Supplementary Information

Dicationic ionic liquids with the difluorophosphate anion

Kentaro Kamada,[a] Kohei Nishimoto,[a] Toshiki Nokami,[b] Hideto Nakajima,[c] Jinkwang Hwang,[a] Kazuhiko Matsumoto[a,]*

[a]Graduate School of Energy Science, Kyoto University, Yoshida-honmachi, Sakyo-ku, Kyoto 606-8501, Japan.

[b] Faculty of Engineering, Tottori University, 4-101, Koyama-cho minami, Tottori, Japan.

[c] Graduate School of Engineering, Kyoto University, Kyotodaigakukatsura, Nishikyo-ku, Kyoto 615-8510, Japan

*Corresponding authors: Kazuhiko Matsumoto

E-mail: matsumoto.kazuhiko.4c@kyoto-u.ac.jp (K.M.)

Tel: +81757535827

Fax: +81757535906

Table S1. Densities (ρ) of dicaionic ionic liquids, $[C_{1O2O1}\text{-}(C_1pyrr)_2][PO_2F_2]_2$, $[C_{1O2O1}\text{-}(N_{221})_2][PO_2F_2]_2$, and $[C_{1O2O1}\text{-}(C_1pyrr)_2][BF_4]_2$ [a]

ρ (g cm^{-3})			
T (K)	$[C_{1O2O1}\text{-}(C_1pyrr)_2][PO_2F_2]_2$	$[C_{1O2O1}\text{-}(N_{221})_2][PO_2F_2]_2$	$[C_{1O2O1}\text{-}(C_1pyrr)_2][BF_4]_2$
278	1.364	1.290	1.319
288	1.356	1.284	1.312
298	1.349	1.277	1.305
308	1.342	1.270	1.299
318	1.335	1.263	1.292
328	1.328	1.256	1.286
338	1.321	1.250	1.279
$A\times10^4$	−7.056	−6.791	−6.560
B	1.560	1.479	1.501

[a]The symbols, ρ and T, denote density and temperature, respectively. The A and B parameters are the constants in Equation 1.

Table S2. Viscosities (η) of dicaionic ionic liquids, $[C_{1O2O1}\text{-}(C_1pyrr)_2][PO_2F_2]_2$, $[C_{1O2O1}\text{-}(N_{221})_2][PO_2F_2]_2$, and $[C_{1O2O1}\text{-}(C_1pyrr)_2][BF_4]_2$.[a]

η (mPa s)			
T (K)	$[C_{1O2O1}\text{-}(C_1pyrr)_2]$ $[PO_2F_2]_2$	$[C_{1O2O1}\text{-}(N_{221})_2]$ $[PO_2F_2]_2$	$[C_{1O2O1}\text{-}(C_1pyrr)_2]$ $[BF_4]_2$
278	11840	24540	107444
288	4542	8908	33090
298	2000	3700	11900
308	985	1714	4933
318	535	856	2280
328	314	469	1162
338	201	275	642
$A_\eta x10^3$ (mPa s $K^{-1/2}$)	10	10	990
B_η (K)	1000	1000	917.7
$T_{0\eta}$ (K)	184.5	189.2	200.5

[a]The symbols, η and T, denote density and temperature, respectively. The A_η, B_η, and $T_{0\eta}$ parameters are the constants in Equation 2.

Table S3. Ionic conductivities (σ) of dicaionic ionic liquids, $[C_{1O2O1}\text{-}(C_1pyrr)_2][PO_2F_2]_2$, $[C_{1O2O1}\text{-}(N_{221})_2][PO_2F_2]_2$, and $[C_{1O2O1}\text{-}(C_1pyrr)_2][BF_4]_2$.[a]

σ (mS cm^{-1})			
T (K)	$[C_{1O2O1}\text{-}(C_1pyrr)_2][PO_2F_2]_2$	$[C_{1O2O1}\text{-}(N_{221})_2][PO_2F_2]_2$	$[C_{1O2O1}\text{-}(C_1pyrr)_2][BF_4]_2$
278	0.078	0.044	0.026
288	0.203	0.102	0.062
298	0.425	0.222	0.132
308	0.791	0.452	0.288
318	1.443	0.859	0.567
328	2.303	1.503	1.061
338	3.478	2.420	1.813
A_σ (mS cm^{-1} K$^{-1/2}$)	10000	15000	12000
B_σ (K)	1200	1100	1250
$T_{0\sigma}$ (K)	170	180	175

[a]The symbols, σ and T, denote ionic conductivity and temperature, respectively. The A_σ and B_σ parameters are the constants in Equation 3.

