Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

TDDFT studies on chiroptical properties of chiral inorganic polythioanion Möbius strip

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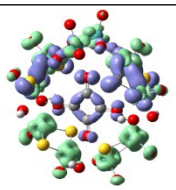
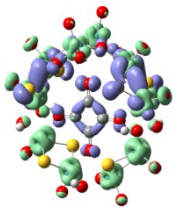
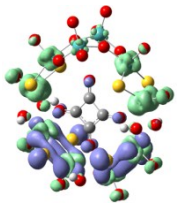
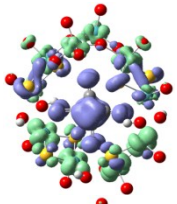
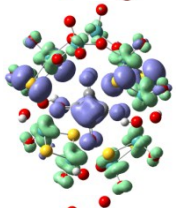
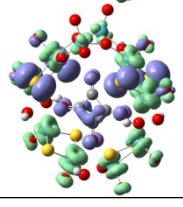
General Comments

Table S1. Relative energy (Δ*E*) of 1a and 1b with various basis sets and functionals

		PBE0		B3LYP	BP86
	6-31G*	6-31+G*	6-31++G*	6-31+G*	6-31+G*
Δ*E* (kal·mol^{-1})	0.628	-1.255	-0.628	-2.510	-1.883

*$\Delta E=E_{1a}-E_{1b}$

Table S2. The EDDMs for crucial transitions contribute to the ECD spectra of 1a (Electron densities move from the purple area to the green area)

Excitation state	MO	Coefficient	EDDM
1	252 ->262, 252 ->265	0.28096, 0.20580	
	253 ->259, 253 ->263	0.14543, 0.23475	
	253 ->264, 253 ->268	0.30278, 0.14565	
	253 ->269, 253 ->279	-0.10211, 0.10796	
	254 ->262, 254 ->265	-0.20042, -0.14489	
	251 ->261, 252 ->269	-0.10466, -0.18631	
17	252 ->271, 252 ->274	0.12325, 0.20717	
	252 ->279, 253 ->261	-0.11736, -0.14758	
	253 ->265, 253 ->275	-0.17912, -0.19254	
	253 ->276, 253 ->277	-0.16837, -0.19346	
	253 ->280, 254 ->269	0.16456, 0.14619	
	254 ->274	-0.14243	
27	248 ->256, 248 ->268	-0.12082, -0.19159	
	248 ->269, 248 ->271	0.21437, 0.10210	
	248 ->273, 249 ->257	0.17774, 0.11737	
	249 ->265, 249 ->266	0.17210, -0.10851	
	249 ->270, 249 ->275	-0.22064, 0.22097	
	249 ->277, 255 ->259	-0.11218, 0.16739	
31	246 ->257, 247 ->256	0.12723, 0.14895	
	251 ->262, 252 ->278	-0.13127, 0.11879	
	253 ->261, 253 ->262	-0.11359, 0.11742	
	253 ->276, 253 ->277	-0.17578, 0.11943	
	254 ->260, 255 ->256	0.12119, 0.25517	
37	246 ->258, 250 ->259	0.11511, -0.11207	
	250 ->263, 250 ->264	-0.22866, -0.14850	
	251 ->267, 251 ->270	0.28785, -0.10229	
	255 ->259, 255 ->264	0.11645, 0.24994	
38	250 ->267, 250 ->270	0.28227, -0.10006	
	251 ->259, 251 ->263	-0.13394, -0.22905	
	251 ->264, 251 ->268	-0.19942, -0.12826	
	251 ->269, 251 ->274	-0.11152, -0.10285	
	253 ->260, 255 ->267	0.11473, -0.22652	

