Supporting Information for

Unravelling the Unusual Chemistry of the Hydrogen Peroxide-Driven Hypergolic Ignition of a Cyanoborohydride Ionic Liquid as Next-Generation Green Space Propellant

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S1. Experimental methods

S1.1. Ultrasonic levitator apparatus: In the acoustic levitator apparatus used in the present experiment, ultrasonic sound waves with a frequency of 58 kHz are produced by a piezoelectric transducer and they are reflected from a concave plate mounted vertically upwards thus generating a standing wave. The soundwaves produce acoustic radiation pressure, which allows a liquid droplet or a tiny solid particle to levitate slightly below one of the pressure minima of the standing wave.[1-3] The distance between the transducer and reflector is set to 2.5 times the wavelength of the soundwave used in the set up (or 14.8 mm) producing five pressure nodes in total, although only the second and third pressure nodes above the ultrasonic transducer are suitable for levitation. The largest diameter of droplets or particles that can be held steadily while levitated in the present apparatus is approximately 3 mm, whereas the smallest could be as low as 15 μm. Here, the droplets loaded in the pressure nodes before merging were oblate spheroidal shaped and their horizontal and vertical diameters measured in the ranges of 1.8-3.0 mm and 1.0-2.1 mm, respectively.

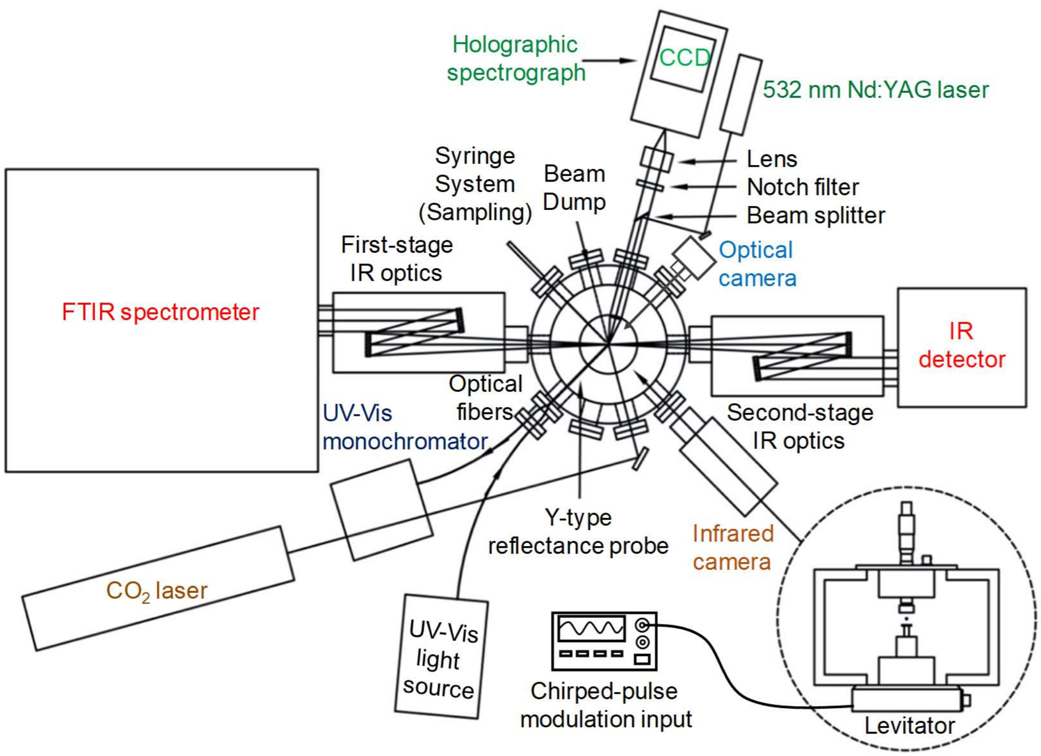

Figure S1. Schematic top view of the complete levitator apparatus displaying the ultrasonic levitator, process chamber, carbon dioxide laser, Raman, FTIR and fiber optic UV-Vis spectrometer along with high-speed infrared and optical camera.

S1.2. Process chamber and sampling system: The levitator assembly is enclosed within a pressure-compatible process chamber with a total volume of about 15 liters made of stainless steel to permit levitation in an inert gas or a highly reactive gas to investigate chemical reactions (Figure S2). The process chamber is also surrounded by spectroscopic (FTIR, Raman and UV-Vis spectrometers) as well as visualization tools (high-speed optical and infrared cameras) to identify any characteristic chemical or physical alterations of the levitated sample(s). In the present experiments, the chamber was filled with pure argon at the temperature and total pressure of 298 K and 900 Torr, respectively. To load chemically distinct droplets in adjacent pressure nodes of the levitator, two syringes are attached to an outside port on the chamber. Each syringe is connected via chemically inert PTFE tubing to one of two microneedles inside the chamber. The pair of needles is attached to the end of a wobble stick. This dual droplet deposition system enables either needle tip to be precisely positioned within the second or third pressure minimum to load a droplet before being withdrawn to a rest position prior to the experiments.

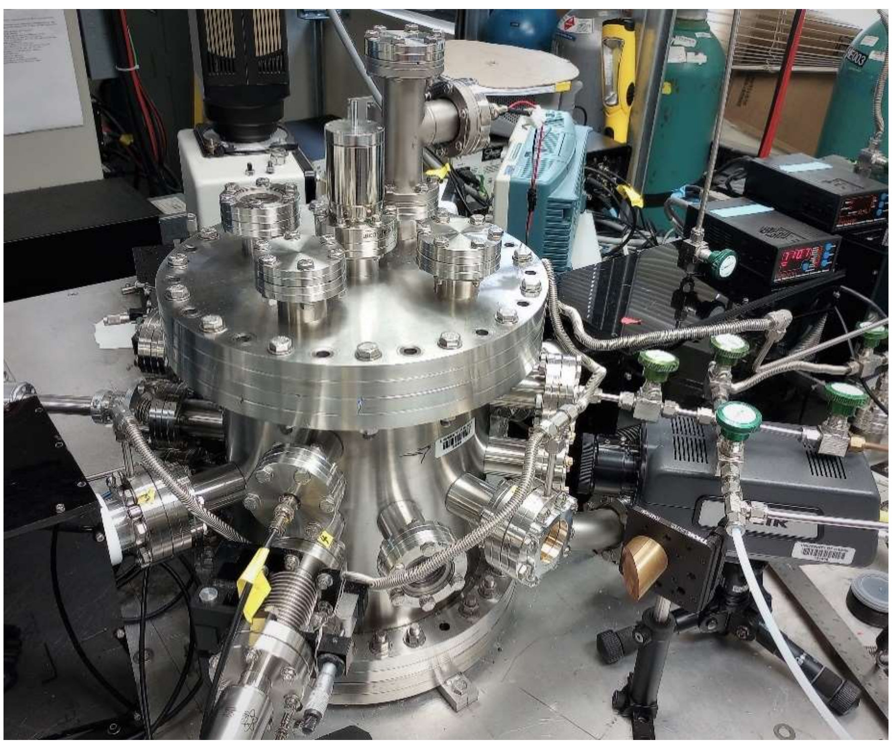

Figure S2. Side view of the levitator experimental setup containing the levitation device.

S1.3. Droplet merging: First, one droplet of the ionic liquid ([EMIM][CBH]) was loaded in the second pressure minimum above the ultrasonic transducer; hereafter the droplet of the oxidizer, hydrogen peroxide (H_2O_2) was dispensed into the pressure minimum above. Second, the chirped pulse of 1 s duration with the modulation voltage of typically 600-900 mV was applied to tune in for the resonant frequency (Figure S3). Initially the droplets undergo only non-axisymmetric oscillations, which were not sufficient to de-trap or dislocate them out of the acoustic potential wells. Third, as soon as the resonant frequency for the axial oscillations was attained in the chirp, there occurs a deformation in one of the droplets, making it a prolate spheroid from an oblate one along the vertical axis. The oscillation was further amplified due to the significantly high value of modulation voltage applied. Due to this excitation to the resonant normal mode of the droplet, it initiated vertical oscillation and further merged with the other droplet positioned at the alternate pressure node driven by the surface tension. The merging motion can be initiated in either of the droplets, depending upon the size and mass.[2, 4]

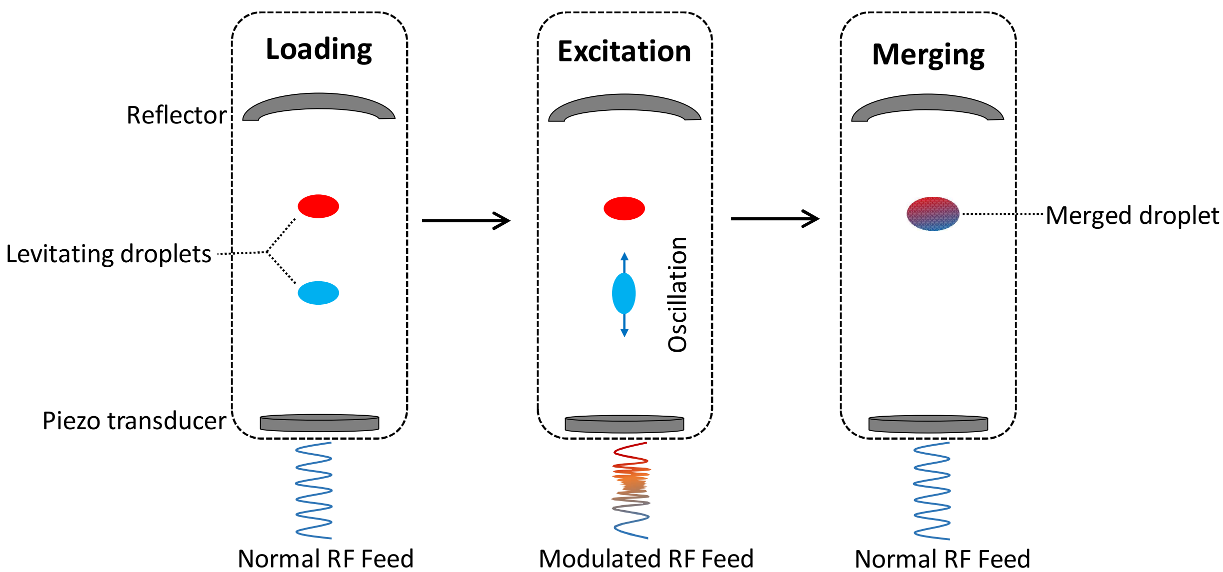

Figure S3. Schematic of droplet merging approach in the ultrasonic levitator utilizing an externally triggered chirped pulse in the range of 1-50 Hz to match the modulation frequency.

S1.4. UV-Vis emission spectroscopy: In the UV-Vis spectrometer system, the end of a fiber-optic probe is attached to an x, y, z manipulator located inside the process chamber. The manipulator enables the probe to be precisely aligned on the droplets at approximately 10-15 mm. The electromagnetic radiation emitted by the flame upon ignition due to droplet merging is collected by the optical fiber, exits the chamber via a conflat fiber-optic feedthrough, and finally enters a StellarNet SILVER-Nova UV-Vis spectrometer. The spectrometer operates in the 200-1100 nm spectral range with a resolution at full-width half-maximum (fwhm) of 2 nm and is capable of measuring emission spectral traces resulting from flame in a millisecond temporal resolution.

S1.5. FTIR spectroscopy: The gases produced by the merging of the droplets followed by ignition were identified by collecting an FTIR absorbance spectrum in the 400-4000 cm^{-1} wavenumber region through the full width of the process chamber. The FTIR spectrometer system combines a Nicolet 6700 FTIR spectrometer (Thermo Scientific) with two stages of copper mirror optics. The infrared incident beam from the spectrometer was focused into a diameter of 4 mm around the levitated sample before re-collimating prior to detection by a liquid nitrogen cooled MCT-B (mercury cadmium telluride, wide band) detector. The acquisition time for each spectrum was 10 s at a spectral resolution of is 4 cm^{-1} for the instrument. In the experiment, to get the FTIR spectrum for the newly generated gaseous products, first a background spectrum was recorded immediately after loading the droplets, which was then subtracted from the spectrum acquired after ignition event. The number densities or number of moles of the major gases (for hydrogen cyanide (HCN), carbon dioxide (CO_2), carbon monoxide (CO) and methane (CH_4)) evolved during merging events followed by ignition are evaluated from the recorded calibration curves obtained by taking different pressures of the respective gases individually in the process chamber maintaining the identical experimental conditions (Figures S10-S13).

S1.6. Raman spectroscopy: In the Raman spectrometer, the allowed vibrational transitions were excited by the 532 nm line of a diode-pumped, Q-switched Nd:YAG laser (CrystaLaser, model QL532-1W0) having a beam diameter of 0.35 mm and a divergence angle of 3.8 mR. The average power output from the laser was about 200 mW and its pulse width was 13.5 ns operating at 1 kHz repetition rate. The laser beam was introduced into the chamber through an antireflection coated window from a mirror (Edmund Optics, model NT45-991, >99% reflectance) followed by a dichroic beam splitter (Semrock, RazorEdge, model LPD01-532RU-25 × 36 × 2.0). A plano-convex lens with a focal length of 60 mm focused the laser beam onto the sample to form a spot with a diameter (1/e2) of approximately 20 μm. The Raman-shifted photons, backscattered from the droplet are then passed through an ultra-steep long-pass edge filter (Semrock, model LP03-532RE-25) which cuts down the elastically scattered 532 nm laser light. Further the resultant backscattered photons were focused by a 50 mm f/1.8 camera lens (Nikon, Nikkor 2137) into a HoloSpec f/1.8 holographic imaging spectrograph (Kaiser Optical Systems, model 2004500-501 and Holoplex HPG-532) equipped with a PI-Max 2 ICCD camera (Princeton Instruments) through a slit (width = 100 μm). The CCD detector is composed of 1024 × 256 pixels each having a spatial resolution of 26 μm. The spectra were collected over the Raman-shift ranges of 200-2450 cm^{-1} and 2400-4000 cm^{-1} simultaneously which are obtained by dispersing the total signal by the two overlaid holographic transmission gratings. The resolution of the Raman spectrometer is 9 cm^{-1}. Both the excitation laser and the detector are operated at 1 kHz repetition rate and they are externally triggered and synchronized via a pulse generator, Quantum Composer Plus, model-9518. In order to accumulate only Raman scattering signal, the pulse width for the ICCD detector is kept typically around 50 ns and accumulation time for each spectral trace was kept in the range of 5-50 seconds. For the experiments presented here a typical gate delay in the range of 480-500 ns was used and gates per exposure was fixed at 1000 shots. For the ionic liquid sample, some background fluorescence was observed in the Raman spectral traces. To suppress the fluorescence, a pre-treatment of photoprocessing for the sample was performed. The photoprocessing was essentially the exposure of the levitating ionic liquid droplet with a loosely focused (about 2 mm beam diameter) 532 nm laser at 200 mW until the point where the fluorescence background in the Raman spectrum had completely diminished. As verified by FTIR and Raman scans, this treatment did not destroy or chemically modify the ionic liquid. The Raman spectrometer was calibrated, i.e. pixel versus wavenumber by recording Raman spectra for levitating droplets of cyclohexane (C_6H_{12}), toluene ($C_6H_5CH_3$) and acetonitrile (CH_3CN).

S1.7. The optical and infrared movies and snapshots: To record high-speed events, a Phantom Miro 3a10 camera operating at repetition rate up to 1 kHz combined with a Navitar Zoom 6000 modular lens system was aligned on the levitated sample via an optical viewport. Infrared thermal imaging videos of the merging events were recorded using an FLIR A6703sc camera. The camera was set to a repetition rate of 250 Hz and the infrared camera was also partially used to determine temperature changes of the levitated droplets while merging. Both optical and IR cameras were triggered externally by the pulse generator synchronized with the UV-Vis spectrometer.

S1.8. Pulse sequence: The droplet merging, and the successive ignition event occur at a few milliseconds time regime; therefore, each spectroscopic as well as visual detection methods needed to be synchronized. For this purpose, all the data collection tools except the FTIR spectrometer and Raman spectrometer were synchronized and externally triggered by a pulse generator, (Quantum Composer Plus, model-9518) operating at 1 kHz repetition rate. A schematic of the typical pulse sequencing is depicted in Figure S4. The merging-up chirp, which was generated by the waveform/function generator was triggered in a single-shot mode, spanning 1 s. The UV-Vis spectrometer to detect the intermediate species formed during the ignition was also triggered in single-shot mode with a typical delay of 100 ms since trigger (T_0), enabled to capture 127 consecutive spectral traces with a temporal resolution of 2 ms. On the other hand, the optical and infrared camera were operated in burst mode which implies the number of pulses were limited to a certain value. As the infrared camera was only capable of operating up to one-fourth of the trigger repetition rate, it was synchronized by providing 3 milliseconds wait time with respect to T_0, which captured thermal images every fourth pulse from T_0, thus, it was synchronized with the optical video frames.

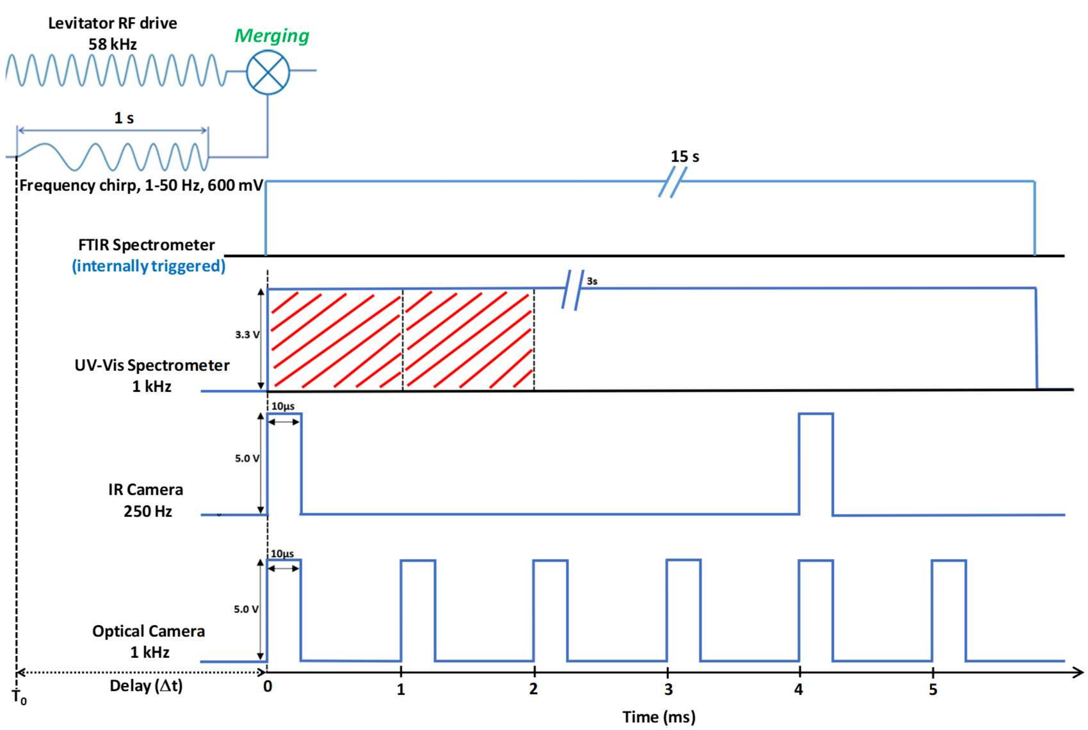

Figure S4. Typical pulse sequence used for operation of the ultrasonic levitator, droplet merging and data recording.

S1.9. Chemicals and gases: The sample 1-ethyl-3-methylimidazolium cyanoborohydride was synthesized in house[5] while concentrated hydrogen peroxide (H_2O_2) was enriched from 30% w/v stock (Fisher) by vacuum distillation (Supporting Information S1.9.1). Characteristic Raman spectra of the ionic liquid were always recorded prior to experiments to ensure the structural integrity of the sample. Argon (99.9999%, Ar) gas to fill the levitator process chamber was procured from Airgas. The gases for calibration purposes were supplied by Matheson Tri-gas: carbon dioxide (CO_2, purity: 99.999%) hydrogen cyanide (HCN, diluted 5% in helium), methane (CH_4, purity: 99.999%), carbon monoxide (CO, purity: 99.999%).

S1.9.1. Enrichment of H_2O_2

Vacuum distillation of 30% H_2O_2 was performed to reach concentrated H_2O_2 (> 90%).[6] A pump was attached to maintain a sufficient pressure gradient throughout the distillation process. All of the glassware were properly cleaned with acid solution (sulfuric acid) and rinsed with dilute (3%) H_2O_2 before use. To obtain a concentration of ~ 90% H_2O_2 starting from a concentration of 30%, multiple rounds of distillation were performed by stepwise removal of wastewater. Each cycle takes around 2-3 hours. A quantity of 40 ml of H_2O_2 of 30% concentration was introduced into the 100 ml volume glass flask. The heating nest maintained the heating temperature constant (approximately 74 - 77ºC) throughout the distillation process.