Table S4. Molar concentrations (C) of dicaionic ionic liquids, $[C_{1O2O1}\text{-}(C_1pyrr)_2][PO_2F_2]_2$, $[C_{1O2O1}\text{-}(N_{221})_2][PO_2F_2]_2$, and $[C_{1O2O1}\text{-}(C_1pyrr)_2][BF_4]_2$ [a]

C (mol dm^{-3})			
T (K)	$[C_{1O2O1}\text{-}(C_1pyrr)_2][PO_2F_2]_2$	$[C_{1O2O1}\text{-}(N_{221})_2][PO_2F_2]_2$	$[C_{1O2O1}\text{-}(C_1pyrr)_2][BF_4]_2$
278	2.963	2.778	3.053
288	2.946	2.765	3.037
298	2.930	2.750	3.021
308	2.915	2.735	3.007
318	2.900	2.720	2.991
328	2.885	2.705	2.977
338	2.870	2.692	2.961

[a]The symbols, C and T, denote molar concentration and temperature, respectively.

Table S5. Molar ionic conductivities (Λ) of dicaionic ionic liquids, $[C_{1O2O1}\text{-}(C_1pyrr)_2][PO_2F_2]_2$, $[C_{1O2O1}\text{-}(N_{221})_2][PO_2F_2]_2$, and $[C_{1O2O1}\text{-}(C_1pyrr)_2][BF_4]_2$. [a]

Λ (S cm^2 mol^{-1})			
T (K)	$[C_{1O2O1}\text{-}(C_1pyrr)_2][PO_2F_2]_2$	$[C_{1O2O1}\text{-}(N_{221})_2][PO_2F_2]_2$	$[C_{1O2O1}\text{-}(C_1pyrr)_2][BF_4]_2$
278	0.026	0.016	0.0085
288	0.0689	0.0369	0.020
298	0.145	0.0807	0.0437
308	0.271	0.165	0.0958
318	0.498	0.316	0.190
328	0.798	0.556	0.356
338	1.212	0.889	0.612

[a]The symbols, Λ and T, denote molar ionic conductivity and temperature, respectively.

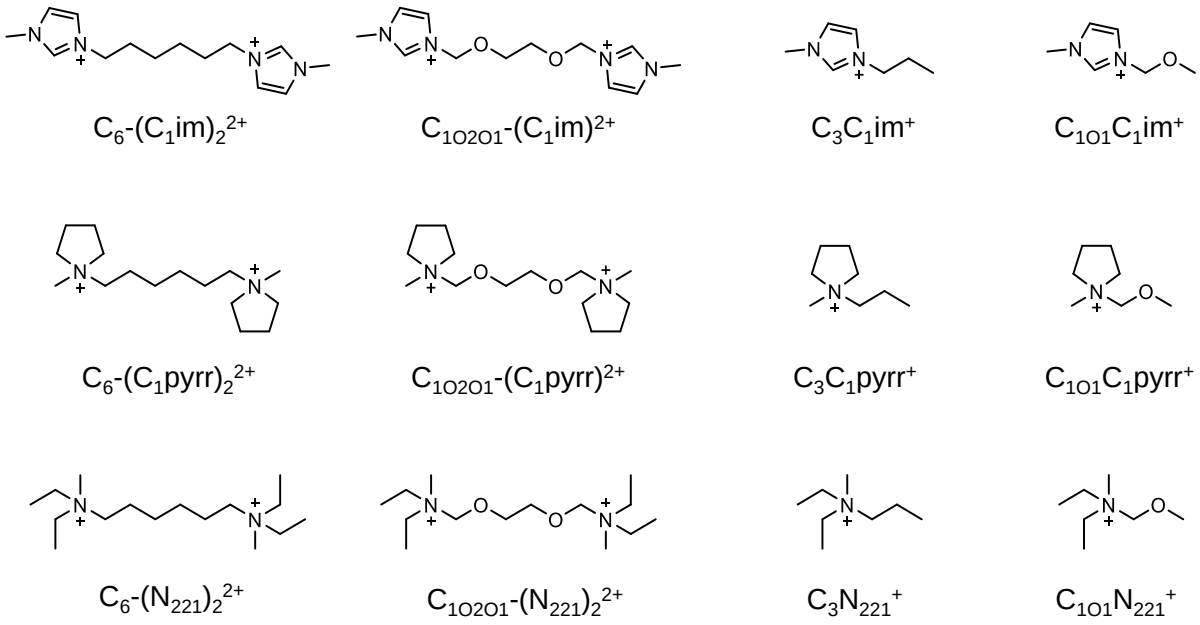

Figure S1. Structures of 12 cationic species whose structures were optimized at PBE1PBE/aug-cc-pVDZ in this study. See the following data for the atomic coodicates of the optimized structures.

