Supporting Information

Molecular Dynamics Simulations and Product Vibrational Spectral Analysis for the Reactions of NO_2 with 1-Ethyl-3-methylimidazolium Dicyanamide ($EMIM^+DCA^-$), 1-Butyl-3-methylimidazolium Dicyanamide ($BMIM^+DCA^-$) and 1-Allyl-3-methylimidazolium Dicyanamide ($AMIM^+DCA^-$)

Jianbo Liu,[*†] Wenjing Zhou,[†] Steven D. Chambreau,[‡] and Ghanshyam L. Vaghjiani[§]

[†]Department of Chemistry and Biochemistry, Queens College and the Graduate Center of the City University of New York, 65-30 Kissena Blvd., Queens, New York 11367, USA; [‡]ERC, Inc., Air Force Research Laboratory, California 93524, USA; [§] In-Space Propulsion Branch, Rocket Propulsion Division, Aerospace Systems Directorate, Air Force Research Laboratory, AFRL/RQRS, Edwards Air Force Base, California 93524, USA

Table of Contents

Computational Methodologies

Direct dynamics simulations VENUS[1-2] was used to set up initial trajectory conditions. Trajectories started at the equilibrium geometries of reactants. Vibrational modes of reactants were sampled using the quantum Boltzmann probability distribution:[3]

$$P(n_i) = \exp(-\frac{n_i h\upsilon_i}{k_B T})\,[1 - \exp\left(-\frac{h\upsilon_i}{k_B T}\right)] \quad (1)$$

where ν_i and n_i are the frequency and the quantum number of the i-th vibrational mode, respectively; k_B is the Boltzmann constant, and T is temperature. Vibrational states were simulated by giving individual atoms displacements from equilibrium geometries and momenta that were appropriate to initial rovibrational states, with random phases for different modes. Molecules had the zero point energies (ZPEs) in all vibrational modes. Reactant rotational energy (E_{rot}) was sampled from a classical Boltzmann distribution. Collision energy (E_{col}) was added as relative translational energy. Initial separation between the centers of mass of randomly oriented reactants was set at 9.0 Å where the inter-molecular interaction was negligible. All trajectories were calculated for head-on collisions, *i.e.* at zero impact parameter.

The Hessian-based predictor-corrector algorithm,[4] as implemented in Gaussian 09,[5] was used for numerical integration of the classical equations of motion, with the Hessian matrix updated every five steps. Trajectories were propagated with a step size of 0.25 amu$^{1/2}$Bohr (corresponding to a step size of ~ 0.4 fsec in trajectory time), which was small enough to ensure that energy conservation was met. Because millions of gradient and Hessian evaluations were required, a compromise was made between accuracy and computational cost when selecting a level of theory for simulations. The B3LYP method has been used successfully in calculating energetics of dialkylimidazolium-[6-10] and triazolium-based[11] ILs, with negligible basis set superposition errors for the ion pairs.[9] In our recent work the B3LYP/6-31G(d) level of theory was utilized for dynamics simulations of $EMIM^+DCA^-$,[12] $EMMIM^+DCA^-$[12] and MAT^+DCA^-,[13] and the trajectory outcomes were in good agreement with the experiments.[14-15] We therefore expected that B3LYP/6-31G(d) would be able to provide a reliable description of $EMIM^+DCA^-$

+ NO_2 and used it for the present work. An initial guess of molecular orbital for each trajectory step was obtained from the previous step, and the total energy of the system was checked at each step to ensure that the energy was conserved to better than 10^{-4} Hartree. A quadratically convergent SCF procedure[5, 16] was adopted for trajectory integration. Trajectories were terminated after a preset length of time (~ 3 psec) or when product separation exceeded 8.0 Å. All calculations were completed on a Linux computer cluster. gOpenMol[17] was used for trajectory visualization. Analyses of individual trajectories and trajectory ensembles were carried out with custom programs written for these purposes.

An issue with using quasi-classical direct dynamics methods is that vibrational energy (E_{vib}) is not quantized in the molecules. Lack of quantization may affect how energy is distributed between vibrational modes.[18-19] It is possible to have trajectories where the product E_{vib} is below ZPE. Such unphysical trajectories were found to be of minor occurrence in the IL trajectories, presumably because we were looking at high internal energy conditions, for which the errors associated with treating the motion classically were minimalized.

In a previous work,[13] we compared the performance of the B3LYP method vs. the M06 method using the reaction of MAT^+DCA^- + NO_2 as a sample system. The two theories produced similar PESs for the $MAT^+DCA^- \rightarrow [MAT^+ - H_{C5}^+]$ + HDCA reaction, and the maximum energy difference between the two PESs was less than 0.2 eV. Trajectories of MAT^+DCA^- + NO_2 calculated at the M06/6-31G(d) level of theory were found to follow similar pathways and revealed similar dynamics as the B3LYP/6-31G(d) trajectories. We also computed a few trajectories of MAT^+DCA^- + NO_2 at the MP2/6-31G(d) level of theory. But the MP2 computational cost was significantly higher than that of B3LYP and M06, because the computational requirements for MP2 scales as N^5, whereas DFT scales only as N^{3-4} where N is a measure of the problem size.[20]

Electronic structure and PES calculations Using trajectory results as a guide, structures of reactants, intermediates, TSs and products along all of the reaction pathways were optimized at the B3LYP/6-311++G(d,p) level of theory. TSs were verified to be first-order saddle points by frequency

calculations, and the vibrational mode with an imaginary frequency corresponded to the associated reaction pathway. IRC calculations were carried out to confirm that TSs were located between correct minima. Cartesian coordinates for all of the reactants, intermediates, TSs and products are provided in the Supporting Information. Reaction ΔH and ΔG were evaluated at 298 K, including thermal corrections for which ZPEs were scaled by a factor of 0.981.[21]

To simulate reactant and product IR and Raman spectra in a condensed-phase IL environment, structures were re-optimized at the M06/6-311++G(d,p) level of theory using a parameterized SCRF-based SMD[22] method (*i.e.* the generic ionic liquid solvation model SMD-GIL)[23] and the solvent parameters that were consistent with the experiment.

References

(1) Hase, W. L.; Bolton, K.; de Sainte Claire, P.; Duchovic, R. J.; Hu, X.; Komornicki, A.; Li, G.; Lim, K.; Lu, D.; Peslherbe, G. H.; Song, K.; Swamy, K. N.; Vande Linde, S. R.; Varandas, A.; Wang, H.; Wolf, R. J. *Venus 99: A General Chemical Dynamics Computer Program*, Texas Tech University Lubbock, TX, 1999.

(2) Hu, X.; Hase, W. L.; Pirraglia, T. Vectorization of the General Monte Carlo Classical Trajectory Program Venus. *J. Comput. Chem.* **1991,** *12*, 1014-24.

(3) Peslherbe, G. H.; Wang, H.; Hase, W. L. Monte Carlo Sampling for Classical Trajectory Simulations. *Adv. Chem. Phys.* **1999,** *105*, 171-201.

(4) Bakken, V.; Millam, J. M.; Schlegel, H. B. Ab Initio Classical Trajectories on the Born-Oppenheimer Surface: Updating Methods for Hessian-Based Integrators. *J. Chem. Phys.* **1999,** *111*, 8773-8777.

(5) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; J. A. Montgomery, J.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Rev. B. 01. **2009**.

(6) Kroon, M. C.; Buijs, W.; Peters, C. J.; Witkamp, G.-J. Quantum Chemical Aided Prediction of the Thermal Decomposition Mechanisms and Temperatures of Ionic Liquids. *Thermochimica Acta* **2007,** *465*, 40-47.

(7) Emel'yanenko, V. N.; Verevkin, S. P.; Heintz, A. The Gaseous Enthalpy of Formation of the Ionic Liquid 1-Butyl-3-Methylimidazolium Dicyanamide from Combustion Calorimetry, Vapor Pressure Measurements, and Ab Initio Calculations. *J. Am. Chem. Soc.* **2007,** *129*, 3930-3937.

(8) Verevkin, S. P.; Emel'yanenko, V. N.; Zaitsau, D. H.; Heintz, A.; Muzny, C. D.; Frenkel, M. Thermochemistry of Imidazolium-Based Ionic Liquids: Experiment and First-Principles Calculations. *Phys. Chem. Chem. Phys.* **2010,** *12*, 14994-15000.

(9) Hollóczki, O.; Gerhard, D.; Massone, K.; Szarvas, L.; Németh, B.; Veszprémi, T.; Nyulászi, L. Carbenes in Ionic Liquids. *New J. CHem.* **2010,** *34*, 3004-3009.

(10) Clough, M. T.; Geyer, K.; Hunt, P. A.; Mertes, J.; Welton, T. Thermal Decomposition of Carboxylate Ionic Liquids: Trends and Mechanisms. *Phem. Chem. Chem. Phys.* **2013,** *15*, 20480-20495.

(11) Gao, Y.; Gao, H.; Piekarski, C.; Shreeve, J. n. M. Azolium Salts Functionalized with Cyanomethyl, Vinyl, or Propargylsubstituents and Dicyanamide, Dinitramide, Perchlorate and Nitrate Anions. *Eur. J. Inorg. Chem.* **2007**, *31*, 4965-4972.

(12) Liu, J.; Chambreau, S. D.; Vaghjiani, G. L. Dynamics Simulations Amd Statistical Modeling of Thermal Decomposition of 1-Ethyl-3-Methylimidazolium Dicyanamide and 1-Ethyl-2,3-Dimethylimidazolium Dicyanamide. *J. Phys. Chem. A* **2014,** *118*, 11133-11144.

(13) Liu, J.; Zhou, W.; Chambreau, S. D.; Vaghjiani, G. L. Computational Study of the Reaction of 1-Methyl-4-Amino-1,2,4-Triazolium Dicyanamide with NO_2: From Reaction Dynamics to Potential Surfaces, Kinetics and Spectroscopy *J. Phys. Chem. A* **2019,** *123*, 2956-2970.

(14) Chambreau, S. D.; Schenk, A. C.; Sheppard, A. J.; Yandek, G. R.; Vaghjiani, G. L.; Maciejewski, J.; Koh, C. J.; Golan, A.; Leone, S. R. Thermal Decomposition Mechanims of Alkylimidazolium Ionic Liquids with Cyano-Containing Anions. *J. Phys. Chem. A* **2014,** *118*, 11119-11132.

(15) Brotton, S. J.; Lucas, M.; Chambreau, S. D.; Vaghjiani, G. L.; Yu, J.; Anderson, S. L.; Kaiser, R. I. Spectroscopic Investigation of the Primary Reaction Intermediates in the Oxidation of Levitated Droplets of Energetic Ionic Liquids. *J. Phys. Chem. Lett.* **2017,** *8*, 6053-6059.

(16) Bacskay, G. B. A Quadratically Convergent Hartree-Fock (QC-SCF) Method. Application to Closed Shell Systems. *Chem. Phys.* **1981,** *61*, 385-404.

(17) Laaksonen, L. *Gopenmol*, 3.0; Center for Scientific Computing: Espoo, Finland, 2005.

(18) Untch, A.; Schinke, R.; Cotting, R.; Huber, J. R. The Vibrational Predissociation of *cis*-Methyl Nitrite in the S_1 State: A Comparison of Exact Quantum Mechanical Wave Package Calculation with Classical Trajectory Calculations and Detailed Experimental Results. *J. Chem. Phys.* **1993,** *99*, 9553-9566.

(19) Miller, W. H.; Hase, W. L.; Darling, C. L. A Simple Model for Correcting the Zero Point Energy Problem in Classical Trajectory Simulations of Polyatomic Molecules. *J. Chem. Phys.* **1989,** *91*, 2863-2868.

(20) Sun, R.; Siebert, M. R.; Xu, L.; Chambreau, S. D.; Vaghjiani, G. L.; Lischka, H.; Liu, J.; Hase, W. L. Direct Dynamics Simulation of the Activation and Dissociation of 1,5-Dinitrobiuret (HDNB). *J. Phys. Chem. A* **2014,** *118*, 2228-2236.

(21) Zheng, J.; Alecu, I. M.; Lynch, B. J.; Zhao, Y.; Truhlar, D. G. Database of Frequency Scale Factors for Electronic Model Chemistries, Version 2. http://comp.chem.umn.edu/freqscale/version2.htm: 2010.

(22) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009,** *113*, 6378-6396.

(23) Bernales, V. S.; Marenich, A. V.; Contreras, R.; Cramer, C. J.; Truhlar, D. G. Quantum Mechanical Continuum Solvation Models for Ionic Liquids. *J. Phys. Chem. B* **2012,** *116*, 9122-9129.

(24) Brotton, S. J.; Lucas, M.; Jensen, T. N.; Anderson, S. L.; Kaiser, R. I. Spectroscopic Study on the Intermediates and Reaction Rates in the Oxidation of Levitated Droplets of Energetic Ionic Liquids by Nitrogen Dioxide. *J. Phys. Chem. A* **2018,** *122*, 7351-7377.

(25) Lucas, M.; Brotton, S. J.; Shukla, S. K.; Yu, J.; Anderson, S. L.; Kaiser, R. I. Oxidation of a Levitated Droplet of 1-Allyl-3-Methylimidazolium Dicyanamide by Nitrogen Dioxide. *J. Phys. Chem. A* **2019,** *123*, 400-416.

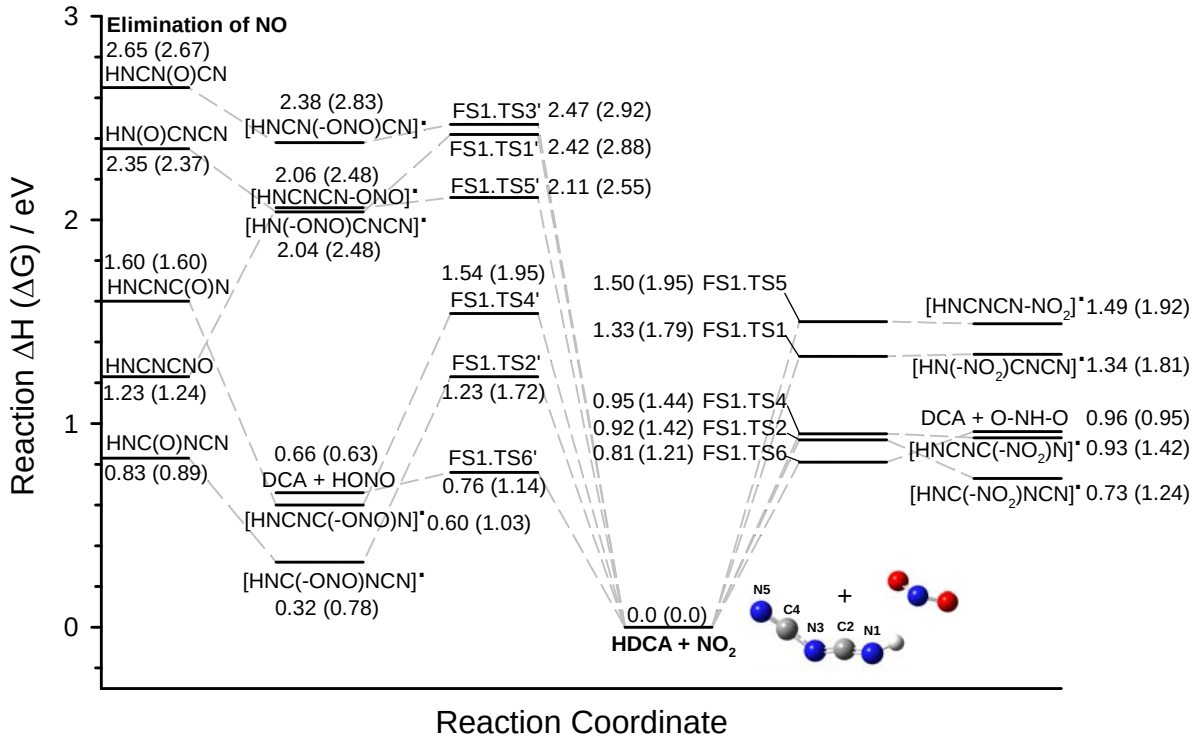


Figure S1 Schematic reaction coordinates for the reaction of HDCA with NO_2. Reaction enthalpies ΔH (eV) and changes of free energy ΔG (eV, in parentheses) were calculated at the B3LYP/6-311++G(d,p) level of theory, including thermal corrections at 298 K. Cartesian coordinates of stable structures and TSs are provided on page S14.

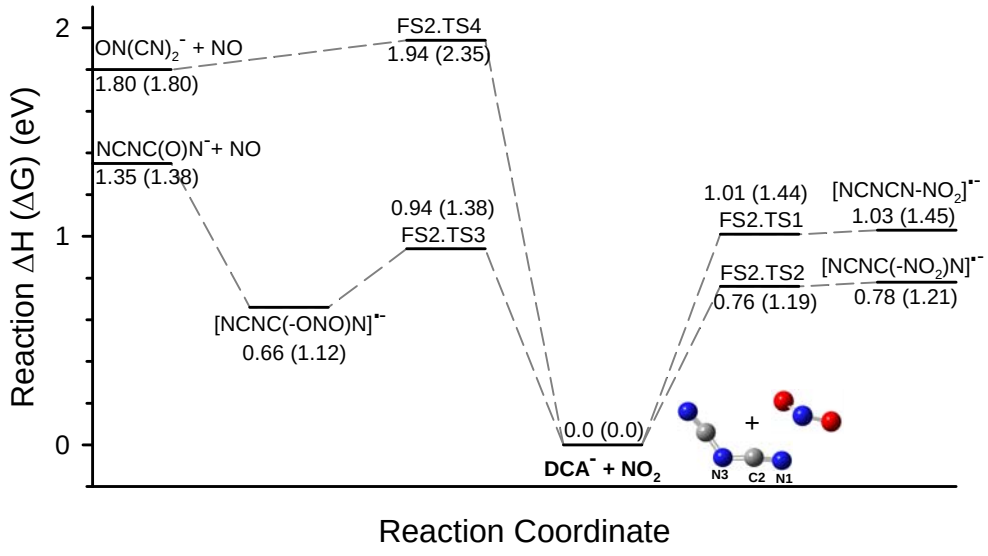


Figure S2 Schematic reaction coordinates for the reaction of DCA^- with NO_2. Reaction enthalpies ΔH (eV) and changes of free energy ΔG (eV, in parentheses) were calculated at the B3LYP/6-311++G(d,p) level of theory, including thermal corrections at 298 K. Cartesian coordinates of stable structures and TSs are provided on page S18.

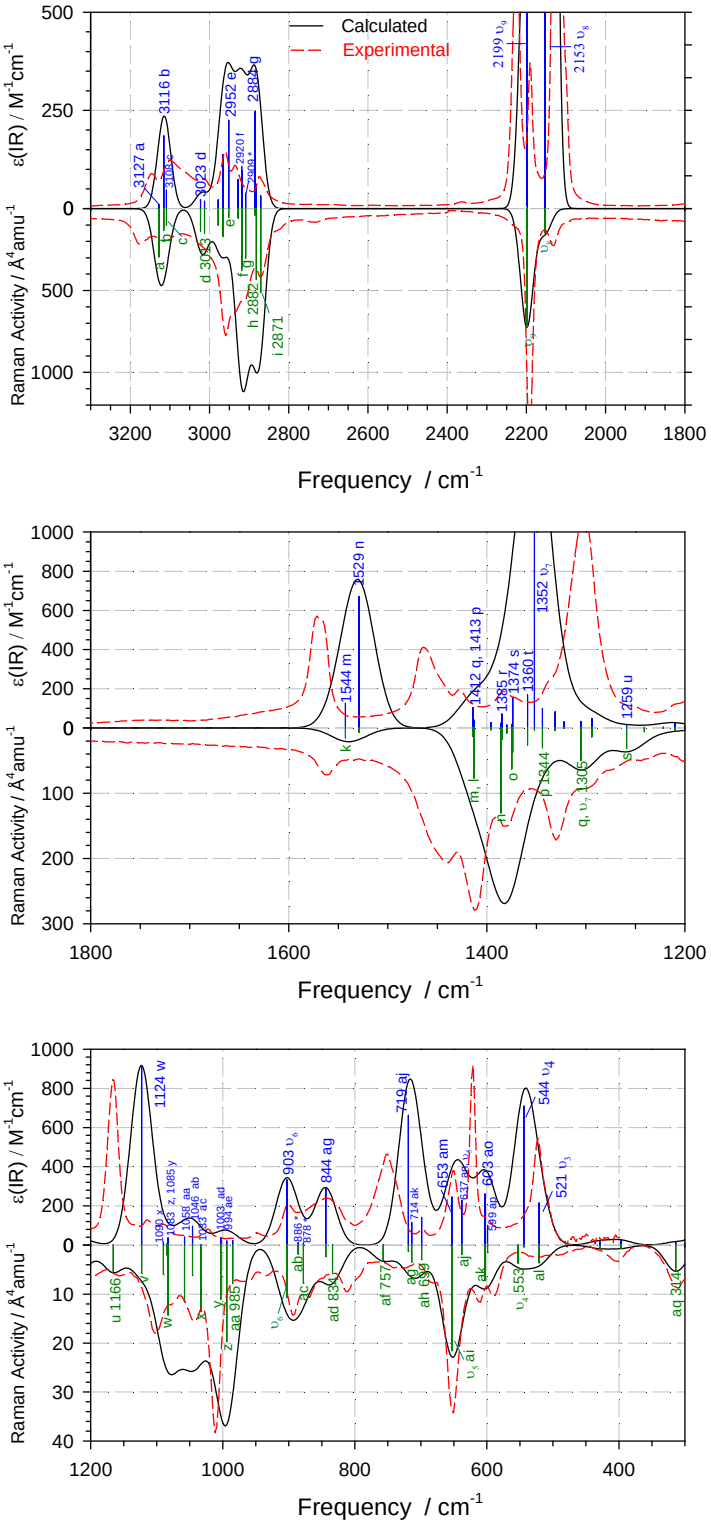


Figure S3 Comparison of the SMD-GIL//M06/6-311++G(d,p)-calculated harmonic infrared (top frame in each figure) and Raman (bottom frame in each figure) spectra of $BMIM^{+}DCA^{-}$ with the experimental spectra available in Ref [24]. Calculated frequencies were scaled by a factor of 0.957. See Tables S1 and S2 for assignments.

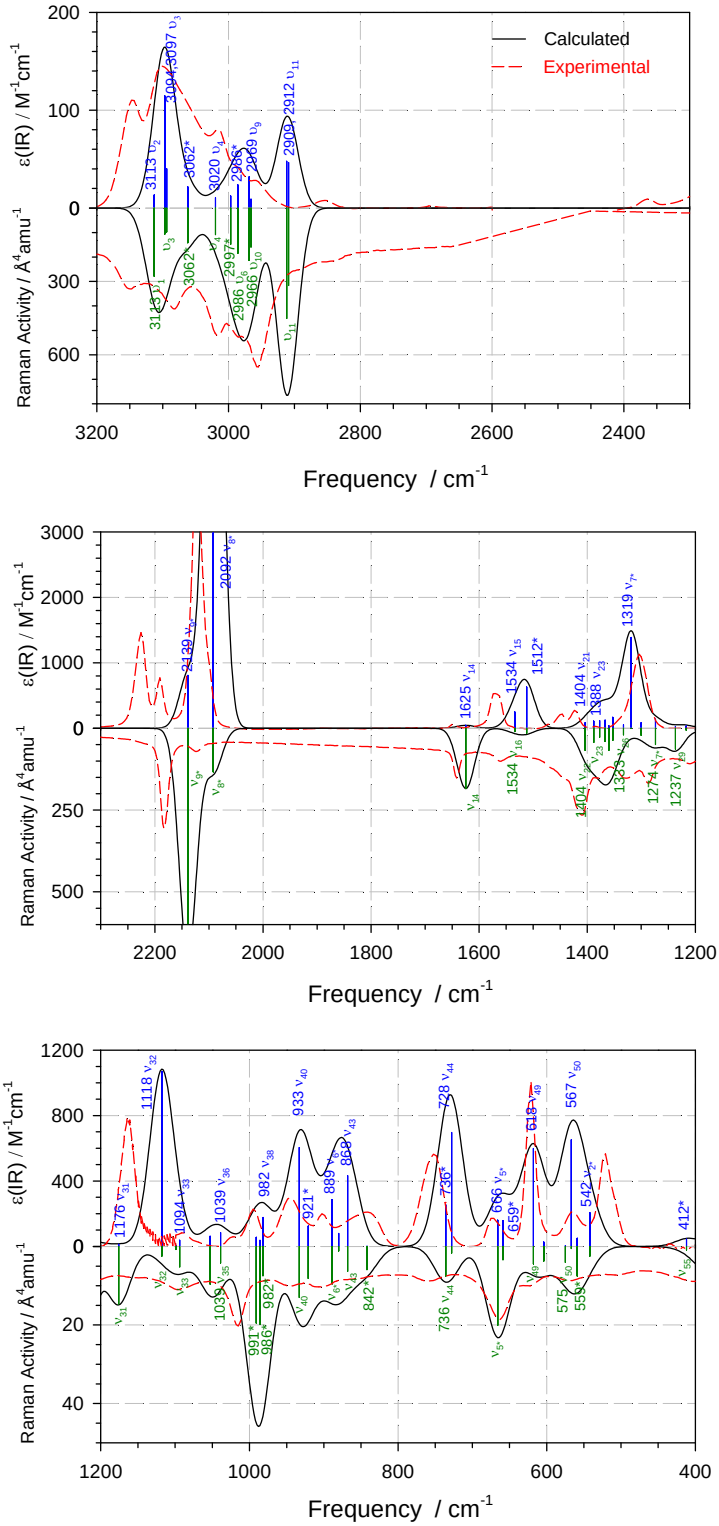


Figure S4 Comparison of the SMD-GIL//M06/6-311++G(d,p)-calculated harmonic infrared (top frame in each figure) and Raman (bottom frame in each figure) spectra of $AMIM^{+}DCA^{-}$ with the experimental spectra available in Ref [25]. Calculated frequencies were scaled by a factor of 0.957. See Tables S3 and S4 for the assignments.

Table S1 Comparison of SMD-GIL//M06/6-311++G(d,p)-calculated infrared frequencies of $BMIM^+DCA^-$ with the experimental values

	Vibrational modes [a]	Calculated frequencies (cm^{-1})	Experimental IR (cm^{-1}) [a]
a	C(4)-H, C(5)-H out-of-phase and in-phase stretch	3127	3149
b	C(2)-H stretch	3116	3105
c	no assignment	3108	3078
d	CH_3(Me) asym stretch	3023	3015
e	CH_2 asym stretch	2952	2963
f	CH_2 asym stretch	2919	2936
g	CH_3(Bu) symmetric stretch	2884	2875
ν_9	C≡N symmetric stretch	2199	2191
ν_8	C≡N asym stretch	2153	2123
m	no assignment	1544	1617
n	N(1)C(2)N(3) asym stretch, C(2)-H rocking	1529	1569
p	CH_2(Me) asym bend, CH_2 symmetric bend	1413	1450
q	CH_3(Me) symmetric bend	1412	1426
r	CH_2 wagging	1385	1383
s	C(2)N(1)C(5) stretch, CH_2 wagging	1374	1370
t	(N-Bu), (N-Me) stretch	1360	1326
ν_7	(N-C) asym stretch,	1352	1302
u	(CH_3) twisting, (C2-H) rocking	1259	1250
w	(N-Bu), (N-Me) stretch, (C-H) rocking	1124	1167
x	(CH_3), [CH_3(Bu)] twisting	1090	1112
y	(CH), (CH_3), [CH_3(Bu)] twisting	1085	1090
aa	C-C stretch	1058	1028
ab	ring bend	1046	1021
ac	breathing, N-Me stretch, N-Bu stretch	1033	1010
ad	out-of-plane C-H	1003	988
ae	C-C asym stretch	994	975
ν_6	N-C symmetric stretch	903	903
ag	(C4-H), (C5-H) out-of-plane	844	839
aj	CH_2 rocking	719	751
ak	CH_2 rocking	714	737
am	(N-Me) stretch, (N-Bu) stretch	653	663
an,ν_5	(N-Bu) out-of-plane, (N-Me) out-of-plane, CNC bend	637	651
ao	out-of-plane (N-Bu) ring puckering	603	621
ap	N(1)-C(2)-N(3) bend	599	600
ν_4	out-of-plane symmetric N-C≡N bend of DCA^-	544	523
ν_3	out-of-plane asym N-C≡N bend of DCA^-	521	510

[a] Ref [24].

Table S2 Comparison of the SMD-GIL//M06/6-311++G(d,p)-calculated Raman frequencies of $BMIM^+DCA^-$ with the experimental values

	Vibrational modes [a]	Calculated frequencies (cm^{-1})	Experimental Raman (cm^{-1}) [a]
a	C(4)-H, C(5)-H in-phase stretch	3127	3183
b	C(4)-H, C(5)-H out-of-phase stretch	3116	3163
c	C(2)-H stretch	3108	3116
d	CH_3(Me) asym stretch	3013	2986
e	CH_2 asym stretch	2952	2960
f	CH_2 asym stretch	2919	2937
g	CH_3(Me) symmetric stretch, CH, CH_3 asym stretch	2909	2910
h	CH_2 symmetric stretch, CH_3(Bu) symmetric stretch	2882	2869
i	CH_2 symmetric stretch	2871	2832
ν_9	C≡N symmetric stretch	2199	2192
ν_8	C≡N asym stretch	2153	2131
k	N(1)C(2)N(3) asym stretch, C(2)-H rocking	1544	1563
l	CH_2(Me) asym bend, CH_2 symmetric bend	1413	1445
m	CH_2 symmetric bend	1412	1438,
o	C(2)N(1)C(5) asym stretch, CH_2 wagging	1375	1381
p	breathing, (N-Me) stretch, (N-Bu) stretch	1344	1329
q, ν_7	CH_2 twisting, and wagging, N-C asym stretch	1305	1270, 1299
s	CH_2 twisting, C(2)-H rocking	1259	1239
u	(N-Me) stretch, (N-Bu) stretch, C-H rocking	1166	1159
v	[CH_3(Bu)], CH_2 rocking	1124	1102
w	C-C stretch	1083	1077
x	C-C stretch	1033	1044
y	breathing, (N-Me) stretch, (N-Bu) stretch	1003	1011
z	C-C asym stretch	994	963
aa	[CH_3(Bu)], CH_2 rocking, C(2)-H stretch	985	934
ν_6	N-C symmetric stretch	903	894
ab	C-C stretch	886	871
ac	no assignment	878	850
ad	C-C-C symmetric stretch	834	812
af	CH_2 rocking	757	740
ag	(N-Me) stretch, (N-Bu) stretch, CH_2 rocking	714	722
ah	(N-Me) stretch, (N-Bu) stretch	699	686
ai, ν_5	(N-Bu) out-of-plane, (N-Me) out-of-plane, CNC bend	653	652
aj	(N-Bu) out-of-plane ring puckering	637	611
ak	N(1)-C(2)-N(3) bend	603	589
ν_4	out-of-plane symmetric N-C≡N bend of DCA^-	553	525
al	C-C-C, N-C-C bend	521	490
aq	C-C-C bend	314	312

[a] Ref [24].

Table S3 Comparison of SMD-GIL//M06/6-311++G(d,p)-calculated infrared frequencies of $AMIM^+DCA^-$ with the experimental values

	Vibrational modes [a]	Calculated frequencies (cm^{-1})	Experimental IR (cm^{-1}) [a]
2	ν(C4−H, C5−H) out-of-phase	3113	3153
3	ν(C2H)	3094, 3097	3097 ± 3
4	ν_{as}(CH2(C = C))	3020	3014
9	ν_{as}(CH2)	2969	2956 ± 3
11	ν_{s}(CH3)	2909	2856 ± 2
6* + 7*	DCA^- combination		2227
9*	ν_{s}(C≡N)	2139	2191
8*	ν_{as}(C≡N)	2092	2122
14	ν(CC) + β(CH)	1625	1647
15	ν(CC)	1534	1569
19	β_{as}(CH2)		1471 ± 3
20	β_{s}(CH3)		1448
21	B(CH2)	1404	1423
23	R_{as} + β(CH)	1388	1385
7*	ν_{as}(C−N)	1319	1303
31	ν(CC) + β(CH)	1176	1164
32	β(CH) + R_{as}	1118	1110 ± 20
33	β(CH) + R_{as}	1094	1090 ± 20
36	R_{as} + ν(CN)	1039	1022 ± 2
38	ω(CH)	982	995
40	ν(CC)	933	945
6*	ν_{s}(C−N)	889	902
43	ω CH)	868	847
44	ν(CN) + β(CCN) + τ(CH)	728	754
5*	β_{s}(CNC)	666	669
49	τ(Ring)	618	621
50	τ(CH) + τ(Ring) + ν(CN)	567	565
2*	β_{as}(NCN)	542	520

[a] Ref [25]; abbreviations: ν, stretching; β, bending; R, ring; ω, wagging; τ, torsion; s, symmetric; as, antisymmetric.