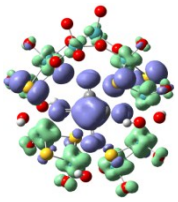
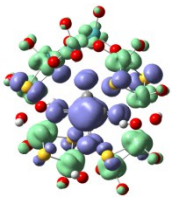
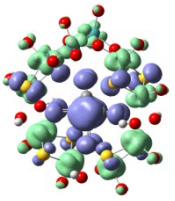
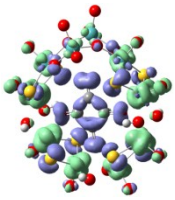
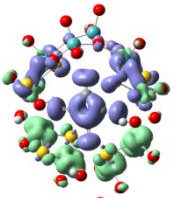
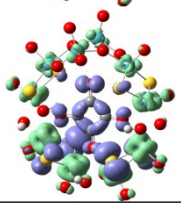
50	246 ->271, 247 ->258	-0.10597, 0.13972	
	250 ->262, 250 ->276	-0.13286, -0.16383	
	251 ->264, 251 ->269	-0.10664, 0.10087	
	251 ->271, 251 ->273	0.11297, -0.13740	
	251 ->274, 254 ->258	0.12688, -0.14138	
	254 ->266, 255 ->258	0.11245, 0.16058	
	255 ->265, 255 ->267	0.17085, 0.14056	
66	246 ->259, 247 ->262	-0.10359, 0.11812	
	247 ->266, 250 ->262	-0.11626, 0.12270	
	250 ->265, 250 ->272	0.10451, 0.10618	
	250 ->275, 251 ->268	-0.10659, -0.18044	
	254 ->257, 254 ->262	-0.14417, -0.11530	
	255 ->262, 255 ->265	0.26440, 0.11039	
	255 ->266, 255 ->275	-0.14357, 0.12379	
67	246 ->265, 246 ->266	0.14628, -0.16996	
	246 ->272, 247 ->259	-0.10365, -0.10699	
	247 ->263, 254 ->256	0.12679, 0.20127	
	255 ->263, 255 ->268	0.11179, 0.15303	
	255 ->269, 255 ->273	-0.15130, -0.18708	
	255 ->274	-0.13828	
83	232 ->256, 242 ->262	-0.15104, -0.13642	
	242 ->270, 242 ->275	0.10167, -0.14933	
	243 ->273, 244 ->268	0.13011, -0.12481	
	244 ->273, 244 ->274	0.11209, 0.11263	
	245 ->275, 252 ->268	-0.12035, 0.10633	
	252 ->273, 254 ->268	-0.12891, 0.17089	
	254 ->273, 254 ->284	-0.16315, -0.12552	
	255 ->268, 255 ->269	-0.12033, -0.11204	
94	242 ->272, 244 ->271	0.10100, 0.11527	
	252 ->256, 252 ->274	0.25098, 0.10526	
	253 ->257, 254 ->271	-0.20664, -0.12989	
	254 ->274, 255 ->268	0.15486, -0.19386	
106	246 ->259, 247 ->265	0.11195, -0.15640	
	247 ->266, 247 ->272	0.16841, 0.13525	
	249 ->256, 254 ->267	0.13079, 0.10723	
	254 ->270, 254 ->272	0.16567, 0.18024	

Table S3. Spin density and atomic charges for [1a]$^{-}$

Atom	Spin density[a]	q [b]	q [c]
Mo^{V}_{3}	0.204	0.389	0.747
Mo^{V}_{4}	0.187	0.379	0.718
Mo^{V}_{5}	0.187	0.379	0.718
Mo^{V}_{6}	0.204	0.389	0.747

Table S4. Spin density and atomic charges for [1a]$^{2-}$

Atom	Spin density [a]	q [b]	q [c]
Mo^{V}_{1}	0.375	0.435	0.841
Mo^{V}_{2}	-0.031	0.291	0.635
Mo^{V}_{3}	0.204	0.289	0.732
Mo^{V}_{4}	0.187	0.263	0.699
Mo^{V}_{5}	0.204	0.263	0.699
Mo^{V}_{6}	0.187	0.289	0.732
Mo^{V}_{7}	-0.031	0.291	0.635
Mo^{V}_{8}	0.375	0.435	0.841
Mo^{VI}_{1}	0.134	1.453	1.717
Mo^{VI}_{2}	0.134	1.453	1.717

[a] Spin densities computed for the Mo atoms; [b] Natural charges computed for the Mo atoms; [c] Mulliken charges computed for the Mo atoms