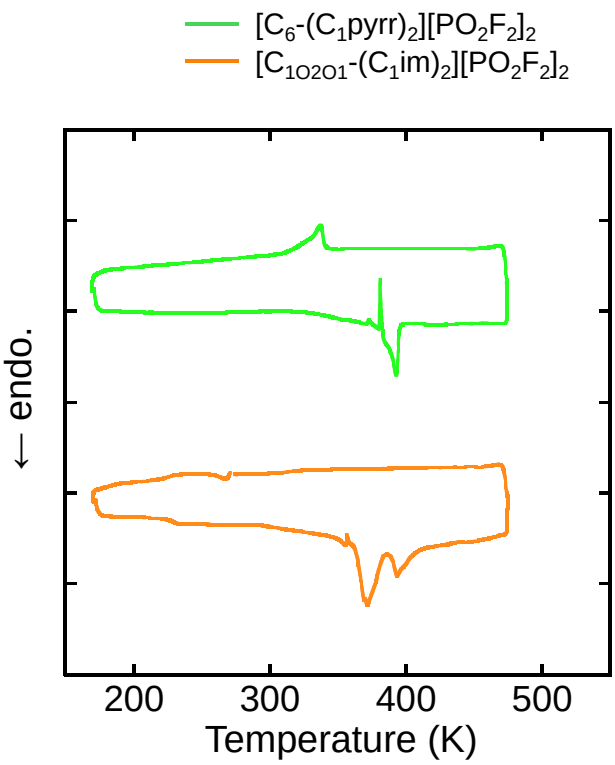

Figure S2. DSC curves $[C_6\text{-}(C_1pyrr)_2][PO_2F_2]_2$ and $[C_{1O2O1}\text{-}(C_1im)_2][PO_2F_2]_2$ under Ar atmosphere. Scan rate: 5 K min^{-1}. Melting point: 394 K for $[C_6\text{-}(C_1pyrr)_2][PO_2F_2]_2$ and 393 K for $[C_{1O2O1}\text{-}(C_1im)_2][PO_2F_2]_2$.

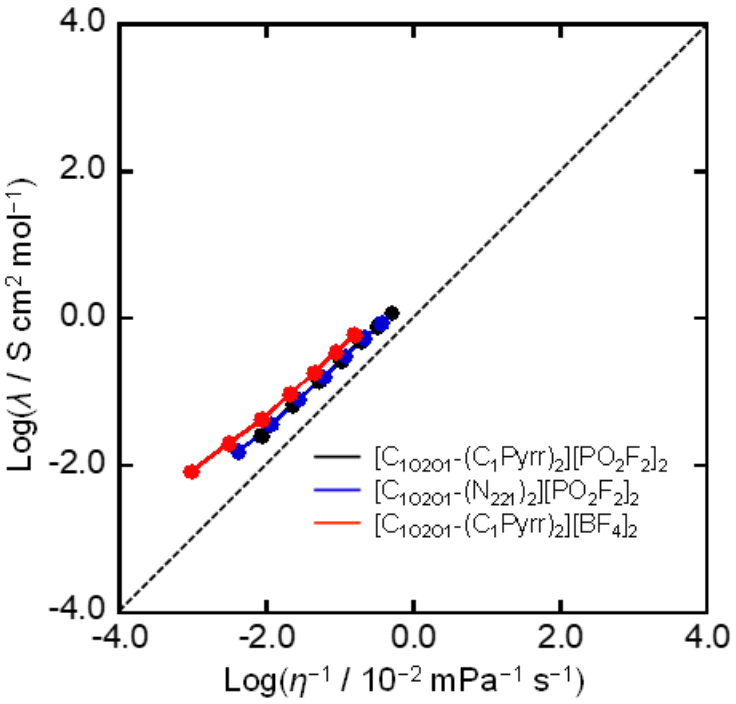

Figure S3. Walden plot of the dicaionic ionic liquids, $[C_{10201}\text{-}(C_1pyrr)_2][PO_2F_2]_2$, $[C_{10201}\text{-}(N_{221})_2][PO_2F_2]_2$, and $[C_{10201}\text{-}(C_1pyrr)_2][BF_4]_2$ based on the viscosity and molar ionic conductivity data in Tables S2 and S5. The plot is close to or slightly above the diagonal line, suggesting normal ion transport mechanism in these dicationic ionic liquids. Further discussion requires more data of related ionic liquids.