Table S4 Comparison of the SMD-GIL//M06/6-311++G(d,p)-calculated Raman frequencies of $AMIM^{+}DCA^{-}$ with the experimental values

	Vibrational modes [a]	Calculated frequencies (cm^{-1})	Experimental Raman (cm^{-1}) [a]
1	ν(C4−H, C5−H) in-phase	3113	3148
3	ν(C2H)	3094, 3097	3085
4	ν_{as} (CH2(C = C))	3020	3016
6	ν_{s} (CH2(C = C))	2986	2987
10	ν_{s} (CH2)	2996	2957
11	ν_{s} (CH3)	2909	2841 ± 3
9*	ν_{s} (C≡N)	2139	2182
8*	ν_{as} (C≡N)	2092	2123
14	ν(CC) + β(CH)	1625	1641
16	ν(CC)	1534	1560
20	β_{s} (CH3)		1439 ± 3
22	β (CH) + ν(CN)	1404	1410
23	R_{as} + β (CH)	1388	1378
26	R_{s}	1333	1327
7*	ν_{as} (C−N)	1274	1286
29	ν(CN) + β (CH)	1237	1210
31	ν(CC) + β (CH)	1176	1162
32	β (CH) + R_{as}	1118	1098 ± 4
33	β (CH) + R_{as}	1094	1081
35	R_{s} + β (CH)	1039	1015
40	ν(CC)	933	947 ± 2
6*	ν_{s} (C−N)	889	904 ± 2
43	ω (CH)	868	870 ± 10
44	ν(CN) + β (CCN) + τ (CH)	736	759
5*	β_{s} (CNC)	666	664
49	τ (Ring)	618	622
50	τ (CH) + τ (Ring) + ν(CN)	575	571 ± 6
2*	β_{as} (NCN)		504 ± 6
55	β (CNC,CCC)	412	406 ± 2

[a] Ref [25]; abbreviations: ν, stretching; β, bending; R, ring; ω, wagging; τ, torsion; s, symmetric; as, antisymmetric.

Cartesian coordinates for the structures in Figure S1, calculated at B3LYP/6-311++G(d,p)

HDCA
H1 2.845933 -0.520152 0.613874
N2 -0.063423 0.580084 0.017050
C3 1.059336 0.083233 0.020988
C4 -1.271048 0.041734 0.003509
N5 2.201703 -0.269510 -0.122870
N6 -2.363375 -0.343381 -0.002874

NO_2
N1 0.000000 0.000000 0.321839
O2 0.000000 1.099987 -0.140804
O3 0.000000 -1.099987 -0.140804

FS1.TS1
N1 -3.815819 0.282084 0.009667
C2 -2.667584 0.108427 -0.014542
N3 -1.360154 0.034011 -0.051689
C4 -0.507413 -0.871868 0.007547
N5 0.768309 -0.993606 0.065248
N6 1.883260 0.247477 0.004127
O7 3.007106 -0.162152 -0.050506
O8 1.423291 1.343896 0.034985
H9 1.277622 -1.863064 -0.025322

[HN(-NO_2)CNCN]$^\bullet$
N1 3.730018 0.291528 -0.000016
C2 2.586233 0.089322 -0.000008
N3 1.280041 -0.013854 0.000000
C4 0.456543 -0.951868 0.000024
N5 -0.866488 -0.952552 0.000025
N6 -1.769735 0.239120 -0.000003
O7 -2.940538 -0.060974 0.000010
O8 -1.242119 1.314722 -0.000035
H9 -1.412248 -1.804409 0.000051

FS1.TS2
N1 1.084120 1.862411 -0.242899
C2 0.270490 0.988282 0.054405
N3 -0.957190 0.870407 0.497873
C4 -1.898391 0.134202 0.028180
N5 -2.845415 -0.472059 -0.324236
H6 2.035581 1.526673 -0.393216
N7 1.004318 -0.735440 0.033262
O8 0.259945 -1.674205 0.052011
O9 2.206430 -0.693146 -0.033298

[HNC(-NO_2)NCN]$^\bullet$
N1 -1.287607 1.732564 0.000128
C2 -0.419510 0.804923 0.000052
N3 0.902933 1.040191 0.000008
C4 1.874328 0.204665 -0.000065
N5 2.894145 -0.392670 -0.000129
H6 -2.230927 1.331303 0.000152
N7 -0.920898 -0.692929 0.000006
O8 -0.074675 -1.560170 -0.000083
O9 -2.127574 -0.839696 0.000063

FS1.TS4
N1 1.281194 1.848383 -0.192939
C2 0.409266 1.031334 0.032810
N3 -0.892891 0.982703 0.356635
C4 -1.777362 0.185017 0.042589
N5 -2.779834 -0.390516 -0.289889
N6 1.105507 -0.667374 0.021051
O7 0.249022 -1.517269 0.110997
O8 2.288472 -0.785623 -0.082726
H9 -3.089215 -1.287346 0.057430

[HNCNC(-NO_2)N]$^\bullet$
N1 -1.331179 1.764927 0.145334
C2 -0.485365 0.861819 -0.034814
N3 0.840900 0.983456 -0.293325
C4 1.773530 0.220465 -0.035897
N5 2.804330 -0.317856 0.269349
N6 -1.053960 -0.622151 -0.017747
O7 -0.221039 -1.503914 -0.113117
O8 -2.248262 -0.748031 0.096101
H9 3.204774 -1.136770 -0.164881

FS1.TS5
N1 3.747196 0.325316 -0.383125
C2 2.655169 -0.023755 0.002752
N3 1.568348 -0.242841 0.524666
C4 0.292991 -0.147686 0.255129
N5 -0.716947 -0.831870 0.109641
H6 4.433673 -0.291287 -0.799967
N7 -2.067987 0.101357 -0.071878
O8 -3.029558 -0.552883 -0.341455
O9 -1.950055 1.284908 0.091149

[HNCNCN-NO_2]$^\bullet$
N1 3.751730 -0.175167 -0.438794
C2 2.638571 0.007563 -0.013942
N3 1.542620 0.362207 0.403784
C4 0.274365 0.201418 0.035935

N5 -0.746329 -0.025716 0.718213
H6 4.410943 -0.876180 -0.131209
N7 -2.010405 -0.056719 -0.047334
O8 -2.502449 -1.151776 -0.167496
O9 -2.454036 1.013033 -0.388983

FS1.TS6
N1 -4.282713 0.775677 0.339393
C2 -3.338126 0.179522 -0.005456
N3 -2.358993 -0.555431 -0.452752
C4 -1.121266 -0.412965 -0.189252
N5 0.039716 -0.371713 -0.052517
N6 2.889377 0.318865 -0.208376
O7 4.045607 0.563950 -0.232616
O8 2.390298 -0.475925 0.658783
H9 1.257406 -0.475333 0.378663

DCA
N1 0.000023 0.656080 0.000097
C2 -1.147556 0.054284 -0.000075
C3 1.147552 0.054307 -0.000197
N4 -2.240223 -0.374569 0.000041
N5 2.240204 -0.374589 0.000095

HONO (*trans*-conformation)
N1 0.180051 0.486565 0.000068
O2 -1.045306 -0.255258 0.000055
O3 1.102795 -0.225557 -0.000053
H4 -1.720273 0.440558 -0.000488

FS1.TS1′
N1 -4.041721 0.352616 0.319180
C2 -2.958950 0.002810 0.092310
N3 -1.781558 -0.523890 -0.182319
C4 -0.621709 -0.065241 -0.190912
N5 0.589730 -0.405767 -0.380221
N6 2.830884 0.532975 0.155069
O7 3.068322 -0.613574 0.359148
O8 1.582097 0.848468 -0.208973
H9 1.099268 -1.196108 0.008247

[HN(-ONO)CNCN]•
N1 -3.800840 0.552715 -0.248800
C2 -2.728781 0.164307 -0.026333
N3 -1.561608 -0.311590 0.337816
C4 -0.425766 -0.353602 -0.202767
N5 0.695115 -0.814960 0.342937
N6 2.694174 0.482466 -0.316143
O7 2.165850 1.283091 0.294841
O8 1.833094 -0.913429 -0.385720
H9 0.747848 -1.181934 1.290963

FS1.TS2′
N1 -2.713108 -0.333855 -0.430433
C2 -1.738886 0.119109 0.028454
N3 -0.707805 0.624953 0.647964
C4 0.396193 1.036337 0.083349
N5 1.217813 1.947701 -0.005714
N6 1.162648 -1.423968 -0.292435
O7 0.724507 -1.635415 0.794035
O8 1.079313 -0.297964 -0.857210
H9 0.908756 2.830539 0.398904

[HNC(-ONO)NCN]•
N1 2.957232 -0.992372 -0.186702
C2 2.123075 -0.163030 -0.142009
N3 1.303302 0.837348 -0.145212
C4 -0.023244 0.667887 0.202568
N5 -0.869537 1.644752 0.086015
N6 -1.900966 -1.122516 0.156268
O7 -2.435486 -0.484193 -0.596631
O8 -0.395332 -0.523822 0.664417
H9 -0.382659 2.464498 -0.278219

FS1.TS3′
N1 1.001911 2.351777 0.054758
C2 1.216933 1.164851 -0.143898
N3 0.660758 -0.008221 -0.025248
C4 1.305034 -1.178233 -0.040118
N5 1.822231 -2.212612 -0.066093
H6 1.600739 3.100268 -0.272656
N7 -1.751680 -0.127483 -0.462768
O8 -2.824808 -0.219044 -0.031793
O9 -0.783328 -0.161481 0.640819

[HNCN(-ONO)CN]•
N1 0.190850 2.398052 -0.048075
C2 0.925113 1.408147 -0.130587
N3 0.638977 0.102327 0.136075
C4 1.538512 -0.881089 -0.031270
N5 2.290281 -1.749251 -0.167211
H6 0.545161 3.325105 -0.256467
N7 -1.623893 -0.501961 -0.490351
O8 -2.641486 -0.751819 -0.046085
O9 -0.583567 -0.277132 0.697903

FS1.TS4′
N1 -2.457678 -1.422935 0.177758
C2 -1.885417 -0.408041 -0.096637
N3 -1.481932 0.737312 -0.320617
C4 -0.322017 1.298593 -0.016901

N5 0.418976 2.221067 0.114621
H6 -2.445231 -2.305740 -0.311674
N7 1.953178 -0.275023 -0.293143
O8 2.497839 -1.310013 -0.089550
O9 0.834914 -0.172552 0.494871

[HNCNC(-ONO)N]•
N1 3.494167 -0.106598 0.264020
C2 2.317675 -0.291235 0.056257
N3 1.130175 -0.596884 0.003806
C4 0.034147 0.251702 -0.184218
N5 0.075653 1.513314 -0.107118
H6 4.205771 -0.080409 -0.453103
N7 -2.301123 0.106224 0.447207
O8 -3.282025 -0.335058 0.081846
O9 -1.106576 -0.426791 -0.461162

FS1.TS5′
N1 -3.949870 -0.094592 -0.441202
C2 -2.829047 -0.029239 0.008556
N3 -1.717300 -0.194700 0.497183
C4 -0.474116 0.159147 0.257753
N5 0.632197 -0.356738 0.134091
H6 -4.631688 0.652404 -0.405266
N7 2.966304 0.387194 -0.154489
O8 3.167246 -0.773505 -0.183633
O9 1.699172 0.821005 0.003424

FS1.TS6′
N1 -3.836117 0.740424 -0.535995
C2 -2.919528 0.218737 -0.033648
N3 -1.961450 -0.360173 0.636504
C4 -0.841823 -0.751011 0.187276
N5 0.201764 -1.219823 -0.121542
N6 2.332418 0.206495 -0.044694
O7 3.371146 -0.333866 -0.351896
O8 2.132807 1.348706 0.306642
H9 1.380178 -0.493541 -0.099652

O-NH-O
N1 0.000000 0.000000 0.309894
O2 0.000000 1.094283 -0.220195
O3 0.000000 -1.094283 -0.220195
H4 0.000000 0.000000 1.353866

[HNCNCN-ONO]•
N1 -4.007544 0.041825 -0.088221
C2 -2.814030 -0.120879 0.019430
N3 -1.624660 -0.402818 -0.033472
C4 -0.488286 0.319395 -0.017772
N5 0.682026 -0.129325 -0.004924
H6 -4.661258 0.098770 0.679980
N7 3.036169 0.292114 0.011450
O8 3.077744 -0.862318 0.015624
O9 1.656408 0.874513 -0.001094

NO
N1 0.000000 0.000000 -0.612285
O2 0.000000 0.000000 0.535749

HN(O)CNCN
N1 -2.975840 -0.217671 -0.250202
C2 -1.867271 -0.046804 0.034676
N3 -0.637587 0.163419 0.516955
C4 0.400252 0.256486 -0.153248
N5 1.694948 0.370890 -0.102239
O6 2.520688 -0.595807 -0.007089
H7 2.065971 1.291893 -0.383448

HNC(O)NCN
N1 2.436805 -0.398988 -0.257299
C2 1.379209 -0.087186 0.092104
N3 0.187601 0.269191 0.608624
C4 -1.035364 -0.110371 0.008899
N5 -0.706460 1.171918 -0.364622
O6 -1.797241 -1.001000 -0.092843
H7 -1.110768 1.898495 0.229800

HNCN(O)CN
N1 2.139446 -0.718468 -0.166566
C2 1.065790 -0.244746 0.124026
N3 -0.053048 0.386381 -0.007145
C4 -1.209531 -0.362236 0.006869
N5 -2.208460 -0.939518 -0.010985
H6 2.770543 -1.044902 0.567014
O7 -0.131708 1.698504 -0.007440

HNCNC(O)N
N1 -2.549614 0.195423 -0.134112
C2 -1.415796 -0.163300 0.025052
N3 -0.293446 -0.675542 0.046514
C4 0.898009 -0.019347 0.009650
N5 1.367707 1.158114 0.005877
H6 -3.216186 0.504698 0.557003
O7 2.081298 -0.519348 -0.024145

HNCNCNO
N1 2.921205 -0.287812 -0.127105
C2 1.769061 0.051479 0.023620
N3 0.644690 0.542457 0.016331

C4 -0.573267 0.016118 -0.000330
N5 -1.738517 -0.016964 0.001950
H6 3.545601 -0.515370 0.636186
O7 -2.939002 -0.194248 -0.001770

HNCO
C1 -0.044851 0.021878 -0.000210
N2 1.158127 -0.122263 0.000066
O3 -1.210324 0.013896 0.000085
H4 1.844813 0.613402 0.000122

NCN
C1 0.000000 0.089813 0.000000
N2 1.211058 -0.039982 0.000000
N3 -1.211058 -0.037001 0.000000

HNCN
N1 1.155561 -0.133976 0.000003
C2 -0.109034 0.009343 -0.000010
N3 -1.299271 0.018057 0.000004
H4 1.660174 0.755376 0.000004

NCO
C1 0.000000 0.047048 0.000000
N2 0.624492 1.082804 0.000000
O3 -0.546431 -0.982739 0.000000

Cartesian coordinates for the structures in Figure S2, calculated at B3LYP/6-311++G(d,p)

DCA^-
N1 -0.000014 0.679121 -0.000008
C2 -1.149914 0.058004 0.000028
C3 1.149938 0.058069 -0.000005
N4 -2.233964 -0.389293 -0.000013
N5 2.233958 -0.389319 0.000002

NO_2
N1 0.000000 0.000000 0.321839
O2 0.000000 1.099987 -0.140804
O3 0.000000 -1.099987 -0.140804

FS2.TS1
N1 -1.283945 0.202315 0.000008
C2 -0.428996 -0.766888 0.000004
C3 -2.589175 0.094402 -0.000005
N4 0.796286 -1.071810 0.000007
N5 -3.757869 0.125066 -0.000016
N6 1.812440 0.123243 0.000003
O7 2.980330 -0.225413 0.000019
O8 1.412250 1.273315 -0.000021

$[NCNCN\text{-}NO_2]^{\bullet -}$
N1 -1.252353 0.186243 0.000615
C2 -0.410298 -0.793880 -0.000862
C3 -2.559657 0.083572 0.000362
N4 0.854655 -1.020821 -0.001011
N5 -3.727546 0.120608 0.000333
N6 1.762400 0.107739 -0.000038
O7 2.952445 -0.196582 0.001480
O8 1.342510 1.259766 -0.001016

FS2.TS2
N1 -1.084031 0.876016 0.426036
C2 0.183605 1.027361 0.105712
C3 -1.878426 -0.029414 -0.099371
N4 1.013765 1.940807 -0.053028
N5 -2.696118 -0.775883 -0.502541
N6 1.095613 -0.541408 0.036737
O7 1.992687 -0.686234 -0.783151
O8 0.740354 -1.374316 0.859592

$[NCNC(\text{-}NO_2)N]^{\bullet -}$
N1 -0.948207 1.092610 -0.000028
C2 0.365571 0.946558 0.000121
C3 -1.804238 0.104121 -0.000186
N4 1.345979 1.748416 0.000307
N5 -2.657795 -0.696988 -0.000331
N6 0.931640 -0.564298 0.000051
O7 1.120718 -1.085068 -1.085676
O8 1.120618 -1.085213 1.085726

FS2.TS3′
N1 1.540787 0.586837 0.378700
C2 0.421308 1.129891 0.022193
C3 1.972652 -0.589861 -0.001240
N4 -0.131692 2.130525 -0.410501
N5 2.474603 -1.608735 -0.273891
N6 -1.776873 -0.352597 -0.382518
O7 -0.999828 0.055153 0.599680
O8 -2.639114 -1.121702 -0.013210

$[NCNC(\text{-}ONO)N]^{\bullet -}$
N1 0.974198 -0.529849 0.274408
C2 0.159376 0.519340 0.148487
C3 2.252837 -0.438529 -0.005575
N4 0.300109 1.726347 -0.236083
N5 3.402669 -0.485739 -0.220063
N6 -1.929508 -0.332689 -0.469797
O7 -1.184002 0.203790 0.587488
O8 -3.029191 -0.595211 -0.124579

FS2.TS4′
N1 -0.544933 0.025182 0.074622
C2 -0.934518 1.285770 -0.011630
C3 -1.357861 -0.997793 -0.125846
N4 -1.232220 2.409118 -0.075474
N5 -2.018796 -1.940951 -0.297633
N6 2.098371 -0.663667 0.106354
O7 2.455328 0.196169 -0.648520
O8 0.749336 -0.263124 0.919742

$ON(CN)_2^-$
N1 -0.000069 0.336501 0.000000
C2 -0.000012 -0.330654 -1.151607
C3 -0.000012 -0.330654 1.151607
N4 -0.000012 -0.873522 -2.183473
N5 -0.000012 -0.873522 2.183473
O6 0.000099 1.730206 0.000000

NO
N1 0.000000 0.000000 -0.612285
O2 0.000000 0.000000 0.535749

Cartesian coordinates for the structures in Figure 2, calculated at B3LYP/6-311++G(d,p)

$EMIM^{+}DCA^{-}$

C1 0.682952 -0.378446 -0.028634
N2 1.354262 0.756581 -0.250455
N3 1.549093 -1.398025 -0.021321
C4 0.766584 2.118834 -0.298287
H5 1.249842 2.633255 -1.131039
H6 -0.297219 2.013679 -0.528322
C7 1.192807 -2.812191 0.183745
H8 1.692461 -3.178262 1.081065
H9 1.515224 -3.388105 -0.683965
C10 2.817329 -0.897997 -0.245093
C11 2.694960 0.450011 -0.385879
H12 3.436274 1.206656 -0.575781
H13 3.683008 -1.535785 -0.291348
H14 -0.381260 -0.490502 0.118584
H15 0.108271 -2.879494 0.298640
C16 0.958336 2.870318 1.014482
H17 2.013922 3.001937 1.267693
H18 0.501326 3.857434 0.921428
H19 0.459224 2.351604 1.835580
N20 -3.484218 -0.317496 -0.072027
C21 -2.679972 -1.311819 0.171315
C22 -2.929843 0.848394 -0.287749
N23 -1.963986 -2.215602 0.391020
N24 -2.455150 1.900965 -0.483779

F2.TS1

C1 -0.154332 -0.973647 -0.736041
N2 1.090516 -1.129355 -0.314233
N3 -1.003845 -1.734610 -0.007398
C4 2.834737 -0.213303 -0.969502
H5 3.361338 -1.092397 -0.619802
H6 2.477616 -0.289337 -1.988925
C7 -2.450862 -1.851426 -0.204820
H8 -2.923662 -2.025852 0.761142
H9 -2.674957 -2.684137 -0.874686
C10 -0.248003 -2.410118 0.926408
C11 1.049033 -2.022418 0.726951
H12 1.934317 -2.313622 1.268713
H13 -0.693045 -3.083007 1.639787
H14 -0.484673 -0.323588 -1.530330
H15 -2.832706 -0.915809 -0.613398
C16 3.076552 1.039233 -0.393520
H17 3.869595 1.088751 0.349171
H18 3.017062 1.896016 -1.061257
H19 2.032983 1.382204 0.425726
N20 -1.041527 2.732527 0.282487
C21 -2.022605 2.011901 -0.215958
C22 0.028371 2.206739 0.726955
N23 -2.913699 1.428901 -0.689250
N24 1.045524 1.793825 1.168541

F2.TS2(SN2)

C1 -1.645853 0.223127 0.442210
N2 -2.988990 0.126054 0.310571
N3 -1.056515 -0.880522 0.017817
C4 -3.972187 1.169478 0.637146
H5 -4.784988 0.694979 1.191081
H6 -3.480742 1.865618 1.318883
C7 0.858925 -1.190874 -0.057575
H8 0.903127 -1.044187 -1.120485
H9 0.784035 -2.185768 0.340365
C10 -2.048014 -1.728193 -0.411393
C11 -3.257214 -1.113379 -0.235436
H12 -4.261784 -1.443882 -0.439062
H13 -1.831312 -2.707954 -0.804886
H14 -1.146326 1.090797 0.844028
H15 1.068494 -0.372506 0.607288
C16 -4.498088 1.896950 -0.598358
H17 -5.008332 1.211114 -1.278053
H18 -5.212938 2.664960 -0.294068
H19 -3.686169 2.381975 -1.144391
N20 4.521594 0.133446 0.625381
C21 3.684674 -0.704630 0.154797
C22 4.998888 1.159083 -0.052868
N23 2.910213 -1.537850 -0.174856
N24 5.460861 2.098227 -0.563462

F2.TS3(SN2)

C1 1.623243 -0.714687 -0.029314
N2 1.471336 0.597842 -0.022235
N3 2.934342 -1.045735 0.023183
C4 -0.417234 1.398906 -0.090513
H5 -0.583166 0.853095 -1.000492
H6 -0.622298 0.911399 0.844616
C7 3.486089 -2.398390 0.033616
H8 4.046038 -2.569383 0.954050
H9 4.141336 -2.543594 -0.826280
C10 3.651656 0.132635 0.066381
C11 2.730196 1.144328 0.037651
H12 2.892920 2.209178 0.055552
H13 4.727709 0.145341 0.112187
H14 0.826916 -1.442255 -0.070481
H15 2.666940 -3.113672 -0.020926
C16 -0.065331 2.853799 -0.132730
H17 0.565299 3.079191 -0.994704
H18 -0.985179 3.428945 -0.226213

H19 0.442160 3.164727 0.782205
N20 -3.752716 -0.401224 0.659091
C21 -3.900824 -1.543444 0.016240
C22 -3.150981 0.608697 0.162097
N23 -4.050194 -2.594616 -0.463092
N24 -2.582705 1.584586 -0.195531

F2.TS4
C1 0.360942 -0.520541 0.474723
N2 1.538267 -0.459864 -0.190797
N3 -0.408007 -1.477203 -0.016747
C4 2.604164 0.534557 0.024163
H5 3.294051 0.430490 -0.814517
H6 2.146944 1.523909 -0.049585
C7 -2.550477 -2.107599 0.392314
H8 -2.165089 -2.717523 -0.408352
H9 -3.523536 -1.679979 0.220636
C10 0.296415 -2.064859 -1.038163
C11 1.509415 -1.440560 -1.158718
H12 2.327785 -1.590503 -1.842638
H13 -0.103365 -2.877863 -1.624169
H14 0.096740 0.140648 1.281769
H15 -2.325913 -2.414536 1.400601
C16 3.333055 0.341618 1.351477
H17 3.787367 -0.650136 1.416756
H18 4.124114 1.089672 1.444304
H19 2.656833 0.467658 2.200125
N20 -2.098223 1.854209 -0.489107
C21 -2.347610 0.911318 0.336251
C22 -0.898196 2.391437 -0.569218
N23 -2.628542 0.044885 1.093536
N24 0.144764 2.895964 -0.697157

F2.TS5
C1 -0.275166 -0.863593 0.684606
N2 0.612199 -1.128727 -0.258033
N3 -1.497595 -1.347845 0.358328
C4 2.909159 -0.265307 -0.497792
H5 2.602675 -0.941533 -1.278705
H6 3.143749 0.743398 -0.795853
C7 -2.740294 -1.123194 1.096616
H8 -2.508838 -1.018514 2.156428
H9 -3.396477 -1.983304 0.963268
C10 -1.379664 -1.944571 -0.877494
C11 -0.066951 -1.804654 -1.243959
H12 0.414395 -2.145783 -2.147446
H13 -2.221752 -2.392824 -1.377364
H14 -0.082217 -0.312531 1.590583
H15 -3.219794 -0.210583 0.737772
C16 3.498431 -0.797942 0.731595
H17 3.058514 -1.745033 1.038139
H18 4.561872 -0.980007 0.484754
H19 3.475550 -0.065803 1.537207
N20 -0.215987 2.587022 -0.573879
C21 -1.455508 2.232439 -0.321820
C22 0.784965 2.072403 0.037587
N23 -2.579750 1.963156 -0.165615
N24 1.755773 1.643398 0.558509

MIM
C1 -0.198841 -1.085728 -0.000017
N2 -1.473775 -0.767754 -0.000011
N3 0.609802 0.016269 -0.000002
C4 2.063530 0.031972 0.000003
H5 2.444983 0.537197 0.890258
H6 2.444986 0.537273 -0.890207
C7 -0.227433 1.113238 0.000015
C8 -1.502635 0.606535 0.000009
H9 -2.433645 1.151832 0.000017
H10 0.152958 2.121580 0.000029
H11 0.203987 -2.088022 -0.000031
H12 2.426820 -0.995569 -0.000041

C_2H_4
C1 -0.664423 -0.000003 0.000000
H2 -1.235130 0.922789 0.000003
H3 -1.235200 -0.922750 -0.000002
C4 0.664423 -0.000004 0.000001
H5 1.235158 0.922774 -0.000004
H6 1.235171 -0.922775 0.000001

[$EMIM^+ - H_{C2}^+$]
C1 0.394489 -0.919700 -0.251770
N2 -0.597211 0.017302 -0.331674
N3 1.493046 -0.157435 0.029341
C4 -1.996390 -0.326561 -0.577344
H5 -2.400575 0.373231 -1.315552
H6 -1.988130 -1.319448 -1.026517
C7 2.825053 -0.716443 0.200559
H8 3.212442 -0.495648 1.198789
H9 3.514057 -0.314123 -0.547004
C10 1.197239 1.198318 0.121617
C11 -0.133963 1.309046 -0.105522
H12 -0.768484 2.179726 -0.130807
H13 1.938278 1.953403 0.326627
H14 2.747885 -1.794250 0.074724
C15 -2.843855 -0.318413 0.694786
H16 -2.855520 0.669787 1.162430
H17 -3.876099 -0.593775 0.461154
H18 -2.450133 -1.035462 1.418528

HDCA
H1 2.845933 -0.520152 0.613874
N2 -0.063423 0.580084 0.017050
C3 1.059336 0.083233 0.020988
C4 -1.271048 0.041734 0.003509
N5 2.201703 -0.269510 -0.122870
N6 -2.363375 -0.343381 -0.002874

$HN(CN)_2$
N1 0.000088 0.679993 0.000531
C2 1.182270 0.037906 -0.000489
C3 -1.182354 0.038008 0.000105
N4 2.207784 -0.493440 0.000138
N5 -2.207831 -0.493426 -0.000135
H6 0.000215 1.692623 -0.001436

[$EMIM^+ - H_{ME}^+$]
C1 0.361580 -0.785678 -0.287953
N2 -0.594142 0.212225 -0.358680
N3 1.562276 -0.238531 0.032149
C4 -2.019103 -0.015315 -0.553415
H5 -2.455927 0.937383 -0.860826
H6 -2.138227 -0.706195 -1.393857
C7 2.797273 -0.834316 0.071653
C8 1.323800 1.130651 0.238715
C9 0.004804 1.384976 -0.005875
H10 -0.540343 2.312243 0.051145
H11 2.129077 1.796719 0.490679
H12 0.209357 -1.804391 -0.591414
C13 -2.733509 -0.558173 0.687628
H14 -2.649311 0.139831 1.523853
H15 -3.794643 -0.709036 0.470730
H16 -2.308755 -1.514912 0.998582
H17 3.559056 -0.286697 0.604249
H18 2.803697 -1.913677 0.088063

NCHNCN
N1 -0.209233 0.220721 0.645042
C2 -1.265078 0.472146 -0.263884
C3 1.003973 0.030451 0.090158
N4 -1.425927 -0.743097 -0.111981
N5 2.096996 -0.099665 -0.273310
H6 -1.666214 1.338709 -0.775903

EIM
C1 0.746893 -1.098134 0.015420
N2 -0.123720 -0.088323 -0.287050
N3 1.956188 -0.653831 0.275672
C4 -1.549174 -0.220502 -0.578119
H5 -1.775802 0.382573 -1.461634
H6 -1.724535 -1.263665 -0.850231
C7 1.874612 0.711836 0.141158
C8 0.600029 1.084487 -0.203998
H9 0.155135 2.046247 -0.400131
H10 2.733874 1.346576 0.292859
H11 0.438563 -2.133502 0.021837
C12 -2.444362 0.183187 0.594325
H13 -2.293132 1.230536 0.864996
H14 -3.495759 0.050392 0.325323
H15 -2.233605 -0.429323 1.473918

CH_3DCA
C1 2.732076 0.365549 0.151855
H2 2.616469 0.719655 1.178338
H3 3.488490 -0.419576 0.119423
N4 -0.810853 -0.651689 0.196842
C5 -1.939094 0.021310 0.042180
C6 0.352721 -0.312533 -0.063141
N7 -2.973364 0.536248 -0.053652
N8 1.492224 -0.160785 -0.371755
H9 3.064767 1.187560 -0.483176

C_2H_5DCA
C1 2.170454 -0.374469 0.339848
H2 1.997624 -0.387497 1.419679
H3 2.771260 -1.249872 0.083711
C4 2.889930 0.902457 -0.084958
H5 2.307250 1.787686 0.178128
H6 3.855625 0.962708 0.422620
H7 3.063962 0.910009 -1.162563
N8 -1.488465 -0.732971 0.001861
C9 -2.473436 0.149422 0.035842
C10 -0.269269 -0.545725 -0.127272
N11 -3.396598 0.849473 0.080254
N12 0.899092 -0.518379 -0.356734

MIM^+
C1 -0.231429 -1.077567 -0.000001
N2 -1.514682 -0.736619 0.000001
N3 0.621503 0.042305 -0.000003
C4 2.095585 -0.006620 0.000002
H5 2.435975 -0.530021 0.893675
H6 2.479999 1.010728 0.000044
C7 -0.166749 1.107732 -0.000001
C8 -1.532667 0.592604 0.000001
H9 -2.443782 1.176109 0.000003
H10 0.200060 2.124832 -0.000002
H11 0.155581 -2.088400 -0.000002
H12 2.435985 -0.529950 -0.893709

EIM^+
C1 0.612413 -1.047262 -0.199613
N2 -0.131268 0.142900 -0.274962
N3 1.884926 -0.833509 0.120593
C4 -1.585015 0.236200 -0.581718
H5 -1.771863 1.268444 -0.877564
H6 -1.758634 -0.398091 -1.453054
C7 2.000868 0.482768 0.260874
C8 0.713525 1.123806 0.008978
H9 0.433983 2.168042 0.028461
H10 2.928293 0.974257 0.523220
H11 0.166061 -2.012949 -0.396737
C12 -2.447393 -0.181411 0.606126
H13 -2.275020 0.463293 1.470138
H14 -3.497464 -0.094889 0.320611
H15 -2.267349 -1.218447 0.897630

C_2H_5
C1 0.793855 0.000000 -0.018080
H2 1.352042 -0.926375 0.039959
H3 1.352060 0.926363 0.039960
C4 -0.693634 0.000004 -0.001996
H5 -1.106561 -0.886455 -0.493045
H6 -1.092314 -0.000317 1.026091
H7 -1.106551 0.886760 -0.492509

CH_3
C1 -0.000001 0.000056 0.000381
H2 0.934041 0.543239 -0.000762
H3 -0.937710 0.536882 -0.000762
H4 0.003673 -1.080454 -0.000762

$EMIM^+$
C1 0.411034 -0.817957 -0.205627
N2 -0.620356 0.023982 -0.319216
N3 1.521645 -0.114817 0.040430
C4 -2.033183 -0.362651 -0.559373
H5 -2.404516 0.282918 -1.356654
H6 -2.015447 -1.382750 -0.944522
C7 2.871821 -0.669693 0.222807
H8 3.239636 -0.409797 1.214862
H9 3.536080 -0.266198 -0.540723
C10 1.187233 1.225212 0.086861
C11 -0.152623 1.311126 -0.136627
H12 -0.800194 2.169926 -0.186048
H13 1.920584 1.993113 0.266462
H14 0.357777 -1.889973 -0.300446
H15 2.825034 -1.752440 0.126048
C16 -2.887719 -0.254781 0.699189
H17 -2.918816 0.768026 1.079968
H18 -3.910312 -0.552930 0.459859
H19 -2.518220 -0.911586 1.489318