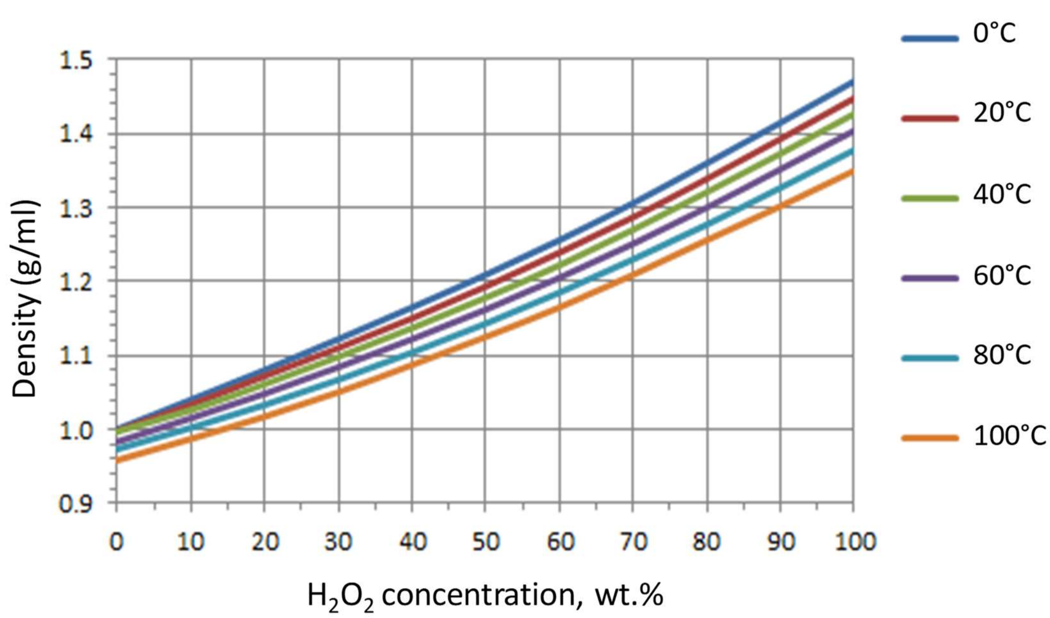

Figure S5: Concentration of the hydrogen peroxide as a function of density[7]

At the beginning of the process, the temperature was increased by 1.2ºC/min and the heating rate of the oven remained constant after reaching the set temperature. When the mentioned temperature was reached, due to the pressure gradient, water vapor is eliminated and moved through the columns with glass cylinders. Water vapor got condensed on the surface of the interior walls of the cold-water flow and was collected in the 100 ml volume glass flask. The remaining concentrated H_2O_2 volume ~ 10 ml. Looking at the characteristic specific gravity value (Figure S5) (1.392 g/ml at 20ºC for 90% H_2O_2), distillation was repeated as per requirement. H_2O_2 thus obtained was stored in the glass vial (Teflon cap) having at least 40% of empty space. Small, clean glass specific gravity bottles were used to determine density with respect to distilled water. After repeated distillation procedures, the concentration of the resultant H_2O_2 achieved was 1.401 g/ml, which corresponds to aqueous solution of 92.3 ± 0.2 % (w/v) of H_2O_2 (Figure S5). This was further diluted to prepare 10-80% (w/v) H_2O_2 as the oxidizer.

S2. Computational method

In recent computational studies,[2, 8] the primary decomposition pathway of the $[CBH]^-$ + HNO_3 reaction was investigated at the B3LYP/6-31G* level of theory[9, 10]. In order to identify non-intuitive reaction pathways, the critical points were searched in an unsupervised manner and ~3,000 of them were found.[8] To find relevant primary decompositions for $[EMIM]^+$/$[CBH]^-$ + HOOH, bimolecular reactions of $[CBH]^-$ + H_2O_2 and $[EMIM]^+$ + H_2O_2 are investigated at the same level of theory. While the unsupervised search of the $[CBH]^-$ + HNO_3 reaction found novel pathways, the initial mechanisms and barriers were largely the same across product formation pathways. Here, an extended analysis of the initial reaction steps is undertaken by examining the effect of an additional H_2O_2. The fact that ignition starts from contact with aqueous H_2O_2 naturally prompts the question of the role of the condensed phase, particularly whether neighboring H_2O_2 stabilizes the reaction barriers or even open new pathways. Previous computational study on the dicyanamide/dicyanoborohydride + HNO_3 reactions suggest that at least the former is true: a second solvent molecule can stabilize rate-limiting transition states.[11]

The follow-up work on secondary reactions of $[CBH]^-$ + HNO_3 with the N-boryl-N-oxo-formamide (BOFA) doublet radical anion ($HCON(O)BH_3^-$) and molecular oxygen[4] suggests that the B3LYP/6-31G* level of theory qualitatively agrees with the CCSD(T)/cc-pVDZ potential energy surface for that reaction[12, 13]. As the current reaction has similar reactants (a boron-containing anion and a protic, oxygen-containing oxidizing agent), B3LYP/6-31G* is thus employed to provide chemically meaningful mechanisms and intermediates. CCSD(T)/cc-pVDZ calculations are too expensive for the $[EMIM]^+ + 2H_2O_2$ reaction system; rather, electronic energies are refined with the double hybrid method B2PLYP/cc-pVDZ.[14] Intermediates and separated reactant/products are confirmed to have 3N-6 (3N-5 for linear molecules) positive vibrational frequencies while transition states are confirmed to have 3N-7 (3N-6 for linear molecules) positive vibrational frequency with a single imaginary frequency. Connections between transition states and their corresponding intermediates are confirmed with intrinsic reaction coordinate (IRC) calculations with the Gonzalez-Schlegel algorithm.[15, 16] Reported intermediates often have multiple similar conformers, differing by orientation of molecules (e.g., for Van der Waals complexes) or rotations about sigma bonds (e.g., large chain molecules). In these cases, the conformer of the lowest energy is reported on the potential energy surface. All calculations were carried out with NWChem version 6.8.[17]

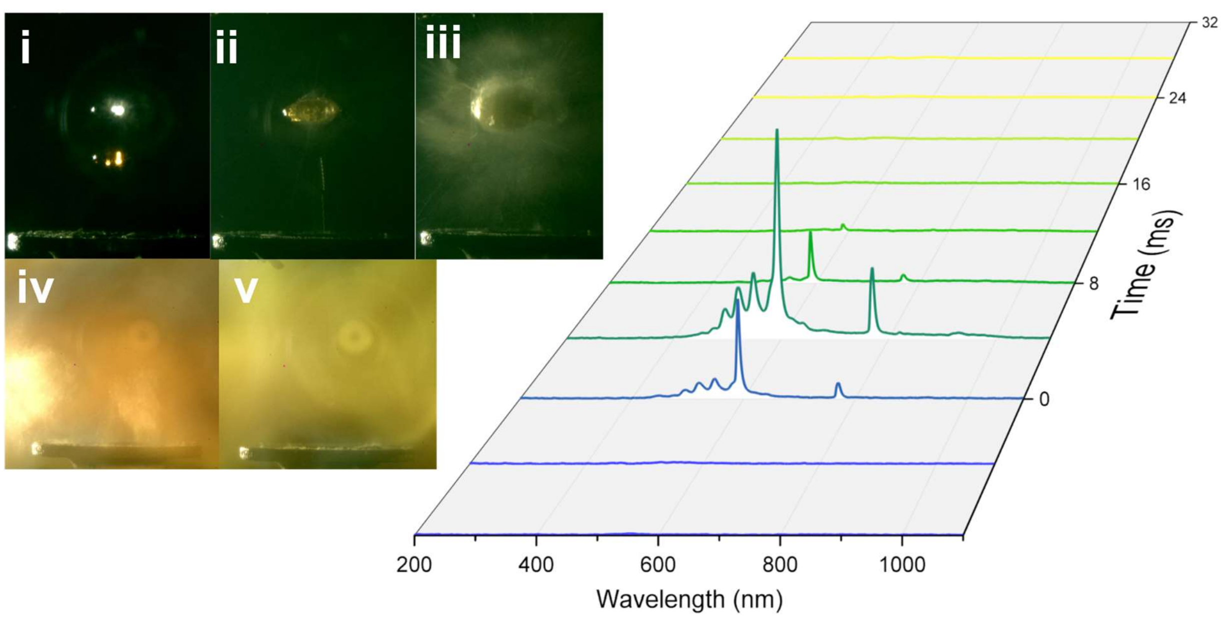

Figure S6: Temporally resolved optical images with simultaneous flame emission spectra for the hypergolic ignition reaction between the ionic liquid [EMIM][CBH] and 80% H_2O_2.

S3. Flame temperature

The relative intensities of the two atomic emission lines (say from *m* and *n* state) incorporating the Boltzmann population distribution can be expressed as-

$$\frac{I_n}{I_m} = \frac{A_n g_n \upsilon_n}{A_m g_m \upsilon_m} exp[-(E_n - E_m)/kT] \quad \text{(Eq. S1)}$$

Where, for *m* and *n*-states: A_m, A_n are the emission transition probabilities of the radiation (s^{-1}); g_m, g_n are the statistical weights of the respective levels [= (2J +1), J represents the total electronic angular momentum]; ($A_m g_m$), ($A_n g_n$) are the weighted transition probabilities (s^{-1}); ν_m, ν_n are the emission frequencies (cm^{-1}); E_m, E_n are the absolute energies (cm^{-1}); respectively and k is Boltzmann constant. If the abovementioned parameters are known,[18] then utilizing the relative intensity ratio of the two atomic emission lines, temperature of the flame, *T* can be determined.

In this work, two emission lines of sodium (Na) have been considered to estimate the flame temperature, which are located at 589 (3p→3s) and 819.5 nm (3d→3p). The required parameters have been adopted from the NIST Atomic Spectra Database.[18] The weighted transition probabilities used for 589 and 819.5 nm bands are 2.46×10^8 and 3.08×10^8 s^{-1}, respectively.

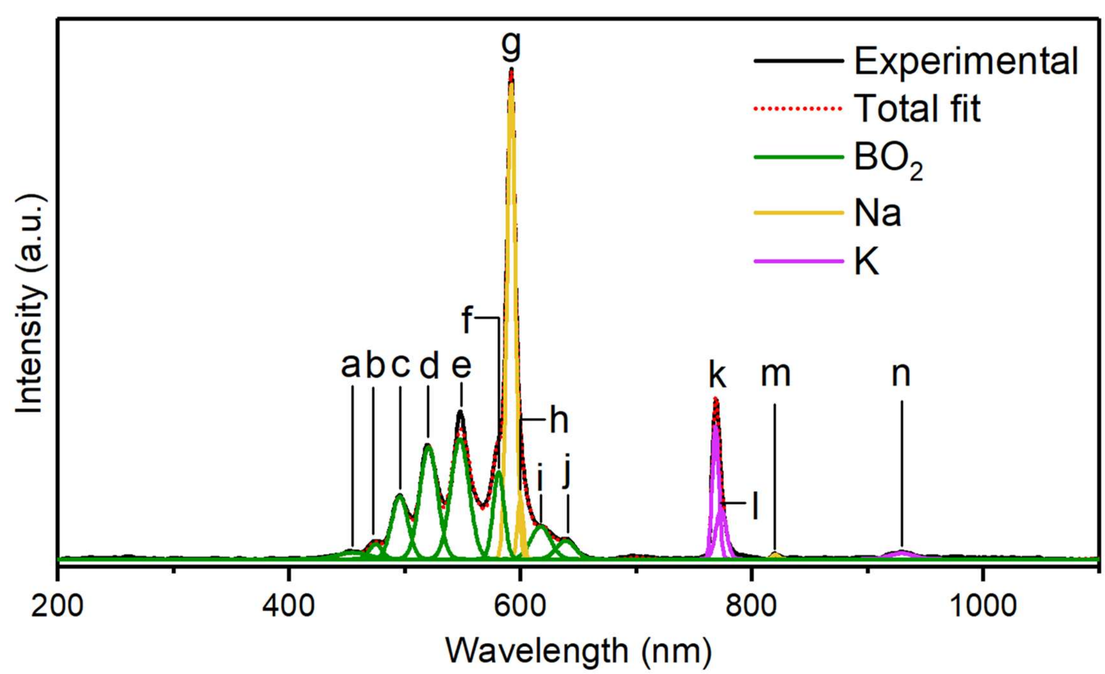

Figure S7: Deconvolution of the most intense flame emission spectrum for the hypergolic ignition reaction between the ionic liquid [EMIM][CBH] and 80% H_2O_2.

Table S1. Mean droplet sizes, number of moles and molar ratios of the reactants for different experimental sets. The errors originate from the volume measurement of the levitating oblate spheroid droplets.

Percentage concentration of H_2O_2	Mean volume of H_2O_2 droplet (μl)	Number of moles for H_2O_2 ($\times 10^{-5}$)	Mean volume of [EMIM][CBH] droplet (μl)	Number of moles for [EMIM][CBH] ($\times 10^{-5}$)	Molar ratio [EMIM][CBH]: H_2O_2
10 %	9.1 ± 3.4	2.8 ±1.0	7.5 ± 2.8	4.7 ± 1.8	1 : 0.6 ± 0.3
20 %	10.2 ± 5.2	6.5 ± 3.3	8.1 ± 4.1	5.1 ± 2.5	1 : 1.3 ± 0.5
30 %	9.6 ± 4.4	9.6 ± 4.4	9.2 ± 4.2	5.8 ± 2.6	1 : 1.7 ± 0.7
40 %	10.5 ± 4.6	14.6 ± 6.4	9.7 ± 4.5	6.1 ± 2.8	1 : 2.4 ± 0.9
50 %	9.4 ± 3.5	16.9 ± 6.3	10.9 ± 4.7	6.9 ± 3.0	1 : 2.5 ± 1.2
60 %	7.9 ± 3.1	17.7 ± 6.9	8.9 ± 3.8	5.6 ± 2.4	1 : 3.2 ± 1.4
70 %	8.4 ± 3.5	22.7 ± 9.5	7.9 ± 2.8	5.0 ± 1.8	1 : 4.6 ± 1.9
80 %	9.2 ± 4.1	29.4 ± 13.1	10.7 ± 3.8	6.8 ± 2.4	1 : 4.4 ± 2.1
92 %	9.1 ± 4.0	34.8 ± 15.3	11.4 ± 4.6	7.2 ± 2.9	1 : 4.8 ± 1.8

Table S2. Peak/band assignments for the deconvoluted flame emission spectra of [EMIM][CBH] – 92% H_2O_2 ignition reaction.[4, 18-20]

Peak /band	Peak wavelength / band center (nm)	Species	Reference wavelength (nm)	Transition	Branch; spin-orbit components; vibrational quantum numbers: (ν', ν") or (ν1',ν2',ν3') - (ν1",ν2",ν3")
a	450.8 ± 0.5	BO_2	448.8 [x]	$A\ ^2\Pi_u – X\ ^2\Pi_g$	(n,2,m)-(n-2,2,m); (n,3,0)-(n-1,3,m)
b	473.5 ± 1.1	BO_2	469.6 [x]	$A\ ^2\Pi_u – X\ ^2\Pi_g$	(n,2,m)-(n-1,2,m); (n,1,m)-(n-2,1,m)
c	495.2 ± 0.8	BO_2	492.7 [x]	$A\ ^2\Pi_u – X\ ^2\Pi_g$	(n,0,m)-(n-2,0,m); (n,1,m)-(n-1,1,m)
d	519.4 ± 0.5	BO_2	518.1 [x]	$A\ ^2\Pi_u – X\ ^2\Pi_g$	(n,0,m)-(n-1,0,m), (n,1,m)-(n,1,m)
e	547.5 ± 0.8	BO_2	546.5 [x]	$A\ ^2\Pi_u – X\ ^2\Pi_g$	(n,0,m)-(n,0,m)
f	581.2 ± 0.7	BO_2	581.2 [x]	$A\ ^2\Pi_u – X\ ^2\Pi_g$	(n,0,m)-(n+1,0,m)
g	590.3 ± 1.5	Na	589.0 [y]	$2p^63p\ ^2P^o$ - $2p^63s\ ^2S$	3/2 - 1/2
h	591.1 ± 1.3	Na	589.6 [y]	$2p^63p\ ^2P^o$ - $2p^63s\ ^2S$	1/2 -1/2
i	621.2 ± 1.1	BO_2	620.2 [x]	$A\ ^2\Pi_u – X\ ^2\Pi_g$	(n,0,m)-(n+2,0,m)
j	642.5 ± 1.5	BO_2	644.2 [x]	$A\ ^2\Pi_u – X\ ^2\Pi_g$	(n,0,m)-(n+3,0,m)
k	767.8 ± 0.6	K	766.5 [y]	$3p^64p\ ^2P^o$ - $3p^64s\ ^2S$	3/2 - 1/2
l	771.5 ± 0.5	K	769.9 [y]	$3p^64p\ ^2P^o$ - $3p^64s\ ^2S$	1/2 - 1/2
m	819.4 ± 0.4	Na	818.3, [y] 819.5 [y]	$2p^63d\ ^2D$ - $2p^63p\ ^2P^o$	5/2 - 3/2; 3/2 - 3/2; 3/2 - 1/2
n	932.6 ± 1.8	K	934.7 [y]	$3p^68p\ ^2P^o$ - $3p^63d\ ^2D$	1/2 - 3/2

x- reference 19, 20; *y* - reference 18.

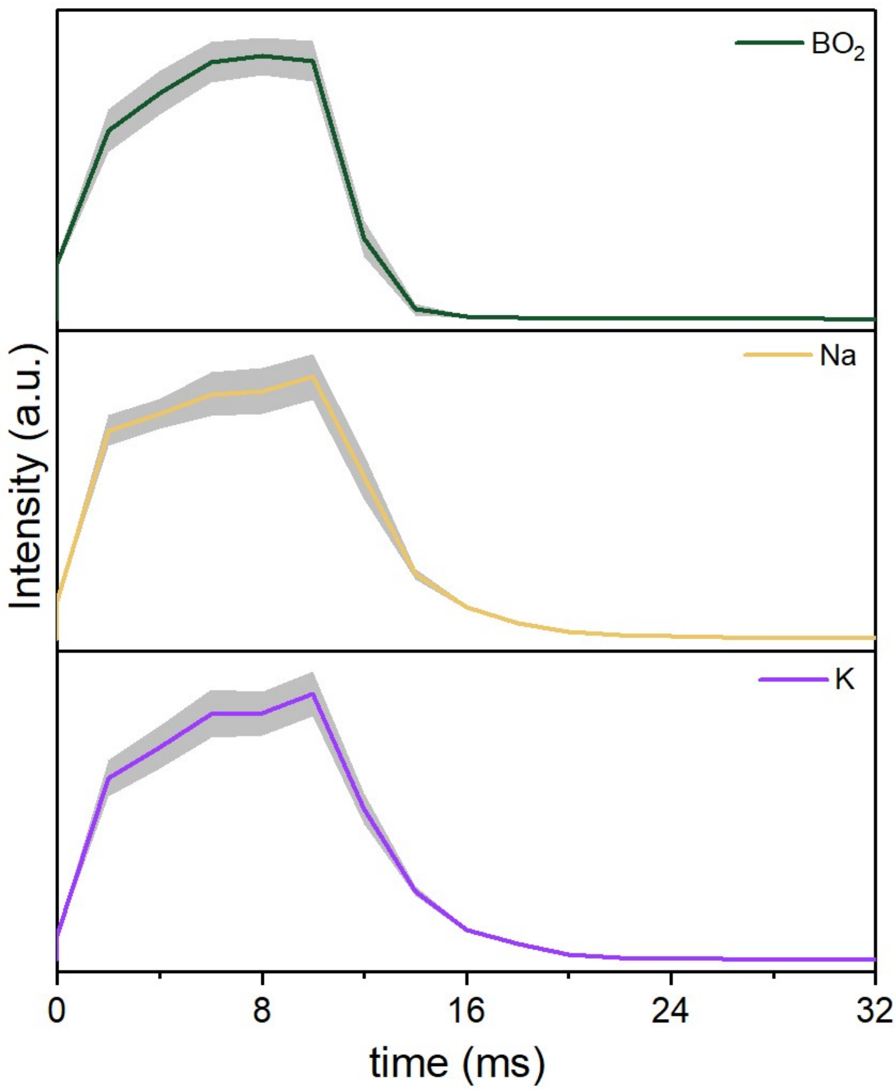

Figure S8: Temporal profiles of the key emitting intermediate – boron dioxide (BO_2) along with trace impurities – sodium (Na) and potassium (K) during the hypergolic ignition reaction between the ionic liquid [EMIM][CBH] and 92% H_2O_2.

