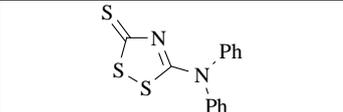
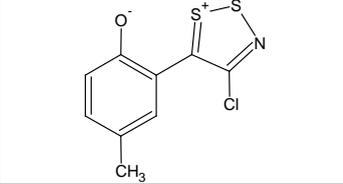
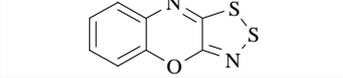
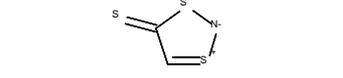
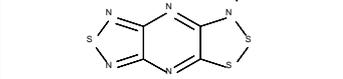
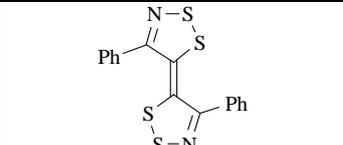
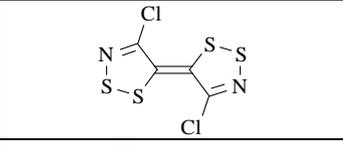
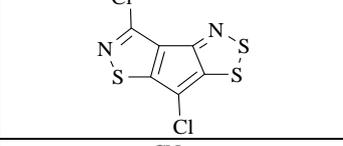
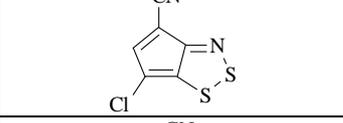
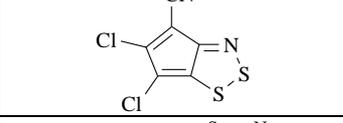
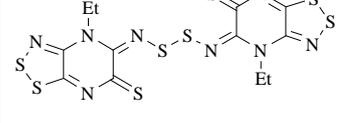
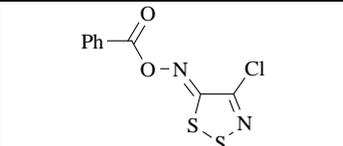
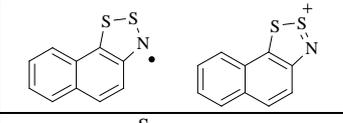
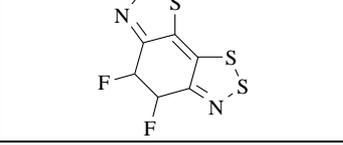


**Bond orders and electron delocalization indices
for S–N, S–C and S–S bonds in 1,2,3-dithiazole systems**

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Table S1 The sample of molecules.

N	Name of compound	Structure formula	Refcode in the Cambridge Structural Database (CSD)
1	4-Methylmercapto-5-phenyl-1,2-dithiole-3-thione [1]		ABOKAE
2	4-Methyl-5-(2-pyrazinyl)-3H-1,2-dithiole-3-thione [2]		BIXSOQ10
3	[1,3]Dithiolo[4,5-b]pyrazine-2-thione [3]		DILCOS
4	4-Methyl-5-(2-(2-pyrazinyl)vinyl)-3H-1,2-dithiole-3-thione [4]		DUVHUX10
5	[1,3]Dithiolo[4,5-f][1,10]phenanthroline-2-thione [5]		MIHNOI
6	5-Amino-4-cyano-3H-1,2-dithiole-3-thione [6]		MOHGUM
7	5-(Pyridin-4-yl)-5H-[1,3]dithiolo[4,5-c]pyrrole-2-thione [7]		OJOVUF
8	2-Sulfanylidene-2H-[1,3]benzodithiole-4-carbonitrile [8]		PIYMIW
9	4-(3-thioxo-3H-1,2-dithiol-4-yl)-5,6-dihydro-3H,4H-[1,2]dithiolo[3,4-b][1,4]thiazine-3-thione [9]		PUJRIV
10	4,5-Dichloro-1,2,3-dithiazolium [10]		HIDFAB