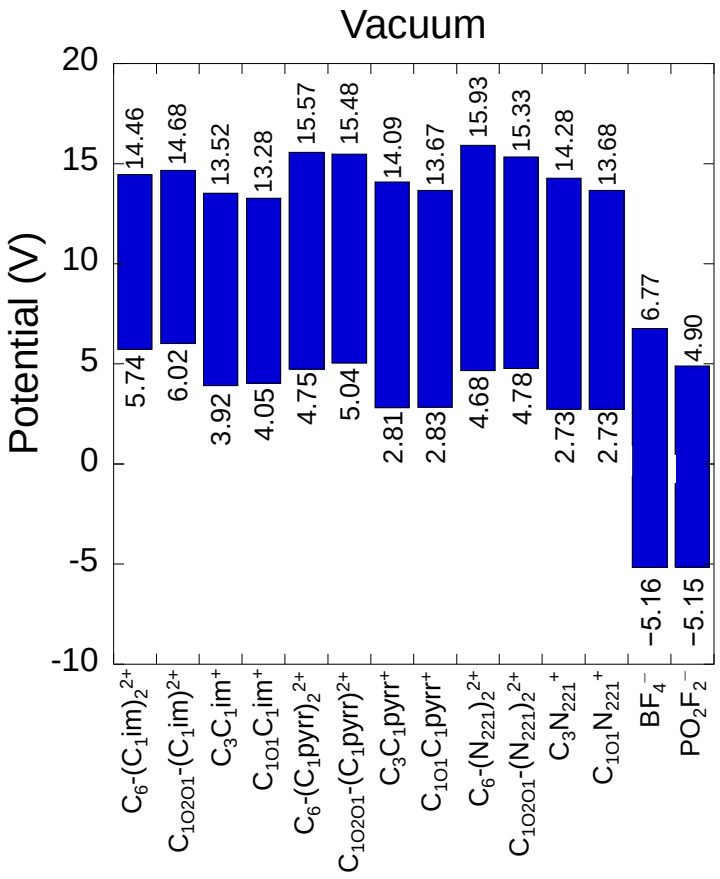

Figure S4. Electrochemical stabilities of the dications, monocations, and anions in this study calculated at the PBE1PBE/aug-cc-pVDZ level under vacuum. See Figure S1 for the structures of the chemical speices and Figure 6 for the data under vacuum.

Atomic coordinates of the calculated dicationic, monocationic, and anionic species.

C_6-(C_1im)$_2^{2+}$

Atom	X	Y	Z
C	-4.91962	-1.38172	-0.11699
C	-6.19331	-1.13536	0.30258
H	-5.16864	1.82843	-0.53318
H	-4.37018	-2.31283	-0.18322
H	-6.95805	-1.80772	0.67350
C	-5.29772	0.77513	-0.31484
N	-4.37846	-0.17584	-0.49896
N	-6.40632	0.21652	0.17085
C	-7.64702	0.91652	0.49294
H	-7.51596	1.98356	0.29394
H	-8.45756	0.52508	-0.13087
H	-7.88376	0.76790	1.55167
C	-3.02130	0.03245	-1.01657
H	-2.99890	1.03740	-1.45478
H	-2.87401	-0.68569	-1.83328
C	-1.94881	-0.12378	0.05589
H	-2.02230	-1.12517	0.50572
H	-2.13339	0.60114	0.86247
C	-0.54987	0.07883	-0.52382
H	-0.48114	1.08044	-0.97662
H	-0.38323	-0.64185	-1.33975
C	0.54987	-0.07917	0.52393
H	0.38320	0.64145	1.33991
H	0.48118	-1.08080	0.97668
C	1.94881	0.12353	-0.05575
H	2.13335	-0.60118	-0.86251
H	2.02235	1.12503	-0.50534
C	3.02134	-0.03298	1.01663
H	2.99908	-1.03808	1.45448
H	2.87401	0.68487	1.83358
C	4.91976	1.38188	0.11830
C	5.29771	-0.77517	0.31415
C	6.19348	1.13585	-0.30137

H	4.37040	2.31299	0.18541
H	5.16855	-1.82866	0.53149
H	6.95832	1.80854	-0.67149
N	4.37846	0.17567	0.49901
N	6.40645	-0.21615	-0.17072
C	7.64664	-0.91616	-0.49475
H	7.87719	-0.77525	-1.55594
H	8.45981	-0.51828	0.12146
H	7.51898	-1.98185	-0.28655