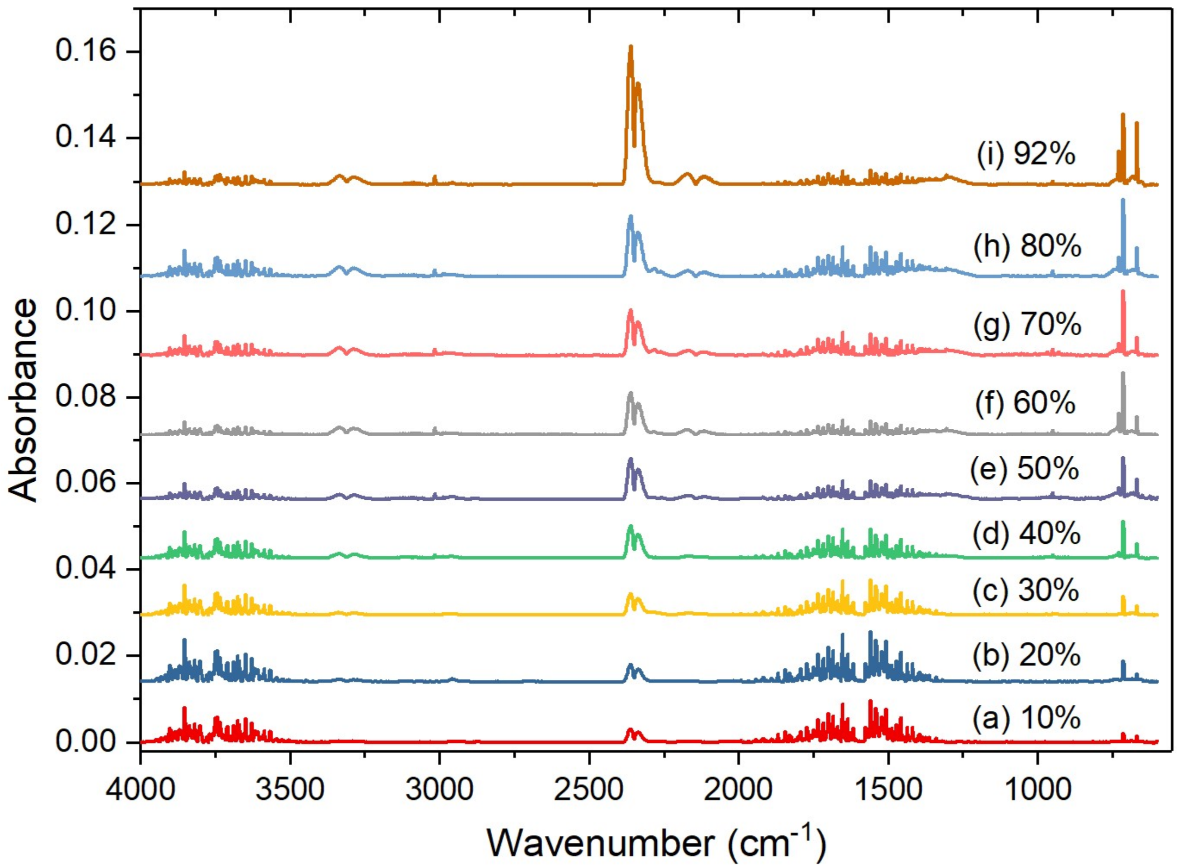

Figure S9: FTIR spectra of the gas phase products formed during the reaction of ionic liquid [EMIM][CBH] and different concentrations of H_2O_2. The top two traces are the outcome of hypergolic reactions with 80 and 92% of H_2O_2.

Table S3. Assignments of the bands in the infrared spectra for the detection of [EMIM][CBH] – H_2O_2 reaction products in the gas phase. The literature wavenumbers of the respective band centers are mentioned in parentheses.[21]

Experimental wavenumber (cm^{-1})	Literature wavenumber (cm^{-1})	Carrier	Vibrational mode
3950 - 3490	3950 - 3510 (3657)	H_2O	O-H stretching
3765 - 3685 3660 - 3580	3760 - 3690 3660 - 3570	CO_2	O-C-O asymmetric stretching + Fermi doublet of O-C-O symmetric stretching and bending
3880 - 3280	3900 - 3300 (3444), (3337)	NH_3	N-H asymmetric stretching, N-H symmetric stretching
3400 - 3210	3390 - 3230 (3311)	HCN	C-H stretching

3150 - 2870	3150 - 2880 (3019), (2917)	CH_4	ν_3 C-H stretching, ν_1 symmetric C-H stretching
2390 - 2300	2385 - 2300 (2349)	CO_2	O-C-O asymmetric stretching
2300 - 2220	2310 - 2220 (2269)	HNCO	C=N, C=O asymmetric stretching
2220 - 2030	2230 - 2040 (2143)	CO	C-O stretching
1910 - 1320	1900 - 1320 (1595)	H_2O	H-O-H bending
1510 - 1330	1500 - 1320 (1412)	HCN	1^{st} overtone of bending
1360-1210	1370-1210 (1306)	CH_4	ν_4 deformation
1070 - 840	1120 - 850 (950)	NH_3	ν_2 deformation (N-H wagging)
780 - 630	790 - 630 (712)	HCN	bending
750 - 630	760 - 630 (667)	CO_2	bending

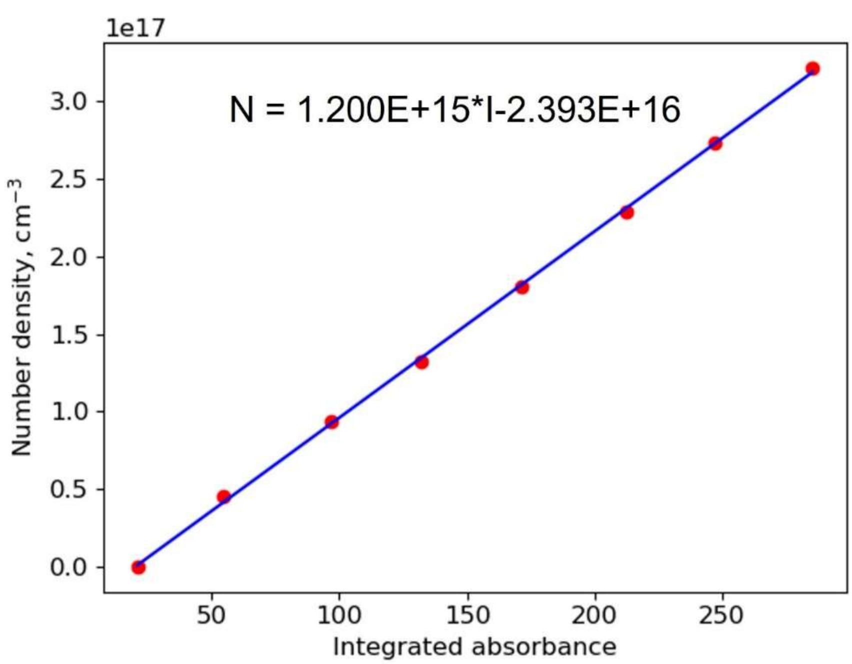

Figure S10. Calibration of FTIR signal for carbon dioxide (CO_2). Integrated area for the CO_2 antisymmetric stretch band in the 2170-2460 cm^{-1} range was used.

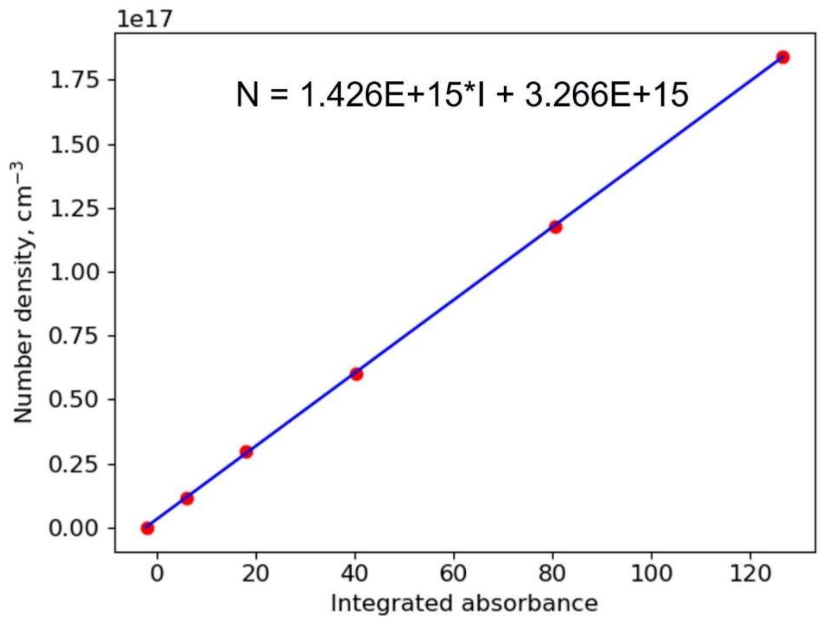

Figure S11. Calibration of FTIR signal for hydrogen cyanide (HCN). Integrated area for the CH stretch band in the 3280-3430 cm^{-1} range was used.

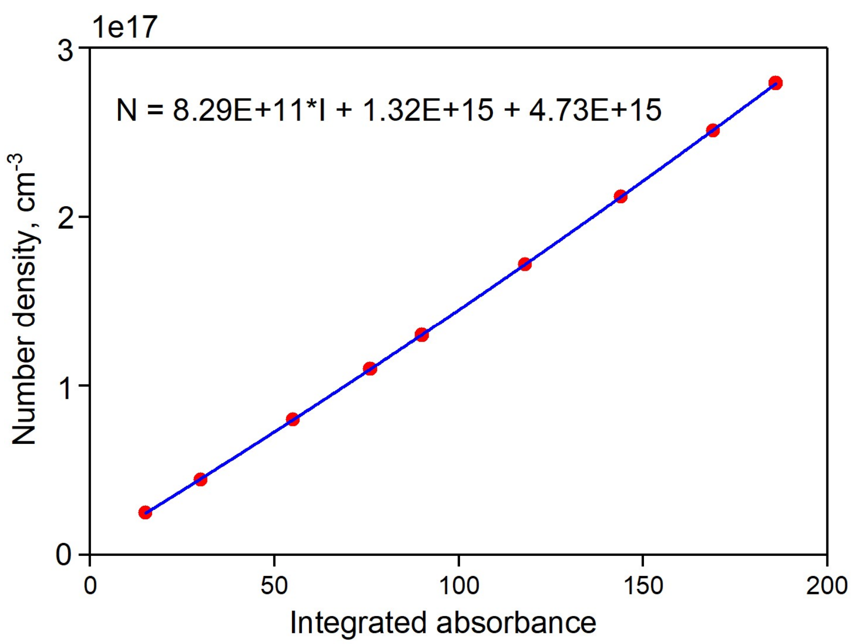

Figure S12. Calibration of FTIR signal for carbon monoxide (CO). Integrated area for the CO stretch band in the 2050-2220 cm^{-1} range was used.

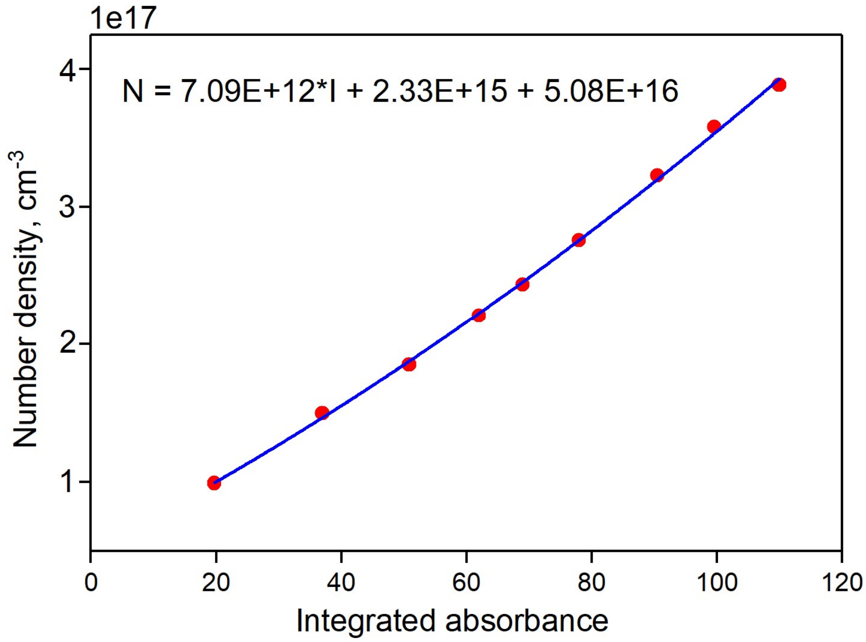

Figure S13. Calibration of FTIR signal for methane (CH_4). Integrated area for the CH stretch band in the 2860-3170 cm^{-1} range was used.

Table S4. Percentage yield of carbon dioxide (CO_2) from the [EMIM]$^+$ cation during the reaction. The errors in the number of moles of the [EMIM]$^+$ and H_2O_2 originate from the volume measurement errors of the droplets. The errors in number of moles of CO_2 is consisted of the uncertainties in the FTIR measurements and calibration curves.

Percentage concentration of H_2O_2	Number of moles for H_2O_2 ($\times 10^{-5}$)	Number of moles for [EMIM]$^+$ ($\times 10^{-5}$)	Number of moles of CO_2 ($\times 10^{-5}$)	Percentage yield from [EMIM]$^+$
10 %	2.8 ±1.0	4.7 ± 1.8	1.2 ± 0.2	4.2 ± 0.7
20 %	6.5 ± 3.3	5.1 ± 2.5	1.9 ± 0.3	8.5 ± 1.2
30 %	9.6 ± 4.4	5.8 ± 2.6	3.1 ± 0.4	11.5 ± 1.6
40 %	14.6 ± 6.4	6.1 ± 2.8	5.2 ± 0.7	13.3 ± 1.9
50 %	16.9 ± 6.3	6.9 ± 3.0	6.1 ± 0.8	16.2 ± 2.1
60 %	17.7 ± 6.9	5.6 ± 2.4	6.6 ± 0.8	26.1 ± 3.3
70 %	22.7 ± 9.5	5.0 ± 1.8	7.2 ± 0.9	34.1 ± 3.9
80 %	29.4 ± 13.1	6.8 ± 2.4	8.9 ± 1.2	40.5 ± 5.4
92 %	34.8 ± 15.3	7.2 ± 2.9	16.3 ± 2.0	59.5 ± 6.4

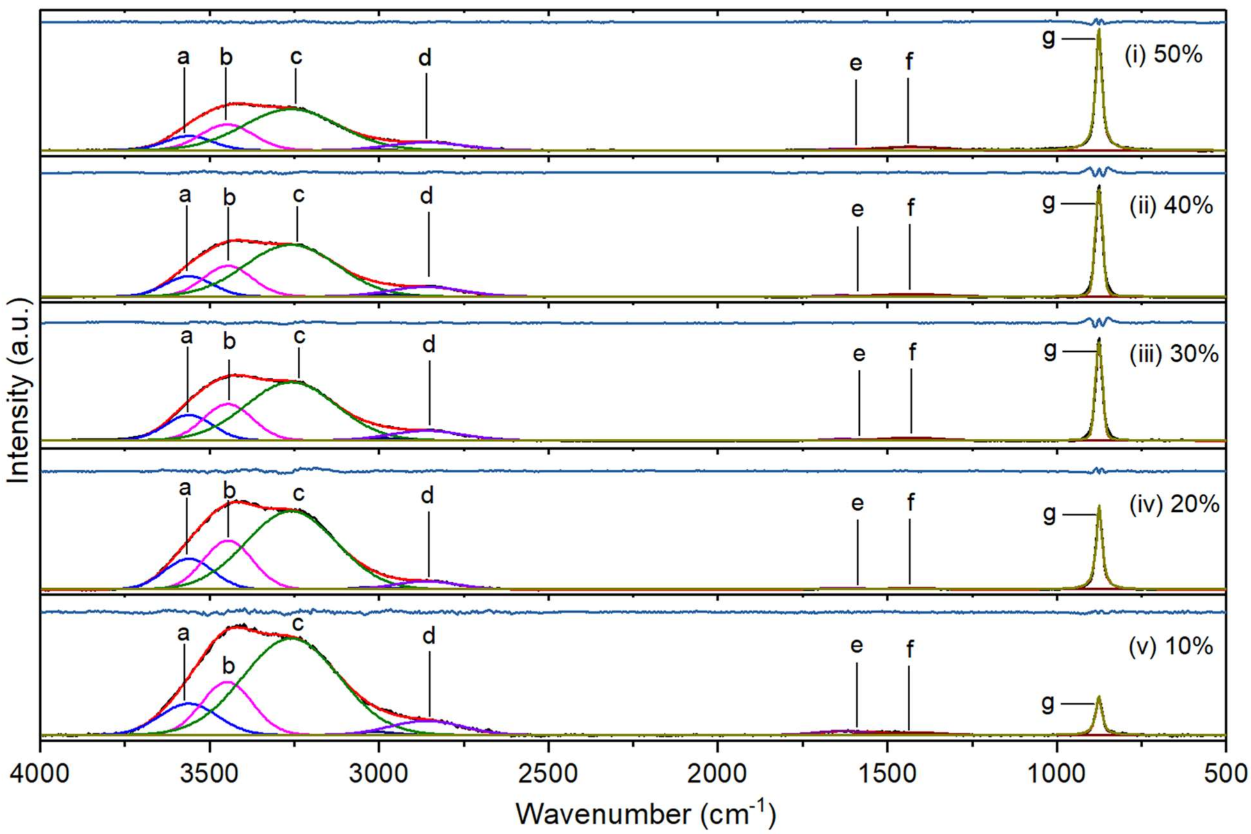

Figure S14: Deconvoluted Raman spectra of the 10-50% H_2O_2 levitating droplets.

Table S5. Assignments of the Raman bands for dilute H_2O_2 solutions.[22, 23]

Band	Wavenumber (cm^{-1})	Literature wavenumber (cm^{-1})	Assignment
a	3551	3540	OH···OO hydrogen bonds from H_2O to H_2O_2
b	3432	3430	Symmetric –OH stretch of H_2O
c	3254	3250	Asymmetric –OH stretch of H_2O
d	2852	2850	H_2O_2 bend overtone ($2\nu_6$)
e	1637	1640	ν_2 bending of H_2O
f	1436	1430	H_2O_2 bending (ν_6)
g	875	875	O-O stretching band of H_2O_2

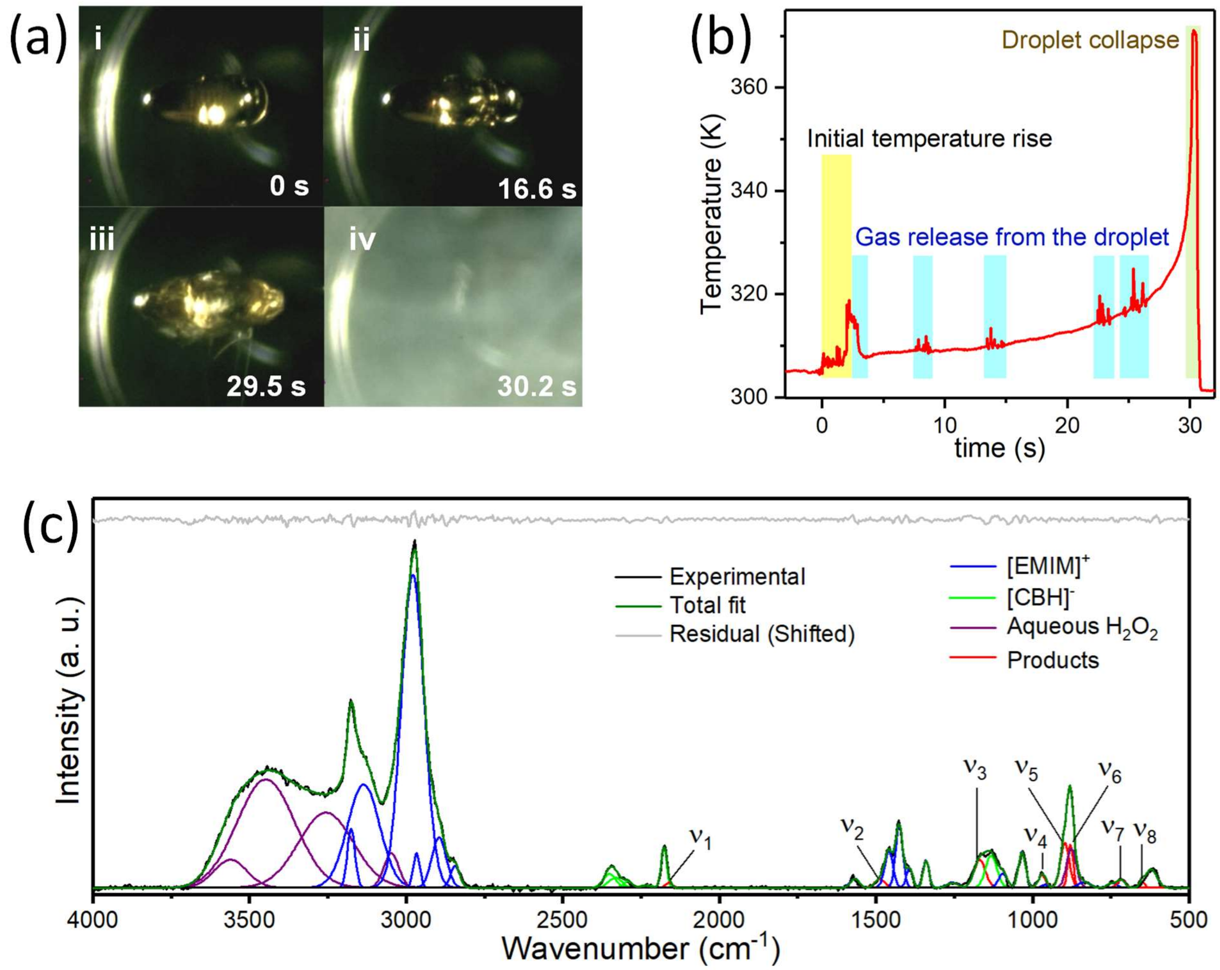

Figure S15. (a) Optical camera images of the (i) merged droplet showing (ii) expansion via the generation of gas bubbles, (iii) gas release and (iv) collapse of the droplet generating smoke for the reaction between [EMIM][CBH] and 50% w/v H_2O_2 (Movie S5). (b) Temperature profile as a function of time since merging instance. The spikes shaded in blue indicate temperature jumps due to rapid gas bubble formation and sequential gas release from the droplet until the collapse (shaded green) after reaching the maximum temperature. (c) Deconvoluted Raman spectra of the merged droplet reveal new peaks (Figure S16, Table S6) of intermediates and product formed *in situ*.