DCA^-
N1 2.234249 -0.389194 0.000000
C2 1.150169 0.058130 0.000000
N3 0.000000 0.678737 0.000000
C4 -1.150169 0.058130 0.000000
N5 -2.234249 -0.389194 0.000000

Cartesian coordinates for the structures in Figure 3, calculated at B3LYP/6-311++G(d,p)

NO_2
N1 0.000000 0.000000 0.321839
O2 0.000000 1.099987 -0.140804
O3 0.000000 -1.099987 -0.140804

HONO
N1 0.180080 0.486576 -0.000020
O2 1.102800 -0.225570 0.000015
O3 -1.045330 -0.255252 -0.000016
H4 -1.720324 0.440540 0.000142

[$EMIM^+ - H_{C2}^+$]
C1 0.394489 -0.919700 -0.251770
N2 -0.597211 0.017302 -0.331674
N3 1.493046 -0.157435 0.029341
C4 -1.996390 -0.326561 -0.577344
H5 -2.400575 0.373231 -1.315552
H6 -1.988130 -1.319448 -1.026517
C7 2.825053 -0.716443 0.200559
H8 3.212442 -0.495648 1.198789
H9 3.514057 -0.314123 -0.547004
C10 1.197239 1.198318 0.121617
C11 -0.133963 1.309046 -0.105522
H12 -0.768484 2.179726 -0.130807
H13 1.938278 1.953403 0.326627
H14 2.747885 -1.794250 0.074724
C15 -2.843855 -0.318413 0.694786
H16 -2.855520 0.669787 1.162430
H17 -3.876099 -0.593775 0.461154
H18 -2.450133 -1.035462 1.418528

F3.precursor for [$EMIM^+ - H_{C2}^+$] + NO_2
C1 0.020997 0.303102 0.152253
N2 -1.176304 -0.185925 -0.260952
C3 -2.079771 0.833920 -0.537357
C4 -1.425579 1.998188 -0.303011
N5 -0.145294 1.649669 0.112210
C6 -1.474362 -1.618992 -0.346735
H7 -2.043620 -1.789910 -1.264762
H8 -0.515527 -2.126589 -0.447162
C9 -2.237544 -2.137516 0.871092
H10 -3.201066 -1.633884 0.987223
H11 -2.426347 -3.208916 0.763553
H12 -1.655397 -1.981472 1.781872
H13 -3.086213 0.652137 -0.876029
H14 -1.753492 3.019737 -0.400931
C15 0.900483 2.601080 0.470964
H16 0.620793 3.157712 1.368685
H17 1.071014 3.302378 -0.348888
H18 1.813391 2.040644 0.659605
N19 2.268214 -0.837655 -0.280040
O20 2.126498 -2.033145 -0.315161
O21 3.164104 -0.178500 0.182046

F3.TS1
C1 -0.218212 -0.059372 0.334642
N2 0.970722 -0.335447 -0.276173
C3 0.953582 -1.617646 -0.808295
C4 -0.266955 -2.143265 -0.540704
N5 -0.980676 -1.176035 0.154553
C6 2.152636 0.535915 -0.237000
H7 2.701249 0.376362 -1.168531
H8 1.788985 1.561758 -0.237451
C9 3.041468 0.261794 0.975732
H10 3.411224 -0.767147 0.979828
H11 3.903996 0.933335 0.961507
H12 2.489760 0.434237 1.902360
H13 1.800702 -2.041200 -1.321095
H14 -0.681470 -3.109016 -0.775963
C15 -2.309952 -1.380575 0.724212
H16 -2.251803 -2.040956 1.593481
H17 -2.965138 -1.824808 -0.026910
H18 -2.713047 -0.414637 1.014334
N19 -1.046597 1.552552 -0.233831
O20 -2.238730 1.634992 0.020701
O21 -0.286770 2.492942 -0.411316

F3.TS2
C1 0.325850 -0.170601 0.209527
N2 -0.265655 0.961099 -0.288114
C3 0.698778 1.929161 -0.542966
C4 1.903462 1.393525 -0.230686
N5 1.669218 0.098172 0.215077
C6 -1.710960 1.151176 -0.425661
H7 -1.855760 1.968680 -1.135892
H8 -2.123356 0.245157 -0.870750
C9 -2.402415 1.447682 0.903312
H10 -2.001790 2.354019 1.365250
H11 -3.474191 1.589617 0.739943
H12 -2.267953 0.611404 1.590820
H13 0.445762 2.906784 -0.917013
H14 2.892064 1.816992 -0.282155
C15 2.677438 -0.818820 0.723576
H16 2.876265 -0.637223 1.783791
H17 3.600784 -0.694705 0.156183
H18 2.318921 -1.838021 0.592385
N19 -0.867018 -2.418055 -0.390410

O20 0.099498 -1.592725 -0.750491
O21 -1.739433 -1.957770 0.300360

F3.TS3
C1 -1.067358 0.932098 0.398310
N2 -1.855398 -0.155255 0.250127
C3 -1.336553 -1.088549 -0.656693
C4 -0.170419 -0.579514 -1.111906
N5 -0.018522 0.651018 -0.479280
C6 -3.131730 -0.317171 0.952039
H7 -3.172287 -1.333865 1.353482
H8 -3.100544 0.375235 1.792567
C9 -4.338264 -0.034663 0.058900
H10 -4.378990 -0.717462 -0.794004
H11 -5.261133 -0.157336 0.631571
H12 -4.302100 0.988672 -0.320862
H13 -1.827340 -2.019805 -0.886821
H14 0.556801 -0.980973 -1.797233
C15 1.089828 1.508444 -0.617209
H16 0.863114 2.502647 -0.239072
H17 1.526064 1.488609 -1.616381
H18 2.010800 1.112761 0.086273
N19 3.443439 -0.462924 -0.009729
O20 4.376266 -1.079462 0.422489
O21 3.101979 0.577934 0.742762

[O_2N-EMIM$^+$ – H_{C2}^+]$^\bullet$
C1 -0.310465 0.115519 -0.117812
N2 0.780549 -0.697567 -0.320505
C3 0.352830 -2.013212 -0.232015
C4 -0.979091 -2.012285 0.003625
N5 -1.403994 -0.695597 0.079322
C6 2.201702 -0.320888 -0.452957
H7 2.683751 -1.176067 -0.932815
H8 2.256967 0.537251 -1.115875
C9 2.856731 -0.002778 0.888654
H10 2.776679 -0.842268 1.584788
H11 3.917238 0.211299 0.731222
H12 2.395476 0.880681 1.331829
H13 1.038166 -2.834331 -0.349627
H14 -1.667126 -2.831557 0.117150
C15 -2.805243 -0.302384 0.260249
H16 -3.380211 -1.221453 0.376291
H17 -3.162648 0.251525 -0.605985
H18 -2.915067 0.326831 1.139291
N19 -0.320781 1.483110 -0.119596
O20 -1.414627 2.067091 0.178406
O21 0.760573 2.093489 -0.409566

[O-EMIM$^+$ – H_{C2}^+]
C1 -0.366511 0.645924 -0.149567
N2 0.669926 -0.265228 -0.313860
C3 0.186859 -1.565463 -0.182506
C4 -1.141586 -1.489571 0.052107
N5 -1.490830 -0.140847 0.073024
C6 2.051348 0.140411 -0.533608
H7 2.489009 -0.532021 -1.277325
H8 2.011017 1.140071 -0.969267
C9 2.887332 0.152962 0.747465
H10 2.928330 -0.838746 1.206010
H11 3.911018 0.466732 0.524875
H12 2.465642 0.851487 1.473368
H13 0.826588 -2.426271 -0.275189
H14 -1.866987 -2.271212 0.198889
C15 -2.811824 0.414788 0.288067
H16 -3.200733 0.131072 1.269927
H17 -3.508208 0.080000 -0.485767
H18 -2.720894 1.499422 0.240405
O19 -0.302769 1.868460 -0.193978

[EMIM$^+$ – H_{C2}^+ – H_{ME}]$^\bullet$
C1 0.394510 -0.919754 -0.251686
N2 -0.597217 0.017253 -0.331668
C3 -0.133998 1.309022 -0.105594
C4 1.197251 1.198323 0.121579
N5 1.493067 -0.157430 0.029403
C6 -1.996385 -0.326659 -0.577324
H7 -2.400556 0.373007 -1.315688
H8 -1.988102 -1.319642 -1.026326
C9 -2.843917 -0.318299 0.694768
H10 -2.855720 0.670025 1.162199
H11 -3.876144 -0.593828 0.461135
H12 -2.450162 -1.035160 1.418715
H13 -0.768545 2.179712 -0.130937
H14 1.938295 1.953448 0.326559
C15 2.825105 -0.716385 0.200548
H16 3.212848 -0.494892 1.198505
H17 3.513893 -0.314627 -0.547548
H18 2.747847 -1.794297 0.075498

[BMIM$^+$ – H_{C2}^+]
C1 -1.387947 -0.817467 0.455953
N2 -0.524218 0.241872 0.463127
N3 -2.506570 -0.277043 -0.112897
C4 0.851151 0.140520 0.944300
H5 1.081441 1.036290 1.531027
H6 0.876583 -0.716415 1.618640
C7 -3.731735 -1.031180 -0.327271
H8 -3.994729 -1.049513 -1.388343

H9 -4.560124 -0.595996 0.238346
C10 -2.345898 1.063518 -0.446663
C11 -1.082792 1.392479 -0.082831
H12 -0.554209 2.328443 -0.159592
H13 -3.123757 1.659499 -0.895072
H14 -3.556305 -2.047928 0.017676
C15 1.871594 -0.037666 -0.183944
H16 1.802797 0.809535 -0.877141
H17 1.601980 -0.932399 -0.755428
C18 3.307488 -0.160920 0.336808
H19 3.368106 -1.007187 1.031486
H20 3.562036 0.731931 0.921368
C21 4.336243 -0.346787 -0.782320
H22 4.324425 0.500033 -1.475697
H23 5.349650 -0.433605 -0.381169
H24 4.128998 -1.251474 -1.361903

F3.precursor [$BMIM^+ - H_{C2}^+$] + NO_2
C1 -1.043551 -0.250131 0.131883
N2 0.012975 -0.841503 -0.482264
C3 -0.213134 -2.195625 -0.700455
C4 -1.454159 -2.458621 -0.221602
N5 -1.942902 -1.256265 0.276892
C6 1.250468 -0.131415 -0.816366
H7 1.583243 -0.475278 -1.800684
H8 0.989464 0.923847 -0.900656
C9 2.353547 -0.331959 0.226599
H10 2.575443 -1.401456 0.326535
H11 1.977233 0.003388 1.199116
H12 0.506814 -2.842569 -1.173508
H13 -2.018463 -3.376079 -0.199659
C14 -3.254014 -1.082214 0.891922
H15 -3.310290 -1.629247 1.836158
H16 -4.036540 -1.441780 0.220181
H17 -3.399938 -0.020311 1.076931
N18 -1.730572 2.167175 -0.272122
O19 -0.762711 2.842763 -0.514082
O20 -2.718735 2.434464 0.362997
C21 3.635022 0.429934 -0.128248
H22 3.996467 0.099177 -1.109821
H23 3.403170 1.496236 -0.231500
C24 4.744947 0.247057 0.910819
H25 5.021125 -0.806973 1.014737
H26 5.645353 0.800375 0.631166
H27 4.427226 0.604850 1.894839

F3.TS1
C1 -0.993774 -0.049123 0.278359
N2 -0.029313 -0.548083 -0.548231
C3 -0.383123 -1.814856 -0.992603
C4 -1.591425 -2.104011 -0.450240
N5 -1.960464 -1.010378 0.321853
C6 1.266555 0.092782 -0.802779
H7 1.570857 -0.180946 -1.817005
H8 1.098602 1.168758 -0.785460
C9 2.337568 -0.315374 0.213619
H10 2.460297 -1.405291 0.201528
H11 1.986813 -0.048983 1.216510
H12 0.248075 -2.394596 -1.644822
H13 -2.208442 -2.982104 -0.540164
C14 -3.150836 -0.959652 1.166775
H15 -3.014346 -1.586424 2.052047
H16 -4.014646 -1.312608 0.601150
H17 -3.321168 0.071937 1.461253
N18 -1.628058 1.680192 -0.190858
O19 -2.706091 1.981020 0.299881
O20 -0.769817 2.465273 -0.565723
C21 3.685106 0.360052 -0.063130
H22 4.022301 0.100677 -1.074249
H23 3.551362 1.447904 -0.055736
C24 4.766133 -0.028641 0.949468
H25 5.713756 0.469280 0.727967
H26 4.473581 0.250816 1.966110
H27 4.947851 -1.107940 0.941443

F3.TS2
C1 -1.121772 0.075851 0.199639
N2 -0.285562 -0.749189 -0.506885
C3 -0.885546 -1.989342 -0.691014
C4 -2.114681 -1.933942 -0.123502
N5 -2.260168 -0.657872 0.407301
C6 1.079216 -0.404878 -0.905137
H7 1.349222 -1.069151 -1.730743
H8 1.066202 0.616356 -1.288556
C9 2.088536 -0.521892 0.240116
H10 2.075613 -1.546458 0.631599
H11 1.764169 0.136570 1.051388
H12 -0.388574 -2.796496 -1.202065
H13 -2.885017 -2.682406 -0.047989
C14 -3.402625 -0.183251 1.172381
H15 -3.321674 -0.474516 2.223709
H16 -4.319890 -0.597911 0.751979
H17 -3.442836 0.901924 1.100293
N18 -0.926115 2.622055 -0.358981
O19 -1.596217 1.515978 -0.630115
O20 0.172477 2.483870 0.114883
C21 3.508258 -0.149258 -0.199193
H22 3.816531 -0.794367 -1.031714
H23 3.506316 0.875315 -0.588489
C24 4.530542 -0.260702 0.935636

H25 5.532904 0.012590 0.595233
H26 4.269365 0.401125 1.766727
H27 4.578934 -1.281827 1.326886

F3.TS3
C1 0.033848 0.902728 -0.408476
N2 0.818612 -0.167176 -0.153644
C3 0.279751 -1.022978 0.815661
C4 -0.896442 -0.480527 1.201433
N5 -1.034289 0.693229 0.466197
C6 2.109367 -0.384056 -0.810784
H7 2.165365 -1.433349 -1.117680
H8 2.095899 0.229167 -1.712094
C9 3.301469 -0.015078 0.076040
H10 3.274656 -0.609495 0.997398
H11 3.200343 1.033547 0.375997
H12 0.766133 -1.930784 1.132337
H13 -1.638379 -0.824992 1.901835
C14 -2.146153 1.555984 0.505898
H15 -1.910687 2.516403 0.053095
H16 -2.607078 1.617209 1.492247
H17 -3.048779 1.102011 -0.185858
N18 -4.486866 -0.461733 -0.003249
O19 -5.408692 -1.111529 -0.410001
O20 -4.123537 0.515855 -0.826423
C21 4.642793 -0.229692 -0.634098
H22 4.727590 -1.278163 -0.944807
H23 4.661930 0.364221 -1.555421
C24 5.845493 0.142386 0.237519
H25 5.874949 -0.460094 1.150684
H26 6.785902 -0.017587 -0.296127
H27 5.807028 1.194462 0.535509

[O_2N-BMIM$^+$ – H_{C2}^+]$^\bullet$
C1 -1.126063 0.121911 -0.154287
N2 -0.176279 -0.802893 -0.521114
C3 -0.701726 -2.065333 -0.293632
C4 -1.957886 -1.922679 0.187364
N5 -2.233241 -0.567974 0.282199
C6 1.224767 -0.573663 -0.920158
H7 1.536732 -1.487111 -1.433943
H8 1.240387 0.253723 -1.624066
C9 2.142050 -0.277621 0.268750
H10 2.080263 -1.097844 0.994569
H11 1.781009 0.628951 0.762287
H12 -0.131833 -2.954435 -0.499586
H13 -2.686214 -2.664304 0.464881
C14 -3.531676 -0.029038 0.699481
H15 -4.158841 -0.880873 0.963564
H16 -3.992178 0.532492 -0.111596
H17 -3.413199 0.634182 1.551914
N18 -1.008949 1.483185 -0.220171
O19 -1.958368 2.182551 0.266277
O20 0.041233 1.973961 -0.751765
C21 3.596703 -0.079256 -0.171304
H22 3.946452 -0.974187 -0.701509
H23 3.642211 0.744736 -0.892005
C24 4.535512 0.216659 1.001802
H25 4.534983 -0.603171 1.727050
H26 5.564259 0.357227 0.659803
H27 4.232249 1.126399 1.528052

[O-BMIM$^+$ – H_{C2}^+]
C1 1.275883 -0.614489 -0.231927
N2 0.383334 0.424973 -0.462905
C3 0.975241 1.643013 -0.136307
C4 2.233521 1.389644 0.285902
N5 2.428309 0.011000 0.229929
C6 -0.981043 0.205995 -0.920606
H7 -1.244296 1.016959 -1.607074
H8 -0.972486 -0.725077 -1.491538
C9 -1.998709 0.113555 0.222144
H10 -1.962800 1.035216 0.815732
H11 -1.700572 -0.702922 0.888320
H12 0.453912 2.578878 -0.241961
H13 3.005933 2.064329 0.612811
C14 3.630659 -0.714541 0.587262
H15 3.880449 -0.564203 1.641287
H16 4.475760 -0.399993 -0.031338
H17 3.436750 -1.772613 0.414367
O18 1.088272 -1.813411 -0.400726
C19 -3.426178 -0.121444 -0.282490
H20 -3.713366 0.693552 -0.958574
H21 -3.449721 -1.038720 -0.882690
C22 -4.451303 -0.228517 0.850190
H23 -4.477079 0.686984 1.449650
H24 -5.458522 -0.398661 0.460398
H25 -4.210057 -1.057546 1.522239

[BMIM$^+$ – H_{C2}^+ – H_{ME}]$^\bullet$
C1 -1.421321 -0.871661 0.422013
N2 -0.584976 0.199447 0.467962
C3 -1.159281 1.364772 -0.038122
C4 -2.414945 1.039527 -0.420609
N5 -2.568270 -0.322390 -0.139604
C6 0.792567 0.105137 0.947951
H7 1.007710 0.989138 1.557267
H8 0.829617 -0.768545 1.599658
C9 1.813756 -0.028587 -0.185628
H10 1.733165 0.835684 -0.856119

H11 1.555898 -0.911549 -0.780145
H12 -0.641109 2.308723 -0.075292
H13 -3.199780 1.640187 -0.848441
C14 -3.711943 -1.055870 -0.375485
H15 -4.564262 -0.561941 -0.813807
H16 -3.692662 -2.098514 -0.108481
C17 3.251434 -0.145856 0.331719
H18 3.323142 -1.007725 1.005802
H19 3.495219 0.735944 0.937145
C20 4.280990 -0.292362 -0.792448
H21 4.258600 0.570507 -1.465484
H22 5.295567 -0.376434 -0.393906
H23 4.084077 -1.185474 -1.393042

[AMIM$^+$ – H$_{C2}^+$]
C1 0.917072 -0.984962 -0.120389
N2 -0.170488 -0.178199 -0.313826
C3 0.144498 1.175448 -0.249979
C4 1.476127 1.238872 -0.010020
N5 1.920469 -0.077251 0.065618
C6 -1.512582 -0.702399 -0.565180
H7 -1.869173 -0.350348 -1.538549
H8 -1.390605 -1.786236 -0.620925
H9 -0.586039 1.958144 -0.368605
H10 2.126141 2.090152 0.109275
C11 3.301900 -0.460293 0.313154
H12 3.643264 -0.076851 1.278429
H13 3.957088 -0.079126 -0.474722
H14 3.345318 -1.547276 0.322102
C15 -2.492031 -0.335299 0.516150
H16 -2.195844 -0.605843 1.527170
C17 -3.660832 0.261862 0.298771
H18 -3.978160 0.545099 -0.700779
H19 -4.346772 0.481054 1.109019

F3.precursor [AMIM$^+$ – H$_{C2}^+$] + NO$_2$
C1 -0.508364 -0.339388 0.079344
N2 0.805607 -0.402291 -0.262238
C3 1.230194 -1.713441 -0.449566
C4 0.147422 -2.497484 -0.226672
N5 -0.899850 -1.639113 0.091374
C6 1.658246 0.782934 -0.409492
H7 2.067161 0.807665 -1.423831
H8 0.992404 1.640184 -0.292231
H9 2.243183 -1.970096 -0.709928
H10 0.037168 -3.568528 -0.265765
C11 -2.256189 -2.067596 0.413655
H12 -2.262715 -2.659687 1.331980
H13 -2.669036 -2.664765 -0.402505
H14 -2.865349 -1.177098 0.552004
N15 -2.071013 1.717242 -0.242707
O16 -1.415776 2.724574 -0.178790
O17 -3.159630 1.467121 0.204399
C18 2.765583 0.823499 0.607084
H19 2.450384 0.771324 1.646711
C20 4.055473 0.939247 0.303562
H21 4.395583 0.994438 -0.726549
H22 4.817066 0.995505 1.072747

F3.TS1
C1 -0.584312 -0.064191 0.380448
N2 0.636703 -0.253166 -0.199922
C3 0.708044 -1.511839 -0.783558
C4 -0.488278 -2.112333 -0.572623
N5 -1.275882 -1.214277 0.136424
C6 1.752265 0.702154 -0.140495
H7 2.076674 0.929167 -1.159578
H8 1.343078 1.619393 0.282312
H9 1.597912 -1.871845 -1.270936
H10 -0.838497 -3.092167 -0.850538
C11 -2.605558 -1.513545 0.661229
H12 -2.531939 -2.180648 1.524178
H13 -3.205729 -1.989213 -0.116038
H14 -3.080560 -0.580107 0.949608
N15 -1.477993 1.515064 -0.180294
O16 -2.682736 1.525793 0.019181
O17 -0.762553 2.497076 -0.303947
C18 2.899280 0.183146 0.682563
H19 2.655769 -0.103896 1.703029
C20 4.150669 0.089795 0.241462
H21 4.419401 0.372221 -0.772269
H22 4.953742 -0.258328 0.880752

F3.TS2
C1 -0.725910 -0.022442 0.244813
N2 0.513462 -0.391756 -0.218826
C3 0.523115 -1.746756 -0.533297
C4 -0.718084 -2.226841 -0.283265
N5 -1.484421 -1.164264 0.180407
C6 1.673294 0.499122 -0.314165
H7 2.011952 0.534493 -1.354292
H8 1.313216 1.491158 -0.037950
H9 1.410174 -2.248095 -0.880527
H10 -1.114740 -3.223020 -0.382707
C11 -2.860482 -1.250641 0.642960
H12 -2.907004 -1.591825 1.681369
H13 -3.415241 -1.944130 0.009306
H14 -3.315881 -0.265181 0.566132
N15 -1.478679 2.413128 -0.300722
O16 -1.532272 1.148837 -0.696849

O17 -0.573459 2.708657 0.434806
C18 2.795018 0.076202 0.593860
H19 2.540406 -0.003395 1.648158
C20 4.035648 -0.172774 0.183278
H21 4.314730 -0.099019 -0.863879
H22 4.820109 -0.445914 0.879609

F3.TS3
C1 0.606602 1.124172 -0.435489
N2 1.491230 0.119191 -0.247538
C3 1.059512 -0.826121 0.692321
C4 -0.149573 -0.409790 1.128318
N5 -0.413470 0.778261 0.451795
C6 2.765175 0.030763 -0.969805
H7 2.787886 -0.899531 -1.544992
H8 2.754548 0.866063 -1.672587
H9 1.643448 -1.689473 0.964098
H10 -0.834935 -0.847261 1.834585
C11 -1.596046 1.534700 0.561368
H12 -1.460398 2.532663 0.150948
H13 -2.032079 1.507098 1.560401
H14 -2.474480 1.032867 -0.128918
N15 -3.792064 -0.634646 0.044339
O16 -4.671237 -1.340531 -0.362334
O17 -3.511659 0.381680 -0.765731
C18 3.953583 0.116064 -0.052379
H19 3.994437 0.997644 0.583176
C20 4.926497 -0.789778 -0.005005
H21 5.780714 -0.670838 0.651368
H22 4.909650 -1.678129 -0.629708

[O_2N-AMIM$^+$ – H_{C2}^+]$^\bullet$
C1 -0.644003 0.108501 -0.149108
N2 0.526088 -0.539830 -0.470656
C3 0.301068 -1.903917 -0.367951
C4 -0.989826 -2.093926 -0.013254
N5 -1.589095 -0.852033 0.125065
C6 1.857036 0.033942 -0.769284
H7 2.379239 -0.713239 -1.370885
H8 1.698047 0.932388 -1.360423
H9 1.082860 -2.617249 -0.560862
H10 -1.541064 -3.003744 0.147431
C11 -3.000298 -0.664327 0.478825
H12 -3.431742 -1.658435 0.598262
H13 -3.522702 -0.122845 -0.306693
H14 -3.091529 -0.100511 1.403968
N15 -0.839164 1.460736 -0.096299
O16 -1.990058 1.880326 0.255736
O17 0.141662 2.221747 -0.391161
C18 2.637634 0.360144 0.474553
H19 2.207579 1.138475 1.097867
C20 3.794216 -0.214370 0.792407
H21 4.244214 -0.981261 0.168136
H22 4.342497 0.071441 1.682698

[O-AMIM$^+$ – H_{C2}^+]
C1 0.861172 -0.684826 -0.073222
N2 -0.310391 0.040733 -0.266986
C3 -0.035785 1.407630 -0.247210
C4 1.290126 1.554680 -0.037885
N5 1.847851 0.281643 0.071505
C6 -1.600268 -0.591627 -0.512297
H7 -1.957956 -0.331902 -1.514434
H8 -1.399788 -1.666713 -0.495571
H9 -0.808341 2.146748 -0.368902
H10 1.884445 2.448001 0.048949
C11 3.242569 -0.041791 0.297355
H12 3.591615 0.374830 1.246175
H13 3.868551 0.337836 -0.514934
H14 3.324824 -1.127522 0.332875
O15 0.990701 -1.902156 -0.040014
C16 -2.630252 -0.230956 0.523132
H17 -2.350641 -0.433208 1.554587
C18 -3.822831 0.287621 0.242954
H19 -4.124300 0.501246 -0.778526
H20 -4.544619 0.506914 1.021289

[AMIM$^+$ – H_{C2}^+ – H_{ME}]$^\bullet$
C1 -0.961140 -1.014125 0.098672
N2 0.110640 -0.201446 0.304823
C3 -0.209663 1.155223 0.257053
C4 -1.537677 1.224281 0.013850
N5 -1.989145 -0.096793 -0.083004
C6 1.457745 -0.717727 0.553344
H7 1.804048 -0.378534 1.534735
H8 1.345948 -1.803335 0.588980
H9 0.520214 1.936242 0.388646
H10 -2.190265 2.073867 -0.096955
C11 -3.293314 -0.471914 -0.327803
H12 -4.038907 0.296479 -0.454866
H13 -3.502310 -1.526777 -0.376443
C14 2.435659 -0.318325 -0.517228
H15 2.152329 -0.584373 -1.533054
C16 3.589721 0.301098 -0.284184
H17 3.893845 0.579316 0.720809
H18 4.276652 0.543721 -1.086803

Cartesian coordinates for the structures in Figure 4, calculated at B3LYP/6-311++G(d,p)

CH_3DCA
N1 0.810867 -0.651664 0.196783
C2 -0.352715 -0.312503 -0.063152
C3 1.939135 0.021287 0.042178
N4 -1.492224 -0.160720 -0.371706
N5 2.973408 0.536228 -0.053618
C6 -2.732164 0.365501 0.151816
H7 -3.488411 -0.419797 0.119804
H8 -2.616384 0.719825 1.178210
H9 -3.065100 1.187355 -0.483270

F4.TS1′
N1 4.092136 -0.649516 -0.094369
C2 3.009460 -0.270690 0.085600
N3 1.836919 0.256237 0.372281
C4 0.677383 0.039240 -0.052250
N5 -0.499286 0.486845 -0.026554
N6 -2.518630 -1.027416 -0.242936
O7 -2.631446 -0.780282 0.904015
O8 -1.503737 -0.440468 -0.925393
C9 -1.008956 1.854239 -0.014732
H10 -0.270083 2.462024 0.511903
H11 -1.137539 2.223524 -1.033357
H12 -1.956217 1.880658 0.521820

F4.TS2′
N1 -1.877921 2.263538 -0.363130
C2 -1.008069 1.585187 0.020442
N3 -0.042021 0.888114 0.556288
C4 0.679211 -0.011948 -0.059940
N5 1.809306 -0.453005 -0.217857
N6 -1.343756 -1.658309 -0.206576
O7 -1.561145 -1.331115 0.918515
O8 -0.417862 -1.154899 -0.900137
C9 3.003460 0.295386 0.162094
H10 3.634917 -0.361367 0.762677
H11 3.556709 0.547170 -0.745322
H12 2.773560 1.208184 0.718969

F4.TS3′
N1 1.977076 -0.430171 -0.150398
C2 1.156884 0.438528 0.074630
N3 -0.140907 0.637873 0.010500
C4 -0.734487 1.833031 0.050804
N5 -1.290898 2.846633 0.100508
N6 -1.575940 -1.282792 0.466779
O7 -2.267108 -2.117707 0.046995
O8 -1.100944 -0.448166 -0.633318
C9 3.393076 -0.593523 0.086120
H10 3.888638 -0.829089 -0.856761
H11 3.829727 0.313680 0.511823
H12 3.547902 -1.426615 0.774474

F4.TS4′
N1 -2.304820 -0.121714 -0.243655
C2 -1.341540 -0.742776 0.036793
N3 -0.437020 -1.559252 0.309324
C4 0.849776 -1.457801 0.036063
N5 1.965232 -1.875129 -0.055736
N6 1.937009 1.069767 0.313628
O7 1.876026 2.234964 0.076969
O8 1.120615 0.375077 -0.528366
C9 -3.164951 0.986529 0.077589
H10 -2.861394 1.851436 -0.514360
H11 -4.190694 0.726595 -0.182051
H12 -3.103555 1.230218 1.139983

F4.TS5′
N1 -3.276687 -0.271738 -0.352995
C2 -2.158949 -0.311471 0.067371
N3 -1.023933 -0.569001 0.484669
C4 0.174538 -0.046106 0.305358
N5 1.313996 -0.436485 0.059696
N6 3.572088 0.555153 -0.092234
O7 3.868122 -0.551776 -0.374314
O8 2.280316 0.831295 0.171340
C9 -4.491412 0.490115 -0.158260
H10 -5.280923 -0.185879 0.173504
H11 -4.356666 1.282941 0.580869
H12 -4.793227 0.926053 -1.111346

F4.TS6′
N1 -4.908890 1.017026 -0.269811
C2 -4.030114 0.304719 0.024316
N3 -3.122288 -0.537489 0.438063
C4 -1.927798 -0.615682 -0.014711
N5 -0.825664 -0.812958 -0.375676
N6 3.723673 0.005180 -0.267601
O7 4.882175 0.268559 -0.164786
O8 2.849136 0.456611 0.518744
C9 1.104785 -0.177273 0.051983
H10 0.979984 -0.610565 1.028645
H11 1.450876 -0.789881 -0.762301
H12 0.769590 0.826189 -0.142347

$[CH_3NC(-ONO)NCN]^{\bullet}$
N1 -3.198525 -0.637918 0.253968

C2 -2.202093 -0.027595 0.150495
N3 -1.168402 0.758366 0.090997
C4 0.043160 0.296327 -0.301938
N5 1.124459 1.035197 -0.286418
N6 1.340267 -1.906975 -0.118656
O7 1.945420 -1.417290 0.700691
O8 0.134543 -0.971235 -0.743054
C9 1.059139 2.407232 0.150089
H10 1.464483 3.030602 -0.655013
H11 0.062154 2.753786 0.428244
H12 1.747838 2.527324 0.994555

[CH$_3$NCNC(-ONO)N]$^\bullet$
N1 -2.856678 -0.109116 -0.456209
C2 -1.702252 -0.299423 -0.215823
N3 -0.513019 -0.626861 -0.099434
C4 0.551611 0.241535 0.131509
N5 0.505096 1.503745 0.055243
N6 2.904155 0.112985 -0.385566
O7 3.877897 -0.318656 0.021280
O8 1.696189 -0.420483 0.462802
C9 -4.108604 -0.000326 0.258494
H10 -4.841978 -0.656753 -0.211558
H11 -3.999257 -0.271892 1.310944
H12 -4.472869 1.025786 0.184637

DCA
N1 0.000023 0.656080 0.000097
C2 -1.147556 0.054284 -0.000075
C3 1.147552 0.054307 -0.000197
N4 -2.240223 -0.374569 0.000041
N5 2.240204 -0.374589 0.000095

CH$_3$ONO
N1 -0.690674 0.439610 0.000019
O2 -1.735495 -0.084629 -0.000017
O3 0.368347 -0.513970 0.000013
C4 1.646830 0.138274 -0.000011
H5 2.191217 -0.169951 0.893669
H6 1.508647 1.221500 0.000174
H7 2.191062 -0.169665 -0.893885