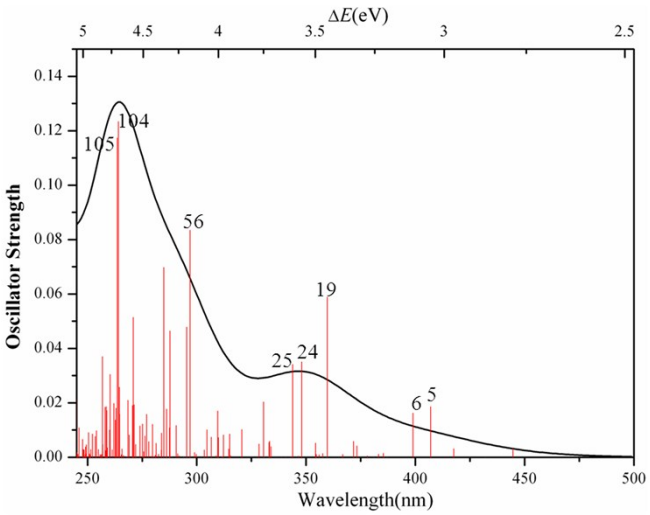


Fig. S1. Calculated UV−vis spectra of **1b**. The half bandwidth of σ = 0.22 eV.

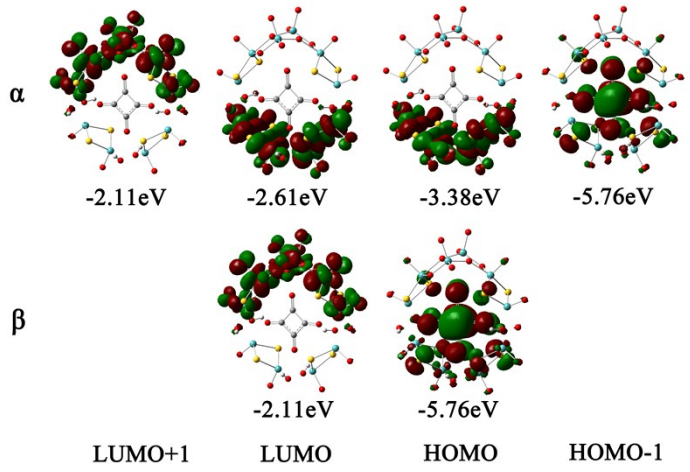


Fig. S2. Frontier molecular orbitals for **[1a]**$^{-}$.

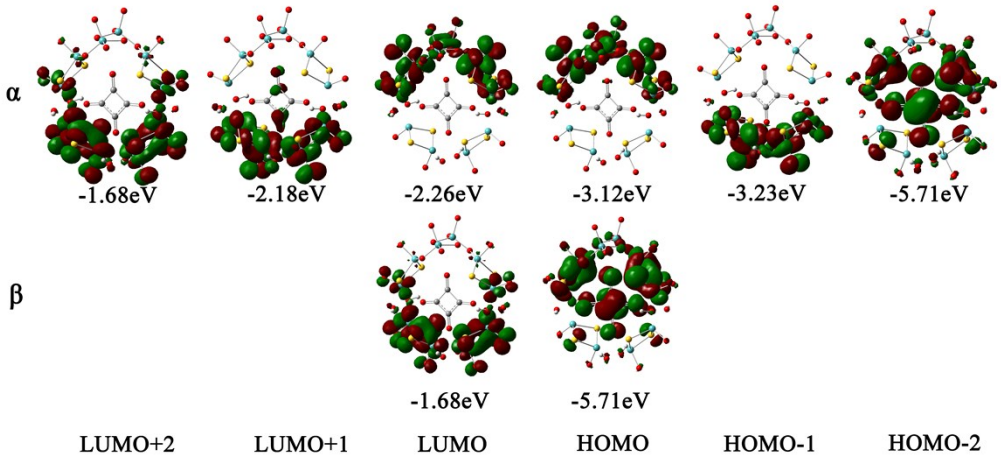


Fig. S3. Frontier molecular orbitals for **[1a]**$^{2-}$.

