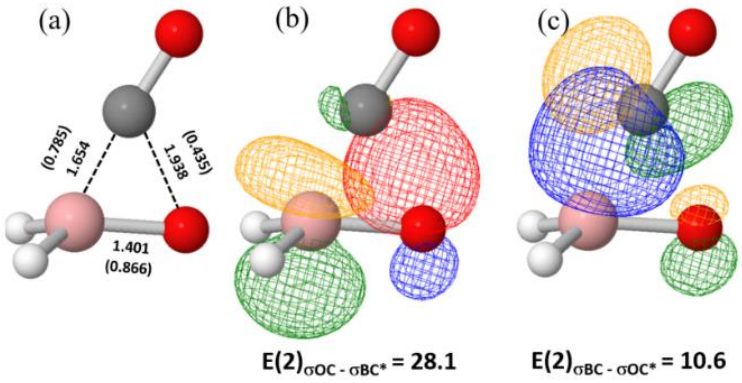


Figure S6. (*a*) Transition state for chelotropic extrusion of CO. distance, Å; Wiberg bond order in parentheses. (*b,c*) Natural bond orbital donor-acceptor interactions with second-order stabilization energy in kcal mol^{-1}. Red/blue, donor; green/orange, acceptor. Isosurface, 0.1 e Bohr^{-3}. M06-2X/6-311++G(2d,p)/PCM and NBO7.

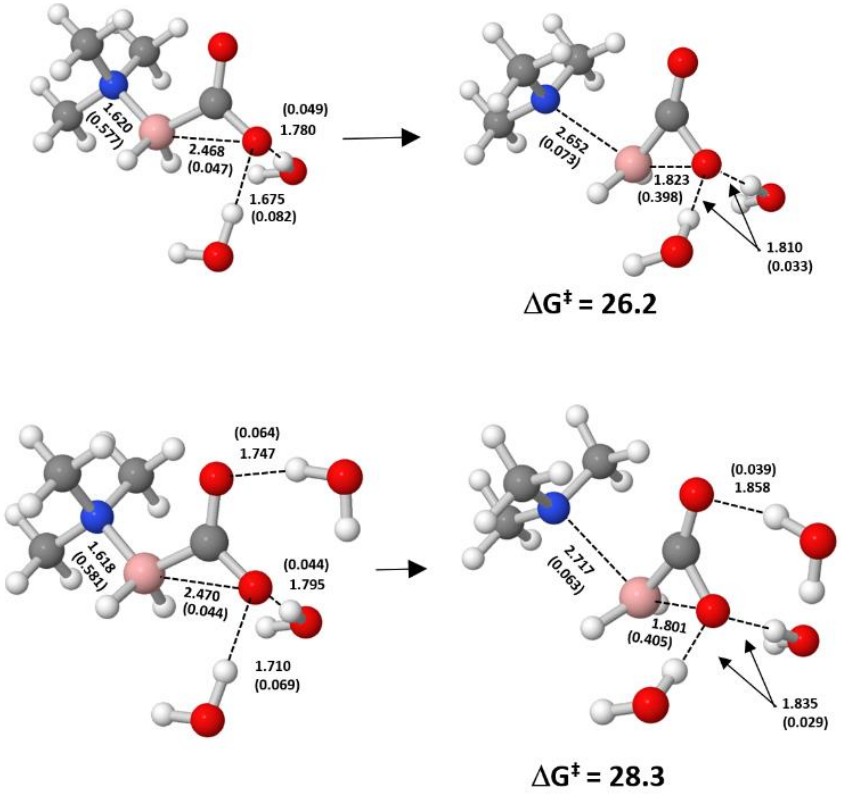


Figure S7. Two- and three-water-TMA-BH_2COO^- complexes and the corresponding S_Ni transition state (C_s symmetry). Distances in Å. Wiberg bond order in parentheses. Gibbs free energy of activation in kcal mol^{-1} at 298.15 K

Figure S8 Plots of activation barriers and S_Ni reaction free energy VS. model chemistry

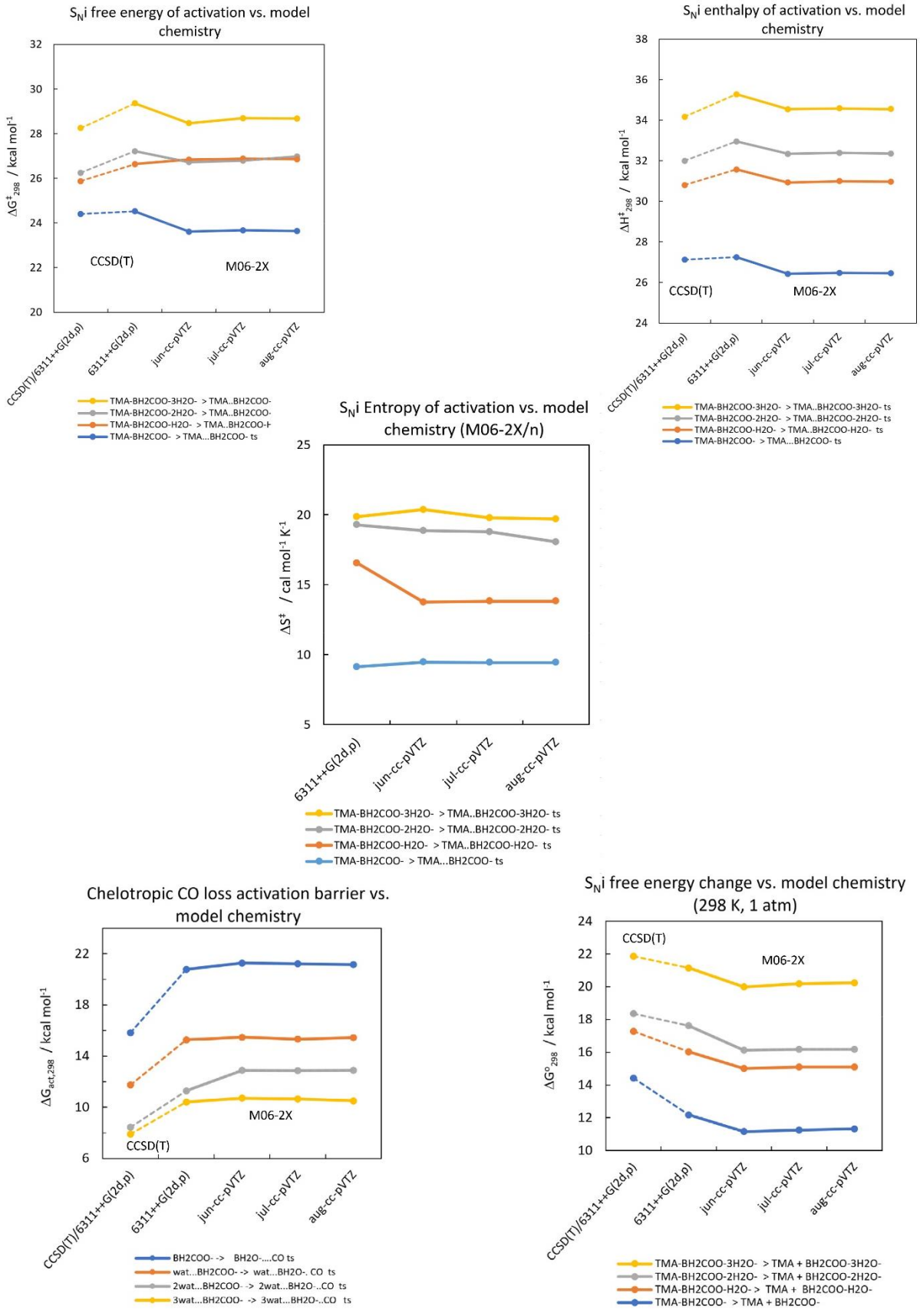


Figure S9. Geometries and energy changes for chelotropic reaction of BH_2COO^- , α-acetolactone, and trans-2,3-di-t-butylcyclopropane

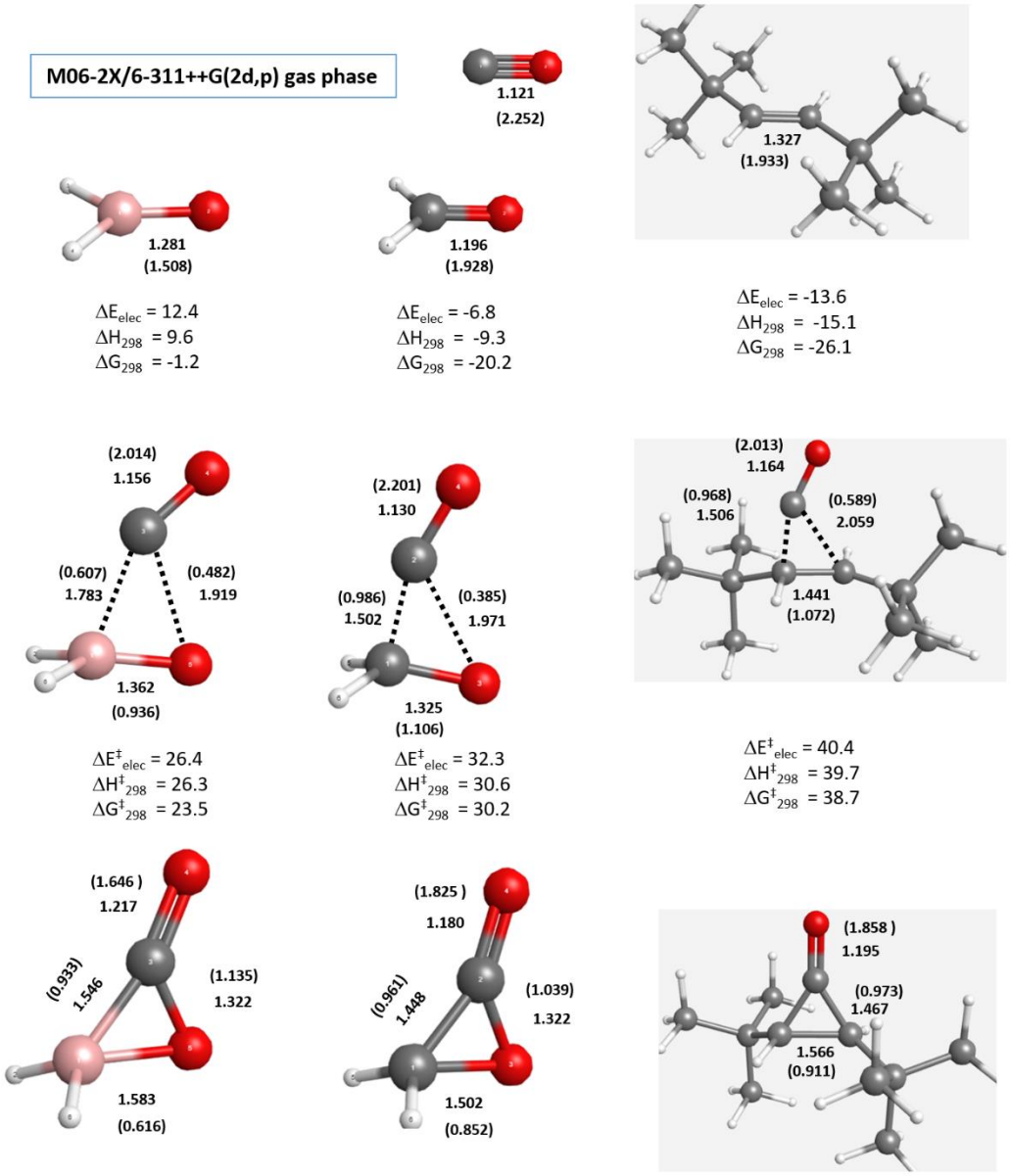


Figure S10. Mulliken atomic charge analysis of TMA-BH2COO- , 2-water complex, and related transition states. The partial charges are displayed using the WebMO graphical interface. The analysis shows that the partial charges on the SNi reacting atoms (O,B,N) decrease going from reactant to transition state, i.e. the transition state is less polar than the reactant.

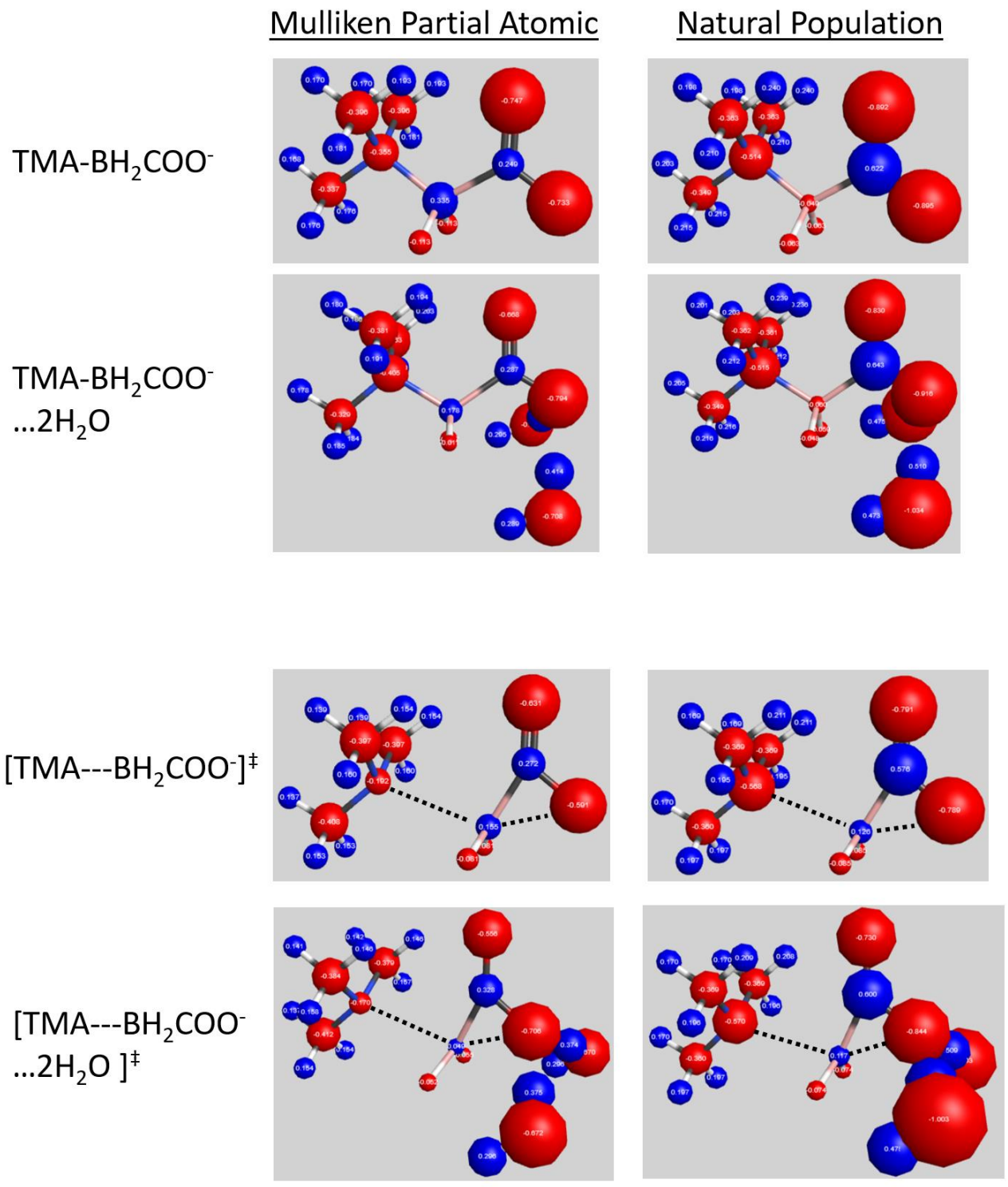


Table S1. Transition state imaginary frequencies (cm^{-1})