[CH$_3$N(-ONO)CNCN]$^\bullet$
N1 3.901103 -0.681405 0.049643
C2 2.820270 -0.256642 0.010836
N3 1.642255 0.322719 0.035724
C4 0.510739 -0.011894 -0.414772
N5 -0.647401 0.609613 -0.239527
N6 -2.452411 -1.079996 -0.143367
O7 -1.896232 -1.376732 0.806197
O8 -1.725950 0.140369 -0.932499
C9 -0.884320 1.824792 0.549564
H10 0.064447 2.126732 0.989083
H11 -1.261648 2.609121 -0.108137
H12 -1.610304 1.620996 1.338393

[CH$_3$NCNCN-ONO]$^\bullet$
N1 -3.319891 -0.018958 -0.360941
C2 -2.148534 -0.195982 -0.213255
N3 -0.955173 -0.514150 -0.185033
C4 0.166687 0.224120 -0.156532
N5 1.343563 -0.192286 -0.027517
N6 3.659212 0.377467 0.092378
O7 3.771122 -0.772229 0.209961
O8 2.283537 0.863712 -0.057225
C9 -4.520978 0.154969 0.422456
H10 -4.928340 1.149793 0.235294
H11 -5.260299 -0.581311 0.104032
H12 -4.325667 0.036497 1.490570

[CH$_3$NCN(-ONO)CN]$^\bullet$
N1 -1.897541 -0.205417 0.066900
C2 -1.068547 0.693285 -0.055815
N3 0.283447 0.640120 0.151264
C4 1.083582 1.699174 -0.044511
N5 1.798660 2.594083 -0.206475
N6 1.261816 -1.470289 -0.495609
O7 1.711125 -2.427360 -0.066271
O8 0.902689 -0.493938 0.692893
C9 -3.334574 -0.205641 -0.100770
H10 -3.703427 0.777882 -0.404032
H11 -3.608852 -0.944598 -0.856391
H12 -3.805691 -0.493284 0.841464

CH$_3$NC(O)NCN
N1 -2.766678 -0.357322 0.216522
C2 -1.661444 -0.220295 -0.098035
N3 -0.407959 -0.087597 -0.568787
C4 0.530102 0.798613 0.025147
N5 0.739439 -0.461104 0.495254
O6 0.870549 1.927810 0.038625
C7 1.785853 -1.323737 -0.060221
H8 1.490817 -2.362295 0.079913
H9 1.976293 -1.118066 -1.116524
H10 2.687821 -1.127450 0.525340

CH$_3$NCNCNO
N1 -2.215128 -0.186173 -0.390784
C2 -1.073308 -0.324553 -0.057677
N3 0.075300 -0.669099 0.249272

C4 1.243568 -0.085573 0.000762
N5 2.396011 0.086331 0.012639
O6 3.576074 0.379741 -0.049806
C7 -3.388106 0.479264 0.141984
H8 -4.187491 -0.255027 0.250777
H9 -3.188962 0.947288 1.108739
H10 -3.718349 1.237578 -0.569370

$CH_3NCNC(O)N$
N1 -1.887977 -0.103890 -0.331132
C2 -0.752206 -0.359887 -0.120762
N3 0.414947 -0.783482 0.002388
C4 1.520750 -0.002648 0.011844
N5 1.877476 1.213128 -0.078018
O6 2.752424 -0.358625 0.145631
C7 -3.163074 0.274707 0.216750
H8 -3.438536 1.258541 -0.165253
H9 -3.915754 -0.444966 -0.107190
H10 -3.129040 0.302106 1.307735

$CH_3N(O)CNCN$
N1 -3.371029 0.111742 -0.302177
C2 -2.263600 0.028258 0.024124
N3 -1.039156 -0.076064 0.554331
C4 0.024286 -0.020756 -0.086681
N5 1.315186 -0.134989 -0.007045
O6 1.910114 -1.258090 -0.106884
C7 2.135712 1.099391 -0.052056
H8 2.637299 1.142378 -1.018035
H9 1.500646 1.973334 0.096001
H10 2.867751 1.002826 0.749020

$CH_3NCN(O)CN$
N1 1.640640 -0.103836 -0.474110
C2 0.517084 0.080865 -0.103537
N3 -0.721005 0.438772 -0.028405
C4 -1.673031 -0.548576 0.023673
N5 -2.513467 -1.339705 0.053961
O6 -1.084714 1.706369 0.105106
C7 2.868815 -0.400343 0.256654
H8 2.698638 -0.498361 1.329936
H9 3.287655 -1.321101 -0.149543
H10 3.571028 0.410225 0.057898

FS4.TS1
N1 -4.000525 -0.096050 -0.042403
C2 -2.840330 -0.052705 0.011116
N3 -1.535159 -0.124974 0.087343
C4 -0.590782 0.690307 0.001145
N5 0.690265 0.683944 -0.043992
N6 1.541378 -0.773277 -0.006890
O7 2.731705 -0.628905 0.017801
O8 0.858287 -1.749042 -0.022746
C9 1.594007 1.833865 -0.001711
H10 2.298389 1.782659 -0.831215
H11 0.988579 2.733116 -0.090942
H12 2.144020 1.851493 0.940019

FS4.TS2
N1 1.215993 -1.333951 0.047120
C2 0.207668 -0.684238 -0.190085
N3 -1.012940 -0.903438 -0.663502
C4 -2.119362 -0.588149 -0.088303
N5 -3.196968 -0.384726 0.341879
N6 0.320024 1.135710 -0.058253
O7 -0.526010 1.683627 0.598052
O8 1.290564 1.598574 -0.605552
C9 2.555740 -0.938990 0.422614
H10 2.913649 -1.634082 1.182442
H11 3.200835 -1.035404 -0.454259
H12 2.622048 0.084971 0.795760

FS4.TS4
N1 2.234434 1.521305 -0.160081
C2 1.153268 0.993985 0.033971
N3 -0.111331 1.318617 0.324399
C4 -1.172450 0.749109 0.012280
N5 -2.270568 0.422461 -0.300600
N6 1.353554 -0.835605 0.023650
O7 0.300012 -1.421103 0.153949
O8 2.451824 -1.285776 -0.115514
C9 -3.283349 -0.562244 -0.002078
H10 -3.903793 -0.713421 -0.884429
H11 -2.823742 -1.507996 0.289871
H12 -3.914577 -0.196107 0.810468

FS4.TS5
N1 -3.097362 0.441980 -0.042048
C2 -2.004158 0.043451 -0.316599
N3 -0.896524 -0.299749 -0.743408
C4 0.350417 -0.181911 -0.359639
N5 1.345564 -0.856457 -0.103681
N6 2.675815 0.105190 0.151607
O7 3.636191 -0.531981 0.467342
O8 2.547623 1.289530 -0.006055
C9 -4.310317 -0.069110 0.563379
H10 -4.498155 0.472638 1.491445
H11 -5.144648 0.114317 -0.114506
H12 -4.235823 -1.138680 0.772639

FS4.TS6
N1 4.387570 1.213201 0.110659
C2 3.561617 0.435998 -0.155528
N3 2.690090 -0.456813 -0.563878
C4 1.650615 -0.826110 0.055521
N5 0.684756 -1.301321 0.562031
N6 -2.953995 0.318660 -0.047174
O7 -3.771889 -0.454776 -0.469874
O8 -3.047876 1.490213 0.206015
C9 -1.157511 -0.481119 0.253608
H10 -0.927743 -0.342604 -0.791574
H11 -1.588647 -1.412882 0.577454
H12 -0.912769 0.283283 0.971915

CH_3NO_2
N1 -0.174686 0.000014 0.010300
O2 -0.732985 1.085795 -0.002760
O3 -0.731707 -1.086467 -0.002664
C4 1.328758 0.000698 0.002992
H5 1.667194 -0.903287 0.501166
H6 1.666849 0.907821 0.495595
H7 1.633735 -0.003443 -1.043415

[$CH_3NC(-NO_2)NCN$]•
N1 1.349570 -1.234434 -0.059212
C2 0.249158 -0.584424 -0.005062
N3 -0.935753 -1.213072 0.046889
C4 -2.078845 -0.609173 0.077484
N5 -3.173067 -0.181854 0.121213
N6 0.231598 0.953715 -0.006587
O7 -0.217062 1.489260 -1.002967
O8 0.693747 1.500632 0.979270
C9 2.641569 -0.600112 -0.108766
H10 3.131805 -0.782751 0.855340
H11 3.238964 -1.120329 -0.861516
H12 2.638018 0.475717 -0.302311

[$CH_3NCNC(-NO_2)N$]•
N1 2.220584 1.487227 -0.079132
C2 1.163350 0.825121 0.041407
N3 -0.097227 1.268067 0.241038
C4 -1.175743 0.706656 -0.023350
N5 -2.281202 0.386883 -0.315093
N6 1.359379 -0.754269 0.013759
O7 0.339068 -1.415529 0.093389
O8 2.488716 -1.167786 -0.090770
C9 -3.348325 -0.507043 0.062613
H10 -3.774617 -0.194278 1.018586
H11 -4.126170 -0.476504 -0.698753
H12 -2.967925 -1.526456 0.151201

[$CH_3N(-NO_2)CNCN$]•
N1 3.956829 -0.049097 0.000072
C2 2.795684 -0.008880 0.000040
N3 1.487614 -0.089361 0.000011
C4 0.552987 0.742164 -0.000061
N5 -0.765100 0.605481 -0.000125
N6 -1.439992 -0.741779 -0.000008
O7 -2.648343 -0.682842 0.000194
O8 -0.720773 -1.702518 -0.000138
C9 -1.686046 1.750202 -0.000004
H10 -2.314472 1.729468 -0.889840
H11 -2.314022 1.729672 0.890157
H12 -1.069793 2.646114 -0.000266

[$CH_3NCNCN\text{-}NO_2$]•
N1 -3.107980 -0.294376 0.100270
C2 -1.987015 0.035028 0.294662
N3 -0.854170 0.374216 0.674778
C4 0.356216 0.061424 0.206027
N5 1.472343 0.508719 0.567851
N6 2.619083 -0.066207 -0.134715
O7 3.321297 0.741264 -0.698140
O8 2.800908 -1.259162 -0.020654
C9 -4.347678 -0.029388 -0.578360
H10 -5.147860 0.044060 0.159305
H11 -4.291097 0.899187 -1.150093
H12 -4.572735 -0.858915 -1.250121

Cartesian coordinates for the structures in Figure 5, calculated at B3LYP/6-311++G(d,p)

C_2H_4
C1 0.000000 0.664420 0.000000
H2 0.000000 1.235163 0.922758
H3 0.000000 1.235163 -0.922758
C4 0.000000 -0.664420 0.000000
H5 0.000000 -1.235163 0.922758
H6 0.000000 -1.235163 -0.922758

F5.TS1
C1 -1.098860 -0.000137 0.667802
H2 -0.998656 0.917526 1.237226
C3 -1.928166 0.000049 -0.452374
H4 -2.221279 -0.926647 -0.930176
H5 -2.221293 0.926902 -0.929860
H6 -0.998625 -0.917996 1.236903
N7 0.734156 0.000006 0.050999
O8 1.216495 -1.088245 -0.141536
O9 1.216370 1.088332 -0.141421

F5.TS2
C1 -1.583486 0.540673 0.361636
H2 -1.773314 1.482824 -0.135905
C3 -2.063222 -0.629826 -0.142145
H4 -1.930653 -1.565427 0.388198
H5 -2.535686 -0.671876 -1.116495
H6 -1.189153 0.592367 1.368167
O7 0.374243 0.494890 -0.493148
N8 1.132351 -0.240646 0.297147
O9 2.298581 -0.197196 0.005530

F5.TS3
C1 1.456860 0.521993 0.214002
H2 1.262820 1.525674 0.569692
H3 0.205110 -0.285585 0.190698
C4 2.531074 -0.120188 -0.172619
H5 3.507744 0.367900 -0.162157
H6 2.512002 -1.150720 -0.515948
N7 -1.787167 -0.299935 -0.052345
O8 -0.666936 -0.979026 0.153400
O9 -1.696202 0.882957 -0.148921

F5.TS5
C1 1.232254 -0.687725 -0.037164
H2 1.470272 -1.313379 -0.902171
C3 2.099281 0.480126 0.163328
H4 2.114577 0.978235 1.122590
H5 2.551608 0.973091 -0.685805
H6 1.060001 -1.304361 0.850923
O7 0.184883 0.227371 -0.285060
N8 -1.488333 -0.419078 0.186615
O9 -2.280801 0.378323 -0.021043

F5.TS6
C1 0.884950 0.042643 0.437136
C2 2.093912 -0.367653 -0.180508
H3 0.811643 -0.139433 1.523601
H4 2.337958 -0.016278 -1.176020
O5 0.141582 1.022849 -0.063870
N6 -1.151485 -0.299540 -0.444847
O7 -2.118124 -0.240109 0.170414
H8 2.741131 -1.091694 0.301351
H9 0.108825 -0.967678 0.072874

F5.TS7
C1 -1.098869 0.203129 0.316554
C2 -2.369318 0.055888 -0.372000
H3 -0.854114 1.239471 0.613662
H4 -2.624046 -0.887973 -0.840395
O5 -0.091952 -0.617546 0.172426
N6 1.491892 0.495991 -0.180278
O7 2.441605 -0.132413 -0.068924
H8 -3.145631 0.792749 -0.201066
H9 -1.807559 -0.170614 1.194412

C_2H_3
C1 0.706758 -0.141745 0.000000
H2 1.605783 0.456868 0.000001
C3 -0.587416 0.029265 0.000000
H4 -1.282946 -0.807508 -0.000001
H5 -1.038888 1.025520 -0.000001

O-NH-O
N1 0.000000 0.000000 0.309894
O2 0.000000 1.094283 -0.220195
O3 0.000000 -1.094283 -0.220195
H4 0.000000 0.000000 1.353866

$[CH_2CH_2\text{-}NO_2]^{\bullet}$
C1 -0.827852 -0.000408 0.664835
H2 -0.860326 0.899526 1.276527
C3 -1.832748 0.000057 -0.416062
H4 -2.156004 -0.931822 -0.860118
H5 -2.156130 0.932321 -0.859214
H6 -0.860182 -0.900957 1.275623
N7 0.607379 0.000023 0.058487
O8 1.109302 -1.086283 -0.171093
O9 1.108772 1.086643 -0.170765

[CH_2CH_2-ONO]$^\bullet$
C1 -1.111722 0.554464 0.104829
H2 -1.425125 1.447660 -0.439531
C3 -2.139682 -0.509140 0.063133
H4 -1.897177 -1.505787 0.409505
H5 -3.137861 -0.308483 -0.301759
H6 -0.856168 0.849910 1.132292
O7 0.120621 0.094924 -0.517444
N8 1.192473 0.092870 0.418741
O9 2.189059 -0.270590 -0.074988

CH_3CHO
C1 -1.168221 -0.148256 0.000006
H2 -1.705007 0.226304 0.878640
H3 -1.704764 0.225827 -0.878982
C4 0.233510 0.396743 0.000007
H5 0.308320 1.506516 -0.000006
H6 -1.163467 -1.238140 0.000279
O7 1.234148 -0.276428 -0.000001

epoxide
C1 -0.733711 -0.373217 -0.000001
H2 -1.270386 -0.590798 -0.919797
H3 -1.270376 -0.590788 0.919803
C4 0.733592 -0.373376 0.000000
H5 1.270101 -0.591184 -0.919835
H6 1.270094 -0.591189 0.919837
O7 0.000160 0.855439 0.000000

[CH_2CHO]$^\bullet$
C1 -0.110121 0.477238 -0.073451
H2 -0.174175 1.359641 0.583972
H3 -0.287260 0.886398 -1.101391
C4 1.208634 -0.206776 0.010638
H5 2.011370 0.204897 0.608789
H6 1.346917 -1.159630 -0.484124
O7 -1.185991 -0.364260 0.096204

Cartesian coordinates for the structures in Figure 6, calculated at B3LYP/6-311++G(d,p)

$BMIM^{+}DCA^{-}$

C1 -1.173803 -0.671632 -0.156318
N2 -0.076109 -1.348485 -0.508270
N3 -2.144807 -1.544444 0.135053
C4 1.234449 -0.749950 -0.859054
H5 1.594136 -1.279118 -1.744574
H6 1.061554 0.296010 -1.121169
C7 -3.507653 -1.180116 0.556430
H8 -3.708166 -1.623233 1.532145
H9 -4.221110 -1.556246 -0.177327
C10 -1.650951 -2.823490 -0.035525
C11 -0.355861 -2.700111 -0.435140
H12 0.379435 -3.448215 -0.675218
H13 -2.255570 -3.697455 0.134588
H14 -1.295845 0.401057 -0.102251
H15 -3.565433 -0.091111 0.617327
C16 2.237368 -0.835408 0.292382
H17 2.387542 -1.881345 0.588728
H18 1.820400 -0.309813 1.158054
N19 -0.942609 3.518469 0.002748
C20 -1.928743 2.708870 0.257114
C21 0.189878 2.979421 -0.371821
N22 -2.827147 1.989515 0.488900
N23 1.214294 2.523135 -0.709303
C24 3.577309 -0.196382 -0.092946
H25 3.991865 -0.717849 -0.964872
H26 3.391990 0.837416 -0.397788
C27 4.592568 -0.229895 1.052360
H28 4.805507 -1.255146 1.373093
H29 5.538047 0.226805 0.749593
H30 4.222934 0.323062 1.920875

F6.TS1

C1 -1.325361 -0.688354 -0.764196
N2 -0.530868 -1.581684 -0.196467
N3 -2.549064 -0.697302 -0.184551
C4 1.510848 -2.065735 -0.583242
H5 1.295677 -3.022660 -0.125717
H6 1.271732 -2.006775 -1.638809
C7 -3.696094 0.129099 -0.567947
H8 -4.320714 0.288892 0.310175
H9 -4.281529 -0.370711 -1.342545
C10 -2.523359 -1.655515 0.805450
C11 -1.264656 -2.192612 0.789206
H12 -0.846537 -2.954109 1.427464
H13 -3.380154 -1.855184 1.426575
H14 -1.062803 -0.012844 -1.562472
H15 -3.337912 1.097077 -0.918809
C16 2.442631 -1.195126 -0.009088
H17 3.017280 -1.642187 0.805941
H18 1.743939 -0.374085 0.772574
N19 0.243430 2.670280 0.559082
C20 -0.882378 2.763340 -0.113282
C21 0.672683 1.563870 1.023041
N22 -1.858060 2.907518 -0.734574
N23 1.134384 0.584168 1.499069
C24 3.220796 -0.222827 -0.906178
C25 4.315866 0.527610 -0.142829
H26 2.525191 0.500311 -1.348323
H27 3.673925 -0.764979 -1.744576
H28 4.844563 1.221927 -0.800656
H29 3.899118 1.101227 0.688152
H30 5.053625 -0.169255 0.267512

F6.TS2(SN2)

C1 -0.693763 -0.528168 0.543485
N2 -1.993907 -0.888429 0.442535
N3 0.084118 -1.426808 -0.033770
C4 -3.148583 -0.115087 0.920066
H5 -3.840958 -0.813408 1.396608
H6 -2.783267 0.557970 1.698764
C7 2.017308 -1.309525 -0.208765
H8 1.965863 -1.019059 -1.241308
H9 2.172192 -2.341083 0.047574
C10 -0.735967 -2.407560 -0.535177
C11 -2.033486 -2.084324 -0.246003
H12 -2.959618 -2.591394 -0.458077
H13 -0.346328 -3.267433 -1.055305
H14 -0.360334 0.372368 1.035093
H15 2.088573 -0.560001 0.558502
C16 -3.844794 0.672561 -0.193345
H17 -4.182784 -0.021150 -0.971174
H18 -3.117375 1.341749 -0.665892
N19 5.358167 0.653221 0.571677
C20 4.686355 -0.266745 0.000258
C21 5.573253 1.844106 0.047072
N22 4.082917 -1.189293 -0.432729
N23 5.801065 2.923906 -0.324768
C24 -5.035805 1.483073 0.331097
C25 -5.741905 2.278803 -0.770098
H26 -4.691222 2.169782 1.113383
H27 -5.753301 0.806977 0.811181
H28 -6.582176 2.847826 -0.365526
H29 -5.058818 2.987986 -1.246499
H30 -6.132638 1.617882 -1.549483

F6.TS3(SN2)

C1 1.750195 0.324839 -0.060124
N2 0.681774 1.047197 0.240135
N3 2.864298 1.093958 -0.055100
C4 -1.158520 -0.103799 0.328620
H5 -0.853764 -0.361354 -0.667387
H6 -0.678351 -0.579503 1.164781
C7 4.220388 0.633313 -0.341164
H8 4.868790 0.816090 0.517135
H9 4.617805 1.150388 -1.216052
C10 2.476537 2.378867 0.267455
C11 1.119697 2.333214 0.448249
H12 0.447382 3.134735 0.708630
H13 3.181981 3.190020 0.336125
H14 1.767760 -0.736766 -0.277234
H15 4.188911 -0.436418 -0.542479
C16 -2.218855 0.921280 0.564156
H17 -1.777865 1.737107 1.149221
H18 -2.971635 0.465718 1.213831
N19 -0.632070 -3.577641 0.388997
C20 0.550852 -3.367573 -0.154090
C21 -1.553858 -2.706863 0.205690
N22 1.625477 -3.177116 -0.566885
N23 -2.376242 -1.863665 0.089113
C24 -2.867997 1.455172 -0.715300
C25 -3.956565 2.493641 -0.435129
H26 -3.292518 0.609960 -1.265068
H27 -2.093669 1.893029 -1.355737
H28 -4.404201 2.854569 -1.364407
H29 -4.758997 2.069379 0.175842
H30 -3.555529 3.361379 0.098802

F6.TS4

C1 -0.448368 -0.595991 0.282303
N2 0.533195 -0.826553 -0.620766
N3 -1.456676 -1.432406 0.105081
C4 1.773590 -0.046968 -0.764105
H5 2.188710 -0.298886 -1.742063
H6 1.494137 1.009134 -0.792787
C7 -3.521335 -1.606222 1.031249
H8 -3.445307 -2.327723 0.234148
H9 -4.418971 -1.011699 1.031005
C10 -1.116511 -2.242875 -0.949867
C11 0.119752 -1.876686 -1.411904
H12 0.719609 -2.247996 -2.225655
H13 -1.769918 -3.018493 -1.318405
H14 -0.402258 0.180001 1.026448
H15 -3.125367 -1.887242 1.993249
C16 2.790922 -0.333819 0.342731
H17 3.017596 -1.406247 0.361133
H18 2.347198 -0.090523 1.314819
N19 -2.614660 2.150614 -0.319941
C20 -2.821312 1.314874 0.624354
C21 -1.392313 2.453873 -0.706391
N22 -3.060920 0.558311 1.503666
N23 -0.336666 2.750870 -1.101539
C24 4.082788 0.470639 0.156021
C25 5.108964 0.212012 1.262540
H26 3.840731 1.538711 0.121265
H27 4.524974 0.225454 -0.817137
H28 6.017581 0.797983 1.102821
H29 4.708301 0.482097 2.244275
H30 5.396019 -0.843459 1.299794

F6.TS5

C1 0.874859 -0.866309 -0.586689
N2 0.062036 -0.949218 0.451507
N3 2.002958 -1.590131 -0.387486
C4 -1.993449 0.379221 0.897872
H5 -1.719210 -0.302007 1.687477
H6 -1.993203 1.429379 1.142839
C7 3.174566 -1.621206 -1.262690
H8 2.850372 -1.489884 -2.294936
H9 3.664995 -2.590117 -1.168848
C10 1.904033 -2.156056 0.864359
C11 0.695297 -1.753788 1.369189
H12 0.257487 -1.994674 2.325570
H13 2.687643 -2.768985 1.276955
H14 0.697237 -0.284894 -1.476633
H15 3.857046 -0.813407 -0.992224
C16 -2.824096 -0.087961 -0.213692
H17 -2.598462 -1.123504 -0.469306
H18 -2.668689 0.548694 -1.085485
N19 1.619885 2.573129 0.463385
C20 2.728716 1.971999 0.096803
C21 0.473054 2.244475 -0.005197
N22 3.753113 1.480327 -0.167849
N23 -0.616227 1.998397 -0.392601
C24 -4.319366 0.031034 0.233122
C25 -5.257190 -0.466070 -0.872518
H26 -4.544632 1.074248 0.471612
H27 -4.483880 -0.550297 1.145798
H28 -6.299406 -0.373969 -0.556428
H29 -5.129314 0.116315 -1.788528
H30 -5.068881 -1.516455 -1.109898

1-C_4H_8

C1 1.860971 0.019112 -0.278585
H2 2.735925 -0.618820 -0.221924
C3 0.723162 -0.297459 0.336126

H4 0.674176 -1.225740 0.905227
C5 -0.538730 0.518307 0.308599
H6 -0.793103 0.816329 1.334024
H7 -0.364678 1.442575 -0.251862
C8 -1.730082 -0.244327 -0.293694
H9 -1.930103 -1.166585 0.260301
H10 -2.638338 0.363876 -0.266657
H11 -1.533993 -0.517127 -1.334057
H12 1.958186 0.931701 -0.859722

[BMIM$^+$ – H$_{C2}$$^+$]
N1 2.506676 -0.276799 -0.113142
N2 0.524199 0.241231 0.463248
C3 -0.851128 0.139254 0.944389
H4 -0.876446 -0.718471 1.617728
H5 -1.081413 1.034315 1.532208
C6 -1.871656 -0.037581 -0.183971
H7 -1.602057 -0.931536 -0.756690
H8 -1.803041 0.810525 -0.876089
C9 3.732044 -1.030475 -0.327980
H10 4.560222 -0.595675 0.238242
H11 3.556749 -2.047593 0.015943
H12 3.995272 -1.047721 -1.389011
C13 1.388165 -0.817910 0.455276
C14 1.082528 1.392380 -0.081816
C15 2.345715 1.063985 -0.445872
H16 0.553710 2.328266 -0.157885
H17 3.123447 1.660485 -0.893809
C18 -3.307491 -0.161651 0.336766
H19 -3.368044 -1.009103 1.030003
H20 -3.561886 0.730201 0.922928
C21 -4.336369 -0.345513 -0.782562
H22 -5.349745 -0.432940 -0.381473
H23 -4.324518 0.502502 -1.474474
H24 -4.129231 -1.249207 -1.363731

[BMIM$^+$ – H$^{\alpha}$$_{BU}$$^+$]
C1 -1.023953 -0.605846 0.035212
N2 -0.441810 0.634318 0.018346
N3 -2.405737 -0.440657 0.101594
C4 0.878522 0.930448 0.101246
H5 1.146370 1.954777 -0.109805
C6 -3.349221 -1.524625 -0.074516
H7 -3.331217 -1.911472 -1.100292
H8 -4.352346 -1.165510 0.156311
C9 -2.674450 0.889941 -0.019612
C10 -1.494240 1.568367 -0.072693
H11 -1.293792 2.624086 -0.106012
H12 -3.682250 1.266707 -0.077618
H13 -0.518890 -1.508011 0.326059
H14 -3.110042 -2.341072 0.611407
C15 1.855620 -0.187062 0.039174
H16 1.663456 -0.827177 -0.849037
H17 1.732129 -0.870978 0.900527
C18 3.312210 0.290722 0.004166
H19 3.448505 0.955265 -0.856995
H20 3.509190 0.897014 0.895275
C21 4.323386 -0.856226 -0.072067
H22 4.170173 -1.460278 -0.971975
H23 5.350600 -0.481182 -0.095263
H24 4.233696 -1.522123 0.792375

[BMIM$^+$ – H$^{\gamma}$$_{BU}$$^+$]
C1 -1.115402 -0.354038 0.764578
N2 -0.490446 0.854104 0.552079
N3 -2.278364 -0.359726 0.019044
C4 0.956995 0.936166 0.765873
H5 1.307841 1.925348 0.473230
C6 -3.116780 -1.529306 -0.156908
H7 -4.073516 -1.226221 -0.582427
H8 -3.301536 -1.997103 0.812210
C9 -2.261454 0.752612 -0.803425
C10 -1.168634 1.490326 -0.488302
H11 -0.833165 2.433587 -0.884589
H12 -3.040556 0.938378 -1.523752
H13 -1.013450 -0.922331 1.677818
H14 -2.640908 -2.263992 -0.817849
C15 1.663872 -0.216643 -0.054610
H16 1.553104 0.004018 -1.123898
C17 3.035899 -0.427770 0.295394
H18 3.268631 -0.685946 1.326896
C19 4.133439 -0.575143 -0.711990
H20 3.884016 -0.068120 -1.651818
H21 5.083067 -0.152388 -0.358995
H22 4.355128 -1.626591 -0.977991
H23 1.160719 0.786908 1.827104
H24 0.904675 -1.063416 0.142545

[BMIM$^+$ – H$^{\delta}$$_{BU}$$^+$]
C1 -1.256658 -0.629413 0.544515
N2 -0.430605 0.453262 0.445867
N3 -2.418126 -0.334716 -0.125886
C4 0.969162 0.490240 0.832165
H5 1.207937 1.521346 1.106951
C6 -3.581976 -1.199211 -0.177713
H7 -4.297039 -0.789158 -0.889312
H8 -4.056357 -1.275278 0.807295
C9 -2.340442 0.968036 -0.568363
C10 -1.116794 1.453258 -0.229929
H11 -0.670862 2.413218 -0.423435

H12 -3.157346 1.444385 -1.083029
H13 -0.970441 -1.605061 0.890890
H14 -3.292152 -2.198322 -0.511175
C15 1.933039 -0.013319 -0.257023
H16 1.913028 0.656975 -1.120578
C17 3.408776 -0.117654 0.279092
H18 3.700081 0.892689 0.606635
C19 4.366958 -0.664963 -0.694773
H20 4.824660 -0.017115 -1.433159
H21 4.399276 -1.732671 -0.880425
H22 1.078548 -0.123010 1.734003
H23 1.611299 -1.001394 -0.602798
H24 3.358088 -0.738277 1.190431

BIM
C1 -1.864313 -1.052737 -0.240546
N2 -1.014005 -0.154324 0.341543
N3 -3.005490 -0.504367 -0.593804
C4 0.347387 -0.412446 0.801598
H5 0.470939 0.044681 1.788097
H6 0.442555 -1.493003 0.937088
C7 -2.897652 0.816872 -0.229878
C8 -1.676402 1.057091 0.347673
H9 -1.232165 1.949329 0.757457
H10 -3.702187 1.516243 -0.396911
H11 -1.594345 -2.090652 -0.370692
C12 1.423859 0.097563 -0.163062
H13 1.303373 1.178121 -0.298346
H14 1.262839 -0.357996 -1.146484
C15 2.842799 -0.207128 0.329180
H16 2.988650 0.240279 1.319976
H17 2.955993 -1.289708 0.464220
C18 3.927542 0.302444 -0.624124
H19 3.864126 1.387342 -0.752068
H20 4.927122 0.070097 -0.247716
H21 3.830244 -0.153846 -1.613837

C_4H_9DCA
C1 0.849163 -1.088590 0.190003
H2 0.757055 -1.128347 1.279824
H3 1.283108 -2.033045 -0.146376
N4 -2.805725 -0.558341 0.099981
C5 -3.539212 0.542033 0.071544
C6 -1.591640 -0.698801 -0.114112
N7 -4.256982 1.452685 0.073264
N8 -0.475524 -0.994169 -0.404992
C9 1.739862 0.080320 -0.239053
H10 1.282152 1.018844 0.091984
H11 1.775919 0.114438 -1.332747
C12 3.158204 -0.038475 0.330352
C13 4.062114 1.124246 -0.089194
H14 3.603346 -0.984734 0.000760
H15 3.109736 -0.086319 1.424723
H16 5.065592 1.014818 0.329523
H17 4.159266 1.176774 -1.177677
H18 3.660501 2.081957 0.254969

BIM^+
C1 -1.667914 -1.005119 0.384369
N2 -1.009520 0.236817 0.322266
N3 -2.882427 -0.964850 -0.151935
C4 0.375606 0.498796 0.791093
H5 0.470374 1.579788 0.899513
H6 0.460475 0.052849 1.784594
C7 -3.043597 0.286129 -0.574112
C8 -1.848448 1.068484 -0.276323
H9 -1.624654 2.108365 -0.468939
H10 -3.943510 0.638343 -1.060375
H11 -1.205740 -1.872638 0.836102
C12 1.422619 -0.068884 -0.173231
H13 1.279694 0.379837 -1.162517
H14 1.273644 -1.148716 -0.288403
C15 2.849488 0.202425 0.326764
H16 2.990461 1.282117 0.449602
H17 2.978069 -0.243232 1.319418
C18 3.911958 -0.350058 -0.627330
H19 3.832276 0.103468 -1.619002
H20 4.913642 -0.141033 -0.247173
H21 3.820621 -1.433552 -0.742518

C_4H_9
C1 2.005163 -0.096572 0.000077
H2 2.488553 -0.384286 -0.926322
H3 2.487974 -0.385178 0.926502
C4 0.644425 0.509073 -0.000002
H5 0.520100 1.152301 -0.880099
H6 0.519932 1.152124 0.880204
C7 -0.504372 -0.533155 -0.000165
H8 -0.396520 -1.180797 -0.876988
H9 -0.396429 -1.181175 0.876375
C10 -1.891014 0.116124 0.000073
H11 -2.033629 0.746715 -0.883143
H12 -2.681861 -0.639154 0.000175
H13 -2.033328 0.746635 0.883398

$BMIM^+$
N1 -2.545604 -0.193364 0.159009
N2 -0.491015 0.149318 -0.473288
C3 0.897435 -0.099246 -0.932637
H4 0.906753 -1.095475 -1.377904

