Recent Progress in Single-phase Molecular Multiferroic Materials with Ferroelectricity and Ferroelasticity

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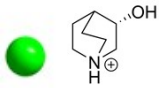
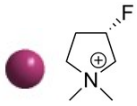
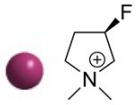
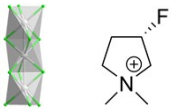
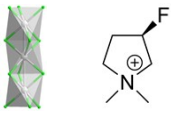
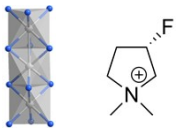
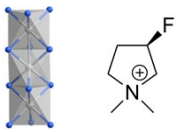
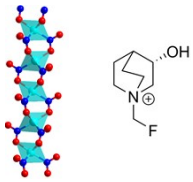
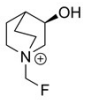
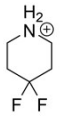
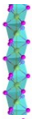
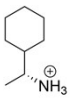
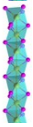
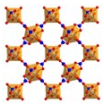
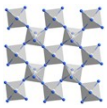
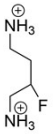
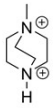
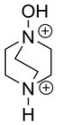
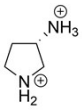
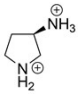
Table S1 Other compounds reported to only exhibit ferroelectric properties

Compound	n-D	component	Phase transition	Polar/ strain axis	P_s (μC·cm^{-2})	ε	Ref.
(*R*)-3-quinuclidinol	0D		**622F6** ($P6_1$ - $P6_122$, T_c = 400 K)	1	6.96		1
(*S*)-3-quinuclidinol	0D		**622F6** ($P6_5$ - $P6_522$, T_c = 396 K)	1	6.72		1
(*R*)-(−)-3 hydroxlyquinuclidinium halides	0D		**432F4** ($P4_1$ - F432, T_c = 340 K)	4	2.4		2
(*R*)-DMFPI iodide DMFPI = (*N,N*-dimethyl-3 fluoropyrrolidinium)	0D		**432F2** ($P2_1$, T_c = 470 K)	6	0.48		3
(*S*)-DMFPI iodide DMFPI = (*N,N*-dimethyl-3 fluoropyrrolidinium)	0D		**432F2** ($P2_1$, T_c = 470 K)	6	0.40		3
(*R*)-3 (Fluoropyrrolidinium) $MnCl_3$	1D		**222F2** ($C222_1$ - $P2_1$, T_c =333 K)	1	5		4
(*S*)-3 (Fluoropyrrolidinium) $MnCl_3$	1D		**222F2** ($C222_1$ - $P2_1$, T_c=333 K)	1	5.8		4
(*R*)-3 (Fluoropyrrolidinium) $CdCl_3$	1D		**222F2** ($C222_1$ - $P2_1$, T_c=303 K)	1	5.63		5
(*S*)-3 (Fluoropyrrolidinium) $CdCl_3$	1D		**222F2** ($C222_1$ - $P2_1$, T_c = 303 K)	1	5.79		5
[(*R*)-FMQ]Ni$(NO_2)_3$ hydroxlyquinuclidinium) FMQ = *N*-fluoromethyl-3-Quinuclidinol	1D		**622F2** ($P2_1$, T_c =405 K)	1	12		6