Table S6: Assignment of the new peaks identified in the Raman spectrum of the merged droplet of [EMIM][CBH] and 50 % H_2O_2 to detect the reaction intermediates.

Peak position (Experimental) (cm^{-1})	Literature wavenumber (cm^{-1})	Assignment	Ref.
2160	2162	Asymmetric N≡C−O stretching	[24]
1487	1482	Symmetric N=C=O stretching	[25]
1168	1167	BOH bending	[26, 27]
970	968	B-OH stretching	[28]
900	901	O-O stretching of >B(O-O)B< linkage	[28]
879	877	(BO_3) stretching	[26, 29]
716	711	B-O stretching of >B(O-O)B< linkage	[28]
650	650	N=C=O bending	[25]

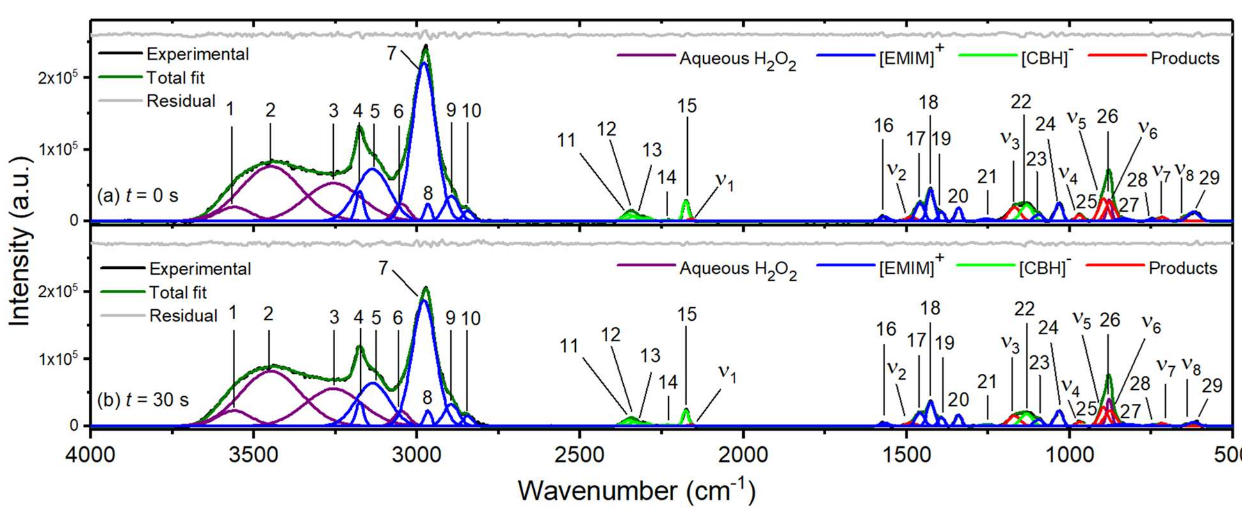

Figure S16: Deconvoluted Raman spectra at (a) the instance of droplet merging and (b) after the progress of the reaction between [EMIM][CBH] and 50% H_2O_2.

Table S7. Assignments of the reactant Raman bands upon droplet merging between [EMIM][CBH] and 50% H_2O_2.[2, 22, 23]

Band	Measured wavenumber (cm^{-1}) (this work)	Vibrational mode description	Literature wavenumber (cm^{-1}), intensity
1	3554	OH···OO hydrogen bonds from H_2O to H_2O_2	3540
2	3436	Symmetric –OH stretch of H_2O	3430
3	3254	Asymmetric –OH stretch of H_2O	3250
4	3175	ν (aro C-H)	3172, m
5	3125	ν (aro C-H)	3122, m
6	3044	O-H stretching mode of OOH···O of H-bonded H_2O_2 - H_2O	3046, w
7	2971	ν_{as} CH_3, CH_2	2971, s
8	2964	ν_{as} CH_3 (Et)	2964, m
9	2892	ν_s CH_3 (Et)	2887, w
10	2843	ν (ali C-H)	2839, vw
11	2350	ν_e (B-H)	2350, m
12	2330	ν_e (B-H)	2334, s
13	2285	ν^{a1} (B-H)	2280, sh
14	2239	ν^{a1} (B-H)	2239, m
15	2177	ν^{a1} (C≡N)	2177, vs
16	1567	ν (C=C), ν_{as}(ring)	1567, w
17	1458	δ_{as} CH_3 (Me)	1456, m
18	1423	δ_s CH_3	1418, s
19	1390	δ_s CH_3 (Et), w CH_2	1381, m
20	1337	ν N-Et, N-Me, breathing	1334, s
21	1255	*r* (aro C-H)	1257, w
22	1133	δ^{a1} (B-H)	1136, m
23	1092	*r* (ring C-H), *r* (ali)	1092, m
24	1031	δ (ring), breathing, ν (C_{ali}-N)	1026, m
25	961	γ (aro C-H)	962, w
26	875	O-O stretching band of H_2O_2	875, s
27	834	γ (C-H)	829, vw
28	745	ν^{a1}BN ($BH_3CNBH_3^-$ isomer)	742, w
29	607	ν N-Et, ν N-Me	599, m

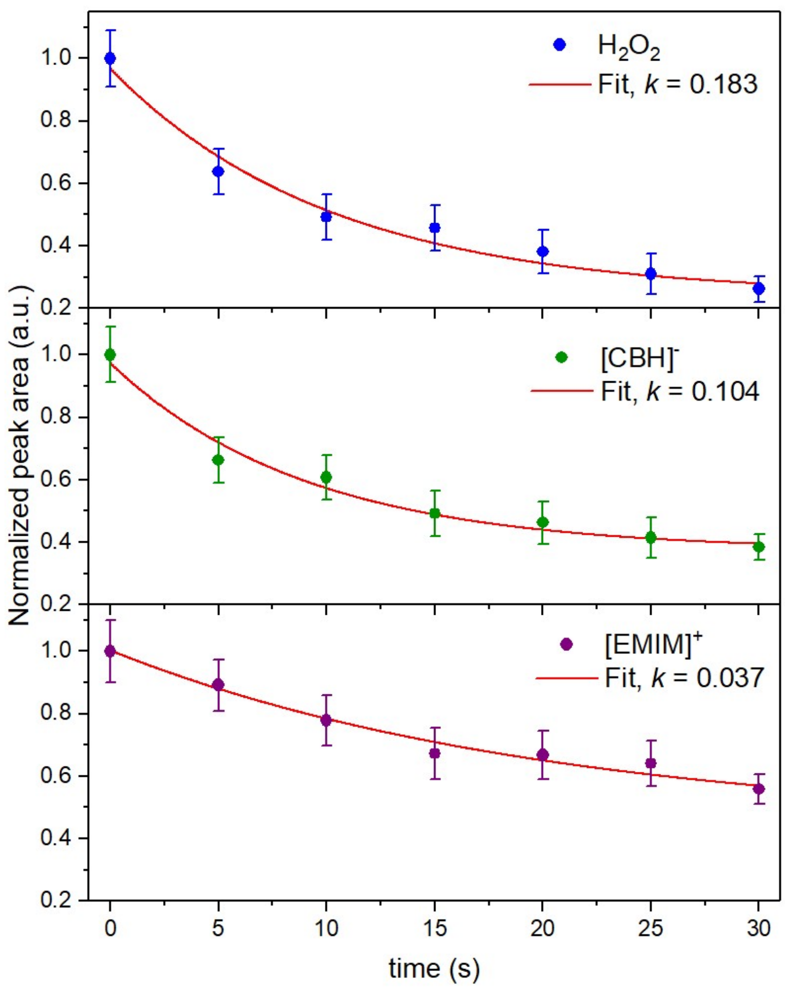

Figure S17: Temporal profiles and the first order decay fittings of the reactant Raman bands as a function of reaction time to determine the rate constants (s^{-1}) for the reaction between [EMIM][CBH] and 50% H_2O_2. The peak areas of the bands at 875, 2175 and 2971 cm^{-1} for H_2O_2, $[CBH]^-$ and $[EMIM]^+$, respectively, were used to extract the kinetic data.

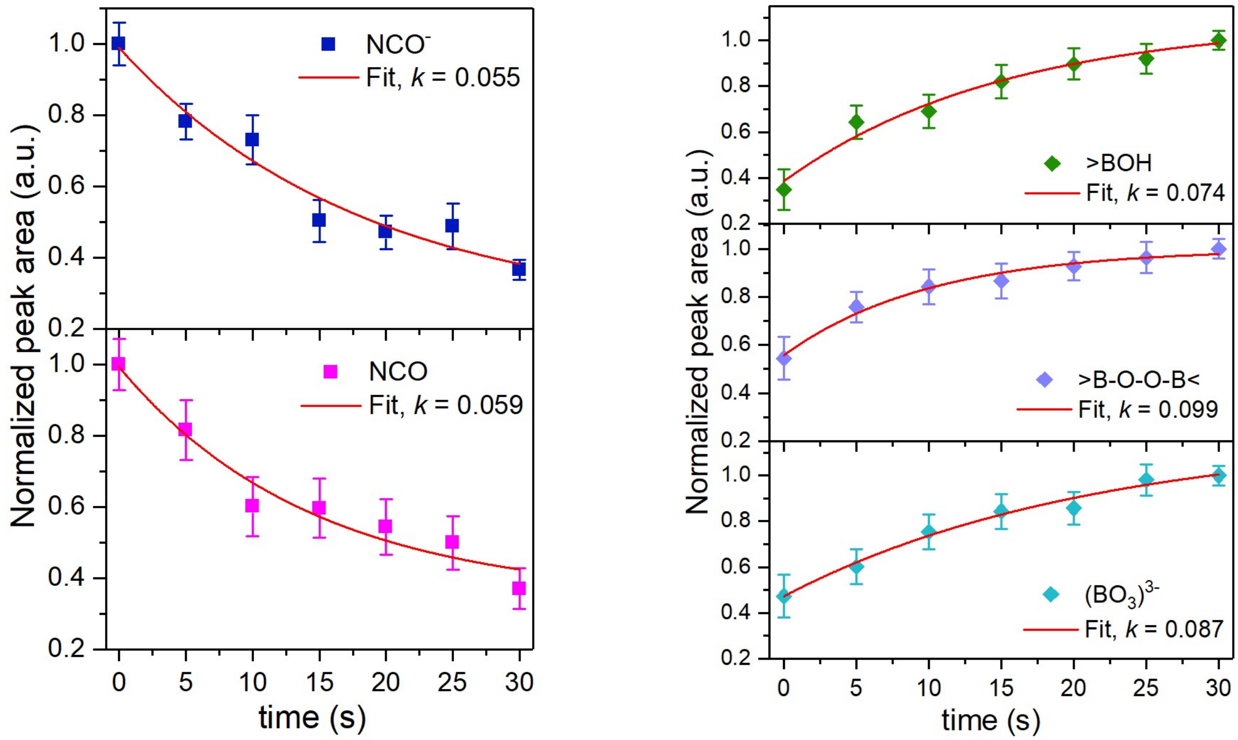

Figure S18: Temporal profiles and the kinetic data fittings of the products/intermediates extracted from the characteristic Raman bands as a function of reaction time to determine the rate constants (s^{-1}) for the reaction between [EMIM][CBH] and 50% H_2O_2.

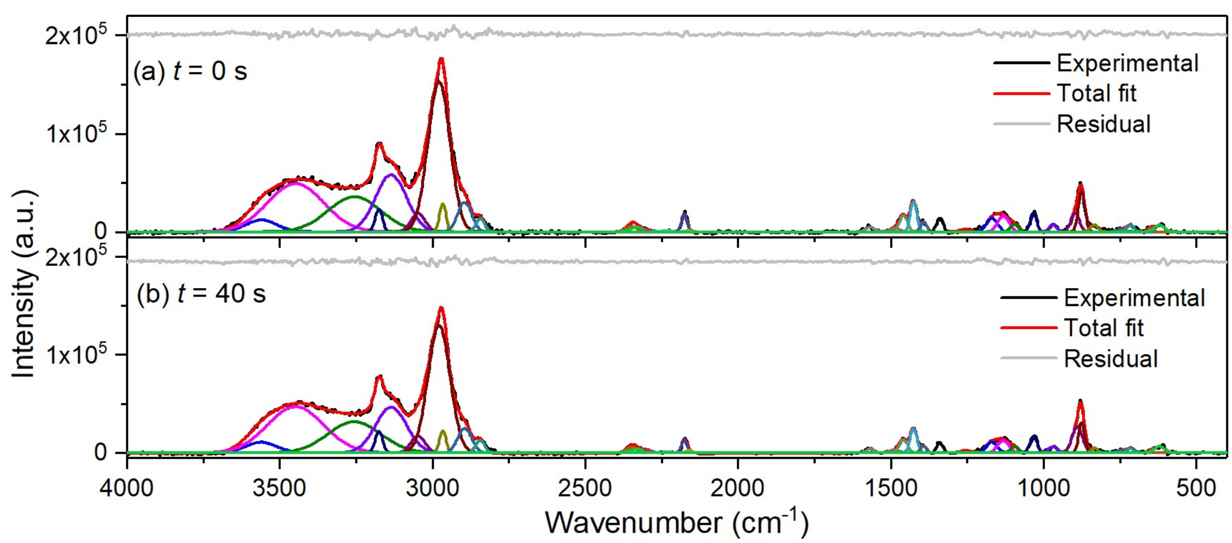

Figure S19: Deconvoluted Raman spectra at (a) the instance of droplet merging and (b) after the progress of the reaction between [EMIM][CBH] and 40% H_2O_2.

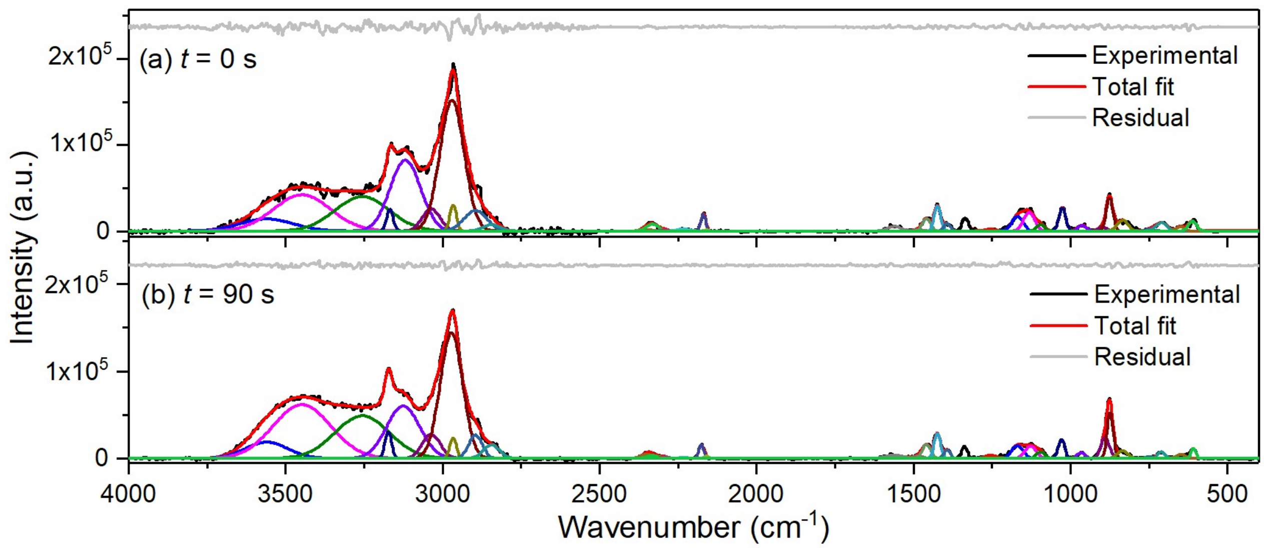

Figure S20: Deconvoluted Raman spectra at (a) the instance of droplet merging and (b) after the progress of the reaction between [EMIM][CBH] and 30% H_2O_2.

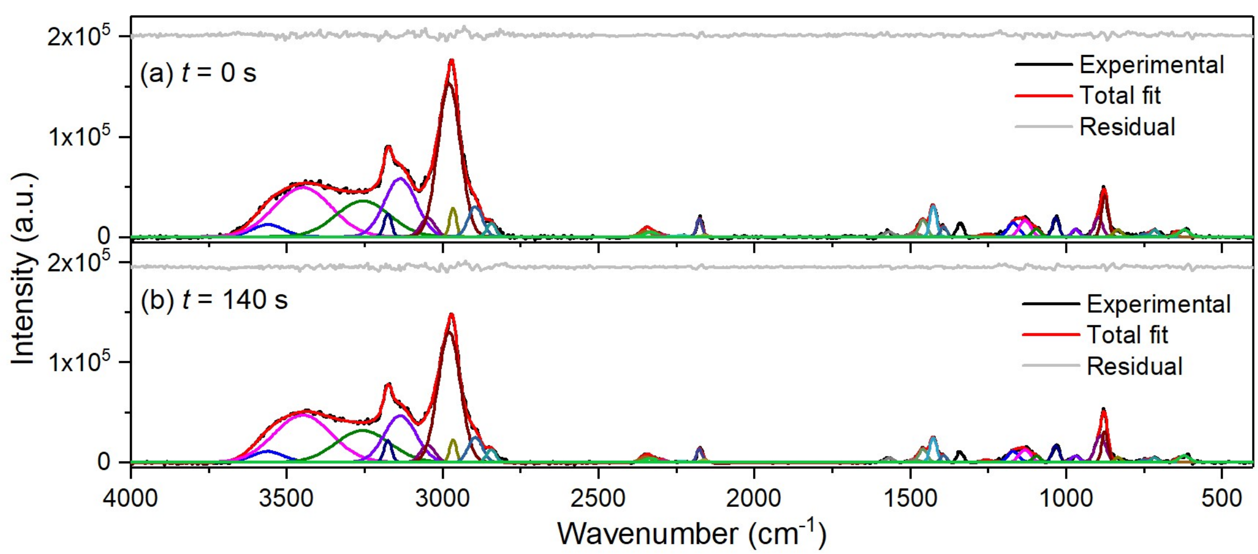

Figure S21: Deconvoluted Raman spectra at (a) the instance of droplet merging and (b) after the progress of the reaction between [EMIM][CBH] and 20% H_2O_2.

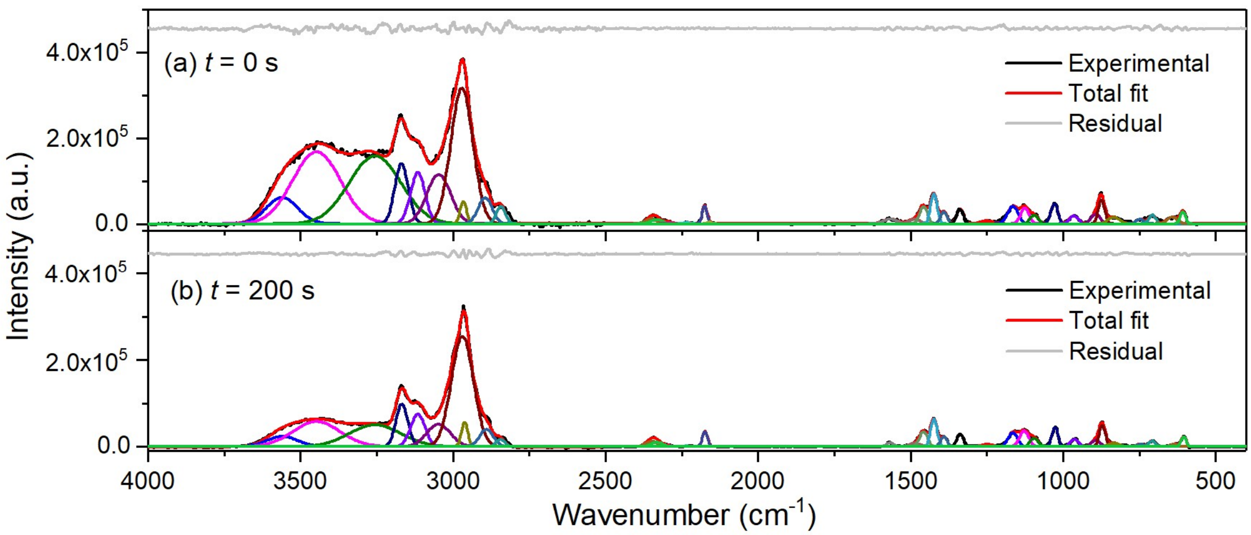

Figure S22: Deconvoluted Raman spectra at (a) the instance of droplet merging and (b) after the progress of the reaction between [EMIM][CBH] and 10% H_2O_2.