H5 1.101571 0.618920 -1.729214
C6 1.921499 0.011835 0.198605
H7 1.664862 -0.701127 0.989978
H8 1.869907 1.011663 0.643368
C9 -3.813094 -0.870211 0.472438
H10 -4.605181 -0.468601 -0.158763
H11 -3.702126 -1.935324 0.279704
H12 -4.057056 -0.715623 1.522982
C13 -1.433113 -0.780994 -0.295437
H14 -1.317405 -1.834247 -0.490708
C15 -1.019178 1.375303 -0.117433
C16 -2.304442 1.162160 0.276576
H17 -0.447595 2.285618 -0.178110
H18 -3.057778 1.850580 0.620418
C19 3.347318 -0.255232 -0.303661
H20 3.394135 -1.256100 -0.747884
H21 3.587545 0.450801 -1.106778
C22 4.391740 -0.139155 0.809782
H23 5.393209 -0.337180 0.423001
H24 4.397454 0.863174 1.247093
H25 4.199050 -0.855521 1.613369

Cartesian coordinates for the structures in Figure 7, calculated at B3LYP/6-311++G(d,p)

$C_2H_5CH=CH_2$

C1	-1.860824	-0.019017	-0.278767
H2	-2.735841	0.618821	-0.221921
H3	-1.957820	-0.931235	-0.860536
C4	-0.723195	0.297252	0.336442
H5	-0.674396	1.225170	0.906148
C6	0.538777	-0.518385	0.308627
H7	0.793344	-0.816516	1.333970
H8	0.364711	-1.442576	-0.251950
C9	1.729937	0.244468	-0.293786
H10	1.929789	1.166823	0.260110
H11	2.638330	-0.363535	-0.266761
H12	1.533717	0.517141	-1.334157

F7.TS1[1]

C1	0.290783	-1.119916	-0.010014
H2	0.379933	-1.319482	1.053872
C3	-0.859053	-0.491027	-0.482344
H4	-1.049350	-0.500177	-1.553198
H5	0.805234	-1.831628	-0.645555
N6	1.778473	0.155847	-0.002244
O7	2.843702	-0.347546	0.264219
O8	1.534405	1.313408	-0.237714
C9	-1.770953	0.335780	0.360021
H10	-1.521451	1.394744	0.191855
H11	-1.575874	0.144881	1.420492
C12	-3.259924	0.122260	0.041521
H13	-3.882778	0.782024	0.650157
H14	-3.472100	0.338204	-1.009435
H15	-3.562897	-0.908980	0.240383

F7.TS2[1]

C1	-0.149214	1.312549	-0.006182
H2	-0.232621	1.701604	-1.013638
C3	-0.992695	0.337564	0.441811
H4	-0.920243	0.033704	1.484338
H5	0.479632	1.862156	0.681265
O6	1.488888	0.064239	-0.645094
N7	2.280287	-0.098467	0.387061
O8	3.309616	-0.669725	0.124932
C9	-1.958390	-0.414673	-0.408935
H10	-1.969456	-0.000450	-1.420915
H11	-1.593534	-1.448040	-0.496849
C12	-3.380926	-0.444240	0.179608
H13	-4.040941	-1.044600	-0.450439
H14	-3.385258	-0.880940	1.182045
H15	-3.800272	0.562526	0.248259

F7.TS3[1]

C1	-0.159753	1.086129	-0.001812
H2	-0.300894	2.144741	0.191323
H3	1.294616	0.851265	0.140321
C4	-0.978555	0.105374	-0.306075
H5	-0.583858	-0.898022	-0.454776
N6	2.907023	-0.371754	0.080336
O7	2.407882	0.838818	0.282478
O8	2.139241	-1.235879	-0.208668
C9	-2.479130	0.262925	-0.459363
H10	-2.741104	-0.004519	-1.490243
H11	-2.759552	1.310762	-0.322360
C12	-3.258805	-0.630146	0.516148
H13	-4.335064	-0.522946	0.357085
H14	-3.002649	-1.684432	0.379234
H15	-3.040188	-0.363771	1.553200

F7.TS5[1]

C1	0.096841	1.013733	-0.185922
H2	-0.171982	1.391025	-1.178734
C3	-0.929029	0.190080	0.469515
H4	-0.827779	0.038366	1.539028
H5	0.524516	1.817512	0.423904
O6	0.927270	-0.127013	-0.237716
N7	2.677535	0.288208	0.078659
O8	3.312301	-0.669552	0.080841
C9	-1.971894	-0.572747	-0.266828
H10	-1.887386	-1.640443	-0.031565
H11	-1.814490	-0.469068	-1.344030
C12	-3.397220	-0.101366	0.102452
H13	-4.140985	-0.695764	-0.434844
H14	-3.585637	-0.213937	1.173412
H15	-3.547761	0.949168	-0.158091

F7.TS6[1]

C1	0.271130	0.260020	-0.330332
C2	-0.919612	0.137183	0.435755
H3	0.191136	-0.065449	-1.384288
H4	-0.949310	0.668852	1.384192
O5	1.204321	1.157740	-0.039438
N6	2.320420	-0.319635	0.431861
O7	3.219120	-0.506566	-0.260971
H8	0.910475	-0.806019	0.106251
C9	-2.081987	-0.704675	0.042525
H10	-1.853169	-1.256514	-0.874864
H11	-2.272925	-1.449629	0.826492
C12	-3.366664	0.129059	-0.157184
H13	-4.203883	-0.523530	-0.416812
H14	-3.630106	0.671551	0.754307
H15	-3.239891	0.859271	-0.959615

F7.TS7[1]

C1 -0.152046 -0.155526 -0.327968
C2 1.096461 -0.217439 0.421701
H3 -0.299663 0.808250 -0.858268
H4 1.203636 -1.039888 1.126692
O5 -1.235669 -0.812953 -0.002516
N6 -2.680196 0.592450 0.051515
O7 -3.714480 0.095542 0.033349
H8 0.476230 -0.776981 -1.105438
C9 2.270184 0.643039 0.125203
H10 2.408989 1.296762 1.001515
H11 2.040271 1.312993 -0.710280
C12 3.582815 -0.117177 -0.131019
H13 4.411193 0.581359 -0.271160
H14 3.831054 -0.770116 0.709830
H15 3.506370 -0.737627 -1.027659

$[C_2H_5CHCH]^\bullet$

C1 -1.927884 -0.056650 -0.293059
H2 -2.341491 0.734399 -0.902417
C3 -0.804415 -0.341313 0.314421
H4 -0.725727 -1.277792 0.871658
C5 0.448273 0.519187 0.312332
H6 0.673289 0.800436 1.348288
H7 0.254711 1.447495 -0.231947
C8 1.657309 -0.208318 -0.291944
H9 2.551225 0.419759 -0.246099
H10 1.872136 -1.134974 0.248370
H11 1.476158 -0.466756 -1.338349

$[C_2H_5CHCH_2NO_2]^\bullet$

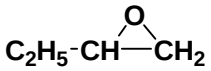
C1 0.567861 -0.736191 0.770609
H2 0.517719 -0.255983 1.748843
C3 -0.732174 -0.734760 0.064151
H4 -0.881650 -1.479927 -0.710886
H5 1.020418 -1.723526 0.833978
N6 1.602788 0.116290 -0.016977
O7 2.392049 -0.479283 -0.730941
O8 1.519699 1.328759 0.101259
C9 -1.708677 0.380538 0.207982
H10 -1.293656 1.286163 -0.265793
H11 -1.803940 0.647645 1.269572
C12 -3.086203 0.076383 -0.390301
H13 -3.758261 0.929647 -0.273996
H14 -3.010695 -0.144260 -1.458865
H15 -3.548280 -0.785414 0.098797

$[C_2H_5CHCH_2(\text{-}ONO)]^\bullet$

C1 0.244851 0.993340 0.035310
H2 0.041231 1.680811 -0.788628
C3 -0.970229 0.260343 0.463120
H4 -0.953574 -0.214084 1.440805
H5 0.712124 1.540067 0.858454
O6 1.260549 0.063473 -0.486910
N7 2.390790 0.018423 0.364140
O8 3.193862 -0.739518 -0.029982
C9 -2.065237 -0.088912 -0.486045
H10 -2.227133 0.745214 -1.181788
H11 -1.736368 -0.928276 -1.123130
C12 -3.383576 -0.470594 0.197829
H13 -4.143720 -0.739465 -0.539681
H14 -3.246839 -1.328244 0.862767
H15 -3.771396 0.358311 0.796085

$C_2H_5CH_2CHO$

C1 -1.462556 0.217900 -0.286979
C2 -0.119085 -0.465192 -0.252536
H3 -1.524967 1.093450 -0.972552
H4 -0.172145 -1.314481 0.433303
O5 -2.425073 -0.108987 0.363084
H6 0.076203 -0.853622 -1.262128
C7 1.012043 0.504469 0.137433
H8 0.824575 0.883936 1.147582
H9 0.991235 1.374812 -0.528786
C10 2.394857 -0.149973 0.081479
H11 3.175942 0.557842 0.370777
H12 2.454677 -1.007184 0.758390
H13 2.623503 -0.506077 -0.927639



C1 1.362763 0.789836 -0.174350
H2 1.211973 1.122472 -1.199126
C3 0.368073 -0.094427 0.447404
H4 0.295058 -0.072603 1.535425
H5 1.977028 1.440896 0.442882
O6 1.619786 -0.613717 -0.024683
C7 -0.878973 -0.545304 -0.273279
H8 -1.083582 -1.585934 0.003001
H9 -0.683017 -0.539962 -1.350046
C10 -2.093732 0.330176 0.056895
H11 -2.986894 -0.032773 -0.457283
H12 -2.306873 0.327879 1.130197
H13 -1.930768 1.368073 -0.247606

$[C_2H_5CHCHO]^\bullet$

C1 -1.378349 0.283907 -0.202825
C2 -0.165147 -0.165198 0.395031
H3 -1.315112 1.213985 -0.801646
H4 -0.219710 -1.081810 0.978013

O5 -2.459919 -0.301012 -0.083940
C6 1.139658 0.535886 0.263419
H7 1.024238 1.427975 -0.360595
H8 1.451610 0.888394 1.257605
C9 2.256857 -0.365662 -0.301209
H10 3.202463 0.180141 -0.342649
H11 2.403630 -1.249322 0.325253
H12 2.014126 -0.704867 -1.310955

F7.TS1[2]
C1 -0.178039 2.072233 0.106550
H2 0.042855 2.411879 1.112329
C3 0.342454 0.865466 -0.374867
H4 0.235178 0.689056 -1.442675
H5 -0.890759 2.644107 -0.474304
N6 -1.082875 -0.426647 0.032377
O7 -1.893655 -0.582171 -0.849889
O8 -1.089652 -0.893922 1.146298
C9 1.542628 0.225763 0.285808
H10 1.328848 0.102059 1.352253
H11 2.368528 0.943955 0.217789
C12 1.974480 -1.105542 -0.333135
H13 2.876349 -1.480701 0.155837
H14 1.200192 -1.868748 -0.226599
H15 2.196252 -0.993848 -1.398676

F7.TS2[2]
C1 0.477862 1.709509 0.105493
H2 0.827142 2.061079 1.070447
C3 0.706959 0.420946 -0.300127
H4 0.408985 0.143771 -1.307076
H5 -0.121054 2.386982 -0.490264
O6 -1.129860 -0.321502 0.480470
N7 -2.109005 0.014028 -0.340838
O8 -3.142169 -0.550112 -0.088436
C9 1.628523 -0.526063 0.406388
H10 1.755771 -0.210188 1.445634
H11 1.164006 -1.515689 0.424576
C12 2.997597 -0.614972 -0.293242
H13 3.636519 -1.337095 0.220347
H14 2.892702 -0.941211 -1.331758
H15 3.509549 0.350550 -0.293377

F7.TS3[2]
C1 -0.431582 1.969941 0.134847
H2 -1.212991 2.732360 0.159679
H3 0.577925 2.288592 0.364287
C4 -0.732784 0.725741 -0.166680
H5 0.361813 -0.212698 -0.188330
N6 2.345202 -0.741452 -0.025084
O7 2.547494 0.402952 0.239891
O8 1.096670 -1.100141 -0.269563
C9 -1.975358 -0.012146 -0.515658
H10 -1.853231 -0.487857 -1.495238
H11 -2.771753 0.738452 -0.632465
C12 -2.390243 -1.065859 0.523478
H13 -3.316159 -1.556852 0.214745
H14 -1.621274 -1.833832 0.633445
H15 -2.554250 -0.606553 1.500917

F7.TS4[2]
C1 0.876043 2.073549 -0.127149
H2 1.780685 2.687955 -0.138919
H3 -0.054856 2.582450 -0.360748
C4 0.935107 0.795086 0.159346
H5 -0.629698 0.160425 0.084178
N6 -1.681249 -0.207912 0.031254
O7 -1.840797 -1.399063 0.222001
O8 -2.530419 0.628525 -0.208804
C9 1.937515 -0.231625 0.514190
H10 2.908187 0.280369 0.614126
H11 1.704248 -0.640081 1.504147
C12 2.049415 -1.377976 -0.505125
H13 2.826968 -2.080535 -0.196891
H14 1.109284 -1.928741 -0.581743
H15 2.305160 -0.996356 -1.496069

F7.TS5[2]
C1 -0.749498 2.040711 0.038827
H2 -0.198369 2.761618 0.626429
C3 -0.689132 0.610044 0.377839
H4 -0.510480 0.415221 1.443060
H5 -1.165316 2.351187 -0.910899
O6 0.526331 0.576855 -0.353837
N7 1.797169 -0.500386 0.386969
O8 2.766829 -0.432904 -0.220599
C9 -1.782159 -0.295324 -0.173959
H10 -2.719016 -0.037447 0.334861
H11 -1.919008 -0.062066 -1.235380
C12 -1.479909 -1.784638 0.004156
H13 -2.284517 -2.398259 -0.408679
H14 -0.553289 -2.059422 -0.505501
H15 -1.371276 -2.044496 1.061645

F7.TS6[2]
C1 -0.481882 -0.752572 0.255528
C2 -0.094085 -1.804893 -0.556980
H3 0.751049 -2.425314 -0.282076
O4 0.353039 -0.249664 1.111444
N5 1.864890 0.027940 -0.047923

O6 2.107462 1.154364 -0.292034
H7 1.281646 -0.594774 -0.771070
C8 -1.812014 -0.044752 0.087338
H9 -2.415817 -0.581787 -0.649309
H10 -2.335294 -0.126070 1.046998
H11 -0.724170 -2.143648 -1.369009
C12 -1.673645 1.436260 -0.291381
H13 -2.655628 1.913849 -0.329925
H14 -1.063917 1.967908 0.441039
H15 -1.206338 1.552393 -1.273496

F7.TS7[2]
C1 -1.193527 1.830292 0.341715
H2 -0.696184 2.753059 0.067368
C3 -0.646916 0.582285 -0.103817
H4 -0.010368 0.616976 0.971845
H5 -1.989763 1.856059 1.077165
O6 0.309413 0.573788 -1.027241
N7 1.684221 0.470648 0.316078
O8 2.380184 -0.427671 0.193725
C9 -1.528283 -0.678015 0.000432
H10 -2.213142 -0.576420 0.848884
H11 -2.143280 -0.685490 -0.905983
C12 -0.737419 -1.981369 0.099131
H13 -1.410880 -2.841107 0.062799
H14 -0.030213 -2.066038 -0.727589
H15 -0.175614 -2.039672 1.036321

$[C_2H_5CCH_2]^\bullet$
C1 1.939095 -0.180551 0.121656
H2 2.230014 0.267719 1.077699
H3 2.710253 -0.746766 -0.393888
C4 0.731100 -0.033733 -0.361942
C5 -0.557248 0.599512 -0.037414
H6 -0.796386 1.343723 -0.806403
H7 -0.445334 1.159707 0.906641
C8 -1.721780 -0.398280 0.087622
H9 -2.650275 0.125993 0.327457
H10 -1.868876 -0.943639 -0.847442
H11 -1.526399 -1.128422 0.876399

$[C_2H_5CH(\text{-}NO_2)CH_2]^\bullet$
C1 -0.616991 1.964627 -0.049141
H2 -0.512983 2.356230 0.955030
C3 0.041139 0.691028 -0.415993
H4 0.069037 0.551179 -1.496583
H5 -1.307614 2.444075 -0.730235
N6 -0.899586 -0.485462 0.041297
O7 -1.517093 -1.069078 -0.833080
O8 -0.965125 -0.719192 1.235960
C9 1.418257 0.486086 0.218148
H10 1.310568 0.543814 1.304564
H11 2.029220 1.341441 -0.087937
C12 2.106911 -0.819943 -0.186080
H13 3.102338 -0.877486 0.260040
H14 1.544918 -1.693935 0.152806
H15 2.223467 -0.891717 -1.271410

$[C_2H_5CH(\text{-}ONO)CH_2]^\bullet$
C1 0.560912 -2.093778 0.041187
H2 0.000966 -2.552471 -0.762524
C3 0.496536 -0.624988 0.258865
H4 0.348115 -0.402908 1.325005
H5 1.246618 -2.695544 0.624552
O6 -0.647665 -0.079831 -0.451791
N7 -1.719392 0.205545 0.435973
O8 -2.650050 0.621839 -0.140308
C9 1.747529 0.131074 -0.230646
H10 2.617676 -0.346539 0.231589
H11 1.840933 -0.023436 -1.309919
C12 1.726389 1.624822 0.100881
H13 2.640965 2.109086 -0.250192
H14 0.879631 2.123211 -0.375505
H15 1.654367 1.790945 1.180258

$C_2H_5C(O)CH_3$
C1 1.885414 -0.509964 0.033043
C2 0.529458 0.170133 -0.019059
H3 1.948920 -1.327252 -0.690884
C4 -0.685772 -0.747092 -0.057753
H5 -0.623370 -1.321292 -0.991990
H6 -0.571932 -1.492397 0.739766
C7 -2.023636 -0.020883 0.046957
H8 -2.851693 -0.731820 -0.007053
H9 -2.101022 0.525446 0.989340
H10 -2.138381 0.705574 -0.759400
O11 0.424802 1.377441 -0.021671
H12 2.674864 0.217598 -0.151798
H13 2.031419 -0.948548 1.026257

$[C_2H_5C(O)CH_2]^\bullet$
C1 1.872579 -0.559759 0.000183
C2 0.595783 0.107005 -0.000056
H3 1.955720 -1.640686 0.000246
C4 -0.661542 -0.758207 -0.000270
H5 -0.612434 -1.422006 -0.872817
H6 -0.612245 -1.422823 0.871641
C7 -1.960618 0.041876 0.000223
H8 -2.823078 -0.629098 0.000085
H9 -2.024523 0.686042 0.879431

H10 -2.024781 0.686738 -0.878453
O11 0.536299 1.339445 -0.000113
H12 2.773739 0.040788 0.000290

Cartesian coordinates for the structures in Figure 8, calculated at B3LYP/6-311++G(d,p)

AMIM$^+$DCA$^-$

C1 0.015870 -0.682689 -0.339088
N2 1.329213 -0.428373 -0.302794
N3 -0.176994 -1.983194 -0.093507
C4 1.958054 0.899525 -0.539182
H5 2.514109 0.838890 -1.477199
H6 1.130989 1.610832 -0.654208
C7 -1.477215 -2.675905 -0.064555
H8 -1.470117 -3.383474 0.763713
H9 -1.622768 -3.208016 -1.005587
C10 1.055586 -2.577162 0.104725
C11 1.997869 -1.604542 -0.023471
H12 3.068695 -1.639746 0.074281
H13 1.151834 -3.626280 0.324501
H14 -0.743394 0.061050 -0.527165
H15 -2.278330 -1.947011 0.089711
C16 2.851495 1.290705 0.600472
H17 2.365664 1.399804 1.566824
N18 -3.099800 1.977778 0.189409
C19 -3.400842 0.713981 0.344410
C20 -1.889553 2.244138 -0.210368
N21 -3.690319 -0.411447 0.490166
N22 -0.801277 2.497150 -0.569372
C23 4.148400 1.554052 0.466135
H24 4.652071 1.471940 -0.492525
H25 4.747508 1.885990 1.305873

F8.TS1

C1 0.250416 -1.187741 0.745977
N2 -0.474272 -1.371714 -0.343847
N3 1.566475 -1.356941 0.480336
C4 -2.598532 -1.269250 -0.459747
H5 -2.498308 -1.330517 -1.538857
H6 -2.613687 -2.224480 0.053111
C7 2.678236 -1.163723 1.411892
H8 3.251063 -0.284581 1.112338
H9 3.310486 -2.052676 1.418600
C10 1.677355 -1.659999 -0.859028
C11 0.402571 -1.670812 -1.357841
H12 0.072604 -1.861024 -2.366439
H13 2.633516 -1.811134 -1.330490
H14 -0.130743 -0.920661 1.718913
H15 2.273211 -1.009178 2.411242
C16 -3.057703 -0.117250 0.129460
H17 -2.099916 0.897063 0.237248
N18 0.733491 2.494897 -0.690684
C19 1.940143 2.092015 -0.355348
C20 -0.325134 2.134606 -0.095906
N21 3.034480 1.766499 -0.126654
N22 -1.361798 1.891881 0.423490
C23 -4.189996 0.398741 0.596104
H24 -5.154941 -0.091326 0.482904
H25 -4.196056 1.376636 1.069572

F8.TS2(S_N2)

C1 -1.220836 0.115221 0.471966
N2 -2.559453 -0.028021 0.331402
N3 -0.592003 -0.960599 0.034842
C4 -3.587074 0.948617 0.732241
H5 -4.169179 0.528912 1.556225
H6 -3.049413 1.819827 1.115875
C7 1.332167 -1.198609 -0.050709
H8 1.363831 -1.069576 -1.116396
H9 1.298833 -2.188275 0.365491
C10 -1.552120 -1.837570 -0.408629
C11 -2.783391 -1.269907 -0.229519
H12 -3.775335 -1.623696 -0.452759
H13 -1.298463 -2.800440 -0.821323
H14 -0.754444 0.995600 0.885722
H15 1.516089 -0.360786 0.597365
C16 -4.481800 1.339761 -0.410609
H17 -3.984278 1.746658 -1.287396
N18 4.948366 0.266285 0.598808
C19 4.140366 -0.606168 0.140260
C20 5.386402 1.301100 -0.091890
N21 3.395318 -1.470221 -0.177590
N22 5.812994 2.250598 -0.613980
C23 -5.806618 1.233820 -0.376021
H24 -6.326003 0.831944 0.488750
H25 -6.420771 1.555953 -1.208463

F8.TS3(S_N2)

C1 -1.460323 -0.397819 0.013958
N2 -1.003753 0.837693 -0.118206
N3 -2.815099 -0.407700 0.019434
C4 1.214721 1.045694 -0.065659
H5 1.100777 0.748624 0.960342
H6 1.124833 0.310807 -0.841583
C7 -3.659909 -1.591785 0.146433
H8 -4.280749 -1.710423 -0.743180
H9 -4.297771 -1.507265 1.027770
C10 -3.236788 0.899979 -0.117506
C11 -2.100195 1.660194 -0.200682
H12 -2.005605 2.728366 -0.311906
H13 -4.280679 1.164710 -0.143370
H14 -0.863564 -1.296896 0.112459
H15 -3.019555 -2.466132 0.253124

C16 1.463662 2.429727 -0.402341
H17 1.591600 2.669016 -1.452461
N18 2.782937 -2.058026 -0.437904
C19 1.690487 -2.643334 0.009155
C20 3.060184 -0.866031 -0.055046
N21 0.698374 -3.170129 0.325306
N22 3.279852 0.261482 0.232261
C23 1.551657 3.386483 0.529026
H24 1.444739 3.158740 1.584349
H25 1.748818 4.418578 0.264188

F8.TS4
C1 0.131857 -0.761426 -0.753057
N2 -1.084638 -0.569964 -0.190815
N3 0.917775 -1.452346 0.053712
C4 -2.156539 0.288382 -0.728006
H5 -2.099300 1.256520 -0.224957
H6 -1.917998 0.449901 -1.782969
C7 3.140040 -1.898502 -0.077589
H8 4.042285 -1.348205 0.127845
H9 3.046630 -2.328219 -1.061538
C10 0.186063 -1.716797 1.185982
C11 -1.061152 -1.168211 1.051200
H12 -1.909045 -1.138946 1.713583
H13 0.591942 -2.267229 2.020315
H14 0.411412 -0.368338 -1.716254
H15 2.739046 -2.465449 0.746542
C16 -3.512746 -0.341262 -0.588850
H17 -3.640567 -1.318410 -1.049558
N18 2.187298 1.988175 0.450910
C19 2.610951 1.048106 -0.301835
C20 0.924522 2.361002 0.455924
N21 3.057267 0.186778 -0.982213
N22 -0.178181 2.732145 0.525772
C23 -4.533411 0.245297 0.030448
H24 -4.429281 1.219073 0.498752
H25 -5.509280 -0.223736 0.081371

F8.TS5
C1 -0.324051 -0.946439 0.519595
N2 0.417536 -1.128571 -0.557710
N3 -1.553991 -1.501704 0.378796
C4 2.757749 0.158851 -0.828719
H5 2.580963 -0.759520 -1.364781
H6 2.537502 1.096808 -1.314727
C7 -2.666829 -1.397007 1.320881
H8 -3.242075 -2.323192 1.303222
H9 -3.296784 -0.545200 1.058719
C10 -1.599724 -2.057886 -0.880651
C11 -0.373149 -1.821106 -1.444846
H12 -0.022617 -2.107946 -2.423926
H13 -2.481275 -2.551665 -1.253913
H14 -0.025285 -0.406313 1.404417
H15 -2.267163 -1.251267 2.324365
C16 3.456376 0.137275 0.392162
H17 3.632718 1.080992 0.892242
N18 -0.876444 2.551186 -0.603351
C19 -2.008221 2.087841 -0.133187
C20 0.264693 2.294585 -0.073197
N21 -3.058855 1.709737 0.207653
N22 1.356029 2.123738 0.342671
C23 3.899585 -1.034154 0.916049
H24 3.656916 -1.983516 0.450417
H25 4.498602 -1.061644 1.819028

CH_2=C=CH_2
C1 1.303450 -0.000059 -0.000089
H2 1.867429 0.696212 -0.612892
H3 1.867485 -0.695715 0.613368
C4 -0.000031 -0.000078 -0.000024
C5 -1.303428 0.000030 0.000023
H6 -1.867487 -0.613133 -0.695844
H7 -1.867367 0.613277 0.695912

[$AMIM^+ - H_{C2}^+$]
C1 0.917570 -0.985335 -0.119886
N2 -0.170780 -0.179709 -0.313649
N3 1.920107 -0.076563 0.065555
C4 -1.512481 -0.705263 -0.564475
H5 -1.869344 -0.355301 -1.538525
H6 -1.389642 -1.789143 -0.618069
C7 3.301914 -0.458112 0.313276
H8 3.643007 -0.073485 1.278176
H9 3.956683 -0.077045 -0.474998
C10 1.474491 1.239096 -0.010730
C11 0.142901 1.174281 -0.250504
H12 -0.588452 1.956176 -0.369374
H13 2.123707 2.091053 0.108073
H14 3.346350 -1.545047 0.323194
C15 -2.491918 -0.336935 0.516075
H16 -2.198048 -0.611180 1.526811
C17 -3.657948 0.265567 0.298549
H18 -3.972434 0.552743 -0.700760
H19 -4.344284 0.485351 1.108305

[$AMIM^+ - H^{\alpha}_{Allyl}{}^+$]
C1 0.897518 -0.900943 -0.008663
N2 -0.237071 -0.147645 -0.002122
N3 1.994613 -0.071330 -0.022603
C4 -1.528756 -0.618741 -0.004934

H5 -1.610587 -1.696523 -0.013332
C6 3.371323 -0.524129 0.023267
H7 3.589100 -1.019197 0.974529
H8 4.029210 0.336997 -0.085738
C9 1.549356 1.215898 -0.008990
C10 0.183647 1.194320 0.001701
H11 -0.514511 2.008598 0.001313
H12 2.223310 2.055723 -0.007392
H13 0.929940 -1.973715 -0.026093
H14 3.569863 -1.221709 -0.794740
C15 -2.668717 0.214694 0.006806
H16 -2.492983 1.289194 0.017548
C17 -3.971141 -0.176911 0.006487
H18 -4.255406 -1.223890 -0.003334
H19 -4.770100 0.552222 0.016267

[AMIM$^+$ – H$^{\beta}_{Allyl}$$^+$]
C1 0.418910 -0.573770 -0.053606
N2 -0.204048 0.596770 -0.036349
N3 1.745702 -0.356473 0.007766
C4 -1.726901 0.703188 -0.107209
H5 -1.991074 1.349844 0.744681
H6 -1.915290 1.254674 -1.036447
C7 2.774187 -1.393410 0.016989
H8 3.354581 -1.338896 0.939186
H9 3.436719 -1.272736 -0.841324
C10 1.962256 1.010481 0.065398
C11 0.733971 1.601686 0.038131
H12 0.457087 2.641677 0.065718
H13 2.950564 1.435329 0.119910
H14 -0.170267 -1.486975 -0.116858
H15 2.288072 -2.365365 -0.041677
C16 -2.319676 -0.667157 -0.114162
C17 -3.635143 -0.736958 0.134594
H18 -4.285938 0.126970 0.353173
H19 -4.161654 -1.690964 0.132919

[AMIM$^+$ – H$^{\gamma}_{Allyl}$$^+$]
C1 0.915941 -0.923272 -0.079359
N2 -0.280603 -0.344897 -0.092665
N3 1.866057 0.028209 -0.011065
C4 -1.650870 -1.048087 -0.151609
H5 -1.847937 -1.194725 -1.214812
H6 -1.468248 -2.017302 0.332603
C7 3.307399 -0.198539 0.069979
H8 3.684220 0.116420 1.044315
H9 3.813407 0.361152 -0.717093
C10 1.230501 1.257751 0.021456
C11 -0.110886 1.018457 -0.028404
H12 -0.974676 1.666183 0.009170
H13 1.780170 2.181038 0.085762
H14 1.101168 -1.982929 -0.123948
H15 3.508535 -1.260065 -0.064861
C16 -2.706431 -0.193708 0.489653
H17 -2.786978 -0.350693 1.572138
C18 -3.437559 0.748338 -0.148116
H19 -3.196414 0.732095 -1.238773

AIM
C1 1.395484 -1.031034 0.102496
N2 0.308284 -0.260148 -0.205763
N3 2.483277 -0.313459 0.266981
C4 -1.050852 -0.730365 -0.470794
H5 -1.324447 -0.499598 -1.504752
H6 -1.025562 -1.820162 -0.375397
C7 2.092117 0.988110 0.056039
C8 0.753452 1.046881 -0.237349
H9 0.091399 1.869341 -0.450726
H10 2.792066 1.806126 0.127750
H11 1.325796 -2.105594 0.189214
C12 -2.062290 -0.151746 0.481281
H13 -1.842546 -0.281337 1.538387
C14 -3.171765 0.473208 0.098165
H15 -3.408946 0.621935 -0.951179
H16 -3.885563 0.854210 0.819145

CH$_2$CH=CH$_2$DCA
C1 1.754052 -0.848993 0.235887
H2 1.702662 -0.699948 1.317692
H3 2.287127 -1.784287 0.044439
N4 -1.918133 -0.648030 0.251480
C5 -2.757749 0.349930 0.030893
C6 -0.712136 -0.743941 -0.013482
N7 -3.562408 1.170959 -0.118495
N8 0.409529 -1.020443 -0.310859
C9 2.465709 0.297620 -0.429799
H10 2.535993 0.245251 -1.512771
C11 3.001237 1.315436 0.235923
H12 2.935156 1.391240 1.316986
H13 3.529470 2.110029 -0.277762

AIM$^+$
C1 1.510965 -1.005777 -0.011891
N2 0.296289 -0.299691 -0.025084
N3 2.568331 -0.199793 -0.007864
C4 -1.069033 -0.917896 -0.067059
H5 -1.265547 -1.190994 -1.106348
H6 -0.994635 -1.834816 0.523305
C7 2.074078 1.033967 -0.018761
C8 0.614847 0.986861 -0.029342

H9 -0.120419 1.778931 -0.036614
H10 2.692058 1.921949 -0.017428
H11 1.541960 -2.087415 -0.004889
C12 -2.122068 0.000778 0.473548
H13 -2.060459 0.235248 1.533432
C14 -3.127889 0.463066 -0.264974
H15 -3.228844 0.222603 -1.318805
H16 -3.901849 1.084887 0.168861

$CH_2CH=CH_2$
C1 1.227842 -0.196146 0.000582
H2 1.295876 -1.278642 -0.000460
H3 2.154855 0.362676 -0.000906
C4 0.000340 0.442167 -0.000429
H5 0.000557 1.530325 -0.000055
C6 -1.228065 -0.195880 0.000031
H7 -1.296981 -1.278380 -0.000956
H8 -2.155008 0.363174 0.001276