C_{1O2O1}-$(C_1im)_2^{2+}$

Atom	X	Y	Z
C	4.54483	1.40463	-0.04117
C	5.78499	1.11074	0.43752
H	4.82089	-1.76288	-0.73163
H	3.99037	2.33510	-0.0463
H	6.52342	1.73904	0.92192
C	4.93884	-0.73394	-0.41296
N	4.03567	0.24045	-0.57240
N	6.00782	-0.22727	0.19279
C	7.22706	-0.95789	0.53163
H	7.39054	-0.90584	1.61312
H	7.11309	-2.00188	0.22774
H	8.07537	-0.51179	0.00179
C	2.72046	0.08248	-1.16868
H	2.72534	-0.8511	-1.75385
H	2.54943	0.9325	-1.84852
C	0.44938	0.00161	-0.60991
H	0.28347	-0.91112	-1.20507
H	0.22960	0.87785	-1.24138
C	-0.44966	-0.00216	0.61053
H	-0.22981	-0.87838	1.24200
H	-0.28382	0.91059	1.20567
C	-2.72074	-0.08278	1.16931
H	-2.72539	0.85084	1.75441
H	-2.54992	-0.93279	1.84922
C	-4.54649	-1.40544	0.04456
C	-4.9378	0.73458	0.41083
C	-5.78604	-1.11108	-0.43544
H	-3.99323	-2.33661	0.05212
H	-4.81864	1.76413	0.72705
H	-6.52521	-1.73968	-0.91831
N	-4.03600	-0.24063	0.57312
N	-6.00720	0.22782	-0.19409
C	-7.22527	0.95925	-0.53539
H	-7.38916	0.90316	-1.61660
H	-8.07423	0.51679	-0.00353

H	-7.10933	2.00425	-0.23573
O	1.78814	0.05275	-0.13306
O	-1.78841	-0.05334	0.13368

$C_3C_1im^+$

Atom	X	Y	Z
C	-3.82916	-0.31998	-0.23304
H	-4.21619	0.41050	0.49034
H	-3.96341	-1.32396	0.19215
C	-2.37010	-0.04824	-0.57282
H	-2.00965	-0.77251	-1.31797
H	-2.26759	0.94989	-1.02338
C	-1.49259	-0.13327	0.66860
H	-1.54114	-1.13057	1.12255
H	-1.80524	0.59237	1.42992
C	0.46794	1.36856	0.11397
C	0.87990	-0.78442	0.25774
C	1.79009	1.17353	-0.15764
H	-0.11727	2.27951	0.14886
H	0.75200	-1.85008	0.40467
H	2.57387	1.88026	-0.40265
N	-0.07882	0.13465	0.37378
N	2.02434	-0.17806	-0.06322
C	3.31053	-0.83487	-0.26603
H	3.66787	-0.63147	-1.28103
H	4.03255	-0.45959	0.46703
H	3.18448	-1.91291	-0.13403
H	-4.44860	-0.25539	-1.13499

$C_{1O1}C_1im^+$

Atom	X	Y	Z
C	-3.59697	-0.30783	-0.38180
H	-4.03364	0.53012	0.18343
H	-3.83044	-1.25716	0.12475
C	-1.53441	-0.09442	0.68755
H	-1.59534	-1.04585	1.24309
H	-1.90290	0.72033	1.33312
C	0.41277	1.38738	0.08261
C	0.82140	-0.76692	0.29867
C	1.72667	1.17454	-0.20544
H	-0.17605	2.29659	0.07950
H	0.68707	-1.82695	0.47774
H	2.50932	1.86580	-0.49429
N	-0.12914	0.16481	0.40357
N	1.95758	-0.17691	-0.06329
C	3.23852	-0.84379	-0.26944
H	3.57403	-0.67385	-1.29792
H	3.97523	-0.44485	0.43594
H	3.11297	-1.91650	-0.09947
H	-4.01284	-0.32243	-1.39256
O	-2.18931	-0.14178	-0.53102

C_6-(C_1pyrr)$_2^{2+}$

Atom	X	Y	Z
C	4.68506	-1.65638	0.77268
C	4.68458	-1.65700	-0.77093
C	4.83012	-0.19724	-1.19516
C	4.82954	-0.19613	1.19577
H	3.76601	-2.10085	1.16728
H	5.51719	-2.24021	1.17958
H	3.76484	-2.10090	-1.16458
H	5.51588	-2.24194	-1.17794
H	5.87291	0.04616	-1.42502
H	4.21363	0.10455	-2.04850
H	5.87199	0.04799	1.42639
H	4.21215	0.10606	2.04833
C	5.23673	1.92293	-0.00061
H	4.98809	2.49930	-0.89735
H	4.98763	2.50018	0.89542
H	6.30327	1.68028	-0.00022
C	2.98990	1.04483	-0.00068
H	2.85894	1.67938	0.88520
H	2.85933	1.67887	-0.88698
C	1.95595	-0.06918	-0.00058
H	2.07362	-0.70701	0.88523
H	2.07334	-0.70683	-0.88655
N	4.45108	0.65274	-0.00019
C	0.54708	0.53308	-0.00033
H	0.42583	1.18103	0.88155
H	0.42568	1.18138	-0.88194
C	-0.54707	-0.53309	-0.00047
H	-0.42571	-1.18138	0.88115
H	-0.42581	-1.18104	-0.88235
C	-1.95594	0.06918	-0.00028
H	-2.07348	0.70714	-0.88601
H	-2.07345	0.70670	0.88578
C	-2.98989	-1.04481	-0.00055
H	-2.85903	-1.67944	0.88529
H	-2.85927	-1.67878	-0.88689