	M06-2X/6-311++G(2d,p)	M06-2X/jun-cc-pVTZ/PCM-H_2O	M06-2X/jul-cc-pVTZ/PCM-H_2O	M06-2X/aug-cc-pVTZ/PCM-H_2O	M06-2X/ 6-311++G(2d,p)/PCM-H_2O
TMA...BH_2COO^-	361.2998*i*	306.9278*i*	307.5277*i*	307.2053*i*	314.6652*i*
TMA…$BH_2COO(H_2O)^-$.	364.1976*i*	278.0357*i*	278.6883*i*	278.1473*i*	289.6412*i*
TMA…$BH_2COO(H_2O)_2^-$.	359.6883*i*	241.0862*i*	241.0247*i*	238.9556*i*	238.9854*i*
TMA…$BH_2COO(H_2O)_3^-$.	301.1473*i*	181.7069*i*	184.7966*i*	184.5482*i*	192.9984*i*
CO…BH_2O^-	491.9006*i*	382.4063*i*	382.3870*i*	382.1343*i*	406.4770*i*
CO…$BH_2O(H_2O)^-$	402.5600*i*	380.1186*i*	380.2659*i*	380.2013*i*	402.7236*i*
CO…$BH_2O(H_2O)_2^-$	364.3893*i*	391.7935*i*	391.3612*i*	391.6203*i*	406.2518*i*
CO…$BH_2O(H_2O)_3^-$	358.8720*i*	407.0097*i*	406.9429*i*	407.5284*i*	413.4166*i*

Table S2. Energies of reactants, intermediates, transition states, and products

		M06-2X/ 6-311++G(2d,p)[a]				CCSD(T)[b]	
	Gas phase	PCM-H_2O				PCM-H_2O	
	G_{298}	E_{elect}	H_{298}	S^d	G_{298}	G_{298}	ΔG_{solv}[c]
T[e]	-174.337916	-174.43519	-174.307831	70.397	-174.34128	-173.986054	-2.111
T-BH_2COOH	-389.547108	-389.700225	-389.516732	92.711	-389.560782	-388.810165	-8.581
T-BH_2COO^-	-388.972556	-389.216801	-389.046886	91.463	-389.090383	-388.339320	-73.938
T-$BH_2COO(H_2O)^-$	-465.405976	-465.664093	-465.466918	105.703	-465.517141	-464.643924	-69.757
T-$BH_2COO(H_2O)_2^-$	-541.834658	-542.106070	-541.881160	123.462	-541.939821	-540.945731	-65.991
T-$BH_2COO(H_2O)_3^-$	-618.264569	-618.550644	-618.297943	141.212	-618.365038	-617.249554	-63.045
T…BH_2COO^- (t.s.)	-388.954776	-389.169540	-389.003471	100.682	-389.051308	-388.300443	-60.575
T…$BH_2COO(H_2O)^-$.. (t.s.)	-465.382584	-465.609793	-465.416604	122.262	-465.474694	-464.602706	-57.800
T…$BH_2COO(H_2O)_2^-$. (t.s.)	-541.806173	-542.049301	-541.828637	142.750	-541.896462	-540.903906	-56.657
T…$BH_2COO(H_2O)_3^-$. (t.s.)	-618.233118	-618.490175	-618.241723	161.070	-618.318253	-617.204535	-53.423
BH_2COO^-	-214.639092	-214.736988	-214.699326	63.922	-214.729698	-214.330286	-56.856
$BH_2COO(H_2O)^-$	-291.063575	-291.175327	-291.110270	84.300	-291.150323	-290.630343	-54.435
$BH_2COO(H_2O)_2^-$	-367.486261	-367.613239	-367.520645	104.848	-367.570461	-366.930427	-52.836
$BH_2COO(H_2O)_3^-$	-443.907906	-444.056543	-443.935518	114.803	-443.990065	-443.228671	-51.556
CO…BH_2O^- (t.s.)	-214.601685	-214.700108	-214.665479	65.475	-214.696588	-214.305080	-59.553
CO…$BH_2O(H_2O)^-$ (t.s.)	-291.035233	-291.148066	-291.086301	83.522	-291.125986	-290.611638	-56.948
CO…$BH_2O(H_2O)_2^-$ (t.s.)	-367.464462	-367.593510	-367.504156	101.725	-367.552489	-366.916971	-55.238
CO…$BH_2O(H_2O)_3^-$ (t.s.)	-443.890899	-444.038715	-443.921067	110.324	-443.973486	-443.216098	-51.824
BH_2O^-	-101.314386	-101.418647	-101.393838	52.741	-101.418897	-101.228573	-65.582
$BH_2O(H_2O)^-$	-177.751913	-177.866293	-177.814253	71.884	-177.848407	-177.535383	-60.551
$BH_2O(H_2O)_2^-$	-254.183762	-254.311506	-254.231871	90.781	-254.275004	-253.840506	-57.255
$BH_2O(H_2O)_3^-$	-330.608428	-330.753226	-330.645307	106.506	-330.695911	-330.139668	-54.896
CO	-113.326619	-113.313299	-113.304817	47.176	-113.327232	-113.133458	-0.385
H_2O	-76.418127	-76.429755	-76.404485	45.074	-76.425909	-76.305603	-4.883

[a]M06-2X energies (a.u.): $H_{298} = E_{elect} + ZPVE + thermal\text{-}correction\text{-}to\text{-}298 + RT$, where T is temperature in K, and R = gas constant. The thermal correction = $E_{tr} + E_{vib} + E_{rot} + E_{elec}$, where $E_{tr} = 3RT/2$, $E_{rot} = 3RT/2$, $E_{elec} \approx 0.000$, $E_{vib} = R\Sigma\theta_i[0.5 + (\exp(\theta_i/T)\text{-}1)]$ with θ_i = vibrational temperature of the *i*th vibration; $G_{298} = H_{298} - TS_{tot}$. [b]CCSD(T) energies (a.u.): $H_{298,CCSD(T)} = E_{elect,CCSD(t)} + (ZPVE + thermal\text{-}correction)_{M06\text{-}2X} + RT$; and $G_{298,CCSD(t)} = H_{298,CCSD(T)} - TS_{tot,M06\text{-}2X}$. [c] Gibbs free energy of solvation (kcal mol^{-1}) = $\Delta G_{solv} = G^o_{298}(PCM\text{-}H_2O) - G^o_{298}$ (gas phase). [d] cal/mol-K [e]T = TMA

Table S3. Cartesion coordinates of all compounds in Tables 1 and S2. M06-2X/6-311++G(2d,p)

	gas	Pcm ("scrf=solvent=water")
TMA	6 0.000000 1.376971 -0.063448 7 0.000000 0.000000 0.392918 6 -1.192492 -0.688486 -0.063448 1 -1.195912 -1.711805 0.314459 1 -2.080423 -0.179788 0.314459 1 -1.256325 -0.725340 -1.165040 6 1.192492 -0.688486 -0.063448 1 1.195912 -1.711805 0.314459 1 1.256325 -0.725340 -1.165040 1 2.080423 -0.179788 0.314459 1 0.884511 1.891593 0.314459 1 0.000000 1.450679 -1.165040 1 -0.884511 1.891593 0.314459	6 0.000028 -0.000506 0.000000 7 0.467870 -1.377686 0.000000 6 0.000001 -2.066257 1.192677 1 0.371420 -3.091781 1.197827 1 0.371400 -1.557904 2.083348 1 -1.101192 -2.096029 1.244375 6 0.000001 -2.066257 -1.192677 1 0.371420 -3.091781 -1.197827 1 -1.101192 -2.096029 -1.244375 1 0.371400 -1.557904 -2.083348 1 0.371528 0.516618 -0.885579 1 -1.101141 0.059163 0.000000 1 0.371528 0.516618 0.885579
TMA-BH2COOH	7 1.084235 0.065305 -0.000058 5 -0.255958 0.980372 -0.000123 6 -1.569422 0.048321 0.000050 8 -1.642389 -1.166343 0.000185 8 -2.712095 0.772377 0.000071 1 -3.442069 0.135133 0.000185 1 -0.214127 1.647492 1.002045 1 -0.214211 1.647225 -1.002471 6 1.148567 -0.790088 1.210929 1 2.088704 -1.345575 1.214852 1 1.092242 -0.147634 2.087539 1 0.303317 -1.472760 1.197202 6 1.148445 -0.790426 -1.210812 1 2.088551 -1.345968 -1.214639 1 0.303160 -1.473050 -1.196841 1 1.092104 -0.148212 -2.087596 6 2.248348 0.979339 -0.000242 1 3.172275 0.397452 -0.000245 1 2.200161 1.607778 -0.886823 1 2.200290 1.607971 0.886209	7 -1.088726 0.065926 0.000005 5 0.251947 0.951777 -0.000035 6 1.579796 0.036562 -0.000020 8 1.691270 -1.175287 -0.000017 8 2.707322 0.793383 0.000038 1 3.464948 0.187515 0.000022 1 0.234346 1.627219 -0.999851 1 0.234447 1.627213 0.999810 6 -1.170258 -0.790366 -1.211894 1 -2.114052 -1.336435 -1.205279 1 -1.118557 -0.150999 -2.090639 1 -0.334551 -1.484089 -1.205370 6 -1.170086 -0.790711 1.211674 1 -2.114238 -1.336156 1.205421 1 -0.334823 -1.484958 1.204476 1 -1.117462 -0.151658 2.090596 6 -2.248793 0.992584 0.000228 1 -3.173257 0.414536 -0.000090 1 -2.199170 1.616781 0.889442 1 -2.198989 1.617479 -0.888485
TMA-BH2COO-	7 -0.013610 0.005101 -0.000028 5 1.377890 0.935198 0.000217 6 2.716066 -0.003785 0.000151 8 2.601689 -1.277515 -0.000059 8 3.800704 0.617549 0.000318 1 1.254459 1.604276 -1.009851 1 1.254325 1.603944 1.010488 6 -1.183481 0.891626 0.000038 1 -2.107411 0.301840 -0.000121 1 -1.142588 1.523902 0.885445 1 -1.142469 1.524191 -0.885157 6 -0.038728 -0.848617 1.206322 1 -0.952150 -1.454385 1.212741 1 0.861260 -1.463955 1.172486 1 -0.014728 -0.198618 2.080363 6 -0.038567 -0.848224 -1.206660 1 -0.951987 -1.453991 -1.213397 1 -0.014453 -0.197941 -2.080485 1 0.861418 -1.463571 -1.172904	7 1.041474 0.067591 -0.000008 5 -0.319010 0.964821 -0.000033 6 -1.697600 0.093918 0.000006 8 -1.699923 -1.175590 0.000047 8 -2.766696 0.778097 -0.000009 1 -0.242241 1.648369 1.002188 1 -0.242252 1.648297 -1.002305 6 2.212813 0.972196 -0.000048 1 3.132109 0.383761 -0.000030 1 2.173390 1.598925 -0.888316 1 2.173399 1.598994 0.888170 6 1.104578 -0.789510 -1.208295 1 2.031389 -1.366243 -1.200166 1 0.238854 -1.445578 -1.197469 1 1.078226 -0.147721 -2.087097 6 1.104591 -0.789420 1.208342 1 2.031399 -1.366156 1.200245 1 1.078252 -0.147565 2.087096 1 0.238865 -1.445486 1.197575
TMA-BH2COO-…H2O	7 1.386733 0.335311 0.000001 5 -0.263870 0.496942 0.000002 6 -1.004586 -0.959044 0.000001 8 -0.317716 -2.024048 -0.000010 8 -2.266252 -0.935965 0.000010 1 -0.485298 1.141558 1.007858 1 -0.485300 1.141560 -1.007853 6 1.995155 1.673651 0.000007 1 3.087293 1.591273 0.000004 1 1.659460 2.210362 -0.885514 1 1.659463 2.210353 0.885533 6 1.820366 -0.401276 -1.207708 1 2.911923 -0.491152 -1.212250 1 1.332604 -1.375025 -1.178226 1 1.487263 0.156830 -2.081782 6 1.820366 -0.401286 1.207703 1 2.911923 -0.491158 1.212247 1 1.487258 0.156810 2.081781	7 -1.386150 0.315429 0.000196 5 0.230511 0.461777 -0.000112 6 1.024472 -0.961513 -0.000213 8 0.435848 -2.074392 -0.000155 8 2.303182 -0.876916 -0.000367 1 0.494881 1.096743 -1.001259 1 0.495245 1.096804 1.000899 6 -1.986313 1.669499 0.000298 1 -3.074608 1.588397 0.000502 1 -1.653369 2.201717 0.888621 1 -1.653702 2.201702 -0.888158 6 -1.850628 -0.407435 1.209836 1 -2.940212 -0.469039 1.201797 1 -1.407202 -1.398934 1.200703 1 -1.519567 0.143749 2.088078 6 -1.851106 -0.407457 -1.209248 1 -2.940688 -0.469055 -1.200780 1 -1.520387 0.143707 -2.087631