[(*S*)-FMQ]Ni$(NO_2)_3$ hydroxlyquinuclidiniu m) FMQ = *N*-fluoromethyl-3-Quinuclidinol	1D			**622F2** (*P*2_1, T_c = 405 K)	1	12	6
$(DFPIP)_4AgBiI_8$	1D			**222F2** (*C*2 - *C*222, T_c = 422 K)	1		7
(*R*-CYHEA)PbI_3	1D			**222F2** (*P*2_1-*P*$2_1$$2_1$$2_1$, T_c=373 K)	1	1.2	8
(*S*-CYHEA)PbI_3	1D			**222F2** (*P*2_1 - *P*$2_1$$2_1$$2_1$, T_c = 373 K)	1	1.2	8
$A_4M^IM^{III}(NO_3)_8$ A = organic cation MI = alkaline metal or ammonium ion	2D			**222F2** (*P*2_1 - *B*222, T_c = 320 K)	1	3.0	9
MIII = rare-earth ion *s*-(FBDA)$CdCl_4$ (*s*-FBDA=(2*s*)-2-fluorobutane-1,4-diamine)	2D			**222F1** (*P*2_1 - *P*222_1, T_c = 391 K)	4	1.67	10
$[C_3H_7FN]_3[SnCl_6]Cl$	3D			**622F2** (*P*6_1 - *P*$6_1$22, T_c = 391 K)	1		11
$A(NH_4)X_3$ A = divalent organic cation X = Cl, Br, or I 1. $MDABCO+NH_4I_3$	3D			**432F3** (*R*3 - *P*432, T_c = 448 K)	4	19	12
2. $ODABCO+NH_4Br_3$	3D			**432F3** (*R*3 - *P*432, T_c = 360 K)	4		12
3. (*R*)-3AP+NH_4Br_3	3D			**432F2** (*P*2_1 - *P*432, T_c = 384 K)	6		12
4. (*S*)-3AP+NH_4Br_3	3D			**432F2** (*P*2_1 - *P*432, T_c = 384 K)	6		12

5. (*R*)-3AQ+NH_4Br_3	3D			**432F2** ($P2_1$ - *P*432, T_c = 493 K)	6	12
6. (*S*)-3AQ+NH_4Br_3	3D			**432F2** ($P2_1$ - *P*432, T_c = 493 K)	6	12

References:

1 P. F. Li, W. Q. Liao, Y. Y. Tang, W. Qiao, D. Zhao, Y. Ai, Y. F. Yao and R. G. Xiong, *Proc. Natl. Acad. Sci*., 2019, **116**, 5878-5885.

2 P. F. Li, Y. Y. Tang, Z. X. Wang, H. Y. Ye, Y. M. You and R. G. Xiong, *Nat. Commun*., 2016, **7**, 13635.

3 Y. Ai, D. J. Wu, M. J. Yang, P. Wang, W. H. He and W. Q. Liao, *Chem. Commun.*, 2020, **56**, 7033-7036.

4 Y. Ai, X.-G. Chen, P.-P. Shi, Y.-Y. Tang, P.-F. Li, W.-Q. Liao and R.-G. Xiong, *J. Am. Chem. Soc.*, 2019, **141**, 4474-4479.

5 Y. Y. Tang, Y. Ai, W. Q. Liao, P. F. Li, Z. X. Wang and R. G. Xiong, *Adv. Mater.*, 2019, **31**, e1902163.

6 B. B. Deng, C. C. Xu, T. T. Cheng, Y. T. Yang, Y. T. Hu, P. Wang, W. H. He, M. J. Yang and W. Q. Liao, *J. Am. Chem. Soc.*, *2020*, **142**, 6946-6950.

7 C. F. Wang, H. Li, M. G. Li, Y. Cui, X. Song, Q. W. Wang, J. Y. Jiang, M. M. Hua, Q. Xu, K. Zhao, H. Y. Ye and Y. Zhang, *Adv. Funct. Mater.*, 2021, **31**,2009457.

8 Y. Hu, F. Florio, Z. Chen, W. A. Phelan, M. A. Siegler, Z. Zhou, Y. Guo, R. Hawks, J. Jiang and J. Feng, *Sci. Adv.*, 2020, **6**, eaay4213.

9 C. Shi, L. Ye, Z.-X. Gong, J.-J. Ma, Q.-W. Wang, J.-Y. Jiang, M.-M. Hua, C.-F. Wang, H. Yu and Y. Zhang, *J. Am. Chem. Soc.*, 2019, **142**, 545-551.

10 W. He, C. Chen, S. Wu, W. P. D. Wong, Z. Wu, K. Chang, J. Wang, H. Gao and K. P. Loh, *J. Am. Chem. Soc.*, 2025, **147**, 811-820.

11 G. P. Li, S. Q. Lu, X. Chen, W. Q. Liao, Y. Y. Tang and R. G. Xiong, *Chem. Eur. J.*, 2019, **25**, 16625-16629.

12 H.-Y. Ye, Y.-Y. Tang, P.-F. Li, W.-Q. Liao, J.-X. Gao, X.-N. Hua, H. Cai, P.-P. Shi, Y.-M. You and R.-G. Xiong, *Science*, 2018, **361**, 151-155.