C	-5.23671	-1.92293	-0.00062
H	-4.98769	-2.50015	0.89546
H	-6.30326	-1.68031	-0.00035
H	-4.98798	-2.49935	-0.89730
C	-4.83003	0.19720	-1.19520
H	-4.21330	-0.10445	-2.04843
H	-5.87272	-0.04638	-1.42532
C	-4.82966	0.19616	1.19572
H	-5.87223	-0.04774	1.42605
H	-4.21256	-0.10618	2.04843
C	-4.68483	1.65702	-0.77095
H	-3.76538	2.10124	-1.16488
H	-5.51647	2.24170	-1.17764
C	-4.68479	1.65636	0.77266
H	-5.51656	2.24050	1.17987
H	-3.76545	2.10048	1.16697
N	-4.45109	-0.65273	-0.00019

C_{1O2O1}-$(C_1pyrr)_2^{2+}$

Atom	X	Y	Z
C	-3.95779	-1.71769	-0.77238
C	-3.95777	-1.71812	0.77175
C	-4.35529	-0.30703	1.19479
C	-4.35599	-0.30657	-1.19454
H	-2.96846	-1.97495	-1.16008
H	-4.67152	-2.43919	-1.18351
H	-2.96856	-1.97611	1.15929
H	-4.67185	-2.43949	1.18247
H	-5.42893	-0.23446	1.40032
H	-3.80924	0.09240	2.05563
H	-5.42982	-0.23420	-1.39916
H	-3.81075	0.09336	-2.05566
C	-5.03639	1.75913	0.00070
H	-4.86492	2.36145	0.89878
H	-4.86534	2.36187	-0.89718
H	-6.06243	1.38157	0.00085
C	-2.71798	1.15926	-0.00005
H	-2.62959	1.78870	-0.90084
H	-2.62925	1.78868	0.90071
N	-4.10312	0.59316	0.00022
C	-0.45360	0.60778	-0.00027
H	-0.26732	1.22172	-0.89604
H	-0.26728	1.22174	0.89549
C	0.45361	-0.60779	-0.00027
H	0.26731	-1.22172	-0.89605
H	0.26729	-1.22175	0.89549
C	2.71798	-1.15926	-0.00007
H	2.62959	-1.78871	-0.90085
H	2.62927	-1.78868	0.90070
C	5.03639	-1.75913	0.00065
H	4.86533	-2.36186	-0.89723
H	6.06243	-1.38156	0.00079
H	4.86494	-2.36146	0.89873
C	4.35530	0.30702	1.19476
H	3.80928	-0.09242	2.05561

H	5.42895	0.23446	1.40026
C	4.35598	0.30658	-1.19458
H	5.42980	0.23421	-1.39921
H	3.81072	-0.09335	-2.05568
C	3.95775	1.71811	0.77173
H	2.96854	1.97608	1.15927
H	4.67182	2.43949	1.18247
C	3.95778	1.71770	-0.77239
H	4.67151	2.43919	-1.18352
H	2.96845	1.97497	-1.16009
N	4.10312	-0.59316	0.00019
O	1.79341	-0.12636	-0.00024
O	-1.79341	0.12636	-0.00023

$C_3C_1pyrr^+$

Atom	X	Y	Z
C	-1.25455	-1.49542	-0.77163
C	-1.25505	-1.49532	0.77171
C	-1.08831	-0.03757	1.19545
C	-1.08850	-0.03763	-1.19536
H	-0.44661	-2.12075	-1.16318
H	-2.19020	-1.89236	-1.17935
H	-0.44780	-2.12117	1.16388
H	-2.19124	-1.89158	1.17884
H	-2.05515	0.41953	1.43268
H	-0.41463	0.12406	2.04348
H	-2.05563	0.41915	-1.43212
H	-0.41524	0.12432	-2.04366
C	-1.04623	2.11831	-0.00003
H	-0.67953	2.62985	0.89547
H	-0.67973	2.62978	-0.89564
H	-2.14019	2.10687	0.00009
C	0.96825	0.78763	-0.00011
H	1.23112	1.37920	-0.88668
H	1.23119	1.37893	0.88662
C	1.73550	-0.52053	-0.00034
H	1.48352	-1.11644	-0.88671
H	1.48289	-1.11717	0.88537
N	-0.54504	0.71415	-0.00003
C	3.23443	-0.23011	0.00028
H	3.53435	0.34086	-0.88857
H	3.53378	0.34005	0.88985
H	3.80106	-1.16826	0.00003