	1 1.332608 -1.375037 1.178210 8 -3.356681 1.493743 -0.000002 1 -2.537724 1.995781 -0.000038 1 -3.011877 0.553852 0.000007	1 -1.407684 -1.398958 -1.200271 8 3.291649 1.535922 -0.000329 1 2.514501 2.102481 -0.000206 1 2.899311 0.608323 -0.000338
TMA-BH2COO-..2H2O	7 -1.893489 0.275829 0.152825 5 -0.312048 0.558509 -0.234562 6 0.503729 -0.836436 -0.450212 8 -0.072147 -1.949700 -0.341030 8 1.739880 -0.712370 -0.727348 1 -0.370559 1.231287 -1.243911 1 0.105429 1.196805 0.713362 6 -2.570878 1.567779 0.343652 1 -3.623071 1.406275 0.599190 1 -2.069909 2.110451 1.143167 1 -2.492034 2.143251 -0.576862 6 -1.976079 -0.509584 1.405065 1 -3.026284 -0.669639 1.669651 1 -1.456796 -1.450449 1.230996 1 -1.472915 0.051941 2.190882 6 -2.557492 -0.468683 -0.940508 1 -3.609393 -0.634702 -0.686440 1 -2.481808 0.126146 -1.849731 1 -2.019314 -1.407335 -1.063321 8 2.704803 1.724213 -0.646510 1 1.955945 2.192823 -0.268263 1 2.326119 0.799712 -0.779227 8 3.845692 -0.323648 1.147530 1 3.744467 0.559241 0.765241 1 3.163270 -0.805574 0.649174	7 -1.697814 0.268463 0.150700 5 -0.128884 0.532772 -0.152903 6 0.666947 -0.779835 -0.694363 8 0.103547 -1.853821 -1.003507 8 1.948175 -0.639581 -0.787192 1 -0.099985 1.414901 -0.986336 1 0.344685 0.915899 0.898409 6 -2.294312 1.512467 0.690931 1 -3.355608 1.353542 0.888129 1 -1.780709 1.778327 1.612114 1 -2.166995 2.308744 -0.039253 6 -1.861384 -0.810869 1.155772 1 -2.920947 -0.942633 1.380507 1 -1.439943 -1.723584 0.744736 1 -1.325201 -0.524762 2.059018 6 -2.424258 -0.103493 -1.089222 1 -3.478842 -0.262921 -0.858428 1 -2.322683 0.710480 -1.804454 1 -1.974262 -1.008802 -1.485966 8 2.787398 1.893517 -0.724254 1 1.998266 2.382922 -0.473057 1 2.470996 0.951025 -0.752081 8 2.621830 -0.657029 1.887833 1 1.933618 -0.084791 2.240753 1 2.437170 -0.665756 0.923772
TMA-BH2COO-..3H2O	7 0.081789 -0.055328 0.030483 5 -1.356491 0.693863 0.313427 6 -2.606848 -0.337394 0.175066 8 -2.415175 -1.568523 -0.036990 8 -3.768443 0.169705 0.293086 1 -1.249992 1.132218 1.441447 1 -1.400686 1.576697 -0.517083 6 1.156753 0.945743 0.136865 1 2.127488 0.472409 -0.039122 1 0.981337 1.727293 -0.599780 1 1.128514 1.384503 1.132539 6 0.093270 -0.637022 -1.331672 1 1.070005 -1.089372 -1.528609 1 -0.704104 -1.375194 -1.380624 1 -0.100597 0.163491 -2.043941 6 0.313532 -1.125403 1.027409 1 1.281444 -1.599491 0.837848 1 0.306800 -0.673254 2.018053 1 -0.504312 -1.837502 0.938934 8 -5.055677 -2.422393 0.399214 1 -4.103024 -2.426671 0.191532 1 -5.163415 -1.463194 0.468155 8 -3.732092 2.788963 0.864485 1 -2.780619 2.926669 0.855746 1 -3.797826 1.801244 0.755236 8 -4.519201 1.999160 -1.854839 1 -4.336638 2.610203 -1.127433 1 -4.349084 1.149669 -1.418065	7 2.058257 -0.073102 -0.024239 5 0.636778 0.613742 0.328463 6 -0.625492 -0.407117 0.258772 8 -0.501622 -1.654136 0.120937 8 -1.786545 0.137539 0.361969 1 0.750046 1.051198 1.454212 1 0.496446 1.512294 -0.475298 6 3.108682 0.972199 0.009236 1 4.078349 0.523063 -0.210300 1 2.873637 1.731392 -0.733212 1 3.123395 1.423229 0.999042 6 2.029445 -0.672321 -1.381841 1 3.011835 -1.082674 -1.620455 1 1.275677 -1.454188 -1.393585 1 1.770945 0.106735 -2.096872 6 2.405173 -1.122261 0.967433 1 3.374699 -1.554288 0.714812 1 2.451763 -0.662244 1.952550 1 1.628250 -1.880502 0.945295 8 -3.100952 -2.434849 0.174860 1 -2.125116 -2.298797 0.136404 1 -3.375879 -1.516276 0.283881 8 -1.718963 2.621332 1.416016 1 -0.779924 2.830235 1.422975 1 -1.746183 1.709710 1.033118 8 -1.993862 1.508244 -2.039367 1 -1.128696 1.924652 -2.097933 1 -1.962238 1.031425 -1.184198
TMA---BH2COO- ts	7 -1.290352 0.071743 -0.000013 5 0.871706 1.194010 -0.000114 6 1.821312 -0.035273 -0.000017 8 1.793117 -1.277165 0.000041 8 2.827580 0.749634 -0.000041 1 0.606488 1.740100 -1.034609 1 0.606500 1.740225 1.034319 6 -2.451914 0.925384 -0.000243 1 -3.398323 0.351097 -0.000303 1 -2.435554 1.565349 0.884764 1 -2.435339 1.565192 -0.885361 6 -1.202010 -0.740821 1.196843 1 -2.063392 -1.428920 1.287292 1 -0.271745 -1.310664 1.157155 1 -1.178985 -0.090129 2.073663 6 -1.201949 -0.741372 -1.196495 1 -2.063188 -1.429702 -1.286518	7 1.353715 0.082318 0.000010 5 -0.977853 1.173748 -0.000106 6 -1.884994 -0.071555 -0.000011 8 -2.020664 -1.297217 0.000087 8 -2.810501 0.832027 -0.000098 1 -0.688037 1.692478 1.036939 1 -0.688008 1.692297 -1.037234 6 2.542760 0.912671 -0.000088 1 3.469276 0.314368 -0.000063 1 2.546219 1.550471 -0.885985 1 2.546264 1.550612 0.885708 6 1.282406 -0.739448 -1.194121 1 2.130330 -1.441416 -1.263420 1 0.350445 -1.306903 -1.179519 1 1.289779 -0.101330 -2.079806 6 1.282436 -0.739213 1.194304 1 2.130363 -1.441167 1.263724

	1 -1.179189 -0.091077 -2.073618 1 -0.271551 -1.310986 -1.156645	1 1.289823 -0.100924 2.079866 1 0.350478 -1.306675 1.179832
TMA---BH2COO-..H2O ts	7 -1.745408 -0.342141 -0.013262 5 0.607255 -0.365191 -0.708414 6 1.072804 0.982519 -0.106011 8 0.700357 1.975835 0.519325 8 2.245012 0.708104 -0.573055 1 0.783687 -1.376832 -0.086207 1 0.280566 -0.428892 -1.857754 6 -2.543140 -1.481646 -0.394464 1 -3.591893 -1.396613 -0.052351 1 -2.540987 -1.581819 -1.481891 1 -2.112382 -2.389133 0.033810 6 -2.212511 0.886805 -0.623417 1 -3.240720 1.137479 -0.303914 1 -1.531756 1.692711 -0.344141 1 -2.199648 0.777983 -1.709873 6 -1.629096 -0.206345 1.425145 1 -2.612677 -0.040269 1.901592 1 -1.187856 -1.115104 1.839583 1 -0.967238 0.633844 1.641466 8 3.755828 -1.454589 0.301440 1 2.985640 -2.024098 0.229871 1 3.378924 -0.591108 0.035512	7 -1.821140 -0.302530 -0.036090 5 0.644369 -0.245659 -0.881667 6 1.182926 0.965396 -0.097966 8 1.042639 1.896532 0.686477 8 2.268974 0.618120 -0.737582 1 0.766656 -1.339774 -0.416118 1 0.220739 -0.097815 -1.987507 6 -2.756729 -1.310003 -0.498945 1 -3.751860 -1.196814 -0.037142 1 -2.871082 -1.236922 -1.581810 1 -2.377288 -2.304174 -0.256592 6 -2.265337 1.032438 -0.393255 1 -3.230484 1.286223 0.076042 1 -1.514220 1.755559 -0.071991 1 -2.379465 1.104126 -1.476426 6 -1.602582 -0.405021 1.395217 1 -2.529335 -0.233526 1.967796 1 -1.225759 -1.400107 1.638679 1 -0.857978 0.333734 1.695635 8 3.655519 -1.520203 0.347828 1 3.004167 -2.227098 0.333557 1 3.185323 -0.749868 -0.027252
TMA---BH2COO-..2H2O ts	7 -2.084216 -0.000039 -0.277629 5 0.356331 -0.000122 -0.593792 6 0.799770 0.000113 0.885227 8 0.446827 0.000292 2.055662 8 2.011106 0.000030 0.394592 1 0.277385 -1.035462 -1.191709 1 0.277362 1.035040 -1.192013 6 -2.889375 -0.000429 -1.475325 1 -3.973117 -0.000452 -1.255066 1 -2.657871 0.884424 -2.071760 1 -2.657734 -0.885579 -2.071266 6 -2.280674 1.197311 0.515774 1 -3.323689 1.288217 0.869032 1 -1.605444 1.163934 1.372083 1 -2.037134 2.074886 -0.086425 6 -2.280504 -1.197008 0.516396 1 -3.323528 -1.287916 0.869631 1 -2.036765 -2.074851 -0.085332 1 -1.605328 -1.163060 1.372721 8 2.874508 -2.443448 -0.687338 1 2.105937 -2.419334 -1.263064 1 2.756194 -1.622684 -0.172708 8 2.874354 2.443381 -0.687655 1 2.105777 2.419092 -1.263366 1 2.756156 1.622671 -0.172910	7 2.198723 0.016171 -0.291625 5 -0.436930 0.028331 -0.582377 6 -0.856090 -0.001276 0.897078 8 -0.638303 -0.022194 2.095764 8 -2.034001 0.000905 0.297248 1 -0.324896 1.078288 -1.139165 1 -0.311111 -0.999104 -1.176778 6 3.123990 0.052264 -1.409104 1 4.175724 0.025550 -1.078256 1 2.948083 -0.804835 -2.061357 1 2.969503 0.965147 -1.986738 6 2.345757 -1.211839 0.469037 1 3.354177 -1.308843 0.904784 1 1.610347 -1.224185 1.274974 1 2.166683 -2.070431 -0.180683 6 2.371432 1.173519 0.568257 1 3.381064 1.211785 1.010366 1 2.213295 2.086901 -0.008105 1 1.635036 1.135025 1.372429 8 -3.016911 2.414520 -0.682936 1 -2.355455 2.662163 -1.335110 1 -2.691254 1.572207 -0.314127 8 -2.935008 -2.442842 -0.689597 1 -2.251100 -2.675358 -1.323982 1 -2.643259 -1.588284 -0.320431
TMA---BH2COO-..3H2O ts	7 0.102230 0.008676 0.092348 5 0.494547 -0.468765 2.600573 6 1.972609 -0.044623 2.658235 8 2.967426 0.378765 2.078982 8 1.848324 -0.367287 3.917861 1 -0.350337 0.337803 2.864447 1 0.207736 -1.611784 2.420465 6 -1.199012 -0.233156 -0.484152 1 -1.230930 0.000651 -1.564801 1 -1.470416 -1.282144 -0.350339 1 -1.945513 0.381383 0.023020 6 1.120584 -0.842471 -0.490697 1 1.234212 -0.662961 -1.575350 1 2.071103 -0.649856 0.008592 1 0.851257 -1.889167 -0.336346 6 0.479496 1.405996 0.015538 1 0.547538 1.756724 -1.030421 1 -0.262931 2.012385 0.538378 1 1.445697 1.538827 0.504235 8 4.766665 0.101742 4.278256 1 4.375293 0.303099 3.410750 1 3.983800 -0.220120 4.740641 8 0.108322 0.846935 5.729005 1 -0.619183 0.806272 5.101441 1 0.872959 0.615440 5.167550	7 -2.653846 0.002842 -0.063305 5 -0.086216 0.123451 -0.944302 6 0.623666 -0.027620 0.409045 8 0.684180 -0.168891 1.622385 8 1.638660 0.073067 -0.428372 1 -0.331841 -0.851124 -1.586359 1 -0.340794 1.215092 -1.351352 6 -3.838417 0.108469 -0.895939 1 -4.767449 0.026187 -0.307177 1 -3.843254 1.070563 -1.410771 1 -3.835882 -0.685724 -1.644262 6 -2.607400 1.077693 0.912305 1 -3.471988 1.050700 1.596581 1 -1.691827 0.991792 1.499376 1 -2.604774 2.040938 0.399045 6 -2.598150 -1.288527 0.598701 1 -3.461278 -1.446961 1.266796 1 -2.589643 -2.085049 -0.147454 1 -1.682078 -1.352223 1.187832 8 3.486894 -0.243064 1.874187 1 2.513557 -0.233526 1.940912 1 3.618398 -0.124285 0.926905 8 2.386446 -2.362188 -1.608052 1 1.599930 -2.611747 -2.101589 1 2.155012 -1.512872 -1.192200