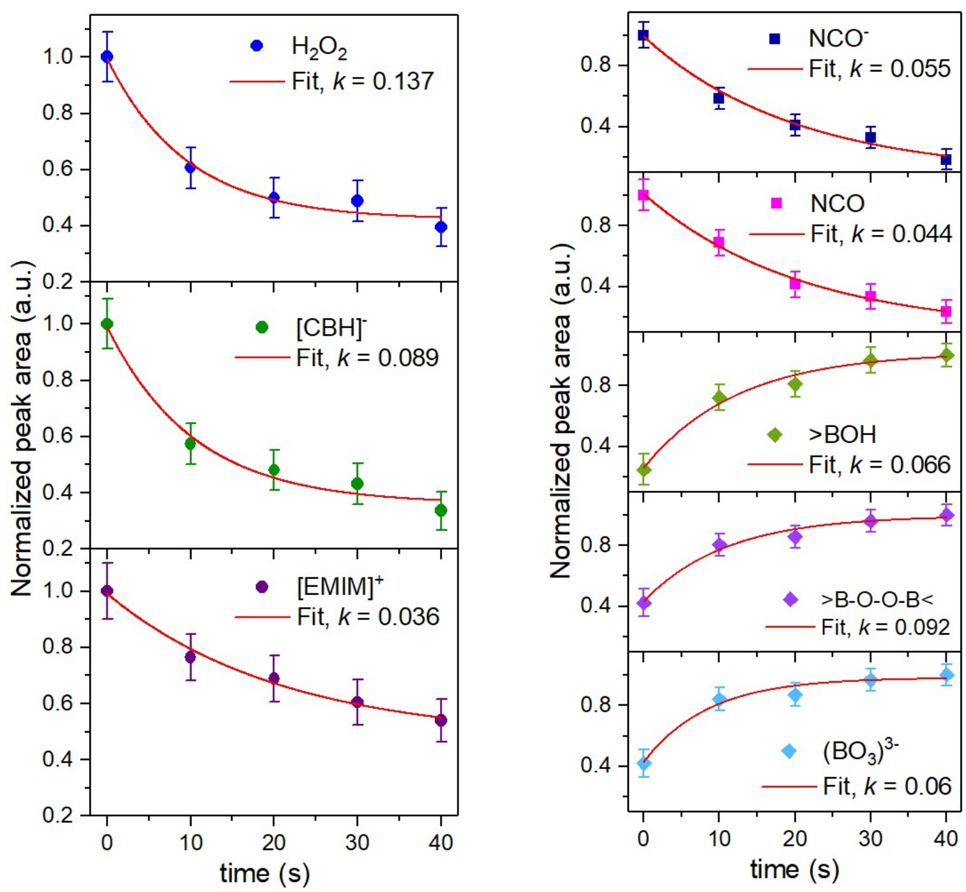

Figure S23: Temporal profiles and the kinetic data fittings of the reactants and the products/intermediates extracted from the characteristic Raman bands as a function of reaction time to determine the rate constants (s^{-1}) for the reaction between [EMIM][CBH] and 40% H_2O_2.

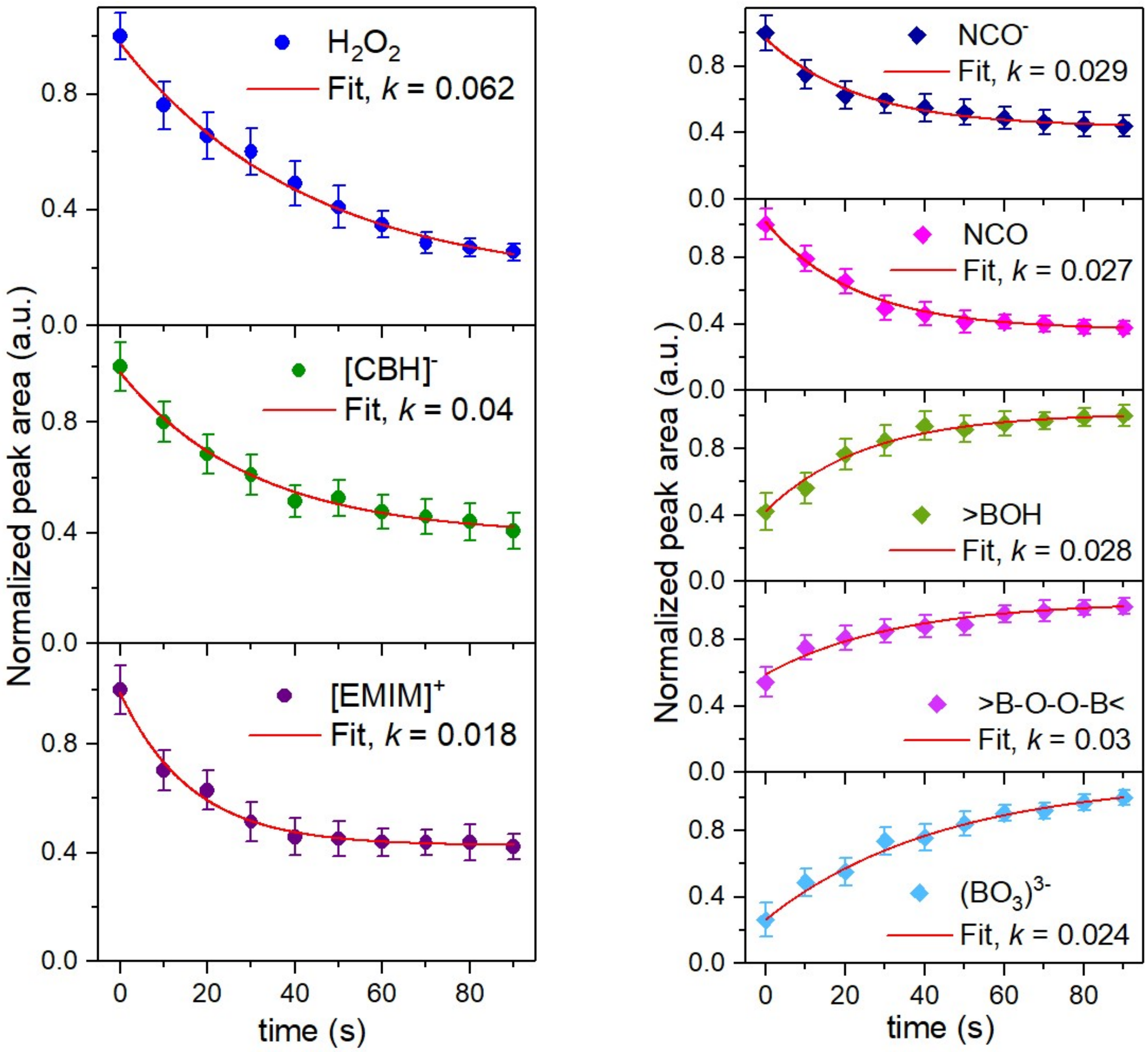

Figure S24: Temporal profiles and the kinetic data fittings of the reactants and the products/intermediates extracted from the characteristic Raman bands as a function of reaction time to determine the rate constants (s^{-1}) for the reaction between [EMIM][CBH] and 30% H_2O_2.

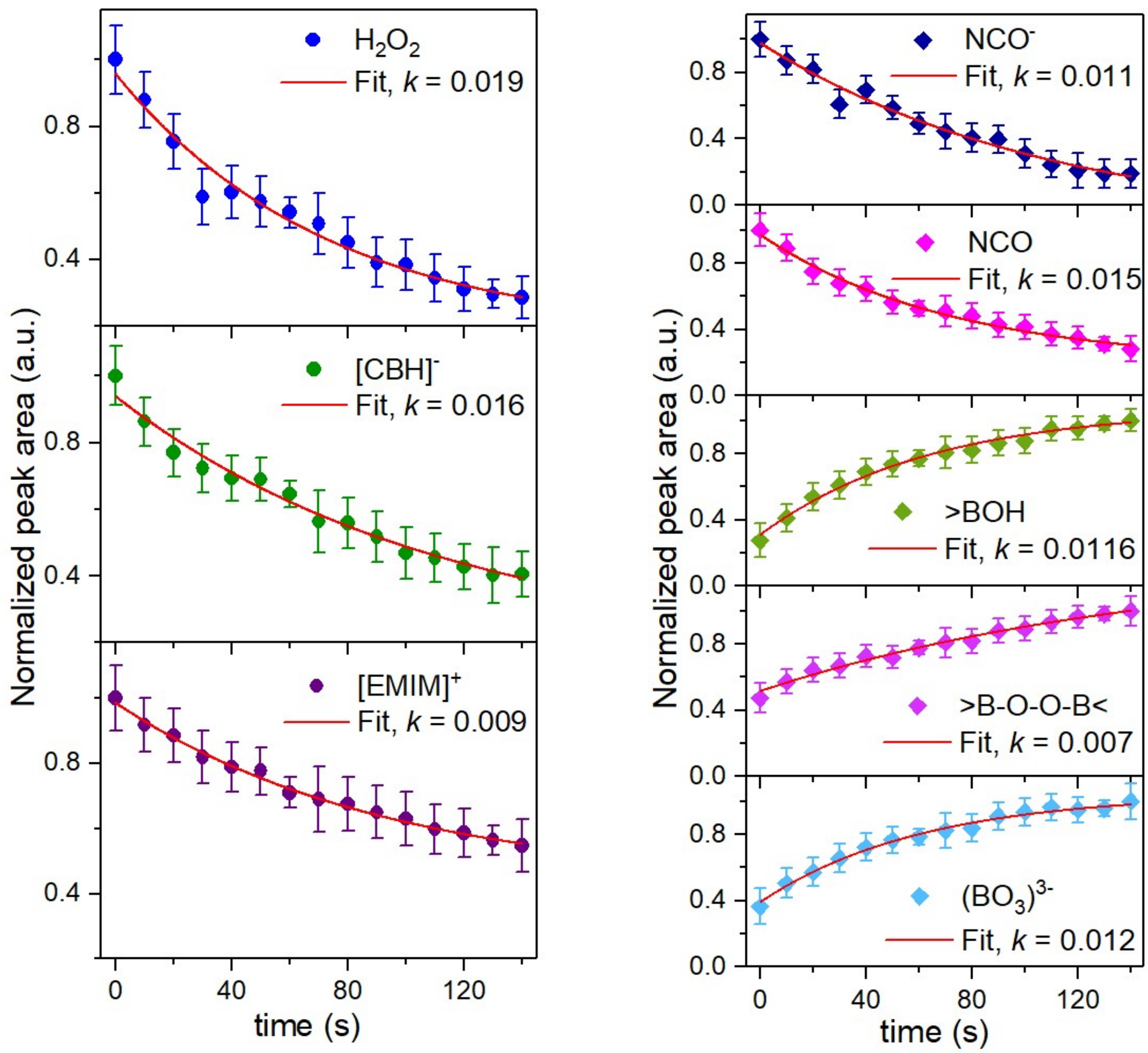

Figure S25: Temporal profiles and the kinetic data fittings of the reactants and the products/intermediates extracted from the characteristic Raman bands as a function of reaction time to determine the rate constants (s^{-1}) for the reaction between [EMIM][CBH] and 20% H_2O_2.

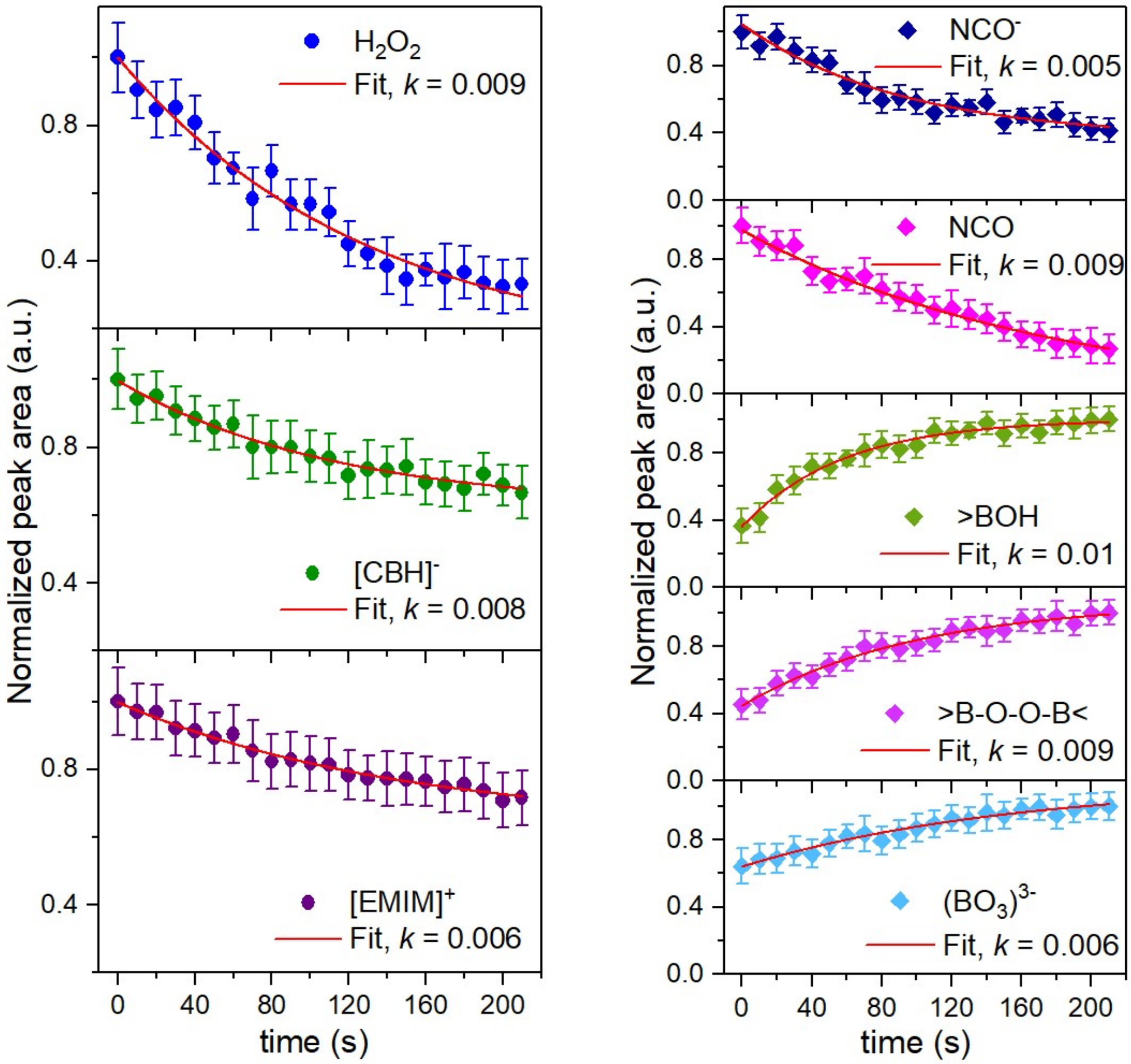

Figure S26: Temporal profiles and the kinetic data fittings of the reactants and the products/intermediates extracted from the characteristic Raman bands as a function of reaction time to determine the rate constants (s^{-1}) for the reaction between [EMIM][CBH] and 10% H_2O_2.

Table S8. Rate constants (s^{-1}) derived from the kinetic data fitting of the characteristic Raman bands of the reactants and products/intermediates.

Species		Mean rate constant (s^{-1})				
		50 % H_2O_2	40 % H_2O_2	30 % H_2O_2	20 % H_2O_2	10 % H_2O_2
Reactants	H_2O_2 (decay)	0.183 ± 0.014	0.137 ± 0.020	0.062 ± 0.020	0.019 ± 0.009	0.009 ± 0.002
	$[CBH]^-$ (decay)	0.104 ± 0.019	0.089 ± 0.014	0.040 ± 0.020	0.016 ± 0.010	0.008 ± 0.003
	$[EMIM]^+$ (decay)	0.037 ± 0.014	0.036 ± 0.014	0.018 ± 0.010	0.009 ± 0.006	0.006 ± 0.003
Products	NCO (decay)	0.059 ± 0.012	0.044 ± 0.014	0.027 ± 0.012	0.015 ± 0.011	0.009 ± 0.005
	NCO^- (decay)	0.055 ± 0.011	0.050 ± 0.021	0.029 ± 0.020	0.011 ± 0.008	0.005 ± 0.003
	BOH (formation)	0.074 ± 0.016	0.066 ± 0.018	0.028 ± 0.011	0.016 ± 0.011	0.010 ± 0.004
	>B(O-O)B< (formation)	0.099 ± 0.020	0.092 ± 0.021	0.03 ± 0.011	0.007 ± 0.005	0.009 ± 0.003
	$(BO_3)^{3-}$ (formation)	0.087 ± 0.019	0.060 ± 0.015	0.024 ± 0.013	0.012 ± 0.008	0.006 ± 0.002

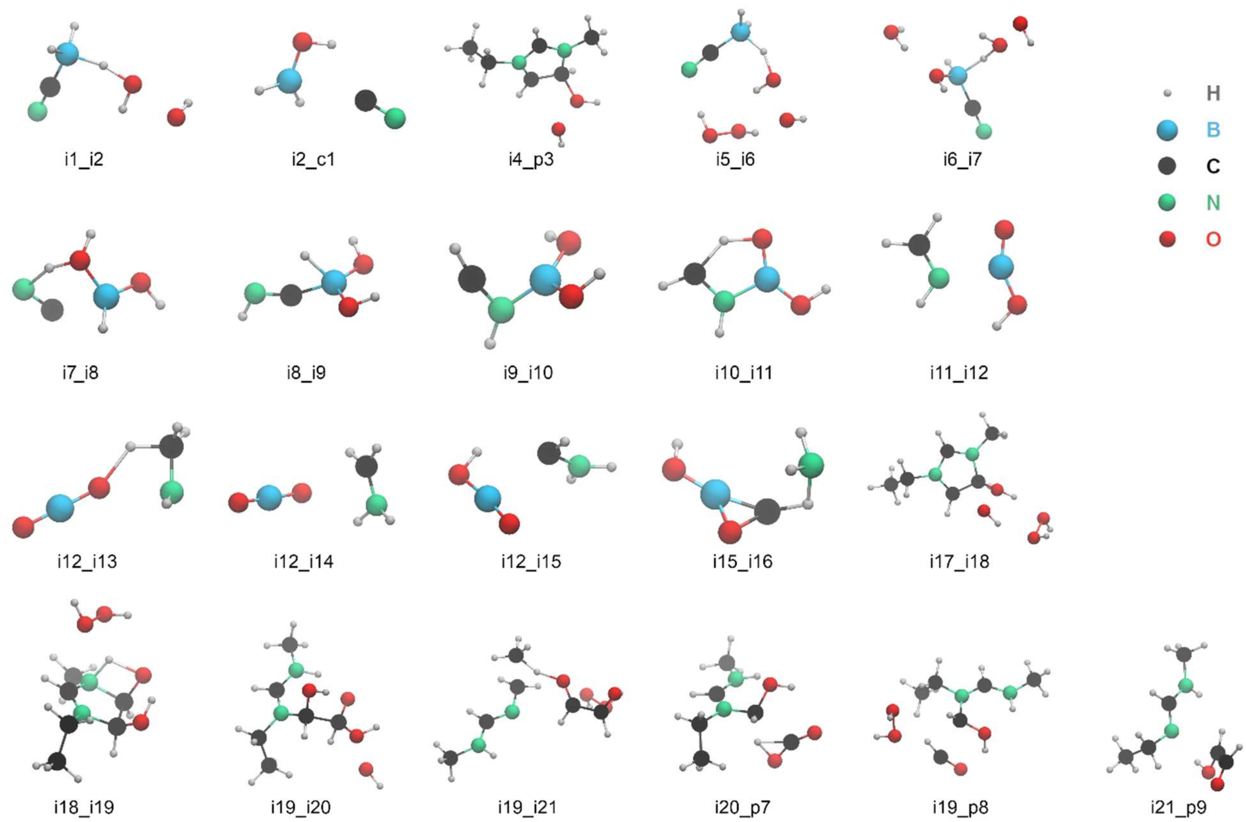

Figure S27: Geometries of transition states presented in the main text (Figures 4 and 5), where a transition state connecting intermediates “X” and “Y” is labeled as “X_Y”.