11	5-(Diphenylamino)-3 <i>H</i> -1,2,4-dithiazole-3-thione [11]		BUTXOF
12	2-(4-chloro-1,2,3-dithiazol-1-ium-5-yl)-4-methylbenzenolate [12]		DASWAV
13	[1,2,3]Dithiazolo[4,5- <i>b</i>][1,4]benzoxazine [13]		DESFEP
14	1,3,2-Dithiazole-4-thione [14]		FUWMIT
15	1,2,5-Thiadiazolo[3,4- <i>b</i>][1,2,3]-dithiazolo(3,4- <i>b</i>)pyrazinyl radical [15]		HEHQUG
16	4-Phenyl-5-(4-phenyl-5 <i>H</i> -1,2,3-dithiazol-5-ylidene)-5 <i>H</i> -1,2,3-dithiazole [16]		HIMRUT
17	<i>trans</i> -4,4'-Dichloro-1,1',2,2',3,3'-tetrathiadiazafulvalenium [17]		LAMQAR
18	4,7-Dichloroisothiazolo[4,5- <i>d</i>]cyclopenta[1,2,3]dithiazole [18]		LAXZAM
19	6-Chlorocyclopenta[1,2,3]dithiazole-4-carbonitrile [18]		LAXZEQ
20	5,6-Dichlorocyclopenta[1,2,3]dithiazole-4-carbonitrile [18]		LAXZIU
21	4-Ethyl-5-[[[4-ethyl-6-thioxo-4 <i>H</i> -[1,2,3]dithiazolo[4,5- <i>b</i>]pyrazin-5(6 <i>H</i>)-ylidene]amino]dithio]imino]-4,5-dihydro-6 <i>H</i> -[1,2,3]dithiazolo[4,5- <i>b</i>]pyrazine-6-thione [19]		LEFHOU
22	5-Benzoyloxyimino-4-chloro-5 <i>H</i> -1,2,3-dithiazole [20]		LOKBIW
23	3 <i>H</i> -Naphtho[1,2- <i>d</i>][1,2,3]dithiazolyl radical or cation [21]		MALJAL
24	4,5-Difluorobenzo(1,2- <i>d</i> :4,3- <i>d'</i>)bis([1,2,3]dithiazole) [22]		MAVQEG

25	trans-4,4'-Dichloro-1,1',2,2',3,3'-tetrathiadiazafulvalene [23]		PIHQUS
26	5-((4-Chloro-5H-1,2,3-dithiazol-5-ylidene)amino)-1,3,4-thiadiazole-2-carbonitrile [24]		PUZXAJ
27	4-Chloro-5-perfluorophenyl-1,2,3-dithiazol-2-ium cation [25]		QACYOI
28	1,2-bis(4-Chloro-5H-1,2,3-dithiazol-5-yl)dinitrogen [26]		QUDWUH
29	Benzo(2,1-d:3,4-d')bis([1,2,3]dithiazole) [27]		REHMIA
30	Benzo(2,1-d:3,4-d')bis([1,2,3]dithiazolyl) [27]		REHMOG
31	1,2,3-Benzodithiazolium cation [28]		RIHHUN
32	Naphtho(2,1-d:6,5-d')bis([1,2,3]dithiazole) [29]		SOBFEU
33	Naphtho(2,1-d:6,5-d')bis([1,2,3]dithiazolium) cation [30]		VEPMAF
34	5H-[1,2,5]thiadiazolo[3,4-e][1,2,3]benzodithiazol-5-ylidenemalononitrile [31]		WURYAL
35	4-(4-(2-Chloroethyl)piperazin-1-yl)-5H-1,2,3-dithiazole-5-thione [32]		XAKBET
36	4-Chloro-5-(3,4-dichloroiso-thiazol-5-yl)-1,2,3-dithiazolium [33]		XOTJAR
37	4,5-Dimethyl-3-phenyl-1,3-thiazole-2(3H)-thione [34]		AJUVEI
38	4-[(1E)-Prop-1-en-1-yl]-1,3-thiazole [35]		ELINAQ