	8 0.562389 -2.084703 5.921282 1 0.272637 -1.205150 6.197113 1 1.075121 -1.878287 5.126823	8 2.369402 2.685556 -1.151936 1 1.598327 2.998494 -1.633520 1 2.140737 1.776671 -0.888486
BH2COO- cyclic	5 0.000072 -0.002007 -0.000013 1 -0.560708 -0.304478 1.028805 6 1.498987 0.377782 0.000007 8 2.715289 0.347177 0.000037 8 0.689938 1.422800 -0.000074 1 -0.560653 -0.304590 -1.028829	5 -1.214188 -0.551911 0.000036 1 -1.764778 -0.841735 1.029181 6 0.280329 -0.168396 -0.000054 8 1.499491 -0.202800 0.000046 8 -0.509683 0.884565 -0.000059 1 -1.764722 -0.842456 -1.028937
BH2COO-…H2O	5 -0.268864 1.313670 -0.201573 6 -1.124185 0.032066 -0.103697 8 -1.967382 -0.822474 -0.255500 8 -0.076233 0.038045 0.724470 1 0.552950 1.425028 -1.085379 1 -0.587585 2.326131 0.368836 8 2.551308 -0.489070 -0.126706 1 1.692491 -0.574396 0.323243 1 2.370030 0.250481 -0.714762	5 -0.435161 1.367836 -0.289428 6 -1.076386 -0.022913 -0.112818 8 -1.762973 -1.016874 -0.231910 8 -0.103502 0.200424 0.767025 1 0.416191 1.526720 -1.123418 1 -0.951253 2.341186 0.184884 8 2.488298 -0.485048 -0.084667 1 1.594376 -0.307590 0.256996 1 2.600222 0.149974 -0.797998
BH2COO-…2H2O	5 0.000302 0.218945 1.297500 6 0.000253 1.256118 0.157134 8 0.000284 2.268558 -0.494651 8 0.000000 -0.023254 -0.276224 1 1.026672 -0.076696 1.859661 1 -1.025973 -0.076466 1.859957 8 2.493297 -1.383607 -0.313708 1 1.672481 -0.957485 -0.611889 1 2.466054 -1.197128 0.629321 8 -2.493925 -1.382912 -0.313591 1 -2.466633 -1.196924 0.629534 1 -1.672888 -0.957020 -0.611490	5 0.000007 0.331662 1.396448 6 -0.000020 1.221293 0.139122 8 -0.000047 2.156172 -0.627110 8 0.000005 -0.088229 -0.165724 1 1.031285 0.098221 1.962593 1 -1.031254 0.098180 1.962607 8 2.525178 -1.335538 -0.360735 1 1.649344 -0.913055 -0.365999 1 2.819227 -1.265362 0.552090 8 -2.525138 -1.335597 -0.360727 1 -2.819192 -1.265413 0.552097 1 -1.649312 -0.913097 -0.365993
BH2COO-…3H2O	5 -1.079160 0.000023 1.399612 6 0.446749 -0.000006 1.203628 8 1.644391 -0.000026 1.373236 8 -0.224632 0.000002 0.039171 1 -1.661591 -1.027388 1.629640 1 -1.661553 1.027457 1.629633 8 2.468648 -0.000054 -1.368654 1 2.413911 -0.000050 -0.397586 1 1.536481 -0.000035 -1.607663 8 -1.463333 -2.442097 -0.879391 1 -1.941073 -2.363980 -0.048765 1 -0.862424 -1.683308 -0.828008 8 -1.463217 2.442153 -0.879399 1 -1.940967 2.364064 -0.048777 1 -0.862346 1.683335 -0.828008	5 -0.191041 -1.615487 1.063977 6 -0.030399 -0.097137 1.256674 8 0.086393 1.017600 1.723531 8 -0.053853 -0.428565 -0.040507 1 0.771150 -2.324637 1.128988 1 -1.282980 -2.104791 1.109374 8 0.311987 2.470278 -0.711270 1 0.250600 2.098780 0.186460 1 0.199828 1.693472 -1.269157 8 2.513490 -0.923858 -1.146677 1 2.754331 -1.754421 -0.726423 1 1.628698 -0.721803 -0.801216 8 -2.651888 -0.468375 -1.197485 1 -3.083020 -1.145053 -0.667469 1 -1.750047 -0.417932 -0.841215
BH2O----CO ts	5 -0.063607 0.004674 -0.000008 1 -0.399467 -0.612610 1.018809 6 1.713568 0.150687 -0.000383 8 2.712243 0.733111 0.000102 8 0.206823 1.339690 -0.000118 1 -0.400190 -0.612711 -1.018501	5 -1.095845 -0.558339 0.000073 1 -1.446617 -1.166113 1.010498 6 0.549374 -0.388110 -0.000245 8 1.588225 0.096014 0.000092 8 -0.953624 0.835572 -0.000007 1 -1.447213 -1.166217 -1.010071
BH2O----CO...H2O ts	5 0.289722 1.282201 0.312872 6 1.288727 -0.071096 0.312454 8 1.746951 -1.071453 -0.014096 8 -0.182093 0.568738 -0.786571 1 -0.342262 1.309845 1.372682 1 0.981661 2.288657 0.185919 8 -2.315135 -0.640510 0.098243 1 -1.505183 -0.219520 -0.338181 1 -2.312980 -0.217608 0.959893	5 0.410488 1.280264 0.338098 6 1.231867 -0.094389 0.262140 8 1.645258 -1.130608 -0.000800 8 -0.177265 0.587071 -0.775806 1 -0.213396 1.364867 1.385294 1 1.123806 2.249025 0.147545 8 -2.277954 -0.595315 0.090315 1 -1.446263 -0.124459 -0.264766 1 -2.428105 -0.213603 0.958924
BH2O----CO...2H2O ts	5 0.414588 0.611600 1.333642 6 -0.296337 1.301184 0.033326 8 -0.823223 1.467093 -0.972398 8 0.187045 -0.492513 0.468531 1 1.552840 1.043897 1.475197 1 -0.268325 0.782089 2.329118 8 2.582554 -0.807562 -0.651197 1 1.646604 -0.800839 -0.309031 1 3.009967 -0.178803 -0.065164 8 -2.266199 -1.375365 -0.052597 1 -2.331365 -0.901132 -0.884817 1 -1.346049 -1.143541 0.247818	5 -0.004806 0.242368 1.295802 6 0.033765 1.434431 0.224540 8 0.066109 2.078155 -0.723274 8 -0.015749 -0.432574 0.026516 1 1.012005 0.223981 1.973124 1 -1.012638 0.275473 1.979036 8 2.420426 -1.269238 -0.402417 1 1.477814 -0.960220 -0.255493 1 2.880581 -1.052107 0.412570 8 -2.480230 -1.181265 -0.411047 1 -2.932597 -0.961323 0.407526 1 -1.528171 -0.904850 -0.261235
BH2O----CO...3H2O ts	5 -1.185797 -0.000080 1.187394 6 -2.378878 -0.000007 0.114536	5 -1.210041 -0.000605 1.239886 6 -2.290678 -0.000163 0.100639

	8 -3.037938 0.000023 -0.821376 8 -0.508092 -0.000062 -0.083259 1 -1.191926 1.014807 1.864756 1 -1.192000 -1.015011 1.864688 8 3.185776 0.000097 -0.194631 1 2.585032 -0.761721 -0.223006 1 2.584970 0.761867 -0.222984 8 1.088763 -2.046266 -0.140874 1 1.010076 -2.332080 0.772235 1 0.429775 -1.286232 -0.202269 8 1.088589 2.046280 -0.140819 1 1.009869 2.332058 0.772299 1 0.429672 1.286185 -0.202239	8 -2.948402 0.000291 -0.840208 8 -0.499765 -0.000273 -0.054553 1 -1.193368 1.016330 1.898284 1 -1.193475 -1.017916 1.897690 8 3.083293 0.000511 -0.158126 1 2.485582 -0.767014 -0.147710 1 2.485203 0.767742 -0.147524 8 1.085356 -2.031304 -0.180042 1 0.976985 -2.521029 0.640158 1 0.409000 -1.283487 -0.142453 8 1.084516 2.031410 -0.179599 1 0.975916 2.520975 0.640666 1 0.408442 1.283319 -0.142154
BH2O-	5 0.000000 0.000000 0.014545 8 0.000000 0.000000 1.296008 1 0.000000 1.040387 -0.687452 1 0.000000 -1.040387 -0.687452	5 0.000000 0.000000 -0.598675 8 0.000000 0.000000 0.693393 1 0.000000 1.035023 -1.276885 1 0.000000 -1.035023 -1.276885
BH2O-….H2O	5 1.432498 0.432485 0.000000 1 0.921074 1.566854 0.000004 1 2.668894 0.441961 -0.000001 8 0.727262 -0.648494 -0.000002 8 -1.767508 0.042426 0.000002 1 -0.812934 -0.313086 0.000001 1 -1.617551 0.990395 -0.000005	5 -1.457968 0.427536 0.000000 1 -0.978476 1.559546 0.000004 1 -2.681913 0.376076 -0.000004 8 -0.710328 -0.637048 0.000000 8 1.761955 0.033040 0.000000 1 0.777793 -0.234750 0.000000 1 1.759426 0.993510 -0.000003
BH2O-…2H2O	5 0.000003 1.324950 -0.000019 1 1.038385 1.989214 -0.000030 1 -1.038374 1.989221 -0.000031 8 -0.000001 0.028480 0.000003 8 2.574542 -0.644857 0.000012 1 1.584296 -0.520751 0.000011 1 2.882821 0.264090 -0.000008 8 -2.574544 -0.644855 0.000005 1 -2.882823 0.264092 -0.000009 1 -1.584298 -0.520750 0.000006	5 -0.000031 1.453339 0.000013 1 -1.038089 2.096042 0.000014 1 1.037994 2.096097 0.000058 8 0.000003 0.146099 -0.000016 8 -2.456174 -0.743933 0.000021 1 -1.510533 -0.410107 -0.000027 1 -3.000424 0.047643 -0.000135 8 2.456190 -0.743913 0.000019 1 3.000484 0.047631 -0.000142 1 1.510570 -0.410028 -0.000024
BH2O-…3H2O	5 -0.823833 -1.222543 -1.115846 8 -0.367410 -0.437666 -0.177585 1 -1.983933 -1.137358 -1.513890 1 -0.141514 -2.083348 -1.648314 8 1.694838 1.560895 -0.663710 1 0.813617 1.154957 -0.679743 1 2.183080 0.889786 -0.166833 8 -2.615436 0.740524 0.749889 1 -3.167126 0.383750 0.050057 1 -1.724911 0.381712 0.507763 8 1.953262 -0.869284 0.929930 1 1.763036 -0.644802 1.843300 1 1.054887 -0.787730 0.478697	5 0.620258 -1.666520 0.749178 8 0.300223 -0.638613 -0.000222 1 1.765127 -1.844607 1.127757 1 -0.207353 -2.488457 1.097858 8 -1.009609 1.756992 0.720182 1 -0.347405 1.052106 0.619565 1 -1.772734 1.355863 0.281530 8 2.480786 0.718208 -0.627957 1 3.164978 0.364769 -0.053466 1 1.660976 0.199845 -0.402676 8 -2.240546 -0.479265 -0.637861 1 -2.346534 -0.552048 -1.590206 1 -1.265189 -0.613454 -0.459378
CO	6 0.000000 0.000000 -0.640461 8 0.000000 0.000000 0.480346	6 0.000000 0.000000 -0.640410 8 0.000000 0.000000 0.480307
H2O	8 0.000000 0.000000 0.116508 1 0.000000 0.763311 -0.466031 1 0.000000 -0.763311 -0.466031	8 0.000000 0.000000 0.117658 1 0.000000 0.761402 -0.470630 1 0.000000 -0.761402 -0.470630

Table S4. Cartesian coordinates of selected compounds. M06-2X/PCM-H_2O with Gaussian 09's calendar versions of the Dunning correlation consistent triple-ζ basis sets.