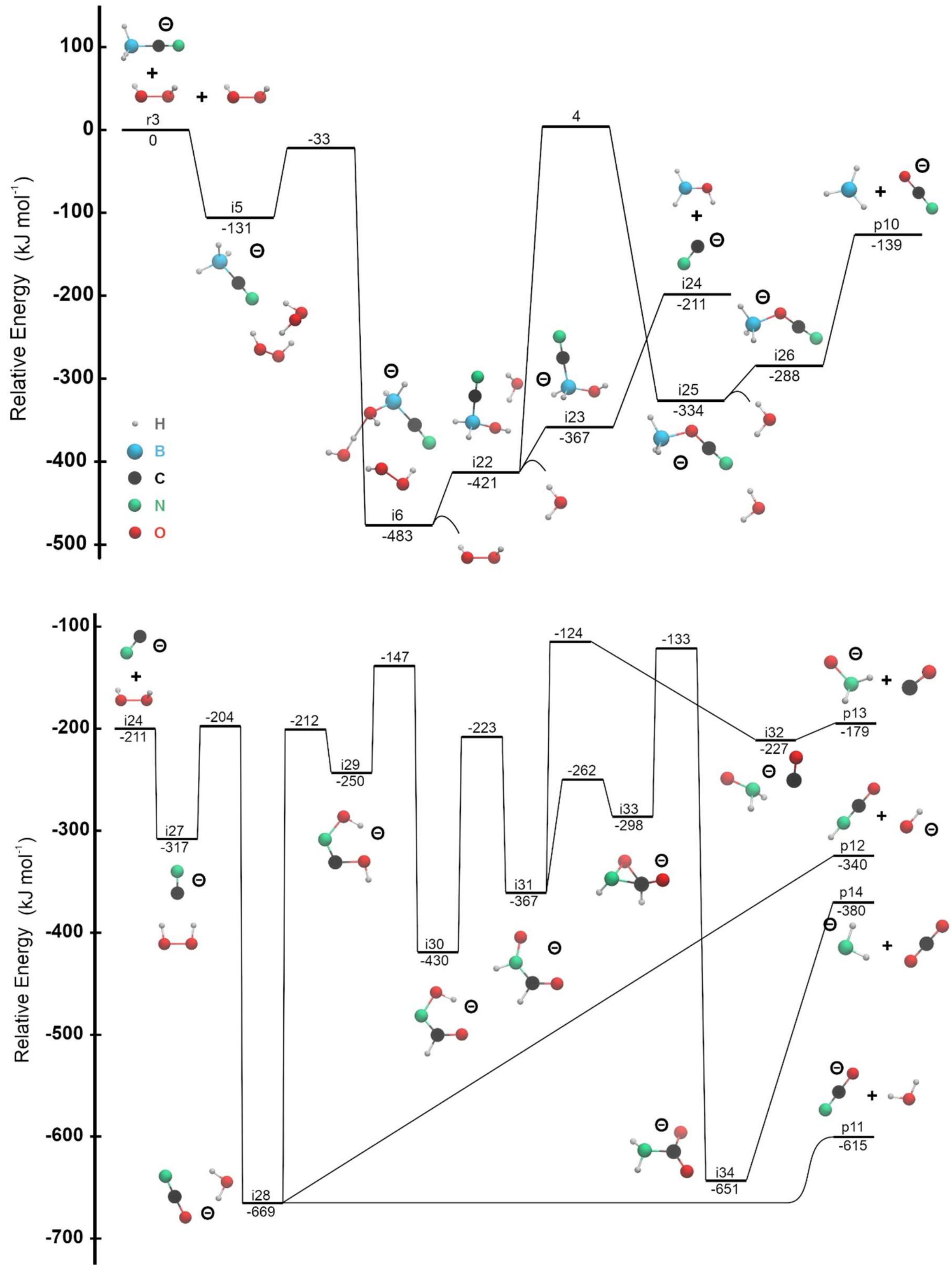

Figure S28: Potential energy profile for the $[CBH]^-$ + 2 H_2O_2 reaction forming CO_2, CO, HNCO and OCN^-. Energies are calculated at the B2PLYP/cc-pVDZ//B3LYP/6-31G* level of theory including zero-point energy corrections, relative to the reactants.

Table S9. Enthalpy changes of the reactant droplets- ionic liquid ([EMIM][CBH]) and oxidizer (H_2O_2) during merging, considering the overall specific heat capacity to be 1.0 ± 0.2 $Jg^{-1}K^{-1}$. The resultant specific heat capacity of the liquid mixture was evaluated using the specific heat capacity values for similar type of ionic liquids containing $[EMIM]^+$ (2.0 $Jg^{-1}K^{-1}$) and that of different concentrations of H_2O_2. The errors in the number of moles and masses originate from the volume measurement errors of the levitating oblate spheroid droplets.

Percentage Concentration of H_2O_2	Mass of [EMIM][CBH] droplet (kg) (× 10^{-6})	Number of moles for [EMIM][CBH] (× 10^{-5})	Mass of H_2O_2 droplet (kg) (× 10^{-6})	Number of moles for H_2O_2 (× 10^{-5})	specific heat capacity of H_2O_2 ($Jg^{-1}K^{-1}$)	Molar enthalpy change (kJ mol^{-1})
20 %	7.7 ± 3.9	5.1 ± 2.5	11.2 ± 5.7	6.5 ± 3.3	3.84	7.9 ± 4.0
50 %	10.4 ± 4.5	6.9 ± 3.0	11.5 ± 4.3	16.9 ± 6.3	3.28	8.4 ± 3.3
80 %	10.2 ± 3.6	6.8 ± 2.4	12.5 ± 5.6	29.4 ± 13.1	2.91	10.6 ± 4.4
92 %	10.9 ± 4.4	7.2 ± 2.9	12.9 ± 5.6	34.8 ± 15.3	2.69	10.9 ± 4.6

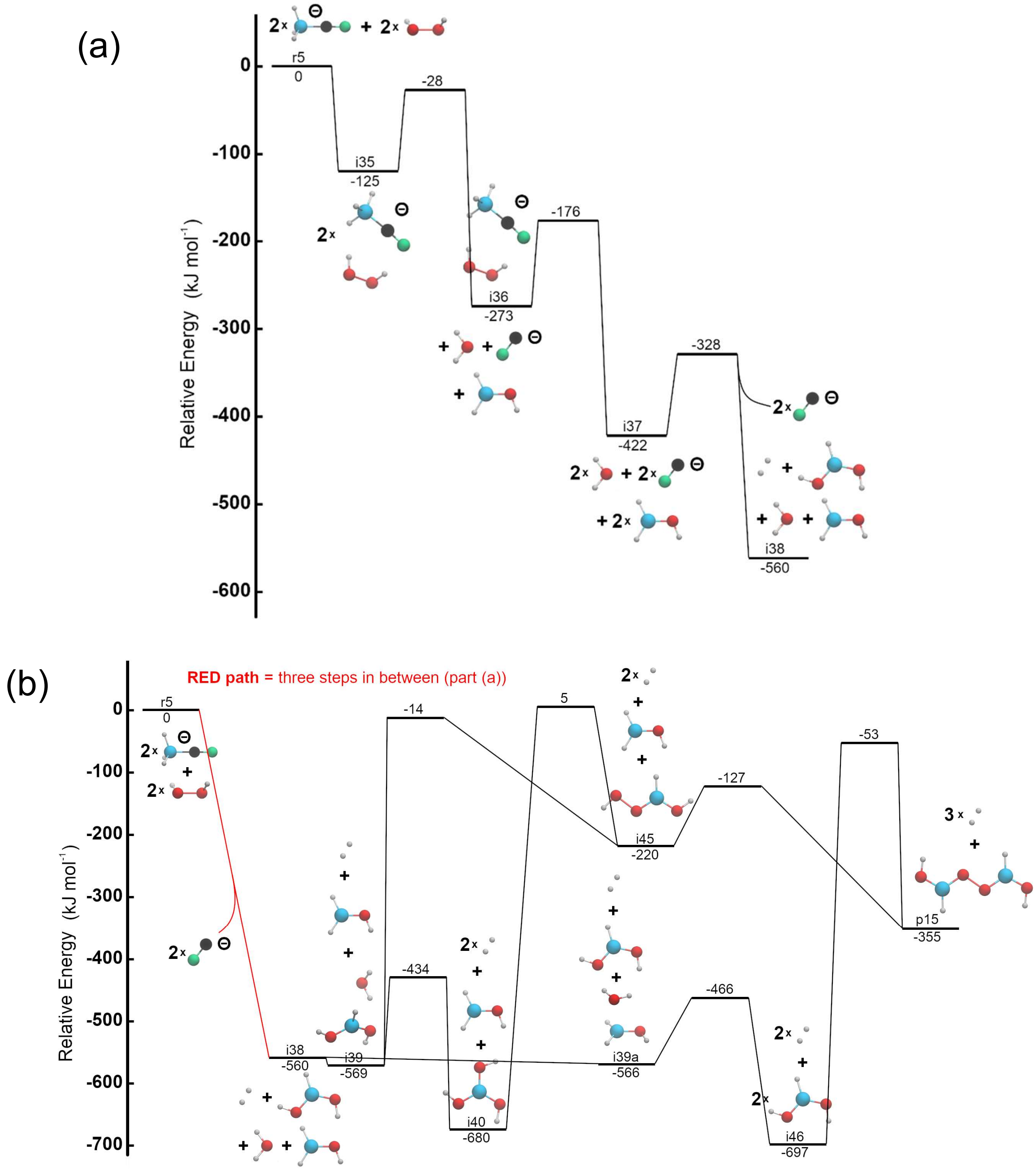

Figure S29: Potential energy profile of the 2 $[CBH]^-$ + 2 H_2O_2 reaction, decomposed into two parts: (a) breaking of the HOOH to form B-O bonds and (b) association of two boron-containing molecules to form a bridging B-O-O-B species. Energies are calculated at the B2PLYP/cc-pVDZ//B3LYP/6-31G* level of theory including zero-point energy corrections, relative to the reactants.

Table S10. Cartesian coordinates for the reactants, intermediates, transition states and products in the abovementioned potential energy profiles.

$[EMIM]^+$			
C	0.41154614	-0.81920262	-0.20781038
N	-0.62197434	0.02305243	-0.32246794
N	1.52317971	-0.11496032	0.04140589
C	-2.03408602	-0.36393566	-0.56117038
H	-2.40709985	0.28274559	-1.35981176
H	-2.01730903	-1.38672552	-0.94546589
C	2.87262347	-0.66932251	0.22407177
H	3.24146260	-0.40704224	1.21779834
H	3.53842261	-0.26462171	-0.54096731
C	1.18749319	1.22597413	0.08906915
C	-0.15485304	1.31142508	-0.13678309
H	-0.80686785	2.16986346	-0.18598426
H	1.92358790	1.99381735	0.27172300
H	0.35912314	-1.89318702	-0.30479373
H	2.82625648	-1.75447176	0.12831258
C	-2.88677133	-0.25311214	0.70098530
H	-2.91262506	0.77245392	1.08200761
H	-3.91287770	-0.54848237	0.46241784
H	-2.51610413	-0.91199436	1.49203997

$[CBH]^-$			
H	-0.58305750	-0.82126062	-1.78110208
H	0.43088551	0.91602642	-1.77855950
H	1.38279156	-0.80462403	-1.35504689
B	0.32603276	-0.18808135	-1.25180156
C	-0.01071191	0.00601836	0.29402673
N	-0.25794043	0.14834980	1.42855473

HOOH			
H	0.84725523	0.86550097	0.43464764
O	0.02314360	0.72743828	-0.06536023
O	-0.02314342	-0.72743419	-0.06535730
H	-0.84725541	-0.86550505	0.43464767

i1			
H	-0.79813836	-0.10553130	-1.71860228
H	-2.02022918	-1.46669869	-0.88797999
H	-2.56915989	0.47142779	-0.99443766
B	-1.64146531	-0.30748916	-0.83973323
C	-0.94741272	-0.03805392	0.56323966
N	-0.37738048	0.16724387	1.56489353
H	1.44617448	0.30342829	0.71828211
O	2.12840250	0.44710463	0.02144354
O	1.83056446	-0.65971302	-0.87529705
H	0.95193168	-0.39512585	-1.22367581

i4			
C	-0.10022689	-0.19591232	0.04504886
N	-0.88640601	0.73459912	0.60255705
N	-0.32386393	-1.36669246	0.65689241
C	-0.95720388	2.15552452	0.19291262
H	-0.87811841	2.75480386	1.10415097
H	-0.06635138	2.34996611	-0.40908229
C	0.34198156	-2.63754316	0.33605129
H	0.76660050	-3.05910967	1.24952145
H	1.13711016	-2.43888944	-0.38334808
C	-1.28474050	-1.17815148	1.63409671
C	-1.63790708	0.13807502	1.59940742
H	-2.34399848	0.69390834	2.19657395
H	-1.62470663	-1.98447646	2.26552167
H	0.60242838	-0.02870476	-0.76542312
H	-0.38464170	-3.33345548	-0.08967667
C	-2.23543818	2.47477030	-0.57990302
H	-3.12935426	2.28892779	0.02364536
H	-2.23109195	3.53368173	-0.85539830
H	-2.30422701	1.88179121	-1.49702863
H	3.53660242	-1.02708520	-1.60627630
O	2.59718969	-1.20356645	-1.80433882
O	2.13487173	0.13058069	-2.14204101
H	2.03969642	0.05115273	-3.11039792

i1_i2			
H	-0.40812555	-0.17999648	-0.88789113
H	-1.79910103	-1.64347127	-0.83577944
H	-2.34550853	0.29455242	-1.28031874
B	-1.74584694	-0.46864459	-0.56184463
C	-1.91690038	-0.17215369	0.96081383
N	-2.04543268	0.04947384	2.10092151
H	2.87060188	-0.18473534	-0.48435864
O	2.61416493	0.75125714	-0.52848075
O	0.78590247	0.14494861	-0.79949999
H	0.73885053	0.67572356	0.01106741

i2			
H	1.01488132	-0.99703711	-1.32035264
H	-1.42322874	-0.76252096	-0.93102638
H	-1.00549887	1.20821517	-1.02450639
B	-0.54902223	0.10108398	-0.75492079
C	-0.23764275	0.08256054	0.84588578
N	-0.00490018	0.03275573	1.99059786
O	0.68506621	-0.11712758	-1.55047475

i4_p3

C	-1.17972070	-0.56678273	0.14902013
N	0.01933004	-0.99831599	-0.29189844
N	-1.23567533	0.76365256	0.07531556
C	0.42338530	-2.42130144	-0.40808050
H	1.40628062	-2.50403140	0.06258208
H	-0.28306454	-2.99488479	0.19648960
C	-2.33977498	1.60060006	0.54565479
H	-2.50592194	2.41026041	-0.16944942
H	-2.10341934	2.01379863	1.52963921
C	0.05238016	1.27662529	-0.30392591
C	0.78684754	0.07083877	-0.62290254
H	1.78752410	-0.02414884	-1.01202694
H	0.00447083	2.08740739	-1.03688881
H	-1.97076072	-1.21040522	0.50422399
H	-3.24521044	0.99547672	0.61068919
C	0.44241877	-2.90222671	-1.85737097
H	1.15574942	-2.33345065	-2.46165247
H	0.74851800	-3.95231596	-1.87682483
H	-0.54739100	-2.82605081	-2.31747084
H	0.55980946	2.94265337	0.94088121
O	0.76286847	1.97284424	0.88338170
O	1.91648469	1.03149583	2.15105850
H	2.68264184	1.58961699	1.90991538

i2_c1

C	-1.14637481	-0.04418017	-0.31859908
N	-2.28564395	-0.08470636	-0.61597677
H	1.09993700	0.28971761	-0.76004448
H	0.66045063	1.21187822	1.37019527
H	1.48882051	-0.59114390	1.97555586
B	1.18599076	0.17107428	1.08253807
O	1.76356367	-0.06828954	-0.13883863

c1

C	-1.11347471	-0.09339482	-1.27598427
N	-2.19944216	0.04107031	-1.69717785
H	0.32945334	-0.28008178	-0.73263777
H	0.70844621	0.66507927	1.48586862
H	2.67829477	-0.01540610	1.33950302
B	1.56860760	0.09155968	0.84490769
O	1.34950621	-0.41591536	-0.35641574

p3

C	-1.19967648	-0.41759846	0.00557338
N	0.00905921	-0.91236248	-0.09882664
N	-1.26517892	0.90819989	-0.04787659
C	0.40099543	-2.33319701	-0.07708294
H	1.22770166	-2.41245480	0.63428122
H	-0.44600218	-2.89297308	0.33018415
C	-2.45348922	1.72207643	0.20928095
H	-2.58018931	2.45177837	-0.59514452
H	-2.34832502	2.23977760	1.16611281
C	0.09360205	1.47146480	-0.04597541
C	0.99158947	0.20535361	-0.30237557
H	1.33822850	0.15735812	-1.33780317
H	0.19785850	2.21986670	-0.83520971
H	-2.08474569	-1.03567319	0.11986802
H	-3.33216063	1.07535077	0.24136059
C	0.80706746	-2.85924312	-1.45341327
H	1.67948601	-2.32971387	-1.84849276
H	1.07760084	-3.91557788	-1.36361716
H	-0.01354097	-2.77715065	-2.17314059
H	0.71275166	2.90347795	1.15464250
O	0.36749078	1.99928916	1.22549515
O	2.08217939	0.12324878	0.52383545
H	1.85249322	0.56643647	1.36467202

i3

C	-2.40202810	0.30081331	-0.64951414
N	-3.35084895	0.97060042	-0.81454751
O	-0.30566098	-1.28075061	-0.10603469
H	-0.36966095	-1.28011385	0.86196091
H	-1.12536410	-0.64858576	-0.38460476
H	1.10263428	-0.68667235	-0.40043307
H	2.06063658	-0.07607936	1.69953976
H	3.76445051	0.44972803	0.60816516
B	2.63247260	0.02308732	0.63441192
O	2.06234290	-0.33401227	-0.51260084

p1

H_2BOH

H	0.84428668	-0.96681327	-0.21565110
H	-1.43106900	-0.77123999	0.34155147
H	-1.06006462	1.29544329	0.24705135
B	-0.69540061	0.16084818	0.15963568
O	0.60661210	-0.02926409	-0.15908297

HCN

H	-1.44860765	-0.63257113	0.05444844
N	0.59130898	0.25822827	-0.02214393
C	-0.46837368	-0.20452357	0.01762084

OH^-

O	0.00000000	-0.09245684	0.07262983
H	-0.00000000	0.68484429	-0.53798205

i5

H	-4.01081582	-1.47806147	-1.07582952
H	-2.86723105	-2.10939547	-2.60627274
H	-2.93503411	-3.16865026	-0.89339120
B	-2.98076777	-2.05447783	-1.39155830
C	-1.76724440	-1.21312644	-0.82330414
N	-0.87063222	-0.58889241	-0.40178408
H	-0.49131050	0.96274474	0.58857627
O	0.07147869	1.68450915	0.97539788

p2

H_2BO^-

H	-1.42489214	-0.81130982	0.31890173
H	-1.06404440	1.24422140	0.28436274
B	-0.56009939	0.09317544	0.11621637
O	0.66188199	-0.12692256	-0.21483563

HCN

H	-1.44860765	-0.63257113	0.05444844
N	0.59130898	0.25822827	-0.02214393

O	0.69222091	0.98415850	2.09409926
H	1.31031174	0.39957816	1.59313930
H	1.00969226	-0.59773755	-0.34229425
O	1.91458698	-0.31542385	-0.04467865
O	2.08099960	0.92353088	-0.79604332
H	1.44490438	1.49561092	-0.30319419

i5_i6

H	-1.90045349	0.04284188	0.73435549
H	-2.96967964	-0.35134828	-0.95100575
H	-3.03857896	-1.60090115	0.68468271
B	-2.37600391	-0.93778037	-0.07773517
C	-1.09005599	-1.67423072	-0.58515919
N	-0.09012652	-2.16517866	-0.93790945
H	0.15977938	2.56938218	1.53837495
O	0.56434220	1.73723670	1.83619686
O	-0.87955881	0.74862115	1.20265612
H	-0.29414983	0.53053667	0.44700561
H	1.53270776	-1.03752061	-0.57407433
O	2.23569037	-0.39718679	-0.32353366
O	1.50387068	0.85579407	-0.47293062
H	1.42438802	1.17851805	0.47671041

i6

H	0.63252723	1.78036462	-0.88828513
H	-0.74228764	-0.22150426	-1.10222831
H	-0.82785561	-0.11959773	0.92783999
B	-0.15109990	0.12514910	-0.06745281
C	1.18273895	-0.78218908	0.01473366
N	2.18450895	-1.37893924	0.07492231
H	2.91342740	0.91113365	1.03532822
O	2.70267235	1.84525054	1.19479552
O	0.18160463	1.57020961	-0.05790056
H	1.75877730	1.87190777	0.92259378
H	-2.41019478	-0.94295962	0.85101664
O	-3.13682950	-1.36514817	0.34458577
O	-3.37929317	-0.33869374	-0.65812012
H	-2.48937609	-0.28956410	-1.07176913

i6_i7

H	0.26768619	1.02838495	-1.38156231
H	-0.41991364	-0.86010150	0.32870124
H	1.38238365	-0.28506656	1.09852143
B	0.81828602	-0.28066040	0.02739669
C	1.39710646	-1.31179316	-1.02249935
N	1.79970976	-2.07167532	-1.81141896
H	1.36829856	2.05931015	2.16290846
O	1.10641685	2.83371242	1.64311680
O	0.61406530	1.05607509	-0.47912114
H	0.86445741	2.41088613	0.79329424
H	-3.56608319	-1.07232369	-0.72453143
O	-3.60090003	-0.62208447	0.13520548
O	-1.70258703	-0.83315849	0.23282797
H	-1.79696450	0.11713569	0.40786071