$C_{1O1}C_1pyrr^+$

Atom	X	Y	Z
C	-0.94332	-1.59996	-0.77192
C	-0.94352	-1.60002	0.77186
C	-1.01975	-0.13577	1.19445
C	-1.02019	-0.13572	-1.19433
H	-0.03210	-2.06575	-1.15553
H	-1.79836	-2.14688	-1.18339
H	-0.03266	-2.06636	1.15567
H	-1.79897	-2.14653	1.18303
H	-2.04991	0.17231	1.40600
H	-0.39152	0.13079	2.05054
H	-2.05056	0.17209	-1.40521
H	-0.39254	0.13113	-2.05076
C	-1.22710	2.02784	0.00012
H	-0.92286	2.57695	0.89710
H	-0.92306	2.57702	-0.89688
H	-2.31205	1.89217	0.00023
C	0.90207	0.91831	-0.00023
H	1.13190	1.51345	-0.90139
H	1.13208	1.51392	0.90057
N	-0.57977	0.68685	-0.00001
C	2.95863	-0.17174	0.00001
H	3.30168	0.35972	-0.90034
H	3.30167	0.36017	0.90010
H	3.36074	-1.18793	0.00027
O	1.53674	-0.30147	0.00004

C_6-$(N_{221})_2^{2+}$

Atom	X	Y	Z
C	-3.09973	-0.00002	-0.68017
H	-3.05827	-0.88086	-1.33020
H	-3.05826	0.88078	-1.33026
C	-1.93432	0.00000	0.29650
H	-1.97359	-0.88400	0.94797
H	-1.97361	0.88400	0.94796
N	-4.47926	0.00000	-0.06739
C	-0.60567	0.00000	-0.46533
H	-0.56075	-0.88132	-1.12385
H	-0.56076	0.88132	-1.12385
C	0.60567	0.00001	0.46532
H	0.56075	-0.88131	1.12385
H	0.56076	0.88133	1.12383
C	1.93432	-0.00001	-0.29650
H	1.97361	0.88399	-0.94798
H	1.97360	-0.88401	-0.94796
C	3.09973	0.00000	0.68017
H	3.05827	-0.88083	1.33023
H	3.05827	0.88082	1.33023
C	5.47368	-0.00014	1.18038
H	5.32777	-0.89059	1.79607
H	6.48246	-0.00018	0.75579
H	5.32788	0.89024	1.79619
N	4.47926	-0.00001	0.06739
C	4.70847	-1.21614	-0.81122
H	4.05475	-1.09094	-1.68078
H	5.74277	-1.12570	-1.16416
C	4.70857	1.21625	-0.81101
H	5.74288	1.12581	-1.16393
H	4.05487	1.09124	-1.68061
C	4.48254	-2.56138	-0.15557
H	5.14188	-2.74263	0.70061
H	3.44154	-2.72166	0.14869
H	4.71937	-3.32899	-0.90281
C	4.48270	2.56139	-0.15513

H	4.71961	3.32912	-0.90222
H	3.44171	2.72168	0.14913
H	5.14203	2.74246	0.70110
C	-4.70849	-1.21612	0.81122
H	-4.05476	-1.09093	1.68077
H	-5.74278	-1.12564	1.16418
C	-4.70855	1.21627	0.81100
H	-4.05485	1.09124	1.68061
H	-5.74285	1.12584	1.16392
C	-4.48265	2.56141	0.15513
H	-4.71954	3.32913	0.90223
H	-3.44165	2.72168	-0.14912
H	-5.14196	2.74249	-0.70110
C	-5.47368	-0.00012	-1.18038
H	-5.32779	-0.89057	-1.79607
H	-6.48247	-0.00013	-0.75579
H	-5.32786	0.89027	-1.79619
C	-4.48261	-2.56137	0.15558
H	-3.44163	-2.72168	-0.14872
H	-4.71944	-3.32896	0.90283
H	-5.14198	-2.74262	-0.70058