	jun-cc-pVTZ	jul-cc-pVTZ	aug-cc-pVTZ
TMA	6 -0.583840 1.246683 0.063782	6 -1.369161 -0.144175 0.063573	6 1.369741 0.138554 0.063573
	7 0.000011 -0.000012 -0.399364	7 -0.000059 -0.000015 -0.398629	7 0.000059 0.000015 -0.398629
	6 -0.787853 -1.128901 0.063781	6 0.559816 1.257896 0.063642	6 -0.564974 -1.255588 0.063642
	1 -0.823378 -1.179690 1.164060	1 0.584270 1.315468 1.163807	1 -0.589664 -1.313059 1.163807
	1 -1.808872 -1.045869 -0.307511	1 1.578190 1.369206 -0.307045	1 -1.583796 -1.362717 -0.307045
	1 -0.357544 -2.058562 -0.307359	1 -0.038509 2.088902 -0.308413	1 0.029935 -2.089042 -0.308413
	6 1.371684 -0.117781 0.063774	6 0.809547 -1.113691 0.063641	6 -0.804969 1.117004 0.063641
	1 1.433407 -0.123249 1.164041	1 0.845771 -1.164716 1.163811	1 -0.840983 1.168178 1.163811
	1 1.810238 -1.043509 -0.307567	1 0.397266 -2.051147 -0.308109	1 -0.388844 2.052760 -0.308109
	1 1.961562 0.719808 -0.307312	1 1.828682 -1.010625 -0.307341	1 -1.824518 1.018122 -0.307341
	1 -0.610044 1.302838 1.164062	1 -1.431609 -0.150945 1.163820	1 1.432217 0.145068 1.163820
	1 -0.001295 2.089300 -0.307442	1 -1.975022 0.681842 -0.307471	1 1.972207 -0.689942 -0.307471
	1 -1.604097 1.339012 -0.307448	1 -1.789839 -1.078066 -0.307796	1 1.794249 1.070711 -0.307796
TMA-BH2COOH	7 -1.090329 0.065613 -0.000001	7 1.090403 0.065531 -0.000004	7 1.090414 0.065566 -0.000004
	5 0.252303 0.949840 -0.000195	5 -0.252281 0.949504 0.000173	5 -0.252354 0.949487 0.000191
	6 1.581218 0.035284 -0.000105	6 -1.581207 0.035131 0.000063	6 -1.581187 0.035058 0.000065
	8 1.695615 -1.176613 0.000004	8 -1.695995 -1.176577 0.000001	8 -1.695978 -1.176622 0.000001
	8 2.706803 0.794618 0.000033	8 -2.706353 0.794802 -0.000034	8 -2.706223 0.794837 -0.000035
	1 3.468049 0.194309 0.000062	1 -3.467444 0.194698 -0.000117	1 -3.467501 0.195222 -0.000123
	1 0.235019 1.625659 -0.999386	1 -0.235012 1.625352 0.999406	1 -0.235146 1.625188 0.999519
	1 0.235018 1.626070 0.998705	1 -0.235049 1.625700 -0.998824	1 -0.235185 1.625572 -0.998878
	6 -1.172779 -0.789840 -1.210630	6 1.172400 -0.790272 1.210169	6 1.172357 -0.790332 1.210186
	1 -2.115316 -1.335902 -1.202778	1 2.115114 -1.336025 1.202402	1 2.114929 -1.336183 1.202190
	1 -1.122871 -0.151412 -2.088730	1 1.121956 -0.152130 2.088450	1 1.121992 -0.152176 2.088359
	1 -0.337845 -1.482706 -1.205420	1 0.337633 -1.483354 1.204252	1 0.337427 -1.483115 1.204038
	6 -1.172248 -0.790095 1.210481	6 1.172675 -0.789416 -1.210765	6 1.172652 -0.789397 -1.210837
	1 -2.114998 -1.335797 1.203169	1 2.115438 -1.335086 -1.203228	1 2.115274 -1.335165 -1.203090
	1 -0.337582 -1.483279 1.204526	1 0.337969 -1.482574 -1.205479	1 0.337785 -1.482258 -1.205378
	1 -1.121471 -0.151905 2.088702	1 1.122320 -0.150657 -2.088605	1 1.122390 -0.150567 -2.088527
	6 -2.247760 0.993183 0.000346	6 2.247517 0.993101 0.000449	6 2.247614 0.993138 0.000489
	1 -3.172140 0.417047 0.000254	1 3.171907 0.416942 0.000397	1 3.171800 0.416836 0.000425
	1 -2.197437 1.616841 0.888485	1 2.197233 1.617196 -0.887407	1 2.197179 1.617168 -0.887297
	1 -2.197569 1.617344 -0.887447	1 2.196985 1.616638 0.888684	1 2.196917 1.616553 0.888692
TMA-BH2COO-	7 -1.042968 0.067072 -0.000002	7 0.013068 -0.006288 -0.000001	7 0.013068 -0.006288 -0.000001
	5 0.319640 0.963413 -0.000115	5 1.374135 0.891821 0.000234	5 1.374135 0.891821 0.000234
	6 1.699054 0.093014 0.000010	6 2.754685 0.023126 0.000155	6 2.754685 0.023126 0.000155
	8 1.702531 -1.176090 -0.000005	8 2.760317 -1.245749 -0.000020	8 2.760317 -1.245749 -0.000020
	8 2.766911 0.778678 0.000009	8 3.821448 0.710277 0.000413	8 3.821448 0.710277 0.000413
	1 0.243457 1.646749 -1.001857	1 1.296994 1.575585 -1.001254	1 1.296994 1.575585 -1.001254
	1 0.243375 1.647083 1.001384	1 1.296889 1.575226 1.001961	1 1.296889 1.575226 1.001961
	6 -1.106799 -0.788883 -1.207166	6 -1.156384 0.897819 0.000062	6 -1.156384 0.897819 0.000062
	1 -2.032819 -1.364838 -1.198634	1 -2.074960 0.310201 -0.000114	1 -2.074960 0.310201 -0.000114
	1 -1.081057 -0.148114 -2.085310	1 -1.117216 1.523759 0.887507	1 -1.117216 1.523759 0.887507
	1 -0.242664 -1.445135 -1.197483	1 -1.117074 1.524067 -0.887159	1 -1.117074 1.524067 -0.887159
	6 -1.106665 -0.788804 1.207220	6 -0.049459 -0.862321 1.206973	6 -0.049459 -0.862321 1.206973
	1 -2.032924 -1.364384 1.199095	1 -0.974918 -1.439204 1.198490	1 -0.974918 -1.439204 1.198490
	1 -0.242792 -1.445396 1.197236	1 0.815320 -1.517747 1.197030	1 0.815320 -1.517747 1.197030
	1 -1.080295 -0.148010 2.085326	1 -0.024184 -0.221510 2.085101	1 -0.024184 -0.221510 2.085101
	6 -2.211264 0.972952 0.000041	6 -0.049287 -0.861931 -1.207259	6 -0.049287 -0.861931 -1.207259
	1 -3.130815 0.386897 -0.000175	1 -0.974737 -1.438832 -1.199087	1 -0.974737 -1.438832 -1.199087
	1 -2.171293 1.598924 0.887391	1 -0.023904 -0.220839 -2.085179	1 -0.023904 -0.220839 -2.085179
	1 -2.171087 1.599271 -0.887054	1 0.815497 -1.517351 -1.197412	1 0.815497 -1.517351 -1.197412
TMA-BH2COO-…H2O	7 1.389258 0.316974 0.000005	7 1.389104 0.316874 0.000008	7 -0.001110 -0.003811 -0.000106
	5 -0.228638 0.460566 -0.000026	5 -0.228754 0.460177 0.000032	5 1.616532 0.141863 -0.000548
	6 -1.022626 -0.963212 -0.000004	6 -1.022671 -0.963503 0.000013	6 2.412601 -1.280660 -0.000286
	8 -0.434407 -2.076253 -0.000087	8 -0.434776 -2.076572 -0.000124	8 1.826463 -2.394588 -0.000006
	8 -2.300476 -0.876741 0.000116	8 -2.300359 -0.876689 0.000151	8 3.690147 -1.191836 -0.000573
	1 -0.494606 1.095428 1.000290	1 -0.494703 1.095065 1.000439	1 1.881453 0.776717 -1.001244
	1 -0.494566 1.095479 -1.000328	1 -0.494722 1.095207 -1.000286	1 1.881932 0.777322 0.999636
	6 1.985817 1.670926 0.000221	6 1.985350 1.670700 0.000265	6 -0.599537 1.349199 0.000061
	1 3.073187 1.592219 -0.000264	1 3.072749 1.591967 -0.000242	1 -1.686694 1.268586 0.000368
	1 1.652213 2.202425 -0.886847	1 1.651679 2.202111 -0.886869	1 -0.266762 1.880616 0.887419
	1 1.653009 2.201771 0.887987	1 1.652505 2.201395 0.888145	1 -0.267264 1.880611 -0.887487
	6 1.854408 -0.404447 -1.208405	6 1.854183 -0.404250 -1.208362	6 -0.464806 -0.725927 1.208304
	1 2.942981 -0.464749 -1.200105	1 2.942771 -0.464400 -1.199901	1 -1.553257 -0.787138 1.200263
	1 1.413323 -1.395738 -1.199828	1 1.413215 -1.395611 -1.199994	1 -0.022657 -1.716688 1.199152
	1 1.523626 0.145524 -2.086077	1 1.523377 0.145959 -2.085896	1 -0.133942 -0.175668 2.085668
	6 1.854431 -0.404800 1.208202	6 1.854277 -0.404703 1.208075	6 -0.465505 -0.725925 -1.208251
	1 2.943050 -0.464263 1.200332	1 2.942909 -0.464026 1.199967	1 -1.553953 -0.787115 -1.199588
	1 1.522821 0.144400 2.086044	1 1.522706 0.144669 2.085845	1 -0.135136 -0.175669 -2.085804
	1 1.414054 -1.396394 1.198910	1 1.414006 -1.396362 1.198937	1 -0.023367 -1.716691 -1.199356
	8 -3.305405 1.530476 -0.000002	8 -3.304214 1.531300 -0.000011	8 4.689534 1.218154 0.000237
	1 -2.535309 2.104466 -0.000392	1 -2.532964 2.103767 -0.000529	1 3.917053 1.788789 0.000047
	1 -2.905274 0.607123 0.000072	1 -2.905524 0.607475 0.000090	1 4.292953 0.293632 -0.000968
TMA-BH2COO-…2H2O	7 -1.722842 0.266528 0.164936	7 -1.721533 0.266354 0.163903	7 -1.720446 0.265717 0.163837
	5 -0.142616 0.512385 -0.101453	5 -0.142992 0.514836 -0.109807	5 -0.142755 0.516886 -0.111397
	6 0.644985 -0.796635 -0.662806	6 0.646249 -0.795535 -0.665524	6 0.647841 -0.791460 -0.669991
	8 0.078706 -1.866875 -0.979605	8 0.081587 -1.868646 -0.975004	8 0.084518 -1.864205 -0.982898
	8 1.924868 -0.655608 -0.761708	8 1.925456 -0.652579 -0.767799	8 1.927044 -0.646961 -0.770477