$AMIM^+$
C1 0.945541 -0.888029 -0.063318
N2 -0.201145 -0.219632 -0.220292
N3 1.948222 -0.009852 0.042569
C4 -1.547610 -0.831007 -0.408177
H5 -1.838975 -0.678288 -1.448976
H6 -1.416969 -1.903387 -0.244951
C7 3.368568 -0.340437 0.235002
H8 3.717947 0.091471 1.172279
H9 3.948681 0.054375 -0.598445
C10 1.421995 1.265038 -0.050579
C11 0.077256 1.133471 -0.214214
H12 -0.696787 1.874767 -0.314714
H13 2.039716 2.145116 0.009673
H14 1.046543 -1.960246 -0.029283
H15 3.478091 -1.422363 0.271883
C16 -2.562209 -0.252789 0.534817
H17 -2.363380 -0.381530 1.595512
C18 -3.675359 0.346529 0.122198
H19 -3.904649 0.472966 -0.931490
H20 -4.408848 0.716838 0.828204

Cartesian coordinates for the structures in Figure 9, calculated at B3LYP/6-311++G(d,p)

[$AMIM^+ - H_{C2}^+$]

C1 0.917072 -0.984962 -0.120389
N2 -0.170488 -0.178199 -0.313826
C3 0.144498 1.175448 -0.249979
C4 1.476127 1.238872 -0.010020
N5 1.920469 -0.077251 0.065618
C6 -1.512582 -0.702399 -0.565180
H7 -1.869173 -0.350348 -1.538549
H8 -1.390605 -1.786236 -0.620925
H9 -0.586039 1.958144 -0.368605
H10 2.126141 2.090152 0.109275
C11 3.301900 -0.460293 0.313154
H12 3.643264 -0.076851 1.278429
H13 3.957088 -0.079126 -0.474722
H14 3.345318 -1.547276 0.322102
C15 -2.492031 -0.335299 0.516150
H16 -2.195844 -0.605843 1.527170
C17 -3.660832 0.261862 0.298771
H18 -3.978160 0.545099 -0.700779
H19 -4.346772 0.481054 1.109019

F9.TS1$^{\gamma}$

C1 2.045859 -0.946411 -0.070918
N2 1.200036 0.095184 -0.339658
N3 3.238763 -0.308075 0.110497
C4 -0.222833 -0.090000 -0.600692
H5 -0.483476 0.340381 -1.573665
H6 -0.375243 -1.172860 -0.671932
C7 4.476551 -1.010496 0.416490
H8 4.887264 -0.671259 1.370936
H9 5.217824 -0.848407 -0.370307
C10 3.140973 1.071373 -0.039817
C11 1.842612 1.330854 -0.324294
H12 1.338910 2.264248 -0.513669
H13 3.981529 1.738089 0.061736
H14 4.245552 -2.071547 0.480015
C15 -1.087764 0.473637 0.481110
H16 -0.772029 0.279085 1.501873
C17 -2.325806 1.067448 0.246694
H18 -2.526813 1.482161 -0.737639
H19 -2.831259 1.572613 1.061006
N20 -3.692185 -0.310562 0.056162
O21 -4.808986 0.070959 0.308120
O22 -3.331775 -1.399305 -0.314220

F9.TS2$^{\gamma}$

C1 -2.038783 -0.916384 0.393566
N2 -1.319293 0.248259 0.383563
N3 -3.253958 -0.506107 -0.071577
C4 0.077377 0.313078 0.791368
H5 0.207159 1.059116 1.581285
H6 0.309840 -0.668509 1.218802
C7 -4.388017 -1.405572 -0.231509
H8 -4.720538 -1.425077 -1.272391
H9 -5.220047 -1.094552 0.405230
C10 -3.291040 0.854439 -0.359134
C11 -2.059097 1.337699 -0.072378
H12 -1.661495 2.336117 -0.149236
H13 -4.169424 1.355808 -0.731044
H14 -4.062535 -2.401073 0.061996
C15 0.999475 0.580190 -0.357238
H16 0.811643 0.010289 -1.263022
C17 2.092085 1.393650 -0.285408
H18 2.252626 2.038814 0.569784
H19 2.701079 1.579197 -1.159691
N20 4.113317 -0.563922 -0.497742
O21 5.038883 -1.262596 -0.175350
O22 3.513522 0.015052 0.520723

F9.TS3$^{\gamma}$

C1 2.318461 -0.008480 -0.963521
N2 1.415739 0.706047 -0.222623
N3 3.164450 -0.483472 -0.005341
C4 0.283153 1.394928 -0.824121
H5 0.247752 2.430506 -0.477830
H6 0.466790 1.392737 -1.900274
C7 4.321599 -1.313885 -0.306828
H8 4.243044 -2.281543 0.195174
H9 5.244349 -0.820346 0.008859
C10 2.801739 -0.086876 1.278659
C11 1.686129 0.667925 1.142661
H12 1.078194 1.162305 1.881875
H13 3.354139 -0.365559 2.160939
H14 4.345415 -1.467157 -1.383454
C15 -1.034096 0.687381 -0.538663
H16 -1.070202 -0.362506 -0.817927
C17 -2.073117 1.284062 -0.003361
H18 -2.251933 2.298342 0.339167
H19 -3.346160 0.550757 0.245936
N20 -4.463674 -1.129017 0.172074
O21 -3.511181 -1.645171 -0.320633
O22 -4.357593 0.152324 0.499358

F9.TS5$^{\gamma}$

C1 2.158945 -0.981818 -0.247134
N2 1.309063 0.078685 -0.407066
N3 3.323126 -0.365214 0.111161

C4 -0.099160 -0.082563 -0.773218
H5 -0.332328 0.550636 -1.634350
H6 -0.205003 -1.125712 -1.080282
C7 4.554911 -1.091400 0.382809
H8 4.897851 -0.901957 1.403280
H9 5.339981 -0.798120 -0.319030
C10 3.203602 1.019518 0.173534
C11 1.920484 1.303912 -0.152643
H12 1.408946 2.249164 -0.227826
H13 4.021154 1.672464 0.431720
H14 4.344396 -2.152014 0.264149
C15 -1.004016 0.231010 0.376159
H16 -0.859638 -0.324243 1.295581
C17 -2.198920 1.075822 0.249542
H18 -2.150778 1.845669 -0.529112
H19 -2.578983 1.499893 1.185191
N20 -4.687242 -0.061611 0.341410
O21 -5.188687 -1.036308 0.012472
O22 -2.900726 -0.079404 -0.157741

F9.TS6$^{\gamma}$
C1 2.341293 -1.016454 -0.053764
N2 1.331196 -0.167286 -0.417851
N3 3.376953 -0.154139 0.158337
C4 -0.010576 -0.638617 -0.745651
H5 -0.269762 -0.347559 -1.769189
H6 0.056393 -1.731628 -0.716259
C7 4.704483 -0.591449 0.566159
H8 4.983489 -0.136858 1.520046
H9 5.448161 -0.324798 -0.189143
C10 3.027653 1.174269 -0.063393
C11 1.724073 1.169400 -0.429007
H12 1.063344 1.981335 -0.683837
H13 3.717393 1.993870 0.053737
H14 4.675532 -1.673149 0.676897
C15 -1.035775 -0.149609 0.225330
H16 -0.832375 -0.261741 1.286392
C17 -2.303586 0.363280 -0.163193
H18 -2.984823 -0.763884 -0.347195
H19 -2.375842 0.718071 -1.207368
N20 -4.281578 -0.555655 0.384664
O21 -5.261609 -0.306129 -0.159956
O22 -3.132505 0.908752 0.720079

F9.TS7$^{\gamma}$
C1 1.991140 0.923437 -0.515792
N2 0.921440 0.713881 0.314657
N3 2.816311 -0.108354 -0.181843
C4 -0.252147 1.574661 0.304567
H5 -0.488815 1.903338 1.320527
H6 0.035854 2.451891 -0.283243
C7 4.119789 -0.315271 -0.797989
H8 4.161977 -1.290216 -1.289743
H9 4.913685 -0.256040 -0.049355
C10 2.286176 -0.925469 0.812605
C11 1.077162 -0.406503 1.129792
H12 0.337261 -0.729631 1.842930
H13 2.801870 -1.785794 1.206184
H14 4.263043 0.468831 -1.538075
C15 -1.425005 0.879049 -0.325629
H16 -1.252038 0.393675 -1.282231
C17 -2.808759 1.075447 0.060839
H18 -2.678566 2.001946 -0.675145
H19 -2.939424 1.560812 1.047567
N20 -2.363910 -1.365485 0.220613
O21 -2.380053 -2.257240 -0.500705
O22 -3.707682 0.228339 -0.347266

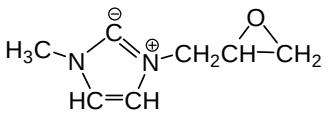
[(MIM^{+} – H$_{C2}^{+}$)CH$_2$CHCH]$^{\bullet}$
C1 0.827399 -0.971312 -0.165895
N2 -0.241987 -0.135809 -0.340994
N3 1.846379 -0.091533 0.059926
C4 -1.589595 -0.626821 -0.607453
H5 -1.975879 -0.173252 -1.523665
H6 -1.485842 -1.701095 -0.769695
C7 3.218441 -0.510637 0.302755
H8 3.559288 -0.170052 1.284056
H9 3.886604 -0.113151 -0.465792
C10 1.428672 1.235496 0.028897
C11 0.098473 1.208367 -0.223635
H12 -0.615177 2.009674 -0.318346
H13 2.094718 2.068475 0.183411
H14 3.240806 -1.597797 0.271289
C15 -2.539258 -0.370853 0.554608
H16 -2.202602 -0.763788 1.514578
C17 -3.685109 0.251829 0.458833
H18 -4.286803 0.735970 -0.297021

[(MIM^{+} – H$_{C2}^{+}$)CH$_2$CHCH$_2$NO$_2$]$^{\bullet}$
C1 -1.937160 -0.927625 0.147176
N2 -1.144468 0.166751 0.361847
N3 -3.145734 -0.356880 -0.130275
C4 0.270511 0.062238 0.691900
H5 0.474441 0.583000 1.636024
H6 0.458059 -1.002896 0.880028
C7 -4.340723 -1.133246 -0.427805
H8 -4.718223 -0.894503 -1.425416
H9 -5.123761 -0.934760 0.308547
C10 -3.108307 1.032973 -0.088602
C11 -1.833866 1.368880 0.223198

H12 -1.375925 2.334907 0.356905
H13 -3.969490 1.653393 -0.275146
H14 -4.067658 -2.185418 -0.388039
C15 1.155902 0.574512 -0.393501
H16 0.824841 0.464206 -1.420193
C17 2.554074 0.975510 -0.138169
H18 2.686044 1.447352 0.837583
H19 2.974974 1.588253 -0.931831
N20 3.486477 -0.271286 -0.071530
O21 4.267692 -0.437881 -0.990923
O22 3.344831 -1.005005 0.892932

[(MIM$^+$ – H$_{C2}$$^+$)CH$_2$CHCH$_2$ONO]$^\bullet$
C1 -2.119848 -0.878693 0.453624
N2 -1.335753 0.239011 0.370195
N3 -3.297331 -0.445153 -0.084808
C4 0.045876 0.270337 0.835552
H5 0.155642 1.028803 1.621621
H6 0.214632 -0.704046 1.313099
C7 -4.471276 -1.295495 -0.215293
H8 -4.765297 -1.390988 -1.263777
H9 -5.309562 -0.888070 0.355863
C10 -3.249145 0.886378 -0.484302
C11 -2.000023 1.323575 -0.195960
H12 -1.542468 2.287613 -0.343901
H13 -4.085787 1.401281 -0.927377
H14 -4.211771 -2.276440 0.176765
C15 1.030738 0.506532 -0.259238
H16 0.821264 0.076206 -1.233338
C17 2.393539 1.018669 0.019596
H18 2.404963 1.724182 0.853903
H19 2.841472 1.489415 -0.859138
N20 4.277630 -0.312181 -0.566403
O21 4.983309 -1.193758 -0.260177
O22 3.289931 -0.069680 0.428867

[(MIM$^+$ – H$_{C2}$$^+$)CH$_2CH_2$CHO]
C1 1.104398 -0.777056 -0.387335
N2 0.287785 0.313487 -0.277695
N3 2.318084 -0.267935 -0.026356
C4 -1.149803 0.248225 -0.526782
H5 -1.517961 1.258231 -0.713866
H6 -1.311127 -0.331135 -1.435386
C7 3.537835 -1.061443 -0.003556
H8 3.979102 -1.062406 0.996522
H9 4.268432 -0.669965 -0.716329
C10 2.260650 1.083870 0.297085
C11 0.966350 1.453298 0.140470
H12 0.488603 2.409691 0.275851
H13 3.122391 1.658447 0.594094
H14 3.273388 -2.079143 -0.282276
C15 -1.900547 -0.390720 0.641397
H16 -1.534873 -1.411300 0.810525
C17 -3.393712 -0.447111 0.454033
H18 -1.706329 0.145525 1.580707
H19 -3.948529 -0.949785 1.275704
O20 -3.988152 0.007324 -0.493633



C1 1.203230 -0.958876 -0.184621
N2 0.210188 -0.066029 -0.484757
N3 2.250467 -0.136246 0.114313
C4 -1.144349 -0.481494 -0.827592
H5 -1.539562 0.158351 -1.621196
H6 -1.076644 -1.500902 -1.208897
C7 3.567667 -0.630689 0.486687
H8 3.852644 -0.263315 1.475959
H9 4.319679 -0.316533 -0.241907
C10 1.925234 1.212034 0.006058
C11 0.625486 1.257925 -0.371464
H12 -0.015967 2.099920 -0.572150
H13 2.628651 2.006985 0.191751
H14 3.517817 -1.717171 0.505997
C15 -2.071914 -0.448002 0.369268
H16 -1.753201 -1.064547 1.207785
C17 -2.964359 0.686453 0.636924
H18 -2.964370 1.541300 -0.035865
H19 -3.288159 0.890516 1.654035
O20 -3.468930 -0.530349 0.068254

[(MIM$^+$ – H$_{C2}$$^+$)CH$_2$CHCHO]$^\bullet$
C1 1.391958 -0.984994 -0.053122
N2 0.322848 -0.201427 -0.394881
N3 2.374683 -0.059040 0.141480
C4 -0.990787 -0.756945 -0.697066
H5 -1.288614 -0.487636 -1.716675
H6 -0.855415 -1.845151 -0.673549
C7 3.734967 -0.412189 0.522428
H8 4.002368 0.055775 1.473141
H9 4.445645 -0.096029 -0.245382
C10 1.937645 1.244700 -0.070155
C11 0.630114 1.157558 -0.410807
H12 -0.084439 1.926304 -0.654183
H13 2.576418 2.106177 0.034844
H14 3.776958 -1.493915 0.628517
C15 -2.034396 -0.347782 0.286258
H16 -1.788128 -0.360866 1.343895

C17 -3.359747 0.021089 -0.086809
H18 -3.579000 0.044434 -1.172616
O19 -4.243379 0.305695 0.726432

F9.TS1$^{\beta}$
C1 -1.634635 -0.925677 0.200540
N2 -0.896514 0.196978 0.464377
N3 -2.866948 -0.404198 -0.062033
C4 0.533575 0.137086 0.747736
H5 0.809495 0.963100 1.405761
H6 0.715299 -0.797349 1.274954
C7 -4.025352 -1.225482 -0.383624
H8 -4.432416 -0.951277 -1.360122
H9 -4.804107 -1.109983 0.374625
C10 -2.896686 0.983866 0.031007
C11 -1.640832 1.368481 0.360976
H12 -1.232397 2.349464 0.537859
H13 -3.788040 1.568007 -0.128064
H14 -3.697465 -2.262352 -0.407274
C15 1.342628 0.189459 -0.539833
H16 1.177727 -0.656423 -1.201333
C17 1.634034 1.418205 -1.142617
H18 1.623292 2.337784 -0.568042
H19 1.979679 1.469587 -2.167351
N20 3.061372 -0.470011 0.063823
O21 3.703377 -1.049407 -0.776159
O22 3.382520 -0.181289 1.192498

F9.TS2$^{\beta}$
C1 -1.753874 -0.942132 0.290520
N2 -1.108780 0.253182 0.466601
N3 -2.995936 -0.541679 -0.106141
C4 0.295116 0.335636 0.856747
H5 0.425722 1.126096 1.600053
H6 0.552812 -0.619110 1.312829
C7 -4.072611 -1.474852 -0.406512
H8 -4.410434 -1.353949 -1.438866
H9 -4.918235 -1.319184 0.268180
C10 -3.120583 0.842248 -0.177307
C11 -1.918429 1.350613 0.182555
H12 -1.586902 2.372285 0.266474
H13 -4.033401 1.339711 -0.461082
H14 -3.683316 -2.481250 -0.269679
C15 1.176569 0.578302 -0.342962
H16 1.134161 -0.185888 -1.111800
C17 1.745191 1.787370 -0.631854
H18 1.729421 2.599903 0.086901
H19 2.294597 1.942475 -1.552086
N20 3.751920 -0.601131 -0.472984
O21 4.673403 -1.262869 -0.078908
O22 2.933705 -0.244231 0.511362

F9.TS3$^{\beta}$
C1 -1.509142 -0.387390 0.891332
N2 -0.763625 0.670054 0.440730
N3 -2.570497 -0.373285 0.035554
C4 0.479558 1.070321 1.082603
H5 0.353667 2.047182 1.574708
H6 0.672564 0.327334 1.858615
C7 -3.658803 -1.337952 0.104260
H8 -3.712969 -1.924902 -0.816139
H9 -4.614008 -0.831077 0.263257
C10 -2.491830 0.648677 -0.905602
C11 -1.342303 1.315973 -0.648744
H12 -0.895105 2.161347 -1.144162
H13 -3.239194 0.811578 -1.664680
H14 -3.458436 -2.001094 0.942854
C15 1.637819 1.172377 0.153470
H16 1.892447 -0.089098 -0.582672
C17 2.477119 2.136379 -0.154553
H18 2.354183 3.140488 0.256829
H19 3.318821 1.987505 -0.823236
N20 2.613649 -1.957321 -0.406981
O21 2.128221 -1.004532 -1.188000
O22 2.723883 -1.709933 0.752113

F9.TS4$^{\beta}$
C1 -1.812221 0.082688 0.984050
N2 -0.904174 0.829976 0.281603
N3 -2.649053 -0.348919 -0.001681
C4 0.186154 1.533951 0.939716
H5 -0.005009 2.619647 0.937486
H6 0.173331 1.202179 1.980110
C7 -3.794049 -1.212609 0.250582
H8 -3.681600 -2.164757 -0.273845
H9 -4.719440 -0.730378 -0.074319
C10 -2.280612 0.109919 -1.262426
C11 -1.170508 0.864537 -1.085249
H12 -0.560051 1.395127 -1.796533
H13 -2.821595 -0.135539 -2.161493
H14 -3.838696 -1.395221 1.321892
C15 1.514856 1.307756 0.321120
H16 1.994560 -0.317933 0.188531
C17 2.474912 2.048926 -0.178431
H18 2.365877 3.133988 -0.257258
H19 3.409980 1.627249 -0.536511
N20 2.511152 -1.289737 0.013037
O21 3.562506 -1.213143 -0.596818
O22 1.970740 -2.284934 0.447451

F9.TS5$^{\beta}$
C1 1.653441 -0.985401 -0.152697
N2 0.988687 0.150787 -0.527949
N3 2.906242 -0.513600 0.111912
C4 -0.430307 0.155870 -0.857187
H5 -0.631658 0.928337 -1.604165
H6 -0.671734 -0.814524 -1.290669
C7 4.003543 -1.369606 0.537206
H8 4.389122 -1.049316 1.508625
H9 4.815906 -1.350310 -0.194085
C10 3.019520 0.858558 -0.088261
C11 1.798097 1.282701 -0.491710
H12 1.451635 2.267105 -0.758813
H13 3.936944 1.404264 0.058683
H14 3.617369 -2.383299 0.618803
C15 -1.314909 0.382111 0.369886
H16 -1.101411 -0.373741 1.133517
C17 -1.437455 1.752785 0.892092
H18 -1.392791 2.595737 0.214618
H19 -1.796751 1.915278 1.898624
N20 -3.553634 -1.188523 0.115709
O21 -4.657557 -1.047228 -0.140029
O22 -2.687103 0.454442 0.047676

F9.TS6$^{\beta}$
C1 1.950819 -0.840602 -0.420603
N2 0.869152 -0.011792 -0.564861
N3 2.906162 0.012769 0.049235
C4 -0.422330 -0.479516 -1.031379
H5 -0.866538 0.254887 -1.710093
H6 -0.251501 -1.391630 -1.606172
C7 4.267518 -0.407311 0.348761
H8 4.506816 -0.222687 1.399177
H9 4.983946 0.126545 -0.280901
C10 2.443820 1.318027 0.188413
C11 1.147010 1.303562 -0.201145
H12 0.423039 2.099777 -0.256859
H13 3.061860 2.130829 0.532860
H14 4.334542 -1.473822 0.145602
C15 -1.444335 -0.808216 0.051772
C16 -1.196579 -0.678595 1.402206
H17 -0.246024 -0.318288 1.768814
H18 -1.899383 -1.093580 2.114644
O19 -2.627205 -1.099947 -0.389032
H20 -2.704356 0.452545 1.080557
N21 -3.622463 0.319015 0.475549
O22 -3.983782 1.193871 -0.227872

F9.TS7$^{\beta}$
C1 -1.139464 0.750845 -0.122799
N2 -0.714327 -0.472488 -0.563871
N3 -2.467366 0.535391 0.097129
C4 0.675619 -0.726116 -0.910980
H5 0.751629 -1.697573 -1.403821
H6 1.018914 0.031850 -1.615461
C7 -3.374314 1.570425 0.572940
H8 -3.827013 1.279499 1.524223
H9 -4.165204 1.755705 -0.158216
C10 -2.856324 -0.769105 -0.193379
C11 -1.739644 -1.411963 -0.612461
H12 -1.595447 -2.427827 -0.941346
H13 -3.869009 -1.121242 -0.087002
H14 -2.793218 2.479266 0.712544
C15 1.641312 -0.729274 0.296014
H16 1.478486 0.472752 0.729741
C17 1.229056 -1.338208 1.519952
H18 0.180890 -1.451212 1.767561
H19 1.979639 -1.557068 2.269178
N20 2.830866 1.194189 0.323699
O21 2.904662 1.864904 -0.599141
O22 2.930173 -0.695331 -0.037337

[(MIM^{+} – H$_{C2}^{+}$)CH$_2$CH(-NO$_2$)CH$_2$]$^{\bullet}$
C1 -1.634635 -0.925677 0.200540
N2 -0.896514 0.196978 0.464377
N3 -2.866948 -0.404198 -0.062033
C4 0.533575 0.137086 0.747736
H5 0.809495 0.963100 1.405761
H6 0.715299 -0.797349 1.274954
C7 -4.025352 -1.225482 -0.383624
H8 -4.432416 -0.951277 -1.360122
H9 -4.804107 -1.109983 0.374625
C10 -2.896686 0.983866 0.031007
C11 -1.640832 1.368481 0.360976
H12 -1.232397 2.349464 0.537859
H13 -3.788040 1.568007 -0.128064
H14 -3.697465 -2.262352 -0.407274
C15 1.342628 0.189459 -0.539833
H16 1.177727 -0.656423 -1.201333
C17 1.634034 1.418205 -1.142617
H18 1.623292 2.337784 -0.568042
H19 1.979679 1.469587 -2.167351
N20 3.061372 -0.470011 0.063823
O21 3.703377 -1.049407 -0.776159
O22 3.382520 -0.181289 1.192498

[(MIM^{+} – H$_{C2}^{+}$)CH$_2$CH(-ONO)CH$_2$]$^{\bullet}$
C1 -1.753874 -0.942132 0.290520
N2 -1.108780 0.253182 0.466601
N3 -2.995936 -0.541679 -0.106141

C4 0.295116 0.335636 0.856747
H5 0.425722 1.126096 1.600053
H6 0.552812 -0.619110 1.312829
C7 -4.072611 -1.474852 -0.406512
H8 -4.410434 -1.353949 -1.438866
H9 -4.918235 -1.319184 0.268180
C10 -3.120583 0.842248 -0.177307
C11 -1.918429 1.350613 0.182555
H12 -1.586902 2.372285 0.266474
H13 -4.033401 1.339711 -0.461082
H14 -3.683316 -2.481250 -0.269679
C15 1.176569 0.578302 -0.342962
H16 1.134161 -0.185888 -1.111800
C17 1.745191 1.787370 -0.631854
H18 1.729421 2.599903 0.086901
H19 2.294597 1.942475 -1.552086
N20 3.751920 -0.601131 -0.472984
O21 4.673403 -1.262869 -0.078908
O22 2.933705 -0.244231 0.511362

[(MIM$^+$ – H$_{C2}^+$)CH$_2$=C=CH$_2$]$^\bullet$
C1 0.925244 -1.003756 -0.019162
N2 -0.193702 -0.242567 -0.219254
N3 1.904476 -0.056686 0.063473
C4 -1.514073 -0.834058 -0.414357
H5 -1.817213 -0.723125 -1.469239
H6 -1.392728 -1.901865 -0.220598
C7 3.305343 -0.380282 0.287289
H8 3.663275 0.072412 1.215740
H9 3.921672 -0.027307 -0.543776
C10 1.415469 1.237973 -0.081019
C11 0.078448 1.120831 -0.262312
H12 -0.681718 1.871633 -0.397713
H13 2.041297 2.114224 -0.038221
H14 3.385543 -1.462680 0.360659
C15 -2.563462 -0.258104 0.448996
C16 -3.742301 0.296431 0.319611
H17 -4.182144 0.481263 -0.665783
H18 -4.341412 0.596006 1.175118

[(MIM$^+$ – H$_{C2}^+$)CH$_2$C(O)CH$_3$]
C1 -1.101548 -1.005014 0.037535
N2 -0.145442 -0.112471 0.448140
N3 -2.197064 -0.207337 -0.101480
C4 1.209214 -0.524807 0.730034
H5 1.494201 -0.252736 1.755719
H6 1.228295 -1.615093 0.673056
C7 -3.494986 -0.706045 -0.529630
H8 -3.809261 -0.218502 -1.456163
H9 -4.250534 -0.530503 0.240818
C10 -1.937818 1.124950 0.211199
C11 -0.631295 1.186483 0.558376
H12 -0.018871 2.025979 0.838611
H13 -2.683642 1.900440 0.154507
H14 -3.397545 -1.775925 -0.700898
C15 2.269553 0.059811 -0.207936
C16 3.627800 -0.605724 -0.129885
H17 3.586831 -1.555183 -0.674874
H18 4.381940 0.032408 -0.588645
O19 2.039453 0.985939 -0.948664
H20 3.904976 -0.837657 0.902398

[(MIM$^+$ – H$_{C2}^+$)CH$_2$C(O)CH$_2$]$^\bullet$
C1 1.000935 -0.537727 -0.791938
N2 0.051048 0.377521 -0.424149
N3 2.077948 -0.148920 -0.049329
C4 -1.309000 0.361676 -0.935060
H5 -1.629732 1.371567 -1.197569
H6 -1.301614 -0.240977 -1.845949
C7 3.368539 -0.820249 -0.109321
H8 3.651770 -1.201287 0.875180
H9 4.143333 -0.136162 -0.464702
C10 1.812244 0.960574 0.746998
C11 0.521140 1.295005 0.512373
H12 -0.082864 2.091249 0.915323
H13 2.546477 1.414426 1.392036
H14 3.275726 -1.650923 -0.805443
C15 -2.355332 -0.224475 0.023787
C16 -1.983004 -1.281530 0.913592
H17 -0.983296 -1.696052 0.920021
H18 -2.742713 -1.687966 1.569378
O19 -3.514149 0.202033 -0.025814

Cartesian coordinates for the structures in Figure 10, calculated at B3LYP/6-311++G(d,p)

CH_2=C=CH_2
C1 0.000000 0.000000 0.000002
C2 0.000000 1.303397 0.000000
H3 -0.655867 1.867368 0.655849
H4 0.655869 1.867361 -0.655854
C5 0.000000 -1.303397 0.000000
H6 0.655867 -1.867368 0.655849
H7 -0.655869 -1.867361 -0.655854

F10.TS1
C1 -1.537892 -0.464729 -0.000051
C2 -0.322160 -1.097588 0.000039
H3 -0.022979 -1.613663 0.909282
H4 -0.022890 -1.613750 -0.909126
C5 -2.499947 0.405045 -0.000142
H6 -3.547618 0.111586 -0.000165
H7 -2.286541 1.474802 -0.000198
N8 1.109542 0.146165 0.000047
O9 0.834483 1.319258 -0.000046
O10 2.199671 -0.374070 0.000145

F10.TS2
C1 -1.448757 0.250713 0.158649
C2 -0.406266 1.104059 0.437011
H3 0.030039 1.028241 1.428993
H4 -0.485422 2.116313 0.052056
C5 -2.234992 -0.681603 -0.281118
H6 -1.873619 -1.456724 -0.958159
H7 -3.281683 -0.739241 0.009934
N8 1.676091 -0.349292 -0.314547
O9 1.246550 -1.078310 0.533927
O10 1.055717 0.760490 -0.561208

F10.TS3
C1 -1.921042 0.265242 -0.100026
C2 -3.016420 -0.304237 0.397271
H3 -3.318385 -0.131981 1.424753
H4 -3.645657 -0.939404 -0.216847
C5 -0.831119 0.723285 -0.549179
H6 -0.500460 1.633691 -1.022622
H7 0.218926 -0.155633 -0.426419
N8 2.195313 -0.413539 0.147668
O9 2.185989 0.744990 0.440616
O10 1.125245 -0.947195 -0.350733

F10.TS4
C1 -1.873790 -0.365826 -0.000021
C2 -2.831780 0.565292 0.000094
H3 -3.236415 0.949811 -0.929485
H4 -3.236377 0.949612 0.929772
C5 -0.898721 -1.161091 -0.000115
H6 -0.682183 -2.216217 -0.000211
H7 0.361742 -0.465988 -0.000071
N8 1.437117 0.109690 -0.000010
O9 1.372517 1.319385 -0.000102
O10 2.422378 -0.596298 0.000142

F10.TS5
C1 1.741471 0.196030 0.119538
C2 0.628966 1.113691 -0.004292
H3 0.806866 1.918848 -0.729317
H4 0.310412 1.548789 0.954043
C5 2.471666 -0.873257 0.091922
H6 2.089200 -1.833744 -0.250190
H7 3.511149 -0.842340 0.416530
N8 -1.942874 0.200561 0.318153
O9 -2.571655 -0.696950 -0.016477
O10 -0.199610 0.095167 -0.466166

F10.TS6
C1 -1.629798 0.052003 0.157289
C2 -0.344302 0.495878 0.463146
H3 0.255284 -0.667284 0.539370
H4 -0.215775 0.804096 1.516002
C5 -2.754927 -0.511626 -0.140467
H6 -3.668932 0.070313 -0.252520
H7 -2.837949 -1.586822 -0.300027
N8 1.530155 -0.560038 -0.296639
O9 2.573277 -0.415361 0.163333
O10 0.443029 1.050663 -0.451603

F10.TS7
C1 -1.026961 0.103047 0.138881
C2 -0.069366 1.167092 0.353955
H3 -0.060994 1.492706 1.411181
H4 -0.951765 1.770105 -0.123343
C5 -2.112754 -0.502712 -0.227019
H6 -2.205694 -1.574163 -0.075133
H7 -2.949620 0.017612 -0.685499
N8 1.601976 -0.806085 -0.296403
O9 0.753896 -1.316635 0.336197
O10 1.022195 1.233107 -0.342108

F10.TS8
C1 1.142254 -0.000006 0.000001
C2 1.432982 -1.275886 0.235422

H3 0.780413 -2.072085 -0.103266
H4 2.292509 -1.536094 0.844416
C5 1.432998 1.275874 -0.235421
H6 2.292502 1.536071 -0.844454
H7 0.780457 2.072081 0.103299
N8 -0.954690 0.000003 -0.000002
O9 -1.469518 1.030879 0.349866
O10 -1.469539 -1.030865 -0.349865

F10.TS9
C1 1.056060 0.207527 0.038299
C2 2.026552 -0.622854 -0.266323
H3 1.851892 -1.678399 -0.425407
H4 3.041498 -0.247456 -0.338337
C5 0.616348 1.485097 0.235029
H6 0.509424 2.165802 -0.601109
H7 0.254425 1.809682 1.203624
N8 -1.547243 -0.610854 0.077274
O9 -1.751103 0.466520 -0.420238
O10 -0.376434 -0.990554 0.367524

F10.TS10
C1 1.094177 -0.131610 0.029530
C2 1.870954 1.087623 -0.132447
H3 1.763642 1.667827 -1.040176
H4 2.356233 1.548085 0.720106
C5 1.373568 -1.436327 0.034025
H6 2.383849 -1.767558 -0.161634
H7 0.610028 -2.177316 0.228344
N8 -1.721044 -0.366801 -0.300080
O9 -2.597977 0.231134 0.103080
O10 -0.039353 0.541173 0.242828

F10.TS11
C1 0.892392 0.075152 -0.164307
C2 2.067724 0.373095 0.550695
H3 2.332881 1.406960 0.735479
H4 2.735900 -0.407243 0.893004
C5 0.654682 -1.331425 -0.419607
H6 1.288928 -2.092104 0.017264
H7 -0.144693 -1.641675 -1.079575
N8 -1.932184 0.486146 -0.097486
O9 -1.906828 -0.406428 0.619527
O10 0.109765 0.985191 -0.580084