39	(4S,5R)- <i>cis</i> -3,4-Dimethyl-5-phenyl-thiazolidinethione [36]		IPUCAY
40	2-(<i>tert</i> -Butylthio)-4,4-dimethyl-1,3-thiazole-5(4 <i>H</i>)-thione [37]		YILWIZ
41	5-Amino-3 <i>H</i> -1,3,4-thiadiazole-2-thione [38]		ATTDZ02
42	3-Methyl-5-(methylsulfanyl)-1,3,4-thiadiazole-2(3 <i>H</i>)-thione [39]		CEGYAQ
43	5-Sulfanyl-1,3,4-thiadiazole-2(3 <i>H</i>)-thione [40]		DMCTDZ01
44	3-(2-Methylphenyl)-1,2,4-thiadiazole-5(4 <i>H</i>)-thione [41]		ZUGFAK
45	4-Trichloromethyl-1,2-dithia-3,5-diazolium chloride [42]		CLMTDZ
46	Dithiadiazolyl bromide [43]		ZALXUF
47	5-Methylsulfanyl-1,2,3,4-thiaziazole [44]		ISEBIR
48	1,3-Thiazolidine-2-thione [45]		CASHOT04
49	4,4-Dimethyl-1,3-thiazolodine-2,5-dithione [37]		YILWEV
50	3- <i>tert</i> -Butylthiazolidine-2-thione [46]		YUFPOE
51	<i>cis</i> -3,4,5-Trimethylthiazolidine-2-thione [47]		ZIKVUK
52	2,4-Dimethyl-1,2,4-thiadiazolidine-3,5-dithione [48]		MTDZDT
53	3,4-Diisopropyl-1,3-thiazole-2(3 <i>H</i>)-thione [49]		DIPTZT
54	1-Thia-2,3,4-triazacyclopent-2-ene-5-thione [50]		QOBFUI
55	1,2,5,6,9,10-Hexathiacyclododecane [51]		DICHEC

56	bis(Pyrazol-1-ylthiocarbonyl)disulfide [52]		AHUFUF
57	Dimethyl disulfide [53]		DEMQIW
58	bis(1,2,3,4-Thiatriazol-5-yl) disulfide [50]		QOBGAP

Table S2 The topological characteristics of electron density at the bond critical points (a.u.), equilibrium interatomic distances (Å) and electron delocalization indices DI(S-S) for S-S bonds.

Refcode in the Cambridge Structural Database (CSD)	R_{AB}	$\rho(r_b)$	$\lambda_1(r_b)$	$\lambda_2(r_b)$	$\lambda_3(r_b)$	DI(S-S)
ABOKAE	2.065	0.150	-0.193	-0.159	0.214	1.218
AHUFUF	2.034	0.159	-0.191	-0.189	0.211	1.279
BIXSOQ10	2.058	0.152	-0.197	-0.162	0.213	1.229
BUTXOF	2.070	0.148	-0.188	-0.158	0.212	1.223
CLMTDZ	2.057	0.155	-0.212	-0.161	0.242	1.259
DASWAV	2.149	0.132	-0.170	-0.136	0.232	1.070
DESFEP	2.104	0.140	-0.181	-0.146	0.214	1.167
DEMQIW	2.040	0.155	-0.179	-0.177	0.207	1.352
DICHEC	2.042	0.154	-0.177	-0.176	0.206	1.335
DUVHUX10	2.058	0.151	-0.196	-0.161	0.212	1.231
HEHQUG	2.119	0.137	-0.176	-0.146	0.218	1.122
HIDFAB	2.049	0.156	-0.210	-0.163	0.225	1.238
HIMRUT	2.095	0.143	-0.184	-0.150	0.217	1.154
LAXZAM	2.113	0.138	-0.180	-0.142	0.219	1.140
LAXZEQ	2.104	0.141	-0.185	-0.145	0.220	1.153
LAXZIU	2.103	0.141	-0.185	-0.145	0.220	1.153
LEFHOU	2.187	0.128	-0.180	-0.137	0.235	0.962
	2.083	0.146	-0.190	-0.151	0.216	1.182
LOKBIW	2.101	0.142	-0.183	-0.148	0.216	1.159
MALJAL	2.049	0.156	-0.210	-0.163	0.225	1.229
MALJAL	2.108	0.139	-0.180	-0.147	0.218	1.129
MOHGUM	2.090	0.142	-0.181	-0.149	0.213	1.189
PIHQUS	2.102	0.142	-0.186	-0.149	0.218	1.138
PUJRIV	2.064	0.147	-0.188	-0.154	0.213	1.207
PUZXAJ	2.089	0.146	-0.190	-0.154	0.222	1.159
QACYOI	2.040	0.159	-0.215	-0.166	0.225	1.251
QOBGAP	2.044	0.154	-0.182	-0.176	0.209	1.293
QUDWUH	2.092	0.144	-0.187	-0.151	0.217	1.171
REHMIA	2.115	0.137	-0.177	-0.143	0.216	1.139
RIHHUN	2.046	0.157	-0.212	-0.164	0.225	1.251
SOBFEU	2.104	0.140	-0.181	-0.146	0.217	1.146
VEPMAF	2.043	0.158	-0.215	-0.166	0.227	1.262
WURYAL	2.094	0.143	-0.187	-0.150	0.219	1.156
XAKBET	2.067	0.150	-0.196	-0.157	0.220	1.185
XOTJAR	2.051	0.157	-0.212	-0.165	0.227	1.216
ZALXUF	2.051	0.157	-0.213	-0.163	0.241	1.276

Table S3 The topological characteristics of electron density at the bond critical points (a.u.), equilibrium interatomic distances (Å) and electron delocalization indices DI(S-C) for S-C bonds.