	1 -0.086123 1.415725 -0.909852	1 -0.091892 1.413405 -0.923982	1 -0.093411 1.416677 -0.924333
	1 0.320208 0.856900 0.967374	1 0.322729 0.867503 0.955160	1 0.323852 0.868604 0.953544
	6 -2.310582 1.508508 0.714913	6 -2.310196 1.509595 0.709339	6 -2.310353 1.506983 0.712706
	1 -3.376759 1.362601 0.888551	1 -3.375266 1.361650 0.888086	1 -3.374910 1.356970 0.892207
	1 -1.812091 1.750204 1.649585	1 -1.808554 1.757632 1.640683	1 -1.807906 1.753486 1.643930
	1 -2.157702 2.314958 0.002785	1 -2.162406 2.312437 -0.007943	1 -2.164301 2.311473 -0.002964
	6 -1.925528 -0.827794 1.144131	6 -1.917562 -0.822949 1.149707	6 -1.913527 -0.826025 1.147678
	1 -2.991016 -0.949331 1.339403	1 -2.982035 -0.946045 1.349509	1 -2.977441 -0.950394 1.349254
	1 -1.506373 -1.737478 0.727206	1 -1.497671 -1.733879 0.736248	1 -1.493606 -1.735474 0.731153
	1 -1.409976 -0.566175 2.065112	1 -1.399276 -0.554803 2.067289	1 -1.393452 -0.559392 2.064604
	6 -2.425825 -0.070538 -1.096442	6 -2.428293 -0.079162 -1.092818	6 -2.428363 -0.078388 -1.092734
	1 -3.487073 -0.215225 -0.893264	1 -3.488395 -0.225234 -0.884662	1 -3.487741 -0.227180 -0.883230
	1 -2.294005 0.752486 -1.794408	1 -2.301107 0.740467 -1.795628	1 -2.303721 0.743115 -1.793683
	1 -1.983916 -0.976080 -1.498659	1 -1.985796 -0.985841 -1.491817	1 -1.984295 -0.983146 -1.494222
	8 2.776352 1.872124 -0.793732	8 2.774194 1.875879 -0.785905	8 2.775168 1.881298 -0.775012
	1 1.994108 2.381529 -0.567129	1 1.990977 2.381417 -0.554014	1 1.991086 2.384445 -0.541010
	1 2.451679 0.932608 -0.776772	1 2.451760 0.935521 -0.774942	1 2.453661 0.940622 -0.769505
	8 2.786318 -0.603502 1.836246	8 2.778535 -0.608189 1.835448	8 2.768521 -0.620158 1.835930
	1 2.183184 0.020124 2.248473	1 2.175570 0.016909 2.245627	1 2.159226 -0.000951 2.245645
	1 2.500576 -0.620820 0.895931	1 2.497681 -0.623202 0.893956	1 2.494258 -0.629756 0.892441
TMA-BH2COO-…3H2O	7 -2.072819 -0.047460 0.020083	7 -2.068171 -0.063106 0.026052	7 -2.068033 -0.063965 0.026165
	5 -0.630678 0.620432 -0.289094	5 -0.638873 0.618199 -0.311416	5 -0.639570 0.618590 -0.311848
	6 0.618694 -0.413005 -0.183407	6 0.622972 -0.401266 -0.221081	6 0.623340 -0.399615 -0.222539
	8 0.482171 -1.658291 -0.036556	8 0.501983 -1.646890 -0.063418	8 0.503999 -1.645316 -0.064731
	8 1.784248 0.119254 -0.271546	8 1.780985 0.142768 -0.330225	8 1.780698 0.145747 -0.332383
	1 -0.705418 1.057439 -1.418124	1 -0.736875 1.049600 -1.440873	1 -0.738333 1.050177 -1.441155
	1 -0.501260 1.517521 0.517388	1 -0.504910 1.520183 0.489126	1 -0.505547 1.520513 0.488792
	6 -3.106646 1.009937 -0.055098	6 -3.114384 0.982408 -0.038495	6 -3.115320 0.980650 -0.037721
	1 -4.087480 0.575880 0.138106	1 -4.086976 0.539171 0.174700	1 -4.087219 0.536510 0.176271
	1 -2.885177 1.772222 0.686650	1 -2.888338 1.752290 0.694027	1 -2.889189 1.750675 0.694484
	1 -3.085422 1.451559 -1.047729	1 -3.114989 1.416975 -1.034507	1 -3.116858 1.415026 -1.033707
	6 -2.097505 -0.638348 1.379753	6 -2.062940 -0.644892 1.389662	6 -2.061659 -0.646092 1.389694
	1 -3.090465 -1.038204 1.585307	1 -3.047622 -1.054622 1.614688	1 -3.045858 -1.056654 1.614947
	1 -1.353231 -1.426693 1.423571	1 -1.308937 -1.424354 1.425621	1 -1.306987 -1.424846 1.424797
	1 -1.858273 0.141322 2.098889	1 -1.820403 0.142447 2.099361	1 -1.819324 0.141271 2.099290
	6 -2.398712 -1.097389 -0.975595	6 -2.399306 -1.123030 -0.956928	6 -2.398487 -1.124094 -0.956910
	1 -3.381231 -1.514428 -0.754675	1 -3.373953 -1.548112 -0.717197	1 -3.372668 -1.549924 -0.716980
	1 -2.404981 -0.644465 -1.963794	1 -2.425957 -0.676999 -1.947943	1 -2.425420 -0.677934 -1.947759
	1 -1.634917 -1.865659 -0.921802	1 -1.627044 -1.883279 -0.910146	1 -1.625478 -1.883485 -0.910067
	8 3.005155 -2.596750 -0.159673	8 3.032687 -2.563468 -0.183187	8 3.033797 -2.560994 -0.185475
	1 2.052378 -2.337804 -0.097841	1 2.078441 -2.309486 -0.122849	1 2.079572 -2.306913 -0.124930
	1 3.413661 -1.730610 -0.254921	1 3.436481 -1.697460 -0.297078	1 3.437522 -1.695079 -0.299929
	8 1.815664 2.501836 -1.530951	8 1.748946 2.588959 -1.462625	8 1.745961 2.592439 -1.459813
	1 0.885454 2.724407 -1.620514	1 0.812654 2.796396 -1.520476	1 0.809413 2.798333 -1.517633
	1 1.800621 1.630247 -1.064137	1 1.759912 1.692928 -1.043999	1 1.758179 1.695671 -1.042586
	8 2.062743 1.689483 1.975238	8 2.063601 1.601368 1.996279	8 2.063086 1.595179 1.998961
	1 1.228690 2.162971 2.026571	1 1.232449 2.078963 2.057444	1 1.229662 2.068363 2.062472
	1 1.975356 1.142931 1.165919	1 1.983960 1.094886 1.161291	1 1.985057 1.091556 1.162153
TMA-BH2COO-ts	6 2.511769 0.931529 -0.000101	6 2.513075 0.930292 -0.000101	7 -0.004009 -0.015376 0.000008
	7 1.349847 0.067901 0.000022	7 1.350440 0.068035 0.000021	5 -2.305376 1.084305 -0.000071
	6 1.288937 -0.749369 -1.194597	6 1.288560 -0.748946 -1.194447	6 -3.235278 -0.144281 -0.000049
	1 2.146353 -1.437463 -1.269013	1 2.145442 -1.437707 -1.269159	8 -3.405333 -1.365248 -0.000021
	1 0.367420 -1.331456 -1.180716	1 0.366601 -1.330353 -1.180375	8 -4.136345 0.783765 -0.000087
	1 1.284467 -0.109092 -2.077167	1 1.284376 -0.108522 -2.076927	1 -2.006005 1.598473 1.036477
	6 1.288992 -0.749104 1.194823	6 1.288615 -0.748682 1.194671	1 -2.005976 1.598411 -1.036642
	1 2.146396 -1.437204 1.269338	1 2.145485 -1.437448 1.269483	6 1.162277 0.842113 -0.000110
	1 1.284592 -0.108634 2.077253	1 1.284500 -0.108066 2.077012	1 2.102512 0.267372 -0.000066
	1 0.367461 -1.331174 1.181130	1 0.366643 -1.330073 1.180786	1 1.150529 1.478606 -0.885233
	1 3.455147 0.361861 -0.000058	1 3.455853 0.359558 -0.000059	1 1.150565 1.478803 0.884872
	1 2.496875 1.568114 -0.885189	1 2.498814 1.566871 -0.885237	6 -0.068814 -0.832308 -1.194457
	1 2.496915 1.568314 0.884843	1 2.498854 1.567070 0.884893	1 0.785560 -1.524058 -1.268904
	5 -0.955018 1.159561 -0.000069	5 -0.955505 1.159490 -0.000071	1 -0.992921 -1.410123 -1.180046
	6 -1.881024 -0.072040 -0.000034	6 -1.881224 -0.072233 -0.000033	1 -0.070784 -0.191850 -2.076822
	8 -2.046063 -1.293794 0.000011	8 -2.047240 -1.293734 0.000014	6 -0.068760 -0.832049 1.194652
	8 -2.785942 0.852281 -0.000086	8 -2.785354 0.852888 -0.000087	1 0.785602 -1.523802 1.269197
	1 -0.657756 1.674860 1.036473	1 -0.657782 1.674627 1.036496	1 -0.070665 -0.191403 2.076880
	1 -0.657721 1.674772 -1.036646	1 -0.657746 1.674535 -1.036674	1 -0.992878 -1.409849 1.180423
TMA-BH2COO-..H2O ts	6 -2.699546 -1.398700 -0.445527	6 -2.698527 -1.404831 -0.438136	7 -1.824129 -0.325078 -0.024352
	7 -1.824843 -0.323972 -0.024103	7 -1.824791 -0.326645 -0.024294	5 0.668170 -0.294658 -0.762689
	6 -2.277134 0.958422 -0.524972	6 -2.275155 0.950908 -0.538469	6 1.152220 1.003012 -0.091971
	1 -3.270102 1.228867 -0.131015	1 -3.269425 1.225056 -0.150348	8 0.974895 2.013325 0.577956
	1 -1.561107 1.727680 -0.235789	1 -1.560019 1.722753 -0.254026	8 2.263022 0.604102 -0.653337
	1 -2.336271 0.927655 -1.613291	1 -2.330655 0.909985 -1.626654	1 0.787885 -1.331283 -0.179421
	6 -1.672709 -0.295454 1.416684	6 -1.676994 -0.284719 1.416411	1 0.282988 -0.272666 -1.891874
	1 -2.628962 -0.103225 1.929437	1 -2.634830 -0.087798 1.924438	6 -2.699359 -1.400503 -0.442398
	1 -1.282949 -1.252775 1.763724	1 -1.288275 -1.238798 1.773449	1 -3.721976 -1.280947 -0.049367
	1 -0.964292 0.487873 1.686431	1 -0.969446 0.501156 1.680990	1 -2.753024 -1.429697 -1.530830
	1 -3.721967 -1.281861 -0.051038	1 -3.722070 -1.283767 -0.047762	1 -2.306561 -2.353880 -0.088411
	1 -2.754460 -1.423853 -1.534061	1 -2.750198 -1.440178 -1.526570	6 -2.274776 0.955591 -0.530640
	1 -2.305596 -2.353257 -0.095829	1 -2.306002 -2.356194 -0.078207	1 -3.268102 1.228006 -0.139136
	5 0.665528 -0.293634 -0.767171	5 0.669585 -0.296061 -0.757155	1 -1.558516 1.725180 -0.243190
	6 1.153124 1.001003 -0.092868	6 1.151522 1.004964 -0.091219	1 -2.332142 0.920555 -1.618858
	8 0.976743 2.009123 0.580915	8 0.971000 2.018010 0.573860	6 -1.673595 -0.291094 1.416331
	8 2.263086 0.604185 -0.657271	8 2.264195 0.605510 -0.648192	1 -2.630318 -0.096438 1.927134
	1 0.786094 -1.332574 -0.188421	1 0.789805 -1.330138 -0.169591	1 -1.284608 -1.247265 1.767185

	1 0.278714 -0.266756 -1.895652	1 0.286991 -0.279130 -1.887318	1 -0.965050 0.492897 1.683535
	8 3.740298 -1.513995 0.319689	8 3.743219 -1.518418 0.314793	8 3.738522 -1.517134 0.317414
	1 3.124578 -2.250626 0.315546	1 3.126522 -2.254212 0.314190	1 3.120162 -2.251457 0.314761
	1 3.219151 -0.757300 -0.012024	1 3.220831 -0.760654 -0.011967	1 3.218863 -0.758543 -0.011822
TMA-BH2COO-..2H2O ts	7 -2.210617 -0.014256 -0.310874	7 -2.209719 -0.014886 -0.308250	7 -2.207602 -0.016166 -0.301558
	5 0.428608 -0.031156 -0.522267	5 0.428445 -0.031733 -0.526355	5 0.428123 -0.032492 -0.539573
	6 0.816342 0.005305 0.965346	6 0.820795 0.004727 0.960017	6 0.830325 0.003355 0.944124
	8 0.578157 0.032570 2.160293	8 0.587863 0.031834 2.155857	8 0.606649 0.029534 2.141638
	8 2.003854 -0.002903 0.388121	8 2.005827 -0.002974 0.377588	8 2.010932 -0.002773 0.352346
	1 0.326808 -1.083626 -1.076030	1 0.324972 -1.084202 -1.079983	1 0.321176 -1.084708 -1.093096
	1 0.318861 0.993013 -1.125142	1 0.316092 0.992508 -1.128780	1 0.309966 0.992118 -1.140341
	6 -3.079491 -0.091577 -1.468031	6 -3.082221 -0.091583 -1.462412	6 -3.087350 -0.090731 -1.450418
	1 -4.145357 -0.065493 -1.188964	1 -4.147173 -0.064841 -1.179844	1 -4.150413 -0.063097 -1.161231
	1 -2.880892 0.746977 -2.135763	1 -2.885205 0.746955 -2.130688	1 -2.893366 0.748282 -2.118851
	1 -2.891126 -1.018687 -2.009671	1 -2.896139 -1.018814 -2.004697	1 -2.905496 -1.017570 -1.994630
	6 -2.390922 1.234431 0.402692	6 -2.386778 1.233683 0.405840	6 -2.379377 1.231794 0.415039
	1 -3.413477 1.338804 0.799948	1 -3.408098 1.338938 0.806060	1 -3.398286 1.337494 0.821014
	1 -1.685798 1.279260 1.232720	1 -1.679235 1.277799 1.233860	1 -1.667077 1.274033 1.238963
	1 -2.195155 2.072503 -0.266621	1 -2.192181 2.071602 -0.264025	1 -2.187551 2.070095 -0.255029
	6 -2.405060 -1.147716 0.571979	6 -2.401596 -1.148203 0.574940	6 -2.395127 -1.150323 0.581605
	1 -3.430607 -1.186046 0.973527	1 -3.425797 -1.186166 0.979978	1 -3.416646 -1.187431 0.993211
	1 -2.214652 -2.073878 0.028931	1 -2.213451 -2.074341 0.031045	1 -2.211574 -2.075894 0.035343
	1 -1.703859 -1.079600 1.403567	1 -1.697562 -1.080503 1.404177	1 -1.685484 -1.084237 1.406089
	8 3.078563 -2.321881 -0.718325	8 3.072651 -2.330569 -0.716417	8 3.061151 -2.351526 -0.707997
	1 2.434427 -2.576489 -1.383296	1 2.426661 -2.586786 -1.378931	1 2.411293 -2.609704 -1.365881
	1 2.705865 -1.519161 -0.310084	1 2.703666 -1.524079 -0.312396	1 2.701377 -1.535608 -0.314656
	8 3.017962 2.333939 -0.737972	8 3.006840 2.345629 -0.734386	8 2.983796 2.373595 -0.721856
	1 2.363208 2.568689 -1.399885	1 2.348151 2.582116 -1.391731	1 2.317956 2.610955 -1.371577
	1 2.669530 1.522855 -0.324638	1 2.664454 1.529578 -0.325959	1 2.655682 1.545683 -0.325699
TMA-BH2COO-..3H2O ts	7 -2.663786 0.003207 0.085432	7 -2.662861 -0.000040 0.085795	7 -2.661954 0.001816 -0.084924
	5 -0.085831 0.634562 0.655974	5 -0.087127 0.634052 0.659317	5 -0.087180 -0.636017 -0.665157
	6 0.610479 -0.233250 -0.401466	6 0.611496 -0.223967 -0.404588	6 0.612263 0.214753 0.403889
	8 0.665530 -1.036737 -1.322447	8 0.668898 -1.020740 -1.331119	8 0.671207 1.006945 1.334194
	8 1.627850 0.344601 0.203936	8 1.627115 0.352059 0.205257	8 1.626714 -0.359841 -0.209226
	1 -0.374497 1.761219 0.392421	1 -0.378811 1.761971 0.404385	1 -0.381234 -1.764823 -0.416888
	1 -0.286857 0.180623 1.740438	1 -0.286632 0.171495 1.740461	1 -0.286441 -0.166400 -1.743323
	6 -3.813307 0.539592 0.786771	6 -3.815123 0.525521 0.790373	6 -3.817918 -0.516596 -0.788926
	1 -4.762537 0.146819 0.387288	1 -4.762261 0.131874 0.386755	1 -4.762527 -0.121584 -0.380955
	1 -3.755346 0.280693 1.844070	1 -3.756906 0.258155 1.845580	1 -3.761389 -0.244484 -1.842916
	1 -3.828394 1.625721 0.695545	1 -3.834802 1.612311 0.708002	1 -3.840926 -1.603587 -0.711414
	6 -2.582989 -1.436806 0.233893	6 -2.575817 -1.440624 0.222577	6 -2.570760 1.442829 -0.215125
	1 -3.461715 -1.945188 -0.195201	1 -3.452085 -1.949318 -0.211160	1 -3.444402 1.952017 0.223102
	1 -1.687798 -1.802120 -0.269318	1 -1.678734 -1.797809 -0.283088	1 -1.671328 1.794458 0.290066
	1 -2.519558 -1.695446 1.291158	1 -2.511888 -1.707466 1.277790	1 -2.508465 1.714266 -1.269185
	6 -2.682425 0.376570 -1.315418	6 -2.681677 0.384771 -1.311720	6 -2.678756 -0.389306 1.310975
	1 -3.565852 -0.025760 -1.837329	1 -3.562813 -0.017048 -1.837888	1 -3.557462 0.012767 1.840832
	1 -2.695005 1.462859 -1.407369	1 -2.698916 1.471732 -1.394626	1 -2.699021 -1.476519 1.388799
	1 -1.785098 -0.004574 -1.802845	1 -1.782168 0.011526 -1.801244	1 -1.776947 -0.020943 1.799799
	8 3.430218 -1.476467 -1.437258	8 3.432443 -1.469728 -1.437833	8 3.432667 1.456049 1.445557
	1 2.459826 -1.387952 -1.493959	1 2.462718 -1.376108 -1.496620	1 2.462955 1.360705 1.501783
	1 3.656814 -0.832708 -0.759396	1 3.661660 -0.828218 -0.758782	1 3.664853 0.817493 0.764853
	8 2.314788 3.018932 -0.323421	8 2.306899 3.032716 -0.293439	8 2.302981 -3.046604 0.257102
	1 1.525149 3.505233 -0.074157	1 1.515463 3.514436 -0.041097	1 1.508566 -3.522476 0.003242
	1 2.091183 2.086848 -0.159178	1 2.085514 2.098437 -0.139353	1 2.083951 -2.109946 0.115067
	8 2.563216 -0.929297 2.519571	8 2.560205 -0.962629 2.498701	8 2.555807 1.007317 -2.472352
	1 1.808838 -0.910065 3.113549	1 1.806267 -0.949823 3.093387	1 1.802710 0.997017 -3.068080
	1 2.253140 -0.486360 1.710659	1 2.252307 -0.503754 1.697955	1 2.252711 0.528399 -1.681606
BH_2COO^-	5 1.215134 -0.548306 0.000011	5 -1.215420 -0.547720 0.000173	5 1.214440 -0.548862 0.000012
	6 -0.281378 -0.171624 0.000025	6 0.281299 -0.171638 -0.001185	1 1.765627 -0.841741 -1.027917
	8 -1.500144 -0.200822 0.000002	8 1.500378 -0.201078 0.000334	6 -0.281019 -0.170786 0.000038
	8 0.510157 0.882412 -0.000018	8 -0.509816 0.882421 0.000335	8 -1.499844 -0.201203 0.000072
	1 1.766343 -0.840665 1.028135	1 -1.768567 -0.840275 -1.026589	8 0.510169 0.882745 -0.000113
	1 1.766149 -0.840789 -1.028208	1 -1.766621 -0.842047 1.027486	1 1.765688 -0.841567 1.027955
BH2COO-…H2O	5 -0.390591 1.358611 -0.248605	5 -0.389077 1.358248 -0.248358	5 -0.387496 1.357961 -0.248409
	6 -1.105224 0.000846 -0.108640	6 -1.105423 0.001239 -0.108474	6 -1.105106 0.001611 -0.108434
	8 -1.854011 -0.945888 -0.237987	8 -1.854939 -0.944786 -0.237713	8 -1.855175 -0.943978 -0.237898
	8 -0.084815 0.126517 0.735234	8 -0.084580 0.125919 0.735126	8 -0.084587 0.125793 0.735458
	1 0.433915 1.510207 -1.110251	1 0.435364 1.509091 -1.110299	1 0.437375 1.507550 -1.110234
	1 -0.828715 2.336439 0.290370	1 -0.825943 2.336729 0.290678	1 -0.823520 2.337141 0.289990
	8 2.525900 -0.491500 -0.090225	8 2.525445 -0.491802 -0.090597	8 2.524226 -0.492453 -0.090963
	1 1.619463 -0.333761 0.225599	1 1.619330 -0.334138 0.225908	1 1.618309 -0.335753 0.226322
	1 2.663045 0.175951 -0.767028	1 2.661763 0.174994 -0.768179	1 2.660244 0.176689 -0.766205
BH2COO-…2H2O	5 0.000001 0.371580 1.375900	5 -0.000025 0.368777 1.375310	5 -0.000005 0.365647 1.374452
	6 0.000023 1.279900 0.133476	6 0.000027 1.279092 0.134128	6 0.000029 1.278118 0.134783
	8 0.000084 2.225935 -0.619425	8 0.000067 2.225609 -0.617943	8 0.000071 2.225914 -0.615653
	8 -0.000008 -0.023594 -0.190753	8 0.000001 -0.024107 -0.191423	8 -0.000004 -0.024441 -0.193002
	1 1.030769 0.128674 1.938687	1 1.030715 0.124696 1.937897	1 1.030809 0.120794 1.936664
	1 -1.030745 0.128927 1.938837	1 -1.030805 0.124719 1.937831	1 -1.030831 0.120894 1.936685
	8 2.450251 -1.421979 -0.344756	8 2.450252 -1.420433 -0.344922	8 2.450258 -1.418807 -0.344913
	1 1.607051 -0.939310 -0.350878	1 1.606486 -0.938972 -0.351905	1 1.605853 -0.938700 -0.354641
	1 2.738987 -1.392184 0.570762	1 2.739477 -1.387904 0.570316	1 2.735659 -1.386514 0.571465
	8 -2.450331 -1.421875 -0.344768	8 -2.450303 -1.420351 -0.344941	8 -2.450325 -1.418712 -0.344924
	1 -2.739063 -1.392049 0.570750	1 -2.739529 -1.387798 0.570296	1 -2.735732 -1.386402 0.571452
	1 -1.607109 -0.939246 -0.350898	1 -1.606519 -0.938921 -0.351927	1 -1.605902 -0.938638 -0.354649