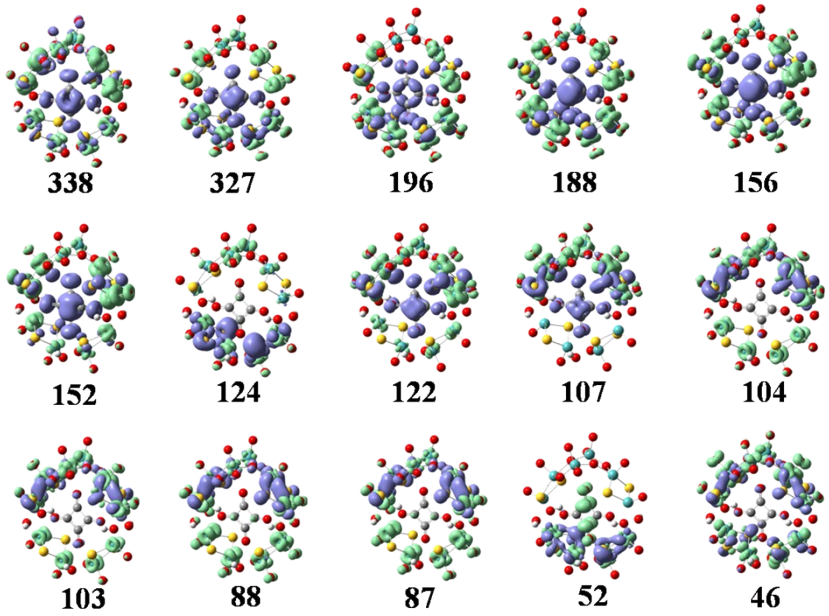


Fig. S4. The EDDMs for crucial transitions contribute to the ECD spectra of **[1a]**$^{-}$.

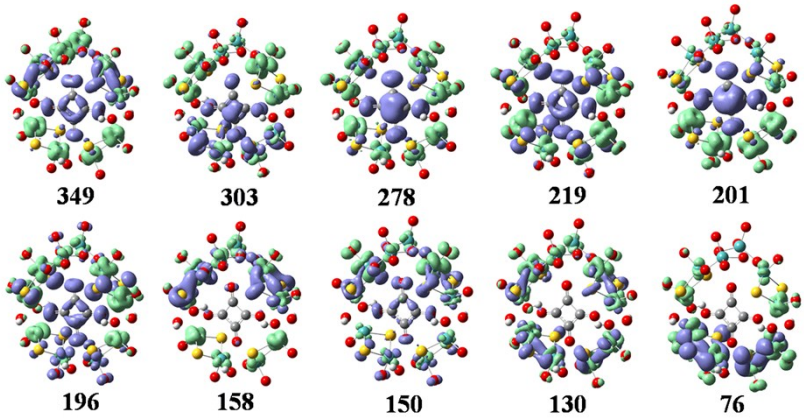


Fig. S5. The EDDMs for crucial transitions contribute to the ECD spectra of **[1a]**$^{2-}$.

Coordinate of 1a

Mo	0.000000	1.751746	-4.440334
Mo	-2.732855	0.39461b	-2.99461b
Mo	-4.241674	-0.219185	-0.630044
Mo	-3.751718	-0.484021	2.662510
Mo	-1.61b386	-0.260898	4.591437
S	-2.823065	1.468038	3.558455
S	-2.214122	-2.134492	3.294642
S	-2.940158	-1.680502	-1.914014
S	-3.601444	1.884460	-1.385902
O	-1.480475	1.937944	-3.324183
O	-0.491691	1.762442	-6.091411
O	0.842579	3.235861	-4.218649
O	-1.264674	-0.400999	-4.203481
O	-3.950437	0.422766	-4.162157
O	-5.807795	-0.441886	-1.222220
O	-4.691173	0.716089	1.213498
O	-4.2431b8	-1.646100	0.960750
O	-2.277407	-0.046996	0.771424
O	-5.103708	-0.796232	3.622545
O	-2.418398	-0.488767	6.072430
O	0.000000	0.000000	2.965710
O	0.199342	-1.189970	5.164522
O	0.000000	0.000000	-1.591787
C	-1.027428	-0.024069	0.704264
C	0.000000	0.000000	-0.1b6273
Mo	0.000000	-1.751746	-4.440334
Mo	2.732855	-0.39461b	-2.99461b
Mo	4.241674	0.219185	-0.630044
Mo	3.751718	0.484021	2.662510
Mo	1.61b386	0.260898	4.591437
S	2.823065	-1.468038	3.558455
S	2.214122	2.134492	3.294642
S	2.940158	1.680502	-1.914014
S	3.601444	-1.884460	-1.385902
O	1.480475	-1.937944	-3.324183
O	0.491691	-1.762442	-6.091411
O	-0.842579	-3.235861	-4.218649