Refcode in the Cambridge Structural Database (CSD)	R_{AB}	$\rho(r_b)$	$\lambda_1(r_b)$	$\lambda_2(r_b)$	$\lambda_3(r_b)$	DI(S-C)
ABOKAE	1.644	0.227	-0.234	-0.219	0.378	1.682
	1.729	0.212	-0.340	-0.277	0.215	1.240
	1.761	0.199	-0.300	-0.265	0.197	1.133
	1.808	0.183	-0.278	-0.255	0.245	1.094
	1.741	0.208	-0.335	-0.279	0.242	1.231
AJUVEI	1.648	0.222	-0.218	-0.207	0.424	1.632
	1.744	0.208	-0.331	-0.277	0.221	1.177
	1.740	0.212	-0.348	-0.280	0.223	1.193
AHUFUF	1.782	0.196	-0.319	-0.255	0.243	1.126
	1.621	0.234	-0.239	-0.227	0.540	1.757
ATTDZ02	1.643	0.222	-0.218	-0.206	0.463	1.655
	1.766	0.202	-0.328	-0.272	0.248	1.124
	1.749	0.207	-0.329	-0.270	0.214	1.123
BIXSOQ	1.734	0.211	-0.342	-0.282	0.236	1.249
	1.738	0.209	-0.336	-0.273	0.217	1.212
	1.649	0.226	-0.231	-0.219	0.346	1.670
BUTXOF	1.773	0.197	-0.315	-0.251	0.235	1.099
	1.777	0.195	-0.312	-0.260	0.267	1.123
	1.639	0.229	-0.240	-0.220	0.428	1.681
CASHOT04	1.819	0.181	-0.272	-0.251	0.246	1.074
	1.758	0.207	-0.337	-0.272	0.225	1.162
	1.641	0.224	-0.226	-0.208	0.445	1.673
CEGYAQ	1.801	0.185	-0.282	-0.263	0.247	1.099
	1.737	0.209	-0.333	-0.261	0.169	1.182
	1.740	0.208	-0.328	-0.272	0.209	1.165
	1.758	0.204	-0.333	-0.274	0.241	1.137
	1.645	0.222	-0.216	-0.207	0.440	1.635
DASWAV	1.739	0.212	-0.349	-0.273	0.221	1.247
DEFEP	1.748	0.207	-0.333	-0.271	0.223	1.174
DEMQUIW	1.810	0.183	-0.281	-0.258	0.249	1.107
DICHEC	1.819	0.181	-0.276	-0.255	0.252	1.074
	1.827	0.178	-0.270	-0.250	0.254	1.059
DILCOS	1.745	0.207	-0.333	-0.275	0.227	1.229
	1.745	0.211	-0.348	-0.284	0.217	1.135
	1.628	0.230	-0.232	-0.222	0.484	1.780
DIPTZT	1.732	0.215	-0.355	-0.283	0.215	1.215
	1.723	0.214	-0.342	-0.286	0.201	1.223
	1.659	0.219	-0.216	-0.203	0.365	1.589
DMCTDZ01	1.762	0.203	-0.330	-0.273	0.245	1.135
	1.745	0.207	-0.326	-0.270	0.217	1.157
	1.747	0.205	-0.327	-0.265	0.190	1.168
	1.638	0.223	-0.219	-0.208	0.484	1.676
DUVHUX10	1.737	0.210	-0.340	-0.281	0.239	1.235
	1.742	0.207	-0.331	-0.274	0.220	1.205
	1.647	0.226	-0.232	-0.220	0.349	1.675
ELINAQ	1.725	0.215	-0.353	-0.282	0.224	1.241
	1.708	0.220	-0.357	-0.291	0.197	1.298
FUWMIT	1.762	0.205	-0.339	-0.280	0.263	1.161
	1.652	0.220	-0.216	-0.206	0.372	1.655
	1.657	0.246	-0.418	-0.314	0.143	1.426
HEHQUG	1.724	0.215	-0.351	-0.286	0.221	1.159
HIDFAB	1.685	0.230	-0.368	-0.284	0.147	1.404
HIMRUT	1.767	0.196	-0.302	-0.257	0.225	1.165
IPUCAY	1.753	0.207	-0.336	-0.272	0.221	1.159