BH2COO- …3H2O bridged	5 -0.979913 0.000017 1.328528 6 -2.009614 -0.000025 0.184729 8 -3.027857 -0.000017 -0.464935 8 -0.745224 0.000017 -0.274906 1 -0.679200 1.031346 1.860464 1 -0.679358 -1.031245 1.860685 8 2.954337 -0.000010 0.253801 1 2.401479 -0.766608 0.036870 1 2.401382 0.766425 0.036544 8 1.095148 -2.084342 -0.455968 1 0.912728 -2.679039 0.276780 1 0.357584 -1.448416 -0.457742 8 1.095128 2.084362 -0.455965 1 0.912876 2.678997 0.276875 1 0.357501 1.448513 -0.457709	5 -0.989179 0.000048 1.330390 6 -2.013284 -0.000037 0.181541 8 -3.027677 0.000001 -0.473853 8 -0.745998 -0.000038 -0.271068 1 -0.690682 1.031267 1.863921 1 -0.691119 -1.031017 1.864465 8 2.962231 0.000022 0.244139 1 2.406959 -0.766495 0.032876 1 2.406950 0.766583 0.033056 8 1.096217 -2.081532 -0.449574 1 0.914507 -2.675963 0.283540 1 0.358550 -1.445660 -0.451445 8 1.096167 2.081510 -0.449594 1 0.914374 2.675975 0.283472 1 0.358537 1.445595 -0.451476	5 -0.996965 0.000026 1.330523 6 -2.016015 0.000001 0.177041 8 -3.027254 -0.000022 -0.483088 8 -0.746660 0.000003 -0.269820 1 -0.701695 1.031335 1.865661 1 -0.701678 -1.031263 1.865690 8 2.969778 -0.000003 0.227988 1 2.411671 -0.766583 0.024740 1 2.411621 0.766522 0.024672 8 1.096417 -2.080558 -0.438187 1 0.914679 -2.665032 0.302803 1 0.361050 -1.442109 -0.445377 8 1.096411 2.080561 -0.438203 1 0.914708 2.665010 0.302816 1 0.361024 1.442135 -0.445400
BH_2O^----CO ts	5 -1.094122 -0.559568 0.000128 1 -1.435487 -1.175185 1.009590 6 0.559736 -0.391622 -0.000044 8 1.591674 0.104645 -0.000159 8 -0.968752 0.832607 0.000065 1 -1.435695 -1.175256 -1.009219	5 -1.093866 -0.559599 0.000129 1 -1.435687 -1.175290 1.009454 6 0.559424 -0.391337 -0.000033 8 1.591376 0.104364 -0.000170 8 -0.968331 0.832719 0.000068 1 -1.435884 -1.175361 -1.009085	5 -1.093866 -0.559599 0.000129 1 -1.435687 -1.175290 1.009454 6 0.559424 -0.391337 -0.000033 8 1.591376 0.104364 -0.000170 8 -0.968331 0.832719 0.000068 1 -1.435884 -1.175361 -1.009085
BH_2O^---- CO…H_2O ts	5 0.424212 1.281104 0.336412 6 1.239503 -0.100331 0.261611 8 1.637015 -1.140680 -0.005950 8 -0.184345 0.599411 -0.769952 1 -0.184013 1.371625 1.392912 1 1.147102 2.242722 0.142575 8 -2.278544 -0.597264 0.091889 1 -1.448940 -0.117414 -0.256358 1 -2.465242 -0.192204 0.941256	5 0.425975 1.281495 0.337798 6 1.237622 -0.102403 0.261465 8 1.632401 -1.143227 -0.007219 8 -0.184004 0.603168 -0.769890 1 -0.182523 1.372398 1.394141 1 1.151811 2.241303 0.145838 8 -2.276079 -0.596402 0.091250 1 -1.447054 -0.115082 -0.256929 1 -2.456388 -0.199993 0.946037	5 0.420967 1.280309 0.336988 6 1.239487 -0.099285 0.261554 8 1.639953 -1.138154 -0.006242 8 -0.185160 0.598110 -0.770536 1 -0.188500 1.368394 1.393053 1 1.141701 2.243940 0.144974 8 -2.279410 -0.596292 0.090916 1 -1.448730 -0.117891 -0.257570 1 -2.449291 -0.209590 0.952172
BH_2O^---- CO…$2H_2O$ ts	5 -0.000025 0.281656 1.301051 6 0.000193 1.425534 0.211590 8 0.000325 2.094400 -0.720353 8 -0.000079 -0.396509 0.005900 1 1.015003 0.261553 1.966996 1 -1.015110 0.261868 1.966917 8 2.443389 -1.247113 -0.398577 1 1.504373 -0.930804 -0.257229 1 2.876319 -1.128450 0.449519 8 -2.443681 -1.246687 -0.398618 1 -2.876637 -1.127858 0.449441 1 -1.504617 -0.930524 -0.257253	5 -0.000021 0.273330 1.302360 6 0.000176 1.418242 0.213527 8 0.000302 2.087550 -0.717790 8 -0.000075 -0.404215 0.006867 1 1.014951 0.252945 1.968450 1 -1.015042 0.253233 1.968384 8 2.449266 -1.235800 -0.401079 1 1.507816 -0.927354 -0.258695 1 2.882286 -1.112706 0.446320 8 -2.449537 -1.235401 -0.401118 1 -2.882569 -1.112209 0.446260 1 -1.508045 -0.927091 -0.258714	5 0.000096 0.274191 1.303131 6 -0.000349 1.417769 0.213096 8 -0.000642 2.086152 -0.718883 8 0.000144 -0.404536 0.008152 1 1.015192 0.254908 1.969015 1 -1.014828 0.254325 1.969259 8 2.448772 -1.235141 -0.401279 1 1.507468 -0.926370 -0.258431 1 2.883370 -1.108580 0.444724 8 -2.448312 -1.235663 -0.401228 1 -2.882211 -1.111627 0.445508 1 -1.507060 -0.926721 -0.258404
BH_2O^---- CO…$3H_2O$ ts	5 -1.216183 0.000000 1.238210 6 -2.291985 0.000000 0.094048 8 -2.937747 0.000000 -0.854421 8 -0.489567 0.000000 -0.043965 1 -1.208756 1.016008 1.899004 1 -1.208756 -1.016008 1.899004 8 3.073995 0.000000 -0.175965 1 2.477255 -0.766902 -0.155059 1 2.477255 0.766903 -0.155059 8 1.082536 -2.043488 -0.169148 1 0.983884 -2.522554 0.657118 1 0.417014 -1.286295 -0.128144 8 1.082536 2.043488 -0.169148 1 0.983884 2.522554 0.657118 1 0.417014 1.286295 -0.128144	5 -1.218150 0.000000 1.237351 6 -2.294412 0.000000 0.093152 8 -2.940149 0.000000 -0.855020 8 -0.491524 0.000000 -0.044782 1 -1.210785 1.015927 1.898386 1 -1.210785 -1.015926 1.898386 8 3.076993 0.000000 -0.178437 1 2.480290 -0.766854 -0.155558 1 2.480290 0.766853 -0.155558 8 1.084728 -2.040288 -0.166605 1 0.982000 -2.522927 0.656977 1 0.418000 -1.284112 -0.126837 8 1.084728 2.040287 -0.166606 1 0.982001 2.522927 0.656977 1 0.418001 1.284112 -0.126837	5 -1.224511 -0.000001 1.237590 6 -2.297437 -0.000001 0.090444 8 -2.940865 0.000000 -0.859295 8 -0.494560 -0.000001 -0.042744 1 -1.219105 1.015888 1.898647 1 -1.219105 -1.015889 1.898647 8 3.080981 0.000001 -0.183242 1 2.484082 -0.766622 -0.157960 1 2.484081 0.766623 -0.157958 8 1.087446 -2.035956 -0.162920 1 0.987435 -2.517083 0.661782 1 0.419400 -1.280957 -0.123294 8 1.087443 2.035957 -0.162920 1 0.987431 2.517083 0.661782 1 0.419399 1.280957 -0.123295
BH_2O^-	5 0.000000 0.000000 -0.599530 1 0.000000 1.034209 -1.278209 1 0.000000 -1.034209 -1.278209 8 0.000000 0.000000 0.694259	5 0.000000 0.000000 -0.599530 1 0.000000 1.034209 -1.278209 1 0.000000 -1.034209 -1.278209 8 0.000000 0.000000 0.694259	5 0.000000 0.000000 -0.599207 1 0.000000 1.034694 -1.278340 1 0.000000 -1.034694 -1.278340 8 0.000000 0.000000 0.694090
BH_2O^- ….H_2O	5 -0.001107 0.000409 0.000085 1 0.464617 1.113968 0.230675 1 -1.223308 -0.055566 -0.047490 8 0.759290 -1.041413 -0.179616 8 3.225807 -0.374837 0.023725 1 2.244308 -0.637957 -0.056780 1 3.218612 0.566800 0.206576	5 0.002466 -0.009339 -0.018911 1 0.469094 1.102723 0.217883 1 -1.219376 -0.061344 -0.076041 8 0.761448 -1.052470 -0.196083 8 3.225946 -0.380849 0.009795 1 2.244970 -0.648235 -0.072192 1 3.212800 0.560948 0.191555	5 0.001692 -0.009314 -0.017264 1 0.467302 1.102342 0.222702 1 -1.220193 -0.063438 -0.070459 8 0.762030 -1.050640 -0.200360 8 3.226175 -0.381030 0.006050 1 2.244536 -0.646743 -0.074717 1 3.215806 0.560258 0.190053
BH_2O^- ….$2H_2O$	5 -0.000069 1.452622 -0.000078 1 1.037584 2.095393 -0.000041 1 -1.037798 2.095269 -0.000035 8 0.000008 0.143968 -0.000155 8 2.454056 -0.742707 0.000118 1 1.508105 -0.407173 -0.000206 1 2.999957 0.046321 0.000172 8 -2.454022 -0.742751 0.000103 1 -2.999818 0.046350 0.000166 1 -1.508024 -0.407349 -0.000190	5 0.000069 1.452622 0.000078 1 -1.037584 2.095393 0.000041 1 1.037798 2.095269 0.000035 8 -0.000008 0.143968 0.000155 8 -2.454056 -0.742707 -0.000118 1 -1.508105 -0.407173 0.000206 1 -2.999957 0.046321 -0.000172 8 2.454022 -0.742751 -0.000103 1 2.999818 0.046350 -0.000166 1 1.508024 -0.407349 0.000190	5 0.000279 1.452717 0.000044 1 1.038025 2.095160 -0.000033 1 -1.037159 2.095657 -0.000060 8 -0.000033 0.144141 0.000230 8 2.452924 -0.742927 -0.000139 1 1.507238 -0.406825 0.000365 1 2.999560 0.045464 -0.000299 8 -2.453061 -0.742749 -0.000120 1 -3.000126 0.045342 -0.000297 1 -1.507572 -0.406096 0.000334
BH_2O^- ….$3H_2O$	5 0.594478 1.767977 -0.636056 8 0.264828 0.677464 0.016192 1 1.747525 1.988673 -0.963109 1 -0.232216 2.607787 -0.940361 8 -0.859572 -1.823912 -0.651601 1 -0.252081 -1.073282 -0.546022 1 -1.669335 -1.460552 -0.270560	5 0.593266 1.778498 -0.611042 8 0.260665 0.671255 0.010686 1 1.749387 2.013038 -0.916876 1 -0.233501 2.621224 -0.906872 8 -0.849930 -1.839336 -0.622512 1 -0.252352 -1.079843 -0.521923 1 -1.667492 -1.482360 -0.252943	5 0.601065 -1.778238 0.612622 8 0.264975 -0.668872 -0.003464 1 1.758391 -2.012138 0.914148 1 -0.223507 -2.623603 0.906862 8 -0.862396 1.836711 0.625616 1 -0.262843 1.078526 0.527997 1 -1.677400 1.478247 0.251965