C_{1O2O1}-$(N_{221})_2^{2+}$

Atom	X	Y	Z
C	-2.84566	0.00284	-0.81600
H	-2.84826	-0.88904	-1.46055
H	-2.84200	0.90393	-1.44684
N	-4.12487	0.00005	-0.04401
C	-0.52313	-0.00409	-0.54909
H	-0.40986	-0.89792	-1.18333
H	-0.41218	0.89216	-1.18019
C	0.52313	-0.00409	0.54909
H	0.40986	-0.89792	1.18333
H	0.41218	0.89216	1.18019
C	2.84566	0.00284	0.81600
H	2.84826	-0.88904	1.46055
H	2.84200	0.90393	1.44684
C	5.24551	-0.05036	1.02783
H	5.21320	-0.99956	1.56786
H	6.19005	0.03545	0.48227
H	5.14967	0.77650	1.73603
N	4.12487	0.00005	0.04401
C	4.19895	-1.19850	-0.89074
H	3.47193	-1.00055	-1.68403
H	5.20356	-1.15257	-1.32722
C	4.24055	1.24312	-0.82542
H	5.15363	1.09221	-1.41338
H	3.38507	1.20239	-1.50633
C	3.94298	-2.54677	-0.25416
H	4.63825	-2.78918	0.55773
H	2.91157	-2.65759	0.09977
H	4.09617	-3.30403	-1.03315
C	4.28889	2.56307	-0.08721
H	4.36457	3.35156	-0.84645
H	3.38027	2.76911	0.49114
H	5.16569	2.66532	0.56156
C	-4.19895	-1.19850	0.89074
H	-3.47193	-1.00055	1.68403
H	-5.20356	-1.15257	1.32722

C	-4.24055	1.24312	0.82542
H	-3.38507	1.20239	1.50633
H	-5.15363	1.09221	1.41338
C	-4.28889	2.56307	0.08721
H	-4.36457	3.35156	0.84645
H	-3.38027	2.76911	-0.49114
H	-5.16570	2.66532	-0.56156
C	-5.24551	-0.05036	-1.02783
H	-5.21320	-0.99956	-1.56786
H	-6.19005	0.03545	-0.48227
H	-5.14966	0.77649	-1.73603
C	-3.94297	-2.54677	0.25416
H	-2.91157	-2.65759	-0.09977
H	-4.09616	-3.30403	1.03315
H	-4.63825	-2.78918	-0.55773
O	-1.79435	-0.00680	0.09016
O	1.79435	-0.00680	-0.09016

$C_3N_{221}^+$

Atom	X	Y	Z
C	-3.16689	-0.00016	0.24243
H	-3.30112	-0.88900	0.87336
H	-3.30120	0.88871	0.87330
C	-1.80129	-0.00013	-0.43946
H	-1.72052	0.88368	-1.08662
H	-1.72044	-0.88397	-1.08655
C	-0.70325	-0.00005	0.60790
H	-0.78541	-0.88074	1.25465
H	-0.78552	0.88065	1.25463
C	1.63863	0.00010	1.24889
H	1.45487	-0.88978	1.85526
H	2.67159	0.00015	0.88657
H	1.45477	0.88995	1.85525
N	0.71312	0.00004	0.08111
C	0.99035	-1.21496	-0.78231
H	0.39039	-1.08614	-1.68896
H	2.04550	-1.13098	-1.07011
C	0.99020	1.21508	-0.78231
H	2.04537	1.13125	-1.07007
H	0.39029	1.08617	-1.68898
C	0.71202	-2.55899	-0.14423
H	1.30751	-2.74283	0.75722
H	-0.34893	-2.71091	0.08472
H	0.99558	-3.32838	-0.87311
C	0.71166	2.55907	-0.14423
H	0.99518	3.32850	-0.87308
H	-0.34933	2.71086	0.08463
H	1.30706	2.74297	0.75726
H	-3.96606	-0.00022	-0.50722

$C_{1O1}N_{221}^{+}$

Atom	X	Y	Z
C	-2.62151	-1.37632	0.13621
H	-2.37009	-2.29622	0.68512
H	-3.20524	-0.70539	0.78437
C	-0.60019	-0.35050	0.69136
H	-0.23546	-1.20625	1.28117
H	-1.05922	0.38250	1.37424
C	1.48163	0.77999	1.16515
H	1.71631	-0.05369	1.83189
H	2.40208	1.17364	0.72340
H	0.97442	1.56588	1.72993
N	0.59271	0.30706	0.06940
C	1.33046	-0.66537	-0.83524
H	0.60153	-0.96277	-1.59496
H	2.11120	-0.06633	-1.31941
C	0.16768	1.47777	-0.80297
H	1.10600	1.94778	-1.12115
H	-0.31226	1.03313	-1.67965
C	1.92513	-1.87816	-0.15324
H	2.69483	-1.62760	0.58543
H	1.16923	-2.52349	0.30921
H	2.41428	-2.47594	-0.93239
C	-0.75556	2.48215	-0.14903
H	-0.90933	3.29479	-0.86982
H	-1.74242	2.05972	0.07017
H	-0.33946	2.93892	0.75669
O	-1.44047	-0.72713	-0.33277
H	-3.20739	-1.62850	-0.75127