C	-0.46837368	-0.20452357	0.01762084

H_2O

O	0.00000000	0.00000000	0.11896417
H	-0.00000000	0.76261769	-0.47829909
H	-0.00000000	-0.76261769	-0.47829909

i17

C	-0.84698418	0.40541530	0.20760056
N	-0.27732651	0.50408484	1.41355332
N	-1.41408984	1.57922058	-0.09899334
C	0.48773292	-0.56683841	2.09507472
H	0.01461227	-0.72678528	3.06827357
H	0.35699497	-1.47017651	1.49642658
C	-2.15497022	1.86190793	-1.33546224
H	-3.22909428	1.85381242	-1.13582748
H	-1.90505212	1.09766579	-2.07186209
C	-1.20291811	2.45738236	0.94873767
C	-0.48943547	1.78408767	1.89492935
H	-0.11879177	2.10428741	2.85603387
H	-1.57308896	3.47077511	0.93055216
H	-0.87401286	-0.47333678	-0.42314585
H	-1.85552560	2.84162830	-1.71192093
C	1.96696760	-0.21758304	2.23511778
H	2.11841667	0.69534830	2.81986996
H	2.47440853	-1.03433570	2.75745527
H	2.42990549	-0.09701709	1.25243792
H	-0.54794865	-1.24640285	-3.83665994
O	-0.32586609	-0.95094357	-2.93350467
O	-1.23570220	-1.76072442	-2.13547402
H	-0.60459423	-2.42693402	-1.77502134
H	1.72348698	-3.31908686	-0.97480065
O	1.00390806	-2.67549513	-0.83511671
O	1.69668144	-1.41446163	-1.04921561
H	1.32530138	-1.15782864	-1.92234376

i17_i18

C	-2.20746805	-0.76578791	-0.25874646
N	-1.94326736	0.46698424	-0.72995341
N	-1.30391452	-1.08761030	0.67723119
C	-2.76610306	1.18705103	-1.72834247
H	-2.07693985	1.56617890	-2.48727840
H	-3.40482554	0.43931331	-2.20447677
C	-1.20123304	-2.38081901	1.35082225
H	-0.93279005	-2.21771920	2.39791990
H	-0.44278999	-3.00225587	0.86913162
C	-0.27789520	-0.08352028	0.72481123
C	-0.81493699	0.94879878	-0.14625444
H	-0.41131558	1.92310665	-0.36441221
H	0.01235589	0.17776853	1.74852649
H	-3.01865483	-1.39356802	-0.59352678

H	-2.17036323	-2.88083922	1.30995019
C	-3.59116427	2.30897051	-1.10111653
H	-2.95242707	3.06266376	-0.63075967
H	-4.17363825	2.80285968	-1.88452570
H	-4.28631466	1.92077577	-0.35053032
H	1.77310901	-0.63979272	0.83342275
O	1.03321885	-0.65549538	0.16536107
O	1.63659586	-0.07936009	-1.56137182
H	2.49298429	0.17651464	-1.15737906
H	4.73133335	-0.52835811	-0.10813139
O	4.08431994	0.14109899	0.18819424
O	3.55224297	-0.50819246	1.37326290
H	3.91053870	0.06874819	2.07460173

i7

H	1.39986287	1.82303534	-2.41332813
H	-0.57303686	-0.53825503	-1.21748131
B	-0.40007952	-0.30100512	-0.05483756
N	-2.11607775	-1.44995989	1.70816768
C	-1.36451686	-0.94261005	0.97993871
H	1.13485550	0.84224400	-0.35371298
O	0.58298677	0.48846380	0.38602846
O	1.98504231	1.35979802	-1.79419220
H	2.33808227	0.60937245	-2.29676642

i7_i8

H	-0.11318733	0.63502617	-1.20244409
H	-0.09172713	1.18043786	1.38640754
B	0.35753828	0.29651074	0.73948387
N	-1.49329194	0.27413625	-1.38912018
C	-1.56654254	-0.17726502	-0.30084425
H	0.77138707	-1.01772700	2.11418552
O	0.98397658	-0.81422295	1.19272400
O	0.86193263	0.67534873	-0.62416708
H	1.43933137	-0.03519969	-0.96453890

i8

H	-1.05381776	0.08467553	-0.84717860
H	0.18806003	0.18744572	2.02992441
B	1.02219570	-0.02179595	1.20276904
N	-1.96419274	0.15917158	-1.29284225
C	-3.01554453	0.24358477	-1.81111868
H	2.53293448	-0.16279611	2.42735014
O	2.33966154	-0.21378926	1.48147663
O	0.62299779	-0.07078730	-0.10893111
H	1.36795840	-0.24560941	-0.70796146

i18

C	-1.35076902	1.28788446	-0.04744008
N	-1.90217165	0.10001980	-0.12164899
N	-0.02667089	1.29044697	-0.11428887
C	-3.33667619	-0.22452331	-0.07828815
H	-3.44609146	-1.03417478	0.64869105
H	-3.85449763	0.65359877	0.31893904
C	0.84274353	2.43604577	0.14301888
H	1.64232117	2.45856149	-0.60152400
H	1.27870357	2.35672081	1.14262227
C	0.47599532	-0.10217161	-0.06690591
C	-0.83196499	-0.93800752	-0.31112659
H	-0.90156587	-1.29616441	-1.34188904
H	1.22500468	-0.25073563	-0.84684711
H	-1.92902941	2.20123023	0.05360577
H	0.26013822	3.35640562	0.06999813
C	-3.89801297	-0.63110386	-1.44081227
H	-3.40965671	-1.53127176	-1.82671553
H	-4.96384932	-0.85489824	-1.33519633
H	-3.78892508	0.17277524	-2.17584338
H	1.93152976	-0.62091350	1.13854691
O	0.97646627	-0.38428918	1.20048824
O	-0.96381199	-2.00507034	0.53978822
H	-0.43150707	-1.79931272	1.33600346
H	4.27823546	-0.52558665	1.42251966
O	3.65802989	-0.89958951	0.76655642
O	3.79083862	0.04507711	-0.32902323
H	4.33924027	-0.47484255	-0.94818950

i8_i9

H	2.24162365	1.75726288	0.98709610
H	-0.88131522	0.76379089	0.36647267
B	-0.29733506	-0.27228633	-0.24561837
N	1.22714113	1.66117261	0.94479965
C	0.75741788	0.72815840	0.32752503
H	-0.78443915	-1.35742849	1.36341426
O	-0.56527416	-1.48214456	0.43064977
O	-0.41172836	-0.27044210	-1.63929806
H	-1.08451558	-0.91955953	-1.88872851

i18_i19

C	-0.05326219	-1.10581450	-0.04092645
N	-1.04076338	-0.47851796	-0.56784743
N	0.41486801	-0.54298680	1.15154658
C	-1.60696074	-0.71705292	-1.91071889
H	-1.55925230	0.25272426	-2.41523894
H	-0.94332093	-1.41380461	-2.42969935
C	0.82359940	-1.43211651	2.27197853
H	-0.03718567	-1.97868057	2.66235103
H	1.25177624	-0.79744943	3.04915878
C	-0.39523506	0.78182513	1.38983872
C	-1.50733296	0.72581017	0.28600423
H	-2.51266139	0.48141542	0.63518681
H	-0.79530822	0.78364003	2.41489077
H	0.44867957	-1.94892967	-0.50444835

i9

H	1.24649880	0.39457365	1.72907678
H	0.15249964	1.98214248	-0.41350670
B	-0.26913190	-0.28659626	-0.31348442
N	1.08563922	1.27952050	1.22182668
C	0.35102281	1.08622122	0.18842340
H	-0.00491594	-1.28179073	1.36283817
O	-0.32471673	-1.41620481	0.45912198
O	-0.75833697	-0.32457942	-1.58274950
H	-1.11037451	-1.20208099	-1.80073821

H	1.58610321	-2.12711597	1.91418059
C	-3.04286442	-1.23731620	-1.84654053
H	-3.71453554	-0.51827161	-1.36896805
H	-3.39998447	-1.39340463	-2.86858044
H	-3.10256595	-2.19190931	-1.31492293
H	1.23641891	0.33885458	0.89010265
O	0.56724503	1.65455539	1.06765863
O	-1.49409172	1.86395696	-0.45524136
H	-0.60648315	2.26699845	-0.24886701
H	2.81914214	1.35263141	-0.10787979
O	2.92569659	0.38684537	0.01070589
O	2.39756130	-0.11415144	-1.24526073
H	3.21823265	-0.42022714	-1.67620726

i9_i10

H	1.24649880	0.39457365	1.72907678
H	0.15249964	1.98214248	-0.41350670
B	-0.26913190	-0.28659626	-0.31348442
N	1.08563922	1.27952050	1.22182668
C	0.35102281	1.08622122	0.18842340
H	-0.00491594	-1.28179073	1.36283817
O	-0.32471673	-1.41620481	0.45912198
O	-0.75833697	-0.32457942	-1.58274950
H	-1.11037451	-1.20208099	-1.80073821

i10

H	0.55863230	1.74103410	-0.45020312
H	0.26403117	2.22560413	1.75020648
B	-0.04413630	-0.35176036	-0.36845106
N	0.22845310	1.00766737	0.18636710
C	0.02306618	1.17821811	1.48063758
H	-0.51328097	-0.81229204	1.36722183
O	-0.47658997	-1.29008781	0.49551559
O	0.16701694	-0.52995116	-1.70110966
H	-0.03608831	-1.43919544	-1.96591600

i19

C	-1.65115332	0.95244900	-0.12147339
N	-1.20851257	-0.29853538	-0.26510969
N	-1.00186638	1.97137737	0.38191816
C	-1.96283256	-1.21766118	-1.16563447
H	-1.97253867	-2.20651424	-0.69820321
H	-3.00017510	-0.87025006	-1.17632115
C	-1.61972436	3.28394735	0.61019395
H	-1.03775214	4.04945838	0.09162127
H	-1.63148043	3.50360161	1.68102632
C	0.18308294	-2.19749710	0.52182397
C	0.12002414	-0.68352087	0.23829771
H	0.26184971	-0.16881309	1.19772338
H	-0.53767167	-2.61399706	1.24591515
H	-2.67150077	1.13412879	-0.45176463
H	-2.64355432	3.28589182	0.23100123
C	-1.39561776	-1.28501049	-2.58247948
H	-0.37573126	-1.67746100	-2.59448069
H	-2.02052848	-1.95192309	-3.18474451
H	-1.39131380	-0.29803915	-3.05547673
H	0.01509586	1.91854836	0.57892636
O	1.03359556	-2.86151218	-0.02019199
O	1.14740932	-0.33369245	-0.64937645
H	1.60215697	-1.17162406	-0.89169418
H	2.01217572	1.18983896	0.11952273
O	1.80647789	1.93506442	0.73103271
O	1.92614915	1.26315809	2.01620698
H	2.70763950	1.71574496	2.38541225

i10_i11

H	0.59427958	1.87166765	-0.34684838
H	0.18940210	2.05874798	1.97695685
B	-0.02751364	-0.35072421	-0.35963872
N	0.26339942	1.07482109	0.19733557
C	0.01917820	1.09867428	1.47247664
H	-0.36525487	-0.27083928	1.47609409
O	-0.43809826	-1.14502471	0.59858902
O	0.19228848	-0.50121554	-1.70086197
H	-0.01060967	-1.40941332	-1.96845177

i19_p8

C	-1.49044679	-1.37322060	0.07149665
N	-0.30630359	-0.77554968	0.09789374
N	-2.55141257	-1.09128742	0.80931734
C	0.77578379	-1.35120396	-0.74553079
H	1.71631839	-1.14713802	-0.22885203
H	0.64600713	-2.43684884	-0.75368863
C	-3.82163307	-1.80914702	0.72060303
H	-4.62179592	-1.12767763	0.41736722
H	-4.07072178	-2.24628429	1.69157081
C	0.35070727	2.25690182	-0.44586269
C	0.04967471	0.40308514	0.88242767
H	0.90490961	0.18344153	1.52309796
H	1.18968585	1.54797429	-0.27225751
H	-1.59527367	-2.19523284	-0.63181441

i11

H	0.52786349	1.87254672	-0.41372126
H	0.28856837	2.26213851	1.84740672
B	-0.08988400	-0.58629922	-0.36557714
N	0.24426335	1.06716812	0.15027274
C	0.11266820	1.28472800	1.39923059
H	-0.19018658	0.41645487	1.98732967
O	-0.41310302	-1.30767090	0.60501235
O	0.09199521	-0.66872366	-1.73087092
H	0.36092782	0.15229011	-2.16034064

i11_i12

H	0.57813289	2.11494381	-0.25476576
H	0.27237428	2.31876821	1.99765021
B	-0.11403770	-0.71593920	-0.37708800
N	0.28495094	1.24883623	0.20844507
C	0.11883176	1.37787287	1.46345754
H	-0.19197233	0.48432459	2.00585012
O	-0.41448819	-1.30730448	0.66414632
O	0.09274301	-0.68068746	-1.71384318
H	0.33344091	0.19612459	-2.03574275

i12

B	-1.87561311	-0.32270838	0.26182919
O	-1.24892177	0.76764998	0.64378871
O	-2.46914107	-1.33177781	-0.08926435
C	1.93924333	-0.38779255	-0.43434950
H	-0.25729931	0.77537752	0.47342955
N	1.41475765	0.63166691	0.11551869
H	2.09512149	1.36613993	0.32584485
H	3.00528562	-0.48149851	-0.66361838
H	1.29945872	-1.23074304	-0.70052952

i12_i13

B	-1.48780419	-0.46074637	0.01555860
O	-0.37722259	-0.48227642	0.66859194
O	-2.53680628	-0.41734189	-0.64212281
C	1.79301574	-0.15848291	-0.27077206
H	0.98010501	0.98474578	1.07227226
N	1.65767280	0.99765799	0.29935308
H	1.81037287	1.86505707	-0.20377057
H	2.21759771	-0.21371606	-1.27019864
H	1.54302171	-1.04634625	0.28736854

H	-3.73980835	-2.61003157	-0.01747176
C	0.79434508	-0.80373386	-2.17283806
H	0.98322606	0.27487713	-2.20492756
H	1.59396973	-1.29396046	-2.73752293
H	-0.14999866	-0.99774173	-2.69218965
H	-2.45263239	-0.31958871	1.46584470
O	-0.67470042	2.78797695	-0.25983610
O	-1.00409904	0.95655580	1.55967772
H	-1.30462390	1.77339859	1.08134508
H	3.98587008	0.49106057	1.33337715
O	3.52285029	0.14645850	0.54527635
O	3.05128893	1.37725732	-0.05468661
H	3.66118327	1.47195160	-0.81101125

i19_i20

C	-1.91893272	0.14299080	-0.01343330
N	-0.97901666	-0.80758193	-0.15617326
N	-1.77792075	1.28183637	0.60259324
C	-1.19430436	-1.90908984	-1.14036030
H	-0.97210475	-2.84904708	-0.62718616
H	-2.26112044	-1.91606345	-1.37981572
C	-2.85625057	2.25721600	0.78112757
H	-2.54567855	3.21517250	0.35675879
H	-3.05993912	2.38395576	1.84774195
C	1.30311564	0.47744827	0.12530099
C	0.23476810	-0.83976044	0.60844754
H	0.81831190	-1.72124877	0.33265527
H	1.30016035	0.30008141	-0.98549470
H	-2.88159625	-0.07140150	-0.47079718
H	-3.76122445	1.90979571	0.27848534
C	-0.35600368	-1.74865399	-2.40769338
H	0.71864371	-1.75479117	-2.19567636
H	-0.56340166	-2.58705673	-3.07992705
H	-0.60178501	-0.82077323	-2.93383477
H	-0.81740817	1.55287528	0.88598596
O	0.92503363	1.58945057	0.58752870
O	-0.06843955	-0.72393730	1.93571202
H	0.74744688	-0.77341321	2.46442645
H	3.02941150	0.68998078	0.96778496
O	2.55095740	-0.04520626	0.52578607
O	3.31108679	0.44371151	-1.36897157
H	4.22667030	0.40714980	-1.72462499

i20

C	-1.45798454	0.22793285	-0.01865538
N	-0.54791646	-0.73553610	-0.14400175
N	-1.31117665	1.38083648	0.58959674
C	-0.90324188	-2.00456104	-0.83660795
H	-0.76604950	-2.81861647	-0.11737533
H	-1.96924499	-1.95780080	-1.07219045
C	-2.36597179	2.39867317	0.68523081
H	-2.01332269	3.33094679	0.23743606
H	-2.61539793	2.56870757	1.73554195
C	1.60191628	0.51122189	0.03445307
C	0.75347246	-0.67884582	0.57193530
H	1.24970239	-1.63323830	0.35594380
O	2.17530943	0.39792167	-1.15673802

i12_i14

B	-1.68640054	0.44627169	-0.08220952
O	-0.43475609	0.08816851	0.04108781
O	-2.86375403	0.77584342	-0.20154405
C	1.89828920	-0.63960126	0.41340219
H	1.44943307	0.56891170	-1.07509384
N	1.65668643	0.61083355	-0.07034433
H	0.70947051	-0.81304607	0.58592043
H	2.18073708	-1.44403412	-0.27734911
H	2.37454480	-0.65525927	1.39598683

i12_i15

B	-1.21311253	-0.62262245	0.08213361
O	-0.90506719	-1.58692516	0.95004902
O	-1.68004171	0.20303397	-0.69384085
C	1.14582317	0.00214448	-0.28161603
H	1.56721905	1.43992525	1.07511506
N	1.66002723	1.14151287	0.10801391
H	2.12334797	1.82805590	-0.49142365
H	1.33824786	-0.10222900	-1.36260163
H	0.07543820	-1.54750658	0.96242439

i15_i16

B	-0.69369015	-0.23948368	-0.19911951
O	-0.09479086	-0.87676034	0.85150942
O	-1.87556389	0.34960649	-0.42864954
C	0.69680068	-0.75844604	-0.34989882
H	1.71742825	1.08756193	0.88670611
N	2.07184040	0.83074363	-0.03702182
H	1.68035171	1.48926535	-0.71239690
H	1.85539313	-0.46770235	-0.31775718
H	-1.95629647	0.70039495	-1.32728585

i13

B	-1.30010644	-0.05806583	-0.30005710
O	-0.41208261	-0.91567920	0.15958762
O	-2.12716000	0.73679651	-0.71478024
C	1.04437230	-0.66335307	0.04000682
H	1.24333986	1.03842488	1.14926451
N	1.47105996	0.66966717	0.23078065
H	1.14826061	1.31180003	-0.48745866
H	1.33495457	-1.01051107	-0.95401814
H	1.47603742	-1.31336905	0.80102480

H	-2.42345907	0.04243409	-0.48125520
H	-3.25549726	2.05531511	0.15413194
C	-0.09153737	-2.24295332	-2.10821715
H	0.97266366	-2.40868478	-1.89626637
H	-0.44978766	-3.15286651	-2.59947019
H	-0.19688614	-1.41341692	-2.81485170
H	-0.41742663	1.60213456	1.02615018
O	1.68265328	1.52101326	0.69932412
O	0.53087180	-0.52508999	1.92967530
H	1.08574979	0.21308615	2.24852274
H	2.05744936	-0.48559409	-1.54910347

i20_p7

C	-1.68147044	0.18050771	0.01292665
N	-0.73304849	-0.74859053	-0.03797609
N	-1.60520771	1.32893494	0.65319579
C	-0.98773115	-2.02536362	-0.76346121
H	-0.81685690	-2.83676391	-0.04913982
H	-2.04844621	-2.04007054	-1.02592155
C	-2.67689159	2.32865157	0.67527643
H	-2.29163392	3.28951779	0.32464975
H	-3.05960972	2.44042600	1.69334385
C	2.28650530	0.60835766	-0.10774952
C	0.59529568	-0.57381816	0.56858743
H	1.03966999	-1.57230925	0.63951827
O	1.95096112	0.72078858	-1.31226275
H	-2.59626063	-0.02493316	-0.53561897
H	-3.48856545	2.01034460	0.01814504
C	-0.12461875	-2.19111658	-2.01231352
H	0.94462193	-2.22169424	-1.77725372
H	-0.37495069	-3.14055527	-2.49534850
H	-0.30487152	-1.38737479	-2.73378531
H	-0.81400652	1.43898372	1.28764382
O	3.00056984	0.81097527	0.79308660
O	0.41551923	0.00978488	1.83947722
H	1.29184545	0.18681676	2.22308569
H	1.05824302	0.11600147	-0.78748469

i19_i21

C	-2.39250428	-1.60085169	-0.27464708
N	-1.35395901	-0.81270639	-0.26857163
N	-2.87872709	-2.16776561	0.82987168
C	-0.96643143	-0.29418430	-1.50472477
H	0.11574087	-0.24558629	-1.63517627
H	-1.44077191	-0.71954263	-2.39852574
C	-3.99865213	-3.10123820	0.87886531
H	-4.78269832	-2.72271179	1.54144922
H	-3.67004728	-4.08191864	1.23698259
C	1.77982008	1.68876346	1.92629882
C	0.80239872	1.05590126	0.92828851
H	0.56329288	-0.01228666	1.01286904
H	2.17730821	0.99973635	2.69474957
H	-2.93109484	-1.86487955	-1.19440284

i14

B	-1.21219843	0.35141414	0.46771538
O	-1.72301689	0.85445950	1.45132766
O	-0.66935299	-0.21314476	-0.60900054
C	1.63583557	0.25711490	-0.23638002
H	0.58528367	-1.38512242	0.38965136
N	0.66502920	-0.81290076	-0.45362354
H	1.68105449	0.87600290	-1.13546301
H	1.42501400	0.89444703	0.63641128
H	2.60723222	-0.22987201	-0.09705077