O	1.264674	0.400999	-4.203481
O	3.950437	-0.422766	-4.162157
O	5.807795	0.441886	-1.222220
O	4.691173	-0.716089	1.213498
O	4.2431b8	1.646100	0.960750
O	2.277407	0.046996	0.771424
O	5.103708	0.796232	3.622545
O	2.418398	0.488767	6.072430
O	-0.199342	1.189970	5.164522
C	1.027428	0.024069	0.704264
C	0.000000	0.000000	1.701375
H	-0.342160	2.057054	4.756416
H	3.660944	2.405937	0.813128
H	-4.461496	1.655949	1.253247
H	-3.660944	-2.405937	0.813128
H	0.342160	-2.057054	4.756416
H	4.461496	-1.655949	1.253247

Coordinate of 1b

Mo	2.231328	-3.398026	0.000081
Mo	-4.783214	-0.452450	0.000070
Mo	1.919747	3.954135	-0.000276
Mo	-0.485145	-4.308834	-0.000239
Mo	3.947545	1.935549	0.000057
Mo	-3.839427	2.720324	0.000042
Mo	-1.418921	4.222122	-0.000233
Mo	-3.550462	-3.030175	-0.000210
Mo	3.759262	-0.953467	-2.318781
Mo	3.757869	-0.953193	2.319540
S	-3.922013	-1.620376	1.832838
S	-3.922028	-1.619929	-1.832917
S	-2.472147	3.223938	1.831812
S	-2.472049	3.223071	-1.831829
S	2.723387	2.757196	-1.826737
S	2.723775	2.758392	1.826693
S	0.752318	-3.548105	-1.823540
S	0.751913	-3.548380	1.823347

O	0.083309	2.202405	0.000725
O	-2.717742	0.691658	0.000550
O	-1.345598	-2.123062	-0.000237
O	1.602575	-0.777061	0.000137
O	-2.240086	-4.165522	1.208454
O	-2.240082	-4.165295	-1.209040
O	-0.284044	-5.988346	-0.000340
O	-4.892767	-4.053262	-0.000357
O	-6.423289	-0.852207	0.000075
O	-4.857947	1.296479	-1.204369
O	-4.858009	1.296596	1.204560
O	-5.001217	3.946397	-0.000195
O	-2.026176	5.793951	-0.000627
O	0.277147	4.500319	-1.211156
O	0.277309	4.501175	1.210419
O	2.814129	5.384081	-0.000889
O	5.367507	2.847341	-0.000218
O	4.383412	0.423189	-1.273521
O	4.381814	0.423518	1.274264
O	4.972221	-1.311129	-3.498338
O	3.476784	-2.460513	-1.322502
O	3.476139	-2.460355	1.323202
O	2.971010	-4.915157	0.000132
O	4.971104	-1.310472	3.498921
O	2.319883	-0.486986	3.150407
O	2.321303	-0.487107	-3.149569
C	-0.231093	0.995002	0.000179
C	0.447240	-0.341297	-0.000018
C	-0.885874	-0.956171	-0.000200
C	-1.511216	0.323669	0.000064
H	-2.077489	-3.780890	-2.083294
H	-2.077532	-3.781400	2.082838
H	0.246803	4.070306	2.077230
H	0.246579	4.068981	-2.077730
H	-4.476663	1.183165	-2.087672
H	-4.476502	1.183292	2.087772