	8 2.448264 -0.704439 0.574969 1 3.133231 -0.339941 0.010279 1 1.631875 -0.171841 0.371756 8 -2.297701 0.412687 0.520065 1 -2.457758 0.536786 1.458278 1 -1.320182 0.578083 0.383011	8 2.457903 -0.697388 0.557623 1 3.139104 -0.324516 -0.006057 1 1.637383 -0.170241 0.358898 8 -2.308839 0.411125 0.493893 1 -2.486470 0.589502 1.419995 1 -1.330774 0.575468 0.363473	8 2.453489 0.705402 -0.560986 1 3.138667 0.335439 -0.000312 1 1.635245 0.175978 -0.357308 8 -2.302953 -0.418889 -0.500506 1 -2.473834 -0.597809 -1.427712 1 -1.324963 -0.578254 -0.364027
CO	6 0.000000 0.000000 -0.640842 8 0.000000 0.000000 0.480632	6 0.000000 0.000000 -0.640765 8 0.000000 0.000000 0.480574	6 0.000000 0.000000 -0.640741 8 0.000000 0.000000 0.480556
H2O	8 0.000000 0.000000 0.117378 1 0.000000 0.761141 -0.469512 1 0.000000 -0.761141 -0.469512	8 0.000000 0.000000 0.117378 1 0.000000 0.761141 -0.469512 1 0.000000 -0.761141 -0.469512	8 0.000000 0.000000 0.117378 1 0.000000 0.761141 -0.469512 1 0.000000 -0.761141 -0.469512

Table S5. Energies of 3-membered ring decarbonylation reactants, transition states and products (gas phase, a.u.)[a,b]

Compound	M06-2X				CCSD(T)	
	E_{elect}	H^o_{298}	S^o cal /mol-K	G^o_{298}	G^o_{298}	G^o_{423}
BH_2OCO^-	-214.646259	-214.608772	63.815	-214.639092	-214.240451	-
$CO…BH_2O^-$ (t.s.)	-214.604234	-214.570118	66.438	-214.601685	-214.211247	-
BH_2O^-	-101.313762	-101.289324	52.748	-101.314386	-101.124955	-
CH_2OCO	-227.791897	-227.748330	62.907	-227.778219	-227.368992	-
$CO…CH_2O$ (t.s.)	-227.740414	-227.699595	64.302	-227.730147	-227.329268	-
CH_2O	-114.489926	-114.458988	52.201	-114.483791	-114.284132	-
CH_2CH_2CO	-191.857831	-191.791513	64.766	-191.822285	-191.446974	-
$CO…CH_2CH_2$ (t.s.)	-191.791775	-191.728033	66.496	-191.759628	-191.392983	-
CH_2CH_2	-78.566232	-78.510912	52.265	-78.535745	-78.370612	-
2,3-di-tbu-CH_2CH_2CO	-506.309730	-506.006305	118.630	-506.062670	-505.023619	-505.049355
CO…2,3-di-tbu-CH_2CH_2 (t.s.)	-506.245396	-505.944626	118.481	-506.000920	-504.967490	-504.993434
Tetra-Me-3-hexene	-393.018674	-392.726091	108.418	-392.777604	-391.944339	-391.968030
CO	-113.312701	-113.304204	47.176	-113.326619	-113.132977	-113.142619

[a]6-311++G(2d,p) [b]See Table S2 for thermodynamic function definitions.

Table S6. Decarbonylation energy changes of 3-membered ring compounds (gas phase, kcal mol^{-1}) [a,b]

Reaction	M06-2X				CCSD(T)	
	$\Delta E^{‡}_{elect}$	$\Delta H^{‡}_{298}$	$\Delta S^{‡}$ cal /mol-K	$\Delta G^{‡}_{298}$	$\Delta G^{‡}_{298}$	$\Delta G^{‡}_{423}$
$BH_2OCO^- \rightarrow CO…BH_2O^-$ (t.s.)	26.371	24.256	2.623	23.473	18.326111	-
$CH_2OCO \rightarrow CO…CH_2O$ (t.s.)	32.306	30.582	1.395	30.166	24.927179	-
$CH_2CH_2CO \rightarrow CO…CH_2CH_2$ (t.s.)	41.451	39.834	1.730	39.318	33.879518	-
trans-2,3-di-tbu-$CH_2CH_2CO \rightarrow$ CO…*trans*-2,3-di-tbu-CH_2CH_2 (t.s.)	40.371	38.704	-0.149	38.749	35.221730	35.091171
	ΔE_{elect}	ΔH_{298}	ΔS^o cal /mol-K	ΔG_{298}	ΔG^o_{298}	ΔG^o_{423}
$BH_2OCO^- \rightarrow CO + BH_2O^-$	12.422	9.566	36.109	-1.200	-10.969394	-
$CH_2OCO \rightarrow CO + CH_2O$	-6.734	-9.326	36.470	-20.200	-30.194053	-
$CH_2CH_2CO \rightarrow CO + CH_2CH_2$	-13.242	-14.811	34.675	-25.150	-35.527106	-
trans-2,3-di-tbu-$CH_2CH_2CO \rightarrow$ CO + tetraMe-3-hexene	-13.582	-15.054	36.964	-26.075	-33.695184	-38.462411

[a]6-311++G(2d,p) [b]See Table S2 for thermodynamic function definitions.

Table S7. Cartesian coordinates of 3-membered ring compounds (M06-2X/6-311++G(2d,p), gas phase)

BH_2COO^-	5 0.000072 -0.002007 -0.000013 1 -0.560708 -0.304478 1.028805 6 1.498987 0.377782 0.000007 8 2.715289 0.347177 0.000037 8 0.689938 1.422800 -0.000074 1 -0.560653 -0.304590 -1.028829	$CO…BH_2O^-$ (T.S.)	5 -0.063607 0.004674 -0.000008 1 -0.399467 -0.612610 1.018809 6 1.713568 0.150687 -0.000383 8 2.712243 0.733111 0.000102 8 0.206823 1.339690 -0.000118 1 -0.400190 -0.612711 -1.018501
BH_2O^-	5 0.000000 0.000000 0.014545 8 0.000000 0.000000 1.296008 1 0.000000 1.040387 -0.687452 1 0.000000 -1.040387 -0.687452		
CH_2OCO acetolactone	6 1.028374 -0.576382 0.000004 6 -0.328105 -0.070783 -0.000066 8 0.605702 0.864521 0.000021 8 -1.504574 -0.156771 0.000017 1 1.494759 -0.889460 -0.925462 1 1.494603 -0.889549 0.925523	$CO…CH_2O$ (T.S.)	6 0.917221 -0.526796 0.000000 6 0.000000 0.662413 0.000000 8 -0.157927 -1.301946 0.000000 8 -0.919459 1.319507 0.000000 1 1.557882 -0.477091 0.898756 1 1.557882 -0.477091 -0.898756
CH_2O	6 0.000000 0.000000 -0.525579 8 0.000000 0.000000 0.670207 1 0.000000 0.940537 -1.104090 1 0.000000 -0.940537 -1.104090		
CH_2CH_2O cyclopropanone	6 0.854899 -0.783929 0.000014 6 0.854897 0.783955 -0.000056 6 -0.382054 -0.000011 -0.000074 8 -1.572211 -0.000003 0.000029 1 1.152347 1.279454 0.915581 1 1.153226 1.280433 -0.914830 1 1.152459 -1.279918 -0.915311 1 1.153206 -1.280028 0.915023	$CO…CH_2CH_2$ (T.S.)	6 -0.831087 0.690088 -0.000002 6 -1.205803 -0.706819 0.000000 6 0.623576 0.341792 0.000008 8 1.615778 -0.251212 -0.000003 1 -1.182885 -1.253796 0.929077 1 -1.182880 -1.253798 -0.929075 1 -1.040280 1.283451 -0.889798 1 -1.040300 1.283465 0.889779
CH_2CH_2	6 0.000000 0.000000 0.661289 6 0.000000 0.000000 -0.661289 1 0.000000 0.923246 -1.228078 1 0.000000 -0.923246 -1.228078 1 0.000000 0.923246 1.228078 1 0.000000 -0.923246 1.228078		
$C_{11}H_{20}O$ di-t-butylcyclopropanone	6 -0.049764 -0.015430 0.146923 6 1.225532 0.137893 -0.749337 6 0.534938 1.293520 -0.165666 8 0.484205 2.479821 -0.035043 1 1.037217 -0.012010 -1.811144 1 4.650532 -0.023195 -0.950108 6 3.643489 0.299025 -1.224877 1 3.468306 0.014626 -2.265037 1 3.598887 1.387978 -1.156920 6 2.903823 0.069319 1.144290 1 3.916985 -0.238731 1.410032 1 2.835922 1.152285 1.270180 1 2.223238 -0.405345 1.853654 6 2.655026 -1.865565 -0.423304 1 3.634560 -2.244368 -0.121831 1 1.897930 -2.330673 0.213084 1 2.471358 -2.179498 -1.453823 6 2.604317 -0.341528 -0.299869 6 -1.387397 -0.500528 -0.408643 6 -2.469404 -0.158108 0.619849 1 -3.448013 -0.497984 0.273032 1 -2.263224 -0.639683 1.578528 1 -2.516472 0.920550 0.783230 6 -1.729862 0.180609 -1.736252 1 -2.717301 -0.144075 -2.070281 1 -1.749608 1.267676 -1.630349 1 -1.019285 -0.078240 -2.523447 6 -1.310969 -2.015091 -0.610909 1 -2.257711 -2.400796 -0.996623 1 -0.522009 -2.271032 -1.322637 1 -1.095298 -2.523796 0.331950 1 0.160146 -0.375640 1.152736	$CO…C_{10}H_{20}$ di-t-butylcyclopropanone (T.S.)	6 -0.583212 0.098373 0.348043 6 0.563146 -0.157244 -0.486011 6 -0.327307 1.573299 0.186612 8 0.190789 2.584320 -0.068104 1 0.427528 -0.042566 -1.555975 1 3.932305 0.590389 -0.312350 6 2.891471 0.739573 -0.612293 1 2.846758 0.705590 -1.703498 1 2.581202 1.736273 -0.294512 6 2.095581 -0.293530 1.518285 1 3.134399 -0.441885 1.819663 1 1.774956 0.673937 1.915966 1 1.499674 -1.079866 1.989254 6 2.489901 -1.719344 -0.485303 1 3.538916 -1.866916 -0.210359 1 1.895253 -2.521779 -0.043719 1 2.409179 -1.798107 -1.571698 6 1.986054 -0.347087 -0.007146 6 -2.016156 -0.341397 -0.015940 6 -3.005509 0.315967 0.943984 1 -4.021751 -0.015365 0.722541 1 -2.782530 0.050933 1.980617 1 -2.976720 1.404139 0.855512 6 -2.346593 0.046086 -1.455774 1 -3.375146 -0.234067 -1.690780 1 -2.251661 1.126432 -1.604190 1 -1.688756 -0.460731 -2.163252 6 -2.056329 -1.861908 0.141604 1 -3.044721 -2.238846 -0.128241 1 -1.312811 -2.334879 -0.501714 1 -1.851826 -2.154547 1.174775 1 -0.406836 -0.089423 1.410415
$C_{10}H_{20}$ di-t-butylethene	6 2.649672 -0.586565 -1.249891 6 1.983614 0.007051 0.000022 6 0.528207 -0.401397 0.000069 6 -0.528188 0.401335 0.000153 6 -1.983640 -0.007055 0.000013 6 -2.649733 0.587368 -1.249489 1 -3.719118 0.362273 -1.256093 1 -2.532034 1.673257 -1.274687 1 -2.203992 0.176092 -2.157296 6 -2.170928 -1.522447 -0.000347 1 -3.235834 -1.764773 -0.000525 1 -1.721637 -1.976876 -0.885980 1 -1.721779 -1.977252 0.885149 6 -2.649916 0.586768 1.249677 1 -3.719385 0.362018 1.255870		1 -2.204617 0.174779 2.157386 1 -2.531879 1.672603 1.275668 1 -0.375114 1.479420 0.000292 1 0.375173 -1.479487 0.000024 6 2.170894 1.522449 0.000574 1 3.235809 1.764753 0.000591 1 1.721627 1.977406 -0.884789 1 1.721741 1.976741 0.886338 6 2.650004 -0.587527 1.249275 1 3.719428 -0.362608 1.255590 1 2.204632 -0.176236 2.157266 1 2.532139 -1.673402 1.274503 1 3.719087 -0.361597 -1.256320 1 2.531828 -1.672418 -1.275915 1 2.204005 -0.174570 -2.157412