H	-4.41480290	-3.21680609	-0.12428049
C	-1.57684831	1.38569148	-1.82429641
H	-1.24924363	1.52545769	-2.85396523
H	-2.63931373	1.16993633	-1.73369953
H	-1.47983414	2.38831383	-1.35372243
H	-2.39700039	-1.95201543	1.69593574
O	2.07957342	2.85281206	1.85049962
O	0.25543533	1.76081335	0.08456551
H	-0.69535058	1.31097698	-0.88411373
H	3.57597983	1.02985830	-0.31202986
O	3.03736263	0.26028026	-0.04087184
O	2.53274353	-0.18583488	-1.32453166
H	3.02463775	-1.02307829	-1.42464950

i15

B	-0.49242966	-0.51515464	0.10051368
O	-0.94534329	-1.47887645	0.94793292
O	-1.01783328	0.43434664	-0.64508412
C	0.70746103	0.19562366	-0.53814302
H	1.21710657	1.47195247	0.96533331
N	1.46386819	1.19225491	0.02373312
H	1.68289117	1.99154206	-0.56254507
H	1.00075677	-0.03705873	-1.55828695
H	-0.22010711	-2.01158739	1.30239289

p4

H_2CNH

C	-0.63844950	-0.07785148	0.00394082
H	1.08429771	0.92671124	-0.06206288
N	0.80558984	-0.06451260	0.00558438
H	-1.01097067	-1.10463175	0.07615204
H	-1.05377157	0.50457570	0.84536353
H	-1.04991851	0.37915307	-0.91346624

BO_2

B	0.00000000	0.00000000	-0.00000070
O	-0.00000000	-0.00000000	1.26474645
O	-0.00000000	-0.00000000	-1.26474575

$H_2O…OH^-$

H	0.05849331	0.10043192	-0.06155875
O	0.09694351	-0.38097487	-1.19799217
H	-0.49168200	-1.13970711	-1.04400055
H	0.86371985	0.00254065	1.40404522
O	0.04565899	0.44742249	1.12346421

i21

C	-1.90530634	-0.62586045	-0.49543721
N	-0.67115575	-1.07921812	-0.49818376
N	-2.29375039	0.50821149	0.05332392
C	-0.25078993	-2.34947707	-1.12153402
H	0.14547185	-2.99282137	-0.32890278
H	-1.14739540	-2.83372978	-1.52011929
C	-3.67444659	0.99832947	0.04464631
H	-3.72480207	1.96316044	-0.46715598
H	-4.03573210	1.11340611	1.07009429
C	2.08485970	1.18310966	1.20628363
C	1.03245979	2.21679796	1.65574233
H	1.39555965	3.08489172	2.23348221
H	3.13692726	1.38748946	1.47058132
H	-2.66506444	-1.23305988	-0.98156117
H	-4.31236999	0.28386970	-0.47946951
C	0.79306618	-2.12567890	-2.21360160
H	1.10217757	-3.09126271	-2.62533776
H	0.39185923	-1.51568135	-3.02888392
H	1.68360219	-1.63186456	-1.81093605
H	-1.59007450	1.08410197	0.51878773
O	1.75839870	0.19283758	0.58899714
O	-0.13762279	2.07232180	1.37899335
H	0.06758654	-0.52141651	-0.05761367

p5

H_2CNH_2

C	-0.70957853	-0.14161344	-0.32073559
H	0.99525915	0.97675806	-0.37541207
N	0.62424477	0.11977266	0.02222381
H	1.25965898	-0.64940757	-0.16432658
H	-1.09115904	-1.11174355	-0.01590354
H	-1.38654504	0.70492408	-0.25167326

BO_2

B	0.00000000	0.00000000	-0.00000070
O	-0.00000000	-0.00000000	1.26474645
O	-0.00000000	-0.00000000	-1.26474575

$H_2O…OH^-$

H	0.05849331	0.10043192	-0.06155875

i21_p9

C	-1.59133143	-0.09364483	-0.45881259
N	-0.30760872	-0.25105558	-0.65048128
N	-2.20340721	1.09604957	-0.51972034
C	0.15736951	-1.64806045	-0.75539560
H	1.15374933	-1.70735239	-0.30097043
H	-0.49935790	-2.32427903	-0.18950261
C	-3.62707541	1.31987356	-0.27586682
H	-4.11165614	1.70053001	-1.18006268
H	-3.76807551	2.04035935	0.53557594
C	1.87663717	0.44707585	2.17147882
C	1.30165238	0.94261421	0.86338272
H	0.37188691	1.50443876	0.82827720
H	1.39328883	0.82277970	3.08836924

O	0.09694351	-0.38097487	-1.19799217
H	-0.49168200	-1.13970711	-1.04400055
H	0.86371985	0.00254065	1.40404522
O	0.04565899	0.44742249	1.12346421

H	-2.25205372	-0.93467758	-0.22269774
H	-4.09598150	0.37557262	0.00707588
C	0.24657304	-2.09810515	-2.21757385
H	0.91185421	-1.44560416	-2.79303867
H	0.64255245	-3.11735812	-2.26820967
H	-0.73827398	-2.08889843	-2.69640046
H	-1.66173086	1.87620445	-0.87685101
O	2.79148675	-0.33985932	2.15533712
O	2.01968216	0.78624303	-0.17770006
H	1.39698019	0.84037689	-0.95936773

P6

HOBCO

B	-0.04613532	0.12049954	-0.21965434
O	0.54065817	-0.50977752	0.85886681
O	-1.32442266	0.37971029	-0.52523350
C	1.46702565	-0.07710501	-0.05834017
H	-1.42542802	0.84623495	-1.36797152

NH_3

N	0.07655746	-0.07654840	-0.07654909
H	0.61518895	0.53524516	0.53524586
H	-0.53524996	-0.61518274	0.53524020
H	-0.53525026	0.53523980	-0.61518315

$H_2O…OH^-$

H	0.05849331	0.10043192	-0.06155875
O	0.09694351	-0.38097487	-1.19799217
H	-0.49168200	-1.13970711	-1.04400055
H	0.86371985	0.00254065	1.40404522
O	0.04565899	0.44742249	1.12346421

p7

C	-0.85582493	0.39736714	-0.14447999
N	-0.04126538	-0.64524917	-0.09722615
N	-0.78720325	1.46394739	0.62535588
C	-0.18869596	-1.76679774	-1.06054048
H	-0.18073400	-2.69546583	-0.48066855
H	-1.18149761	-1.68365334	-1.51130148
C	-1.74618549	2.57273587	0.58366976
H	-1.22787377	3.50062505	0.32851490
H	-2.22700989	2.68187691	1.55921821
H	2.40299390	0.49394865	0.51357681
C	0.97709665	-0.77122475	0.97995933
H	0.45655503	-0.97845433	1.92007717
H	1.60996455	-1.62381664	0.72240258
H	-1.65423745	0.36930293	-0.88219140
H	-2.50987157	2.36754926	-0.16907186
C	0.89807110	-1.77331319	-2.13359005
H	1.90024410	-1.87411490	-1.70279765
H	0.74243481	-2.62762304	-2.79961938
H	0.86730576	-0.86032101	-2.73646501
H	0.03086530	1.55124744	1.22772720
O	1.70261910	0.40805115	1.18181610

CO_2

O	-1.16958709	0.00000030	-0.00000007
C	0.00000149	-0.00000061	0.00000013
O	1.16958559	0.00000030	-0.00000007

H_2O

O	0.00000000	0.00000000	0.11896417
H	-0.00000000	0.76261769	-0.47829909
H	-0.00000000	-0.76261769	-0.47829909

p8

C	-0.93738355	-0.03412243	-0.04497927
N	0.29573444	-0.50473662	0.06918127
N	-1.29226239	1.23094216	0.03127363
C	0.55312239	-1.96778671	0.01073617
H	1.14869802	-2.22245268	0.89337537
H	-0.41104833	-2.47125123	0.11884731
C	-2.66912777	1.71076273	-0.12408751
H	-2.71447154	2.44581794	-0.93177411
H	-3.00803809	2.17205225	0.80733248
H	1.95048381	1.90837879	1.31474048
C	1.45364645	0.39212137	0.17685758
H	2.31861577	-0.22687918	0.43455955
H	1.62792203	0.86651817	-0.80041615
H	-1.72530120	-0.76106164	-0.22341869
H	-3.32336344	0.87197354	-0.36979596
C	1.25078435	-2.40055585	-1.27747825
H	2.23295322	-1.92988877	-1.39238444
H	1.40755808	-3.48337646	-1.25309378
H	0.64545293	-2.16288728	-2.15804614
H	-0.57871098	1.88771632	0.34692265

p9

C	0.19205340	-0.20446975	-0.07825090
N	0.82876409	0.16018023	1.07754227
N	-0.94172474	0.35306324	-0.35897264
C	1.95435667	-0.41483287	1.32500180
H	2.48211866	-0.14335421	2.23773657
H	2.41596447	-1.16409727	0.67049333
C	-1.77572734	0.10146853	-1.53985647
H	-1.89940331	1.03759400	-2.09097108
H	-2.75416059	-0.25897973	-1.21106112
H	-1.29617428	-0.64502269	-2.17399512
H	0.59031864	-0.94379339	-0.78005302
H	-1.27395420	1.03717269	0.32568422

CH_4

C	-0.00000000	0.00000000	0.00000000
H	0.63125636	0.63125636	0.63125636
H	-0.63125636	-0.63125636	0.63125636
H	-0.63125636	0.63125636	-0.63125636
H	0.63125636	-0.63125636	-0.63125636

CHO-CHO

H	1.65832173	0.59124204	0.79561306

O	1.16846255	1.34859645	1.17513769

CO

C	-0.66886384	-0.00000000	-0.00000000
O	0.46886384	0.00000000	0.00000000

HOOH

H	0.84725523	0.86550097	0.43464764
O	0.02314360	0.72743828	-0.06536023
O	-0.02314342	-0.72743419	-0.06535730
H	-0.84725541	-0.86550505	0.43464767

C	0.64079019	0.18002190	0.61184565
C	0.18396294	0.21428277	-0.85863585
O	-0.05213897	-0.25921599	1.49572708
H	0.92487406	0.64385786	-1.56907897
O	-0.89457594	-0.19346918	-1.21193558

HOOH

H	0.84725523	0.86550097	0.43464764
O	0.02314360	0.72743828	-0.06536023
O	-0.02314342	-0.72743419	-0.06535730
H	-0.84725541	-0.86550505	0.43464767

i22

H	0.25510953	-1.22463667	-1.58036064
H	-2.12015852	-0.97374439	-1.16599215
H	-1.73909307	1.00493503	-1.22624626
B	-1.28529149	-0.09426000	-0.94685176
C	-0.98436559	-0.11687329	0.64916386
N	-0.71731800	-0.14224120	1.78705222
H	1.56390761	0.43353338	0.71828005
O	2.11164035	0.51015338	-0.07988806
O	-0.01282353	-0.30429795	-1.71470791
H	1.43196409	0.35725957	-0.77786486

i22_i25

H	-0.62069682	-0.76325310	-2.09324716
H	-2.67077207	-0.53713198	-1.56635990
H	-1.53792128	1.15901283	-1.97418164
B	-1.59414893	0.02756929	-1.53409582
C	-0.50382807	-0.01235733	1.24050090
N	-0.02387272	0.17073427	2.29911680
O	-0.55374253	-0.49117821	-0.74534250
O	2.25216176	0.40371877	-0.09542930
H	1.43566207	0.15620634	-0.56662792
H	1.89577465	0.44144184	0.80958131

i25

H	-3.37224561	-0.79109401	-1.73967947
H	-2.68153048	0.83003861	-0.73259041
H	-1.78509261	0.25027973	-2.45792088
B	-2.40452015	-0.10379398	-1.46781899
C	-0.34337984	-0.72677451	-0.18804371
N	0.70551505	-0.43928165	0.25997122
O	-1.45048374	-1.10239538	-0.63657269
O	3.13946111	0.80914896	1.08837875
H	2.87723097	1.63736315	0.66069727
H	2.36099615	0.24162287	0.88272335

i26

H	-0.90474040	0.47925240	-2.03615979
H	-0.69634971	-1.52853143	-2.23333688
H	-1.96677139	-0.77163028	-0.84531418
B	-0.92751145	-0.60455513	-1.46894788
O	0.28397029	-0.64673404	-0.43278666
C	0.37445234	0.18008582	0.51506371
N	0.52067651	0.91924573	1.42064892

p10

BH_3

H	0.86400166	-0.82863588	0.16065421
H	-0.93296332	0.00471109	0.75478532
H	-0.13510108	0.47712106	-1.09363002
B	-0.06801376	-0.11559827	-0.05939100

OCN^-

N	-0.66032288	-0.39583719	-1.00943118
C	-0.03804449	-0.02274186	-0.05826812
O	0.60456165	0.36255076	0.92395002

i24

H_2BOH

H	0.84428668	-0.96681327	-0.21565110
H	-1.43106900	-0.77123999	0.34155147
H	-1.06006462	1.29544329	0.24705135
B	-0.69540061	0.16084818	0.15963568
O	0.60661210	-0.02926409	-0.15908297

CN-

C	0.36389765	0.44548204	0.27362187
N	-0.31233150	-0.38235496	-0.23484826

HOOH

H	0.84725523	0.86550097	0.43464764
O	0.02314360	0.72743828	-0.06536023
O	-0.02314342	-0.72743419	-0.06535730
H	-0.84725541	-0.86550505	0.43464767

i27

C	-1.03184876	0.76650713	-0.37673219
N	-1.91207629	1.46931794	-0.71000142
O	0.68903266	-0.98593901	1.04494608
H	0.66797559	-0.14845044	-0.63304907
H	-0.11160408	-0.41076128	0.87219827
O	1.35561916	-0.76164393	-0.24209019

i27_i28

C	-1.42592181	0.72654831	-0.05483909
N	-2.28967494	1.33484220	-0.56986934
O	0.19692934	-0.26881449	0.25708617
H	1.91299245	-1.17649330	-0.47664127
H	0.53223351	0.48880984	0.75555430
O	1.89063334	-0.98509779	0.47417761

i28

C	-0.81431959	0.25346974	-0.07676431
N	-0.71637992	1.27820401	-0.68181597
O	-0.85474613	-0.81401896	0.54816152
H	1.60855627	0.31615255	-0.32453655

i28_i29

C	-0.13435603	0.38219784	-1.01580089
N	-0.77626751	0.52518314	0.05993990
O	-0.21300295	-0.36287388	1.35547380
H	1.74906875	0.00721095	-0.94827750

H	1.19551608	-0.89438718	0.41620870
O	2.01385646	-0.46447367	0.09457652

H	-0.82832655	0.05880227	1.97579540
O	0.97419075	-0.56438932	-1.06797696

i29

C	-0.11312728	0.45381860	-0.86251685
N	-0.88325588	0.36803784	0.16615863
O	-0.39376740	-0.50803033	1.31073191
H	1.56986169	-0.16698219	-1.54893970
H	0.45958272	-0.82134458	0.95984294
O	1.12732089	-0.34339464	-0.71173140

i29_i30

C	0.04013703	0.40836329	-0.83590524
N	-0.90308123	0.50213865	0.04244801
O	-0.57909864	-0.30565944	1.24004921
H	1.01061996	0.23684074	-1.58811338
H	0.29589222	-0.67528179	0.97427879
O	1.20562710	-0.39608090	-0.58822842

i30

C	0.57040208	0.14975963	-0.77752792
N	-0.60830536	0.36729559	-0.23035216
O	-0.60145501	-0.23592106	1.09800347
H	0.63085353	0.58869575	-1.80119529
H	0.31593954	-0.60430190	1.11250124
O	1.57268380	-0.46777866	-0.28596561

i30_i31

C	0.28844351	0.28101742	-0.75614800
N	-0.72228575	0.63231569	0.07161984
O	-0.83512590	-0.18461527	1.36195995
H	0.14897878	0.82414523	-1.73331003
H	-1.59623113	0.00568400	0.27275739
O	1.29894491	-0.41152703	-0.57832767

i31

C	0.49353568	0.07377015	-0.62335442
N	-0.71305853	0.33824000	-0.09325959
O	-1.22926776	0.00245138	1.08191947
H	0.52895290	0.54343637	-1.64745806
H	-1.30463424	0.89430312	-0.73406028
O	1.45975665	-0.56082021	-0.15469922

i31_i32

C	1.08941955	0.27582135	-0.70313606
N	-1.04669783	0.35520786	0.21093364
O	-2.19641287	0.30136991	0.72891621
H	0.02866530	-0.16030155	-1.20552226
H	-0.99746747	1.16502445	-0.47628805
O	2.02229278	-0.48371257	-0.64957058

i31_i33

C	0.43360686	0.04762842	-0.58289818
N	-0.91331641	-0.02095380	-0.21786426
O	-0.86712372	0.49635040	1.15041601
H	0.70061468	0.91612063	-1.25600343
H	-1.39863782	0.69074731	-0.78901368
O	1.32104921	-0.73215674	-0.26581227

i32

C	1.22698020	0.20350232	-0.75175011
N	-0.87030237	0.42670161	0.03137917
O	-1.76918060	-0.09683391	0.90962036
H	-1.23558685	0.44657452	-0.95436748
H	-0.69929345	1.45141617	0.19353233
O	1.85212550	-0.66620418	-0.27827717

i33

C	0.31711426	0.08625363	-0.42724236
N	-1.11433049	0.29981931	0.01369386
O	-0.01359720	0.15739931	1.02825898
H	0.77780238	1.08162393	-0.68693999
H	-1.26798379	1.32616187	0.00227420
O	0.73222609	-0.94912415	-1.00144975

i33_i34

C	0.13735416	0.16879164	0.02766735
N	-1.24884706	0.55532366	0.11629454
O	0.63027163	-0.09889360	1.22052466
H	0.56600742	1.24330961	-0.28547505
H	-1.36833450	1.23710485	-0.64933890
O	0.37458416	-0.68256770	-0.96413856

i34

C	0.03257471	0.01518124	-0.03022356
N	-1.19118633	0.54122034	0.61988719
O	0.22087018	0.43715364	-1.19687891
H	-1.89401940	0.71864729	-0.09502717
H	-1.53611153	-0.15080253	1.28221955
O	0.71156950	-0.75485885	0.69128268

p11

OCN^-

N	-0.66032288	-0.39583719	-1.00943118
C	-0.03804449	-0.02274186	-0.05826812
O	0.60456165	0.36255076	0.92395002

H_2O

O	0.00000000	0.00000000	0.11896417
H	-0.00000000	0.76261769	-0.47829909
H	-0.00000000	-0.76261769	-0.47829909

p12

HNCO

H	-1.76739985	0.76455781	-0.00000000
N	-1.15380286	-0.03581015	-0.00000001
C	0.06409129	0.01597497	0.00000002
O	1.23396142	-0.09017718	-0.00000001

OH^-

O	0.00000000	-0.09245684	0.07262983
H	-0.00000000	0.68484429	-0.53798205

p13

H_2BO^-

H	-1.42489214	-0.81130982	0.31890173
H	-1.06404440	1.24422140	0.28436274
B	-0.56009939	0.09317544	0.11621637
O	0.66188199	-0.12692256	-0.21483563

CO

C	-0.66886384	-0.00000000	-0.00000000
O	0.46886384	0.00000000	0.00000000

p14

CO_2

O	-1.16958709	0.00000030	-0.00000007
C	0.00000149	-0.00000061	0.00000013

i40

H_2BOH

H	0.84428668	-0.96681327	-0.21565110
H	-1.43106900	-0.77123999	0.34155147

O	1.16958559	0.00000030	-0.00000007
	NH_2^-		
N	0.14037694	0.03780509	-0.05128386
H	-0.39694758	-0.55905883	0.62648817
H	-0.68231669	0.51663173	-0.49652564

H	-1.06006462	1.29544329	0.24705135
B	-0.69540061	0.16084818	0.15963568
O	0.60661210	-0.02926409	-0.15908297
	H_3BO_3		
O	1.32761265	-0.24270255	-0.24034333
O	-0.82090189	-1.12310865	0.26549503
O	-0.51812282	1.22450152	0.05552029
B	-0.00381139	-0.04711293	0.02689394
H	0.16992621	1.87905357	-0.12966538
H	-1.72844063	-0.83542092	0.43802660
H	1.54715338	-1.18493444	-0.22770072
	H_2		
H	0.00000000	0.37139424	0.00000000
H	-0.00000000	-0.37139424	-0.00000000

i45
HOOBHOH

B	0.51716373	-0.12439006	-0.41318641
O	-1.26620112	1.08685572	0.43462617
O	-0.44192927	-0.10579238	0.56942320
H	1.99787543	-1.17518262	-1.08072236
H	0.59493877	0.75033913	-1.22113762
H	-1.85615426	0.93095415	1.19289341
O	1.34188520	-1.20614244	-0.37242972
	H_2BOH		
H	0.84428668	-0.96681327	-0.21565110
H	-1.43106900	-0.77123999	0.34155147
H	-1.06006462	1.29544329	0.24705135
B	-0.69540061	0.16084818	0.15963568
O	0.60661210	-0.02926409	-0.15908297
	H_2		
H	0.00000000	0.37139424	0.00000000
H	-0.00000000	-0.37139424	-0.00000000

p15
HOBHOOBHOH

O	0.10000869	-0.74533528	-0.22297911
H	-2.25819811	-0.23568182	0.65463683
H	1.34064557	-2.75940062	-0.44967300
B	-1.64973136	0.71304437	0.28268090
O	-0.36698526	0.62991545	-0.22089336
B	1.38244195	-0.82855624	-0.72731682
O	-2.20181600	1.95144641	0.33743549
O	1.93456662	-2.06694421	-0.78200816
H	1.99062373	0.12007829	-1.09997395
H	-1.60762705	2.64397665	0.00572954
	H_2		
H	0.00000000	0.37139424	0.00000000
H	-0.00000000	-0.37139424	-0.00000000

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