[$CH_2C(-NO_2)CH_2$]•
C1 0.737315 0.000001 -0.000001
C2 1.343609 1.238463 -0.000335
H3 0.761397 2.146811 -0.000553
H4 2.423697 1.297820 -0.000400
C5 1.343604 -1.238464 0.000336
H6 2.423691 -1.297825 0.000401
H7 0.761387 -2.146809 0.000556
N8 -0.777369 0.000001 0.000000
O9 -1.342231 -1.082316 -0.000485
O10 -1.342238 1.082316 0.000486

[$CH_2C(-ONO)CH_2$]•
C1 -0.808229 -0.000001 0.157737
C2 -1.326543 1.233642 -0.188894
H3 -0.852904 2.146921 0.143581
H4 -2.229148 1.299839 -0.781831
C5 -1.326455 -1.233706 -0.188801
H6 -2.229048 -1.300012 -0.781745
H7 -0.852758 -2.146928 0.143750
N8 1.647794 0.000045 0.273701
O9 1.587978 -0.000042 -0.885767
O10 0.336603 0.000074 0.970777

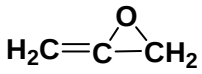
[$CH_2=C=CH_2NO_2$]•
C1 1.472153 -0.614472 -0.000015
C2 0.084138 -1.024599 -0.000007
H3 -0.183998 -1.607696 -0.883621
H4 -0.183982 -1.607701 0.883609
C5 2.346925 0.350781 0.000015
H6 3.416420 0.152478 -0.000001
H7 2.037248 1.397342 0.000057
N8 -0.972548 0.135405 -0.000001
O9 -0.577579 1.284496 -0.000019
O10 -2.134564 -0.228561 0.000018

[$CH_2=C=CH_2ONO$]•
C1 -1.507877 0.217741 0.393785
C2 -0.287461 1.027560 0.369505
H3 0.250293 0.959934 1.318391
H4 -0.508777 2.074940 0.158240
C5 -2.126206 -0.753638 -0.220198
H6 -1.695317 -1.242502 -1.097623
H7 -3.095636 -1.118850 0.108174
N8 1.580739 -0.355333 -0.449076
O9 1.573647 -0.782204 0.646488
O10 0.615543 0.640183 -0.721763

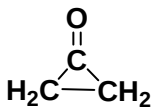
[$CH_2=C=CH$]•
C1 0.115508 0.000012 0.000012
C2 -1.251835 -0.000003 -0.000003
H3 -1.806986 -0.930086 0.000001
H4 -1.807023 0.930056 0.000001
C5 1.338498 -0.000003 -0.000018
H6 2.400983 -0.000009 0.000050

CH_2CHCHO

C1 0.665189 0.596444 0.000005
C2 -0.813292 0.460205 -0.000004
H3 -1.373613 1.417504 -0.000021
H4 1.059694 1.608612 0.000011
C5 1.475928 -0.464248 -0.000002
H6 1.064584 -1.468081 -0.000009
H7 2.554392 -0.358709 -0.000004
O8 -1.409001 -0.594217 0.000004



C1 0.382404 0.000000 -0.000022
C2 -0.857633 0.787546 -0.000014
H3 -1.158904 1.290097 0.913869
H4 -1.158835 1.290329 -0.913791
C5 -0.857633 -0.787546 -0.000014
H6 -1.158835 -1.290329 -0.913791
H7 -1.158904 -1.290097 0.913869
O8 1.579081 0.000000 0.000017



C1 0.264450 -0.065681 -0.000011
C2 -1.070921 -0.594729 -0.000050
H3 -1.523266 -0.942778 0.923421
H4 -1.523313 -0.942186 -0.923731
C5 1.582151 -0.114247 -0.000059
H6 2.172198 0.792998 -0.000265
H7 2.086241 -1.070354 0.000450
O8 -0.733242 0.851282 0.000106

$[CH_2{=}CCHO]^{\bullet}$

C1 -0.570414 -0.135972 -0.000371
C2 0.791345 -0.428607 0.000079
H3 1.051862 -1.500627 0.000500
C4 -1.834960 0.137859 0.000109
H5 -2.392768 0.263784 0.927495
H6 -2.393632 0.263332 -0.926811
O7 1.677340 0.441729 -0.000011

Cartesian coordinates for the structures in Table 3, calculated at B3LYP/6-311++G(d,p)

For the reaction of MIM + NO_2:

TS for PT to [MIM – H_{ME}]• + HONO
N1 -2.688357 0.115356 -0.760429
C2 -1.804145 0.972094 -0.341005
N3 -0.850413 0.379779 0.479217
C4 -1.183399 -0.964653 0.544330
C5 -2.308864 -1.104151 -0.215465
H6 -1.774445 2.028332 -0.564313
C7 0.271443 1.007872 1.029842
H8 1.351675 0.876612 0.158656
H9 0.646278 0.532701 1.931499
H10 0.174072 2.089907 1.083944
H11 -0.588310 -1.666499 1.103427
H12 -2.875600 -2.001537 -0.406361
N13 2.877061 -0.323912 -0.572468
O14 2.279656 0.836615 -0.609484
O15 2.451353 -1.152246 0.179820

TS for PT to [MIM – H_{ME}]• + O-NH-O
N1 2.622041 0.729274 0.658912
C2 1.636527 1.085904 -0.112758
N3 0.938497 -0.009073 -0.607625
C4 1.557247 -1.131054 -0.068973
C5 2.581913 -0.656750 0.696838
H6 1.355171 2.095390 -0.373569
C7 -0.202086 0.029471 -1.407557
H8 -1.414386 0.025141 -0.527080
H9 -0.386933 -0.876873 -1.976864
H10 -0.342814 0.968034 -1.935708
H11 1.208034 -2.126828 -0.284579
H12 3.298486 -1.221082 1.272138
N13 -2.397237 0.010384 0.171880
O14 -2.883732 -1.082711 0.378086
O15 -2.779052 1.089797 0.574189

[MIM – H_{ME}]•
N1 -1.406837 -0.775167 -0.000004
C2 -0.138504 -1.092762 0.000000
N3 0.682249 0.023891 0.000000
C4 -0.174079 1.120357 0.000002
C5 -1.440491 0.605594 -0.000002
H6 0.272656 -2.090969 0.000003
C7 2.057370 0.034275 0.000050
H8 2.576500 -0.910116 -0.000119
H9 2.568550 0.982489 -0.000150
H10 0.203802 2.128772 0.000006
H11 -2.375172 1.143971 -0.000007

[MIM – H_2]
N1 1.352689 -0.759375 -0.000025
C2 0.118010 -1.113075 0.000005
N3 -0.768302 -0.004749 -0.000080
C4 0.088461 1.132662 -0.000052
C5 1.346642 0.652296 0.000054
H6 -0.288079 -2.113510 -0.000050
C7 -2.096106 -0.132604 0.000123
H8 -2.500872 0.897744 -0.000173
H9 -0.319984 2.129065 -0.000030
H10 2.276183 1.199899 0.000211

TS for CH_3 elimination of MIM
N1 -1.670687 -0.724855 -0.000018
C2 -0.403085 -1.108152 -0.000022
N3 0.415368 -0.033159 0.000002
C4 -0.358553 1.102154 0.000022
C5 -1.656597 0.651933 0.000010
H6 -0.054533 -2.128675 -0.000041
C7 2.838509 0.027082 0.000004
H8 2.926969 0.565793 0.932520
H9 2.926969 0.565832 -0.932489
H10 2.971784 -1.044942 -0.000019
H11 0.069117 2.091048 0.000043
H12 -2.574709 1.218941 0.000019

[MIM – CH_3]
N1 1.162282 0.374702 -0.000016
C2 -0.003616 1.097554 -0.000020
N3 -1.164614 0.367286 0.000002
C4 -0.734338 -0.877781 0.000022
C5 0.740035 -0.872945 0.000011
H6 -0.007177 2.179194 -0.000041
H7 -1.399907 -1.731545 0.000043
H8 1.410919 -1.722538 0.000021

TS to [MIM-ONO]•
N1 -0.463930 0.121057 -0.086413
C2 0.532061 -0.784043 -0.061550
N3 1.701102 -0.096021 0.028916
C4 1.414897 1.255290 0.042144
C5 0.061670 1.400140 -0.019114
H6 0.392156 -1.848576 -0.083157
C7 3.029484 -0.695825 -0.000637
H8 3.733473 -0.024152 0.489049
H9 3.353736 -0.874109 -1.028797
H10 3.013360 -1.640935 0.542126
H11 2.192564 1.998517 0.091482

H12 -0.583365 2.260046 -0.020103
N13 -1.869429 -0.216261 0.125587
O14 -2.649053 0.749524 -0.045031
O15 -2.089046 -1.447722 0.015995

[MIM-ONO]•
N1 -0.484594 0.107424 -0.000544
C2 0.528627 -0.803810 -0.014503
N3 1.692696 -0.089189 -0.029294
C4 1.391193 1.255909 -0.011015
C5 0.038762 1.399738 0.002673
H6 0.400263 -1.868271 -0.028877
C7 3.022178 -0.678842 0.027251
H8 3.229010 -1.079686 1.023080
H9 3.757560 0.088588 -0.209384
H10 3.103728 -1.480918 -0.708456
H11 2.161738 2.008097 -0.012759
H12 -0.608842 2.256353 0.005919
N13 -1.830504 -0.217112 0.004529
O14 -2.624562 0.750913 0.013673
O15 -2.071839 -1.447163 -0.003522

TS from [MIM-ONO]• to [O-MIM]
N1 -0.281189 -0.020062 0.787586
C2 0.700096 -0.834649 0.423747
N3 1.721142 -0.099884 -0.073247
C4 1.343656 1.229960 -0.033899
C5 0.080932 1.269046 0.488929
H6 0.683674 -1.908021 0.506574
C7 2.981383 -0.620465 -0.595609
H8 3.821722 -0.151544 -0.082237
H9 3.053148 -0.429168 -1.667674
H10 3.017578 -1.695042 -0.423388
H11 1.991295 2.014852 -0.386732
H12 -0.584398 2.094616 0.671835
O13 -2.550836 0.372132 -1.125785
N14 -2.550291 -0.636797 -0.484475
O15 -1.805045 -0.483613 0.884981

O-MIM
N1 -1.187396 -0.173657 0.004833
C2 -0.056763 -0.900604 -0.016887
N3 1.015394 -0.053869 -0.034278
C4 0.543082 1.233462 -0.009785
C5 -0.822390 1.172434 0.010210
H6 -0.023517 -1.974446 -0.029348
C7 2.408530 -0.466569 0.024799
H8 2.670971 -0.825852 1.023364
H9 3.037996 0.387651 -0.222030
H10 2.595643 -1.258152 -0.702882
H11 1.206576 2.081613 -0.010882
H12 -1.577754 1.937228 0.017310
O13 -2.392582 -0.623462 0.010069

For the reaction of EIM + NO_2:

TS for PT to [EIM – H^{β}]• + HONO
C1 2.132630 -1.151907 0.171398
N2 1.476781 -0.034002 -0.280573
N3 3.418207 -0.944047 0.315596
C4 0.036884 0.107698 -0.483353
H5 -0.132131 0.729590 -1.364188
H6 -0.373801 -0.881166 -0.691377
C7 3.619239 0.371739 -0.042828
C8 2.435744 0.954422 -0.410444
H9 2.191306 1.945165 -0.756771
H10 4.602042 0.816012 -0.025543
H11 1.613959 -2.081413 0.355708
C12 -0.613965 0.711792 0.748233
H13 -0.346015 1.749319 0.951119
H14 -1.843004 0.787740 0.508907
H15 -0.560969 0.089301 1.641441
O16 -3.109624 0.801163 0.235793
N17 -3.400623 -0.508271 -0.035718
O18 -4.549769 -0.640261 -0.299852

TS for PT to [EIM – H^{β}]• + O-NH-O
C1 -2.261968 1.072887 0.318167
N2 -1.492055 0.090060 -0.245343
N3 -3.513195 0.702200 0.452588
C4 -0.047702 0.141409 -0.492548
H5 0.145173 -0.199024 -1.512251
H6 0.249428 1.190984 -0.436129
C7 -3.568336 -0.584454 -0.033554
C8 -2.332671 -0.986493 -0.467343
H9 -1.982144 -1.904126 -0.910250
H10 -4.492040 -1.141458 -0.050029
H11 -1.850519 2.033478 0.591951
C12 0.706583 -0.687842 0.514028
H13 0.786328 -1.759278 0.347190
H14 2.246116 -0.306529 0.265620
H15 0.629702 -0.387851 1.556705
O16 4.196500 -0.763531 0.337241
N17 3.323408 0.028724 0.055439
O18 3.436676 1.137765 -0.427753

[EIM – H^{β}]•
C1 0.753837 -1.093831 0.080105
N2 -0.179410 -0.138186 -0.212194
N3 1.952181 -0.582708 0.249731

C4 -1.603065 -0.349790 -0.462950
H5 -1.846503 -0.003211 -1.474356
H6 -1.756804 -1.439201 -0.476234
C7 1.797870 0.770547 0.060034
C8 0.490005 1.069749 -0.225949
H9 -0.015637 1.998859 -0.430562
H10 2.632395 1.450017 0.138076
H11 0.494875 -2.140047 0.153343
C12 -2.482668 0.305199 0.543447
H13 -3.512638 0.529184 0.297312
H14 -2.140954 0.439415 1.561540

[EIM – CH_3]•
C1 -0.138495 -1.092764 0.000000
N2 0.682262 0.023891 -0.000002
N3 -1.406831 -0.775163 0.000002
C4 2.057349 0.034275 -0.000028
H5 2.568455 0.982504 0.000094
H6 2.576424 -0.910121 0.000064
C7 -1.440484 0.605590 0.000003
C8 -0.174070 1.120357 -0.000001
H9 0.203809 2.128773 -0.000009
H10 -2.375164 1.143970 0.000004
H11 0.272664 -2.090971 0.000000

TS for CH_4 elimination of EIM
C1 0.705177 -1.093800 -0.081203
N2 -0.047012 0.018587 -0.443945
N3 1.879432 -0.771729 0.375845
C4 -1.309831 0.063019 -1.011641
H5 -2.189290 0.611089 -0.342227
H6 -1.647810 -0.941576 -1.271745
C7 1.923190 0.617556 0.335992
C8 0.762128 1.120281 -0.165166
H9 0.424366 2.120883 -0.374582
H10 2.798328 1.155898 0.664153
H11 0.314137 -2.094352 -0.198403
C12 -2.727516 0.040347 0.753731
H13 -2.948553 0.992752 1.237827
H14 -3.622159 -0.476361 0.414513
H15 -2.074851 -0.580750 1.356892

[EIM – CH_4]
C1 -0.038554 -1.099773 -0.000012
N2 0.765417 0.078897 -0.000028
N3 -1.293816 -0.836486 0.000014
C4 2.092982 0.216282 0.000027
H5 2.495850 -0.816076 0.000045
C6 -1.391609 0.572867 0.000013
C7 -0.170280 1.141302 -0.000018
H8 0.177546 2.159586 -0.000004
H9 -2.358250 1.050516 0.000034
H10 0.428414 -2.074970 -0.000032

CH_4
H1 -0.747550 0.665324 0.434296
C2 0.000004 0.000015 0.000000
H3 -0.411643 -0.477535 -0.890262
H4 0.885210 0.576297 -0.272769
H5 0.273961 -0.764175 0.728737

[EIM – C_2H_5]•
C1 0.746006 -1.098116 0.014375
N2 -0.123715 -0.087386 -0.287586
N3 1.955548 -0.654955 0.275430
C4 -1.549255 -0.218135 -0.578884
H5 -1.775735 0.388284 -1.460128
H6 -1.725020 -1.260221 -0.854852
C7 1.875067 0.710891 0.142047
C8 0.600891 1.084800 -0.203254
H9 0.156780 2.047056 -0.398740
H10 2.734771 1.344840 0.294550
H11 0.436889 -2.133257 0.019816
C12 -2.444176 0.181558 0.595144
H13 -2.292429 1.227816 0.869713
H14 -3.495657 0.050219 0.325746
H15 -2.233634 -0.434333 1.472424

C_2H_5
C1 0.793854 -0.000001 -0.018131
H2 1.351981 -0.926407 0.040065
H3 1.352099 0.926328 0.040070
C4 -0.693632 0.000028 -0.001995
H5 -1.106599 -0.885635 -0.494467
H6 -1.092279 -0.002037 1.026111
H7 -1.106535 0.887588 -0.491026

TS from EMIM to 2-thyl-1,3-imidazole
C1 -0.304699 0.506261 0.980777
N2 -0.347430 1.181846 -0.249988
N3 -0.977034 -0.649539 1.003153
C4 1.580721 0.520314 0.033219
H5 1.784486 1.215585 -0.769405
H6 1.988465 0.873565 0.973167
C7 -1.444698 -0.762494 -0.262905
C8 -1.052024 0.335790 -1.034208
H9 -1.241778 0.547520 -2.076026
H10 -2.057585 -1.603333 -0.561502
H11 0.005283 1.013239 1.882491
C12 1.773553 -0.918384 -0.298035

H13 0.964529 -1.278695 -0.947171
H14 2.700887 -1.029201 -0.872465
H15 1.809848 -1.553745 0.585669

2-ethyl-1,3-imidazole
C1 -0.073979 -0.001960 -0.823624
N2 0.603762 1.187581 -0.308289
N3 0.604533 -1.188907 -0.303376
C4 -1.587036 -0.001847 -0.539171
H5 -2.007225 0.877929 -1.033976
H6 -2.006377 -0.884875 -1.028869
C7 1.567926 -0.738413 0.412500
C8 1.567422 0.740681 0.409450
H9 2.267546 1.390045 0.925953
H10 2.268480 -1.385128 0.931733
H11 0.066109 -0.004224 -1.913360
C12 -1.953909 0.002382 0.945957
H13 -1.564081 0.889831 1.449964
H14 -3.040461 0.003008 1.064426
H15 -1.564595 -0.882362 1.455109

For the reaction of C_2H_4 + NO_2,
see structures for Figure 5.

Cartesian coordinates for the structures in the reaction of $CH_2CHCH_2DCA + NO_2$ in Table 4, calculated at B3LYP/6-311++ G(d,p)

CH_2CHCH_2DCA

N1 -3.432763 0.754236 -0.329387
C2 -2.518131 0.153749 0.054129
N3 -1.529405 -0.547922 0.584077
C4 -0.410998 -0.801582 0.114238
N5 0.638533 -1.210525 -0.275924
C6 2.041504 -0.818319 -0.276882
H7 2.582454 -1.591327 0.272379
H8 2.383464 -0.877578 -1.314080
C9 2.326355 0.549770 0.311537
H10 3.053439 0.573448 1.118131
C11 1.762421 1.680866 -0.100484
H12 1.033073 1.708089 -0.904819
H13 2.006110 2.629936 0.361798

F4.TS1′

N1 4.224751 -0.887757 0.143028
C2 3.110908 -0.558940 0.157085
N3 1.894559 -0.059543 0.216602
C4 0.769810 -0.503281 -0.116061
N5 -0.444008 -0.196145 -0.259929
N6 -2.249777 -1.932826 0.062504
O7 -2.399224 -1.362741 1.081685
O8 -1.304384 -1.453272 -0.801291
C9 -1.148113 1.046963 -0.660959
H10 -1.347988 0.972728 -1.734002
H11 -2.097153 1.062622 -0.124049
C12 -0.324020 2.258651 -0.338823
H13 0.605654 2.377485 -0.886594
C14 -0.704646 3.175223 0.546119
H15 -1.626320 3.077050 1.110853
H16 -0.107636 4.060424 0.731048

F4.TS2′

N1 -2.900016 2.119579 -0.002686
C2 -1.913001 1.516790 0.159474
N3 -0.795678 0.904121 0.446837
C4 -0.168232 0.061055 -0.330897
N5 0.927200 -0.284958 -0.754610
N6 -2.025732 -1.747300 -0.013917
O7 -2.002196 -1.423825 1.132623
O8 -1.331289 -1.178598 -0.901143
C9 2.112327 0.581901 -0.627904
C10 3.283509 -0.224341 -0.142666
H11 3.535825 -1.095893 -0.740310
C12 3.994662 0.086878 0.936530
H13 4.851498 -0.504634 1.237478
H14 3.750980 0.945123 1.555136
H15 2.316969 0.967564 -1.633242
H16 1.916603 1.433437 0.032511

F4.TS3′

N1 -1.010685 -0.805776 0.210342
C2 -0.356392 0.193829 -0.021425
N3 0.891848 0.607677 0.020138
C4 1.274511 1.886366 -0.017915
N5 1.650380 2.979833 -0.068297
N6 2.613454 -1.043080 -0.483299
O7 3.440787 -1.754840 -0.083919
O8 2.029439 -0.303235 0.633248
C9 -2.396140 -1.201580 -0.007295
C10 -3.287060 -0.074116 -0.455044
H11 -2.983281 0.436404 -1.365631
C12 -4.389157 0.294550 0.189262
H13 -4.706651 -0.194582 1.105041
H14 -5.016570 1.098143 -0.178622
H15 -2.764078 -1.639311 0.923393
H16 -2.380784 -2.000921 -0.756500

F4.TS4′

N1 1.289791 -1.439654 -0.021283
C2 0.115303 -1.511300 -0.135539
N3 -1.099456 -1.783083 -0.236676
C4 -2.119133 -1.066239 0.196111
N5 -3.260916 -0.897447 0.505797
N6 -1.970124 1.627773 -0.390801
O7 -1.326608 2.630740 -0.391667
O8 -1.418548 0.716006 0.455146
C9 2.492204 -0.807102 -0.548593
C10 2.652493 0.591684 -0.015057
H11 1.825561 1.271357 -0.201966
C12 3.736153 1.003927 0.633639
H13 4.567912 0.337994 0.841851
H14 3.830143 2.027418 0.976603
H15 3.342705 -1.427643 -0.265670
H16 2.417750 -0.802028 -1.641275

F4.TS5′

N1 2.299222 -1.235303 0.373826
C2 1.218793 -0.971031 -0.068967
N3 0.085878 -0.916499 -0.560406
C4 -1.015161 -0.242058 -0.291894
N5 -2.214198 -0.468226 -0.141166
N6 -4.277259 0.848834 0.187596
O7 -4.764731 -0.223913 0.251473
O8 -2.947651 0.942951 -0.011277

C9 3.636412 -0.646320 0.378643
C10 3.735050 0.633816 -0.402841
H11 3.478210 0.568664 -1.457745
C12 4.118781 1.792638 0.123686
H13 4.378514 1.884718 1.173874
H14 4.192456 2.690786 -0.478325
H15 3.923264 -0.493230 1.421438
H16 4.307859 -1.407150 -0.031527

F4.TS6′
N1 -4.613390 -1.297190 0.784328
C2 -3.946418 -0.515928 0.227910
N3 -3.265629 0.331893 -0.498149
C4 -2.242501 0.984474 -0.085596
N5 -1.301978 1.643432 0.183611
N6 3.363365 -0.409173 0.264234
O7 4.505589 -0.743685 0.402712
O8 2.983291 0.777572 0.295759
C9 0.962244 0.885712 0.044458
H10 0.816738 0.654215 1.088242
H11 1.077469 1.925225 -0.210630
C12 0.744450 -0.109888 -0.964030
H13 0.743990 0.211836 -1.999548
C14 0.645336 -1.414115 -0.650685
H15 0.554056 -2.175303 -1.416399
H16 0.641463 -1.751317 0.380060

[$CH_2CHCH_2NC(-ONO)NCN$]•
N1 -2.763454 -2.538095 -0.069454
C2 -1.775610 -1.906734 -0.114423
N3 -0.624179 -1.316362 -0.236060
C4 -0.443842 -0.037138 0.175780
N5 0.669343 0.622642 -0.020291
N6 -1.872849 2.084477 0.339690
O7 -1.324114 2.457197 -0.575524
O8 -1.448743 0.570007 0.832891
C9 1.779539 -0.007852 -0.708264
C10 3.056480 0.240941 0.056692
H11 3.266644 1.278548 0.300513
C12 3.894261 -0.725004 0.419323
H13 3.693544 -1.768920 0.199125
H14 4.814502 -0.504321 0.948132
H15 1.627127 -1.074093 -0.894384
H16 1.854034 0.497252 -1.684170

[$CH_2CHCH_2NCNC(-ONO)N$]•
N1 1.914703 -1.290211 -0.042970
C2 0.824857 -0.840487 -0.248955
N3 -0.321619 -0.517144 -0.587068
C4 -1.322247 -0.051918 0.263530
N5 -1.307627 -0.117788 1.526840
N6 -3.728192 -0.072745 0.104567
O7 -4.591731 0.519805 -0.346915
O8 -2.365656 0.500375 -0.418750
C9 3.282846 -0.790351 0.034424
C10 3.442465 0.614354 -0.476769
H11 3.148754 0.779934 -1.510782
C12 3.916370 1.618425 0.254421
H13 4.210746 1.480944 1.290443
H14 4.029487 2.614430 -0.157707
H15 3.603641 -0.865922 1.076524
H16 3.899867 -1.485746 -0.542646

CH_2CHCH_2ONO
N1 -1.493017 -0.394269 0.334495
O2 -2.516712 -0.539349 -0.211813
O3 -0.740605 0.665263 -0.251196
C4 0.546693 0.800516 0.400040
C5 1.634221 0.162598 -0.410028
H6 1.716286 0.498894 -1.440450
C7 2.475524 -0.748902 0.069987
H8 2.406852 -1.105373 1.093325
H9 3.265397 -1.169703 -0.541472
H10 0.698627 1.879119 0.491110
H11 0.483873 0.364363 1.400108

[$CH_2CHCH_2N(-ONO)CNCN$]•
N1 4.089999 -0.865973 -0.035845
C2 2.962031 -0.587329 -0.018018
N3 1.719772 -0.174198 0.081212
C4 0.631617 -0.598758 -0.398614
N5 -0.587655 -0.126490 -0.170658
N6 -2.221356 -1.984473 -0.171521
O7 -1.640503 -2.268955 0.766132
O8 -1.616098 -0.653135 -0.895342
C9 -0.920301 1.057535 0.663144
C10 -0.996604 2.319849 -0.146798
H11 -1.727960 2.326611 -0.950316
C12 -0.237497 3.386533 0.086536
H13 0.503323 3.398280 0.879899
H14 -0.331442 4.287507 -0.508406
H15 -1.878948 0.831843 1.137487
H16 -0.152969 1.123446 1.435209

[CH_2CHCH_2NCNCN-ONO]•
N1 2.348739 -1.251160 0.223766
C2 1.215463 -0.956256 -0.019652
N3 0.033670 -0.823198 -0.353003
C4 -1.027146 -0.320851 0.300880
N5 -2.185572 -0.156265 -0.153386

N6 -4.417346 0.565515 0.291262
O7 -4.571446 0.240650 -0.812954
O8 -3.060094 0.387061 0.816053
C9 3.678544 -0.661638 0.125227
C10 3.687053 0.703818 -0.503638
H11 3.292776 0.764142 -1.515435
C12 4.149272 1.792834 0.102709
H13 4.544078 1.759445 1.113618
H14 4.153084 2.757177 -0.391801
H15 4.101599 -0.631555 1.132077
H16 4.285246 -1.362577 -0.456871

[$CH_2CHCH_2NCN(-ONO)CN]^{\bullet}$
N1 -0.999371 -0.423672 -0.527696
C2 0.011789 -1.029432 -0.175279
N3 1.307118 -0.591087 -0.168156
C4 2.324906 -1.360008 0.248705
N5 3.221811 -1.998258 0.604365
N6 1.509576 1.736389 0.443323
O7 1.736912 2.767306 0.011212
O8 1.667547 0.654223 -0.698932
C9 -2.397238 -0.841289 -0.549665
C10 -3.180650 -0.204515 0.566856
H11 -2.820880 -0.412417 1.571722
C12 -4.257035 0.553606 0.383523
H13 -4.805814 0.970280 1.220151
H14 -4.631578 0.781311 -0.609864
H15 -2.817055 -0.551258 -1.515525
H16 -2.444909 -1.933929 -0.472418

$CH_2CHCH_2NC(O)NCN$
N1 3.323202 -1.164486 -0.457780
C2 2.385065 -0.643564 -0.023839
N3 1.336248 -0.061223 0.583706
C4 0.605607 0.994846 -0.021321
N5 -0.051245 -0.178466 -0.235085
O6 0.616865 2.164598 -0.179536
C7 -1.198914 -0.579016 0.618433
C8 -2.446740 0.057997 0.072705
H9 -2.500201 1.141624 0.134621
C10 -3.453387 -0.635848 -0.450032
H11 -3.421088 -1.717847 -0.529377
H12 -4.349425 -0.144079 -0.810072
H13 -1.261442 -1.666272 0.577667
H14 -1.009993 -0.267470 1.651890

$CH_2CHCH_2NCNCNO$
N1 1.223132 -1.292344 0.307299
C2 0.144089 -0.929336 -0.070019
N3 -0.983993 -0.746923 -0.545384
C4 -2.041787 -0.127389 -0.031145
N5 -3.121877 0.304428 0.035535
O6 -4.217349 0.799093 0.231619
C7 2.575557 -0.734045 0.282997
C8 2.679794 0.578908 -0.440268
H9 2.382307 0.571063 -1.486520
C10 3.112085 1.702596 0.123890
H11 3.413344 1.738835 1.166469
H12 3.185770 2.626342 -0.438115
H13 2.908237 -0.638648 1.319190
H14 3.209888 -1.490873 -0.188854

$CH_2CHCH_2NCNC(O)N$
N1 0.866714 -1.175360 0.337868
C2 -0.190925 -0.827732 -0.073034
N3 -1.320868 -0.640631 -0.565870
C4 -2.279117 0.143952 -0.016511
N5 -2.502130 0.873885 0.998421
O6 -3.455076 0.409300 -0.472939
C7 2.282002 -0.839822 0.357260
C8 2.620434 0.341173 -0.510142
H9 2.383027 0.239242 -1.566288
C10 3.186142 1.452504 -0.050466
H11 3.428022 1.578651 1.000365
H12 3.431450 2.276104 -0.710628
H13 2.563868 -0.658566 1.396805
H14 2.817012 -1.735540 0.027681

$CH_2CHCH_2N(O)CNCN$
N1 4.039991 -0.709587 -0.177418
C2 2.942029 -0.450429 0.081919
N3 1.694786 -0.237466 0.518981
C4 0.811008 0.367534 -0.111115
N5 -0.398043 0.823699 -0.100477
O6 -0.702135 1.984590 0.334877
C7 -1.453840 0.044155 -0.840781
C8 -2.576707 -0.296506 0.092068
H9 -3.057105 0.545507 0.578650
C10 -2.986888 -1.543077 0.306906
H11 -2.514284 -2.395597 -0.171151
H12 -3.821310 -1.753708 0.965356
H13 -1.775102 0.706845 -1.648249
H14 -0.985874 -0.846348 -1.265214

$CH_2CHCH_2NCN(O)CN$
N1 0.599424 -0.542356 -0.575658
C2 -0.460080 -0.130961 -0.200481
N3 -1.609672 0.443013 -0.085964
C4 -2.716206 -0.349673 0.079982
N5 -3.679852 -0.972428 0.210246

O6 -1.732304 1.765221 -0.034022
C7 1.805855 -0.948801 0.183027
C8 2.703451 0.239049 0.394361
H9 2.282813 1.054554 0.976589
C10 3.943556 0.312273 -0.077432
H11 4.379056 -0.485615 -0.670546
H12 4.569535 1.174604 0.119080
H13 2.306574 -1.714141 -0.408263
H14 1.491697 -1.380097 1.138208

F4.TS1
N1 -4.258158 -0.052646 0.352849
C2 -3.150283 0.043200 0.017883
N3 -1.932859 0.270154 -0.427351
C4 -0.829023 -0.295660 -0.249845
N5 0.407822 -0.226526 -0.457396
C6 1.290132 0.913503 -0.783620
H7 2.210329 0.492411 -1.192851
H8 0.780646 1.463244 -1.579265
N9 1.272185 -1.619786 0.122404
O10 2.460170 -1.537159 0.012669
O11 0.556538 -2.485122 0.510443
C12 1.570025 1.793288 0.400511
H13 2.142260 1.343440 1.207555
C14 1.170287 3.058954 0.483209
H15 0.598547 3.531163 -0.309660
H16 1.404793 3.669907 1.346959

F4.TS2
N1 0.691861 -0.934845 0.356661
C2 -0.402929 -0.553573 -0.036682
N3 -1.475323 -1.082135 -0.610962
C4 -2.689222 -0.992987 -0.195020
N5 -3.831704 -1.018598 0.090585
N6 -0.729100 1.248355 -0.033093
O7 -1.750553 1.611335 0.487771
O8 0.164571 1.903297 -0.512172
C9 1.864621 -0.198211 0.820349
C10 2.877663 -0.063687 -0.287960
H11 2.562438 0.528697 -1.141840
C12 4.090356 -0.605821 -0.245745
H13 4.799895 -0.463382 -1.052558
H14 4.419913 -1.205997 0.596661
H15 1.583546 0.791507 1.195111
H16 2.288987 -0.771642 1.645842

F4.TS4
N1 3.119851 -1.185397 -0.556845
C2 1.965165 -0.852587 -0.355952
N3 0.725338 -1.345525 -0.441999
C4 -0.298658 -1.073297 0.207172
N5 -1.325266 -1.044983 0.809603
N6 1.919567 0.922769 0.133507
O7 0.803910 1.298385 0.421507
O8 2.945462 1.535651 0.139898
C9 -2.511216 -0.199904 0.919800
C10 -3.229276 -0.057889 -0.394990
H11 -3.590710 -0.980591 -0.841389
C12 -3.436896 1.109404 -0.996159
H13 -3.078532 2.042515 -0.572559
H14 -3.976369 1.173011 -1.934031
H15 -3.159743 -0.665059 1.665232
H16 -2.200771 0.775427 1.302419

F4.TS5
N1 2.136244 -1.275105 0.198341
C2 1.086064 -0.920551 -0.255045
N3 -0.005125 -0.703209 -0.792589
C4 -1.192910 -0.309602 -0.406121
N5 -2.032977 0.563477 -0.613601
N6 -3.446198 0.244927 0.196750
O7 -4.243878 1.126175 0.071904
O8 -3.526722 -0.795298 0.793196
C9 3.481451 -0.715823 0.339761
C10 3.636359 0.645051 -0.278207
H11 3.447052 0.707502 -1.347387
C12 3.988388 1.730234 0.404388
H13 4.180309 1.696174 1.472523
H14 4.102681 2.691925 -0.082035
H15 3.712657 -0.691795 1.406996
H16 4.162388 -1.437312 -0.121867

F4.TS6
N1 4.638410 0.559888 -0.999145
C2 3.847064 -0.126700 -0.486380
N3 3.012617 -0.994274 0.032554
C4 1.999339 -0.697375 0.746533
N5 1.054514 -0.542474 1.445258
N6 -2.982980 -0.523958 -0.304050
O7 -3.724027 0.417876 -0.282195
O8 -3.173978 -1.673767 -0.594717
C9 -0.922012 -0.124649 0.375573
H10 -0.686428 -1.052884 -0.119510
H11 -1.302654 -0.179303 1.384117
C12 -0.671793 1.147820 -0.239109
H13 -0.234607 1.149394 -1.232632
C14 -0.987500 2.308073 0.359533
H15 -1.426063 2.332382 1.351249
H16 -0.814712 3.260244 -0.127145

$CH_2CHCH_2NO_2$

N1 -1.063080 -0.017863 0.003183
O2 -1.700259 -0.993175 -0.357127
O3 -1.381698 1.147104 -0.173404
C4 0.242526 -0.268746 0.753553
C5 1.387600 0.423373 0.082210
H6 1.304396 1.501552 -0.007292
C7 2.459130 -0.221876 -0.369005
H8 2.555101 -1.300210 -0.291384
H9 3.282715 0.311304 -0.829099
H10 0.057132 0.132803 1.753098
H11 0.362333 -1.348352 0.796105

$[CH_2CHCH_2NC(-NO_2)NCN]^\bullet$

N1 0.730081 -0.874426 0.458170
C2 -0.449415 -0.442045 0.216522
N3 -1.495628 -1.275978 0.111527
C4 -2.705281 -0.900271 -0.149701
N5 -3.841033 -0.688347 -0.366021
N6 -0.723926 1.060092 0.027889
O7 -1.068715 1.413280 -1.084107
O8 -0.547690 1.767937 1.004118
C9 1.883822 -0.008766 0.595874
C10 3.109035 -0.680164 0.031642
H11 3.295141 -1.690821 0.382736
C12 3.931325 -0.092433 -0.830400
H13 3.752081 0.912208 -1.201025
H14 4.818471 -0.596619 -1.195310
H15 1.749292 0.990317 0.167153
H16 2.012881 0.127877 1.681780

$[CH_2CHCH_2NCNC(-NO_2)N]^\bullet$

N1 3.272684 -0.893884 0.481378
C2 2.101038 -0.619174 0.132768
N3 1.068656 -1.456138 -0.110496
C4 -0.153659 -1.247441 -0.011998
N5 -1.331997 -1.273201 0.143330
N6 1.825459 0.928268 -0.120629
O7 0.684563 1.216819 -0.437023
O8 2.754052 1.685270 0.026030
C9 -2.566908 -0.781205 -0.453821
C10 -2.844216 0.645892 -0.061795
H11 -2.072973 1.365801 -0.320336
C12 -3.960719 1.032897 0.546250
H13 -4.737177 0.325874 0.822063
H14 -4.139590 2.074305 0.786798
H15 -2.479988 -0.871286 -1.542166
H16 -3.376020 -1.432541 -0.121918

$[CH_2CHCH_2N(-NO_2)CNCN]^\bullet$

N1 3.998709 -1.201014 0.061938
C2 2.945271 -0.711907 0.035985
N3 1.814996 -0.046682 0.010401
C4 0.609109 -0.376422 -0.036125
N5 -0.516061 0.319752 -0.064903
N6 -0.530295 1.831267 0.020157
O7 -1.635897 2.309412 0.133089
O8 0.536447 2.378165 -0.031452
C9 -1.858539 -0.316394 -0.050810
C10 -1.769436 -1.761003 -0.446860
H11 -1.370580 -1.964453 -1.436616
C12 -2.202326 -2.756064 0.321819
H13 -2.605533 -2.579510 1.313868
H14 -2.168631 -3.784343 -0.017637
H15 -2.294120 -0.204231 0.944232
H16 -2.481452 0.239398 -0.754152

$[CH_2CHCH_2NCNCN\text{-}NO_2]^\bullet$

N1 2.148108 -1.200678 0.223675
C2 1.052015 -0.960532 -0.166836
N3 -0.085020 -0.874843 -0.657461
C4 -1.219604 -0.385349 -0.148422
N5 -2.315789 -0.196926 -0.730233
N6 -3.381176 0.325321 0.125335
O7 -3.830607 1.392894 -0.222269
O8 -3.762082 -0.383729 1.031093
C9 3.501857 -0.676213 0.308393
C10 3.653514 0.673937 -0.336316
H11 3.410421 0.725717 -1.394870
C12 4.069165 1.756353 0.313411
H13 4.183864 2.708513 -0.191130
H14 4.314931 1.729878 1.370600
H15 3.776479 -0.641192 1.364911
H16 4.151272 -1.415537 -0.170700

Cartesian coordinates for the structures in the reaction of $AMIM^+ + NO_2$ in Table 6, calculated at B3LYP/6-311++G(d,p)

$[MIM^+CH_2CHCH]^\bullet$

C1	0.868266	-0.884019	-0.088038
N2	-0.268820	-0.197062	-0.240308
N3	1.881298	-0.021329	0.039755
C4	-1.620578	-0.785939	-0.436432
H5	-1.932700	-0.576861	-1.459996
H6	-1.505256	-1.866286	-0.325885
C7	3.296404	-0.374044	0.233642
H8	3.645283	0.034353	1.181577
H9	3.886204	0.030255	-0.588351
C10	1.372746	1.262164	-0.033009
C11	0.027617	1.152300	-0.206959
H12	-0.735156	1.906616	-0.296515
H13	2.001778	2.132638	0.046927
H14	0.954794	-1.957963	-0.073481
H15	3.391880	-1.457805	0.249025
C16	-2.615571	-0.244778	0.569575
H17	-2.383047	-0.433046	1.618229
C18	-3.718191	0.376240	0.240575
H19	-4.275278	0.705292	-0.623787

$TS1^\gamma$

C1	2.007832	-0.827158	-0.085634
N2	1.128660	0.156428	-0.303155
N3	3.218042	-0.291984	0.101668
C4	-0.318683	-0.023735	-0.570216
H5	-0.521792	0.333343	-1.582822
H6	-0.508471	-1.103173	-0.567288
C7	4.458821	-1.036137	0.370492
H8	4.867016	-0.724538	1.331332
H9	5.178120	-0.839607	-0.423879
C10	3.108219	1.082553	0.000072
C11	1.800880	1.363343	-0.251919
H12	1.298481	2.304803	-0.394978
H13	3.957661	1.734818	0.113585
H14	1.777388	-1.879753	-0.066694
H15	4.233382	-2.100156	0.400314
C16	-1.173931	0.665912	0.444255
H17	-0.870041	0.591103	1.483973
C18	-2.448413	1.139093	0.126788
H19	-2.657019	1.437942	-0.897526
H20	-2.994984	1.697134	0.877546
N21	-3.640479	-0.365022	0.060738
O22	-4.775971	-0.106338	0.334738
O23	-3.137985	-1.410049	-0.271157

$[MIM^+CH_2CHCH_2NO_2]^\bullet$

C1	1.905683	-0.774272	-0.177994
N2	1.100502	0.277749	-0.361305
N3	3.132959	-0.333354	0.112625
C4	-0.337895	0.204778	-0.693239
H5	-0.499355	0.769921	-1.617211
H6	-0.565146	-0.842388	-0.924898
C7	4.310997	-1.174219	0.380082
H8	4.684221	-0.965997	1.382210
H9	5.082564	-0.961804	-0.359210
C10	3.111743	1.049320	0.115617
C11	1.839752	1.431885	-0.179482
H12	1.405474	2.412383	-0.276222
H13	3.991857	1.635145	0.320795
H14	1.610533	-1.808127	-0.253708
H15	4.021032	-2.220652	0.311329
C16	-1.204421	0.698093	0.417111
H17	-0.831677	0.633236	1.433303
C18	-2.638661	0.960946	0.196724
H19	-2.852584	1.463676	-0.750514
H20	-3.106676	1.512741	1.008632
N21	-3.471843	-0.360077	0.086582
O22	-4.648749	-0.275330	0.345705
O23	-2.875596	-1.361863	-0.282297

$TS2^\gamma$

C1	-2.014266	-0.822331	0.336608
N2	-1.224932	0.257631	0.336271
N3	-3.233020	-0.466739	-0.079313
C4	0.199217	0.287062	0.745003
H5	0.288166	0.926755	1.624931
H6	0.459484	-0.730736	1.051753
C7	-4.392799	-1.362466	-0.219193
H8	-4.730237	-1.358048	-1.255037
H9	-5.193007	-1.023106	0.437669
C10	-3.222958	0.887925	-0.355614
C11	-1.966665	1.341515	-0.096512
H12	-1.543261	2.327670	-0.184039
H13	-4.098352	1.407123	-0.707859
H14	-1.715887	-1.816265	0.627374
H15	-4.096213	-2.371042	0.061247
C16	1.100225	0.737452	-0.365808
H17	0.943528	0.286613	-1.341529
C18	2.185912	1.525751	-0.146013
H19	2.333592	2.042024	0.794780
H20	2.829814	1.813971	-0.966513
N21	4.020436	-0.596929	-0.549854
O22	4.862139	-1.372433	-0.230044
O23	3.419485	-0.056585	0.544627

[MIM$^+$CH$_2$CHCH$_2$ONO]$^\bullet$

C1 -2.063220 -0.824388 0.284844
N2 -1.259354 0.242614 0.330269
N3 -3.284404 -0.430552 -0.089753
C4 0.172887 0.230498 0.709052
H5 0.286099 0.830731 1.617500
H6 0.415020 -0.803244 0.987566
C7 -4.458013 -1.301587 -0.259446
H8 -4.811051 -1.237649 -1.288157
H9 -5.244066 -0.988039 0.426742
C10 -3.259433 0.937138 -0.290651
C11 -1.992123 1.358072 -0.028963
H12 -1.555002 2.341179 -0.068473
H13 -4.133331 1.487007 -0.596866
H14 -1.773509 -1.836675 0.514127
H15 -4.171734 -2.327679 -0.037925
C16 1.057799 0.724061 -0.385521
H17 0.780616 0.505689 -1.411907
C18 2.461296 1.100404 -0.056868
H19 2.506081 1.825137 0.762814
H20 2.975874 1.518797 -0.925251
N21 4.340959 -0.344968 -0.491919
O22 4.908371 -1.285969 -0.141771
O23 3.170309 -0.080292 0.384892

TS3$^\gamma$

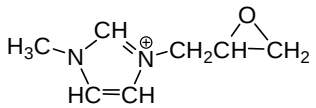
C1 2.421979 0.399355 -0.750821
N2 1.341607 0.680712 -0.014131
N3 3.222684 -0.410661 -0.051976
C4 0.215166 1.557580 -0.425116
H5 0.219685 2.437713 0.218786
H6 0.429892 1.880279 -1.446283
C7 4.510489 -0.956262 -0.509736
H8 4.453013 -2.043832 -0.540725
H9 5.299260 -0.641664 0.172719
C10 2.632456 -0.656919 1.173757
C11 1.455058 0.024528 1.197275
H12 0.694269 0.089136 1.956203
H13 3.092767 -1.289104 1.914250
H14 2.616699 0.767524 -1.744636
H15 4.721218 -0.575314 -1.506874
C16 -1.106564 0.823627 -0.364333
H17 -1.183936 -0.079580 -0.964383
C18 -2.130077 1.252883 0.340120
H19 -2.281939 2.111261 0.986877
H20 -3.513211 0.517658 0.292816
N21 -4.460993 -1.146618 -0.163951
O22 -3.405277 -1.549822 -0.529785
O23 -4.502454 0.086465 0.317883

[MIM$^+$CH$_2$CHCH]$^\bullet$

C1 0.868266 -0.884019 -0.088038
N2 -0.268820 -0.197062 -0.240308
N3 1.881298 -0.021329 0.039755
C4 -1.620578 -0.785939 -0.436432
H5 -1.932700 -0.576861 -1.459996
H6 -1.505256 -1.866286 -0.325885
C7 3.296404 -0.374044 0.233642
H8 3.645283 0.034353 1.181577
H9 3.886204 0.030255 -0.588351
C10 1.372746 1.262164 -0.033009
C11 0.027617 1.152300 -0.206959
H12 -0.735156 1.906616 -0.296515
H13 2.001778 2.132638 0.046927
H14 0.954794 -1.957963 -0.073481
H15 3.391880 -1.457805 0.249025
C16 -2.615571 -0.244778 0.569575
H17 -2.383047 -0.433046 1.618229
C18 -3.718191 0.376240 0.240575
H19 -4.275278 0.705292 -0.623787

TS5$^\gamma$

C1 -2.221039 -0.918585 0.014132
N2 -1.228854 -0.049253 0.223148
N3 -3.382827 -0.255659 -0.008114
C4 0.225264 -0.395789 0.321215
H5 0.550547 -0.166485 1.337078
H6 0.278149 -1.478869 0.187488
C7 -4.711350 -0.849276 -0.220562
H8 -5.154099 -0.436260 -1.126479
H9 -5.346254 -0.633806 0.638201
C10 -3.120811 1.086706 0.194192
C11 -1.773458 1.215112 0.336488
H12 -1.164920 2.087477 0.501399
H13 -3.904094 1.825349 0.219415
H14 -2.104479 -1.981931 -0.115033
H15 -4.603744 -1.926626 -0.328731
C16 1.040569 0.339814 -0.689544
H17 0.929123 0.074796 -1.733611
C18 2.195627 1.157219 -0.285261
H19 2.106019 1.675259 0.676426
H20 2.579554 1.830010 -1.056120
N21 4.797808 0.029517 0.180481
O22 5.212610 -1.018202 0.206497
O23 2.877701 -0.075842 -0.205572



C1 1.253271 -0.861548 -0.133867
N2 0.188110 -0.098485 -0.403299
N3 2.304917 -0.071075 0.099628
C4 -1.173633 -0.595263 -0.695567
H5 -1.523987 -0.120892 -1.613177
H6 -1.093711 -1.667713 -0.882234
C7 3.668907 -0.521162 0.420493
H8 3.973481 -0.096387 1.376268
H9 4.351170 -0.201474 -0.366585
C10 1.898471 1.244443 -0.023742
C11 0.574463 1.227493 -0.336629
H12 -0.113428 2.035368 -0.517931
H13 2.576916 2.069169 0.115498
H14 1.262144 -1.938970 -0.114435
H15 3.676040 -1.607060 0.488496
C16 -2.136672 -0.335674 0.447504
H17 -1.824854 -0.728002 1.415012
C18 -3.114694 0.764013 0.404751
H19 -3.133180 1.443447 -0.444237
H20 -3.512258 1.156679 1.335567
O21 -3.488775 -0.586383 0.104474

TS6$^{\gamma}$
C1 2.428697 -0.908297 0.026281
N2 1.271991 -0.316699 -0.289817
N3 3.388379 0.020651 0.080909
C4 -0.043950 -1.004325 -0.457717
H5 -0.308405 -0.950760 -1.516243
H6 0.132609 -2.053492 -0.205171
C7 4.803533 -0.218068 0.405709
H8 5.065928 0.331706 1.309062
H9 5.425760 0.109322 -0.426496
C10 2.824095 1.248795 -0.209609
C11 1.499670 1.038672 -0.439861
H12 0.710846 1.730188 -0.682601
H13 3.403769 2.156352 -0.224971
H14 2.565881 -1.961629 0.207080
H15 4.953320 -1.282771 0.572629
C16 -1.094085 -0.390074 0.405390
H17 -0.994095 -0.452177 1.484599
C18 -2.258280 0.248608 -0.129578
H19 -3.106391 -0.813384 -0.278201
H20 -2.218160 0.490343 -1.209624
N21 -4.385967 -0.369903 0.319775
O22 -5.278974 -0.067761 -0.312571
O23 -3.034771 0.976021 0.636343

[MIM^{+}CH$_2$CHCHO]$^{\bullet}$
C1 1.405018 -0.878989 -0.021833
N2 0.283365 -0.235255 -0.365408
N3 2.386319 0.014906 0.128111
C4 -1.035618 -0.865854 -0.625525
H5 -1.307077 -0.663619 -1.664405
H6 -0.885585 -1.946881 -0.531155
C7 3.777735 -0.285536 0.504283
H8 4.016350 0.219610 1.439606
H9 4.446565 0.052609 -0.286395
C10 1.875013 1.273721 -0.127538
C11 0.558973 1.118514 -0.435194
H12 -0.192828 1.845954 -0.690871
H13 2.482236 2.161433 -0.070020
H14 1.501470 -1.944121 0.110643
H15 3.884451 -1.360447 0.634634
C16 -2.082944 -0.385942 0.322841
H17 -1.883918 -0.404614 1.390404
C18 -3.375688 0.056832 -0.109634
H19 -3.569693 0.068232 -1.199185
O20 -4.239336 0.414726 0.685428

TS7$^{\gamma}$
C1 2.466434 -0.675985 0.338849
N2 1.249509 -0.642314 -0.212940
N3 3.077387 0.491933 0.112585
C4 0.244341 -1.757205 -0.176616
H5 0.095853 -2.080574 -1.210433
H6 0.730798 -2.570275 0.365360
C7 4.429519 0.860403 0.560207
H8 4.371303 1.733693 1.209102
H9 5.051831 1.078883 -0.307016
C10 2.218927 1.299208 -0.610287
C11 1.074660 0.590853 -0.811368
H12 0.162861 0.860963 -1.315471
H13 2.491151 2.295334 -0.916105
H14 2.887161 -1.508079 0.878799
H15 4.858300 0.026929 1.112815
C16 -1.035100 -1.317311 0.450457
H17 -1.138793 -1.317194 1.530313
C18 -2.252818 -1.114744 -0.355055
H19 -2.207094 -2.291326 -0.136920
H20 -2.068494 -1.040583 -1.444785
N21 -3.570661 1.458332 -0.013059
O22 -4.565939 1.702548 0.459345
O23 -3.359597 -0.659391 0.122044

MIM^{+}CH$_2$CH$_2$CHO
C1 1.175857 -0.799563 -0.117084

N2 0.253194 0.152337 -0.291251
N3 2.370666 -0.222179 0.045634
C4 -1.192175 -0.080633 -0.501836
H5 -1.499926 0.510402 -1.364558
H6 -1.318785 -1.127641 -0.774764
C7 3.647256 -0.923757 0.254312
H8 4.076109 -0.619421 1.208445
H9 4.330951 -0.681047 -0.558496
C10 2.206652 1.147917 -0.028852
C11 0.882654 1.381972 -0.239351
H12 0.347430 2.307787 -0.365121
H13 3.034229 1.830467 0.066421
H14 0.987517 -1.860604 -0.115991
H15 3.463562 -1.996141 0.264966
C16 -2.028400 0.262610 0.730976
H17 -1.689679 -0.292454 1.614472
C18 -3.493450 -0.071713 0.497898
H19 -1.957172 1.324572 0.993775
H20 -4.175483 0.173227 1.333945
O21 -3.894517 -0.572657 -0.520017

TS1$^{\beta}$
C1 -1.669392 -0.793240 0.201876
N2 -0.841710 0.232966 0.431990
N3 -2.871073 -0.313290 -0.129507
C4 0.581403 0.105259 0.818886
H5 0.736696 0.696829 1.722177
H6 0.746453 -0.945078 1.059838
C7 -4.061827 -1.116232 -0.451969
H8 -4.391664 -0.883755 -1.463920
H9 -4.853745 -0.891449 0.261700
C10 -2.810897 1.068079 -0.110411
C11 -1.541435 1.410105 0.239988
H12 -1.084100 2.376574 0.365603
H13 -3.665353 1.681806 -0.340968
H14 -1.407094 -1.836157 0.275277
H15 -3.804293 -2.171387 -0.387646
C16 1.515115 0.543993 -0.296821
H17 1.224719 0.163226 -1.275871
C18 2.044044 1.855192 -0.279366
H19 2.132198 2.408236 0.649073
H20 2.506909 2.278097 -1.160785
N21 2.933431 -0.660830 -0.125552
O22 4.016276 -0.235682 -0.403182
O23 2.605308 -1.780294 0.193669

[MIM^{+}CH$_2$CH(-NO$_2$)CH$_2$]$^{\bullet}$
C1 -1.281835 -0.222970 0.695500
N2 -0.533663 0.813387 0.291039
N3 -2.447433 -0.188756 0.047981
C4 0.829719 1.124851 0.761779
H5 0.911806 2.209735 0.834949
H6 0.945008 0.703566 1.758820
C7 -3.545219 -1.157103 0.204608
H8 -3.736902 -1.642628 -0.751645
H9 -4.439107 -0.637971 0.548665
C10 -2.450770 0.904339 -0.800549
C11 -1.254928 1.532406 -0.648349
H12 -0.867261 2.422614 -1.114218
H13 -3.294085 1.141818 -1.426771
H14 -0.974030 -0.970780 1.406934
H15 -3.252670 -1.904854 0.938669
C16 1.932759 0.607063 -0.163642
H17 1.789365 0.921392 -1.198307
C18 3.287052 0.936693 0.325889
H19 3.488808 0.990502 1.388502
H20 4.112351 0.986059 -0.370489
N21 1.808494 -0.966235 -0.268961
O22 2.196276 -1.466722 -1.298625
O23 1.356757 -1.555766 0.704009

TS2$^{\beta}$
C1 -1.786091 -0.801767 0.361608
N2 -1.054443 0.317418 0.410375
N3 -3.000062 -0.504526 -0.109817
C4 0.349363 0.400242 0.877052
H5 0.394153 1.129690 1.686539
H6 0.608770 -0.576420 1.285249
C7 -4.105085 -1.456246 -0.310078
H8 -4.397920 -1.454364 -1.359407
H9 -4.948974 -1.167629 0.315661
C10 -3.047121 0.852216 -0.372475
C11 -1.829978 1.366432 -0.048308
H12 -1.456816 2.374713 -0.105006
H13 -3.930941 1.330277 -0.760095
H14 -1.450065 -1.782004 0.658015
H15 -3.768896 -2.452219 -0.029277
C16 1.290962 0.759979 -0.248775
H17 1.194121 0.174051 -1.156692
C18 1.968428 1.946828 -0.286277
H19 1.998087 2.610437 0.571309
H20 2.573138 2.211284 -1.144618
N21 3.731596 -0.613582 -0.535409
O22 4.510524 -1.448337 -0.221541
O23 2.789830 -0.451547 0.452266

[MIM^{+}CH$_2$CH(-ONO)CH$_2$]$^{\bullet}$
C1 -1.690360 -0.872989 0.248699
N2 -0.936254 0.198338 0.522660
N3 -2.908279 -0.463959 -0.117610

C4 0.481505 0.160438 0.932944
H5 0.629552 0.922010 1.699233
H6 0.670193 -0.813445 1.384266
C7 -4.036710 -1.334373 -0.483312
H8 -4.359126 -1.101496 -1.497558
H9 -4.857318 -1.177474 0.216049
C10 -2.935815 0.917590 -0.077425
C11 -1.702332 1.331586 0.321382
H12 -1.312777 2.322001 0.480068
H13 -3.819252 1.480550 -0.326963
H14 -1.370306 -1.899343 0.321919
H15 -3.712876 -2.372026 -0.435404
C16 1.455264 0.383885 -0.244953
H17 1.283335 -0.382118 -1.010395
C18 1.395254 1.747713 -0.836951
H19 1.512039 2.611889 -0.192203
H20 1.491899 1.888418 -1.905548
N21 3.495244 -0.913155 -0.447337
O22 4.550323 -1.064226 -0.021324
O23 2.760780 0.160395 0.321354

TS3$^{\beta}$
C1 1.416650 -0.230721 -0.775113
N2 0.879807 0.931635 -0.386449
N3 2.450602 -0.513637 0.019381
C4 -0.335553 1.550779 -0.965597
H5 -0.163207 2.630913 -1.024897
H6 -0.429320 1.176983 -1.987526
C7 3.306614 -1.706682 -0.073590
H8 3.240199 -2.270801 0.856047
H9 4.336450 -1.401017 -0.255296
C10 2.577016 0.499396 0.953533
C11 1.590879 1.401204 0.702955
H12 1.339117 2.322991 1.199000
H13 3.350534 0.494146 1.702726
H14 1.056582 -0.848437 -1.580884
H15 2.959832 -2.326162 -0.897997
C16 -1.557731 1.257263 -0.165561
H17 -1.658363 -0.224303 -0.033515
C18 -2.481821 2.024249 0.366636
H19 -2.402008 3.112803 0.328452
H20 -3.360185 1.620376 0.858390
N21 -2.603740 -2.022960 0.142300
O22 -1.468954 -1.323138 -0.067079
O23 -3.587627 -1.405071 0.335741

[MIM^{+}CH$_2$C=CH$_2$]$^{\bullet}$
C1 -0.914839 -0.890957 0.026916
N2 0.225449 -0.224984 0.233708
N3 -1.917175 -0.011673 -0.062381
C4 1.567320 -0.841393 0.410927
H5 1.841903 -0.744644 1.470590
H6 1.456155 -1.906054 0.192366
C7 -3.332694 -0.337219 -0.296764
H8 -3.663676 0.132769 -1.222266
H9 -3.930284 0.021567 0.540589
C10 -1.397087 1.260247 0.090897
C11 -0.055408 1.126677 0.274352
H12 0.714630 1.865786 0.414399
H13 -2.016467 2.140381 0.052695
H14 -1.010723 -1.960992 -0.055774
H15 -3.438222 -1.416875 -0.380994
C16 2.581499 -0.221504 -0.457385
C17 3.768265 0.311180 -0.328324
H18 4.239307 0.438097 0.650714
H19 4.347119 0.644379 -1.185324

TS4$^{\beta}$
C1 1.256053 -0.302115 -0.656411
N2 0.723803 0.904398 -0.424694
N3 2.363856 -0.428194 0.076169
C4 -0.529077 1.420583 -1.023227
H5 -0.346328 2.458476 -1.327742
H6 -0.713372 0.845242 -1.932628
C7 3.241179 -1.609426 0.109726
H8 3.299369 -1.985732 1.130413
H9 4.233564 -1.334795 -0.246494
C10 2.547392 0.735252 0.803676
C11 1.519340 1.568294 0.493108
H12 1.291436 2.561816 0.839598
H13 3.384861 0.870168 1.467074
H14 0.831143 -1.058333 -1.294831
H15 2.821111 -2.378198 -0.535366
C16 -1.688181 1.358167 -0.098229
H17 -2.163050 -0.296976 0.142532
C18 -2.503942 2.228219 0.444122
H19 -2.371522 3.302587 0.289593
H20 -3.349013 1.937311 1.061692
N21 -2.235664 -1.400534 0.120560
O22 -3.167036 -1.911205 0.686957
O23 -1.325308 -1.944432 -0.491291

TS5$^{\beta}$
C1 1.729626 -0.918135 -0.137797
N2 0.950554 0.115452 -0.475177
N3 2.964703 -0.469638 0.108223
C4 -0.495317 0.042188 -0.770531
H5 -0.695908 0.651153 -1.652764
H6 -0.727461 -0.995196 -1.012616
C7 4.120992 -1.293292 0.492666

H8 4.509387 -0.947455 1.449989
H9 4.892090 -1.217766 -0.273463
C10 2.976025 0.900138 -0.076080
C11 1.716211 1.266003 -0.438193
H12 1.306488 2.233426 -0.670836
H13 3.867272 1.489085 0.059572
H14 1.414662 -1.946978 -0.081440
H15 3.802063 -2.329487 0.584859
C16 -1.361126 0.511178 0.410849
H17 -1.100144 -0.046408 1.321114
C18 -1.483820 1.966632 0.612021
H19 -1.527497 2.621969 -0.248650
H20 -1.831514 2.340857 1.564514
N21 -3.601495 -1.287584 0.120788
O22 -4.697041 -1.117975 -0.083615
O23 -2.718126 0.466840 0.099275

TS6$^{\beta}$
C1 1.819108 -0.602933 -0.491567
N2 0.897875 0.367363 -0.521399
N3 2.935304 -0.122159 0.062923
C4 -0.476614 0.209715 -1.024837
H5 -0.871077 1.205859 -1.232040
H6 -0.440817 -0.326686 -1.973724
C7 4.187067 -0.868553 0.265828
H8 4.433571 -0.879491 1.326954
H9 4.988018 -0.394042 -0.300234
C10 2.721026 1.200569 0.404149
C11 1.445496 1.505227 0.040454
H12 0.892125 2.425055 0.124936
H13 3.484826 1.805247 0.863090
H14 1.680339 -1.607957 -0.854973
H15 4.050274 -1.889388 -0.084824
C16 -1.423222 -0.557460 -0.088118
C17 -1.221778 -0.662068 1.272367
H18 -0.394541 -0.177258 1.773474
H19 -1.804274 -1.372093 1.846725
O20 -2.487556 -0.962625 -0.673304
H21 -2.958855 0.100647 1.149559
N22 -3.842953 -0.090664 0.502709
O23 -4.424651 0.797793 0.021026

MIM^{+}CH$_2$C(O)CH$_2$
C1 0.962173 -0.682420 -0.499070
N2 0.038922 0.287445 -0.493534
N3 2.099974 -0.199322 0.008183
C4 -1.352603 0.149379 -0.953732
H5 -1.643063 1.084617 -1.433867
H6 -1.386094 -0.629205 -1.716533
C7 3.362175 -0.942666 0.156948
H8 3.660448 -0.941976 1.204697
H9 4.132999 -0.472511 -0.452837
C10 1.899853 1.125290 0.349971
C11 0.611026 1.429871 0.036583
H12 0.062589 2.351464 0.136819
H13 2.682070 1.732362 0.773814
H14 0.812991 -1.686676 -0.860929
H15 3.210124 -1.967211 -0.176180
C16 -2.411742 -0.191315 0.120999
C17 -2.082127 -0.336538 1.498600
H18 -1.081333 -0.209318 1.891226
H19 -2.885060 -0.579223 2.183184
O20 -3.558809 -0.326097 -0.301715

TS7$^{\beta}$
C1 1.389931 0.767193 0.255060
N2 0.781605 -0.385168 0.561859
N3 2.656873 0.511960 -0.085745
C4 -0.628512 -0.533009 0.972541
H5 -0.688150 -1.393603 1.638788
H6 -0.915688 0.346742 1.547094
C7 3.664987 1.512077 -0.472278
H8 4.038028 1.282509 -1.469755
H9 4.483791 1.497872 0.246407
C10 2.868878 -0.850869 0.007302
C11 1.696767 -1.411447 0.412339
H12 1.441127 -2.438352 0.612528
H13 3.823562 -1.298595 -0.211894
H14 0.935866 1.743842 0.289217
H15 3.202679 2.497010 -0.476317
C16 -1.668575 -0.754918 -0.160240
H17 -1.647376 0.323253 -0.848122
C18 -1.292735 -1.427774 -1.369333
H19 -0.269896 -1.445173 -1.727007
H20 -2.081322 -1.767923 -2.029510
N21 -3.180760 1.046843 -0.484119
O22 -3.402248 1.865355 0.266248
O23 -2.886639 -0.786671 0.310283

MIM^{+}CH$_2$C(O)CH$_3$
C1 0.834837 -0.470764 -0.507560
N2 0.085227 0.623495 -0.317187
N3 2.062088 -0.235896 -0.039289
C4 -1.341691 0.734237 -0.615540
H5 -1.673761 1.730849 -0.323698
H6 -1.504285 0.641197 -1.693621
C7 3.183181 -1.187784 -0.054923
H8 3.489706 -1.402422 0.968362
H9 4.014570 -0.759877 -0.614088
C10 2.099492 1.045345 0.482313

C11	0.863036	1.581857	0.311731
H12	0.477349	2.552482	0.572657
H13	2.990848	1.460589	0.920844
H14	0.500655	-1.392128	-0.950954
H15	2.857587	-2.108100	-0.535201
C16	-2.173070	-0.358714	0.103097
C17	-3.657339	-0.130791	0.126214
H18	-4.022033	0.238618	-0.836530
H19	-4.169447	-1.053055	0.395033
O20	-1.619105	-1.317039	0.580642
H21	-3.890221	0.634650	0.875396