	1.648	0.224	-0.226	-0.209	0.407	1.647
	1.824	0.181	-0.268	-0.253	0.247	1.035
ISEBIR	1.726	0.212	-0.334	-0.260	0.145	1.221
	1.708	0.221	-0.350	-0.282	0.184	1.249
	1.803	0.185	-0.282	-0.263	0.249	1.092
LAXZAM	1.700	0.224	-0.364	-0.279	0.154	1.286
	1.712	0.216	-0.337	-0.281	0.180	1.265
LAXZEQ	1.706	0.219	-0.341	-0.284	0.176	1.275
LAXZIU	1.704	0.219	-0.341	-0.283	0.171	1.280
LEFHOU	1.651	0.234	-0.260	-0.239	0.271	1.599
	1.731	0.213	-0.347	-0.278	0.214	1.217
LOKBIW	1.753	0.202	-0.318	-0.263	0.225	1.145
MALJAL	1.699	0.224	-0.356	-0.292	0.185	1.342
MALJAL	1.732	0.210	-0.330	-0.275	0.212	1.182
MAVQEG	1.744	0.205	-0.319	-0.269	0.210	1.191
MIHNOI	1.742	0.210	-0.338	-0.282	0.212	1.168
	1.740	0.209	-0.338	-0.276	0.226	1.234
	1.742	0.210	-0.338	-0.282	0.212	1.168
	1.740	0.209	-0.338	-0.276	0.226	1.233
	1.632	0.228	-0.228	-0.219	0.472	1.757
MOHGUM	1.732	0.212	-0.339	-0.269	0.186	1.212
	1.638	0.228	-0.233	-0.217	0.425	1.709
	1.748	0.206	-0.332	-0.278	0.246	1.202
MTDZDT	1.651	0.221	-0.216	-0.205	0.432	1.576
	1.730	0.218	-0.371	-0.292	0.228	1.175
OJOVUF	1.630	0.230	-0.231	-0.221	0.474	1.767
	1.750	0.205	-0.330	-0.268	0.232	1.228
	1.732	0.211	-0.338	-0.285	0.191	1.177
PIHQUS	1.778	0.193	-0.297	-0.248	0.227	1.154
PIYMIW	1.741	0.211	-0.340	-0.282	0.201	1.182
	1.628	0.229	-0.230	-0.221	0.490	1.776
	1.745	0.207	-0.335	-0.275	0.230	1.222
	1.745	0.209	-0.337	-0.275	0.227	1.231
	1.741	0.210	-0.340	-0.284	0.208	1.172
PUJRIV	1.738	0.210	-0.339	-0.281	0.239	1.229
	1.643	0.226	-0.230	-0.217	0.381	1.677
	1.813	0.182	-0.276	-0.258	0.251	1.062
	1.729	0.211	-0.331	-0.272	0.197	1.239
	1.737	0.207	-0.324	-0.261	0.179	1.227
PUZXAJ	1.748	0.206	-0.331	-0.265	0.232	1.199
	1.729	0.213	-0.343	-0.275	0.208	1.188
	1.733	0.214	-0.353	-0.281	0.220	1.155
QACYOI	1.688	0.229	-0.369	-0.291	0.174	1.397
QOBFUI	1.738	0.213	-0.349	-0.284	0.227	1.177
	1.635	0.223	-0.219	-0.206	0.503	1.700
QOBGAP	1.700	0.223	-0.351	-0.280	0.173	1.249
	1.746	0.207	-0.339	-0.275	0.203	1.139
	1.751	0.205	-0.327	-0.268	0.198	1.146
	1.704	0.222	-0.348	-0.280	0.178	1.258
QUDWUH	1.753	0.203	-0.323	-0.264	0.231	1.149
REHMIA	1.745	0.205	-0.319	-0.270	0.212	1.191
RIHHUN	1.706	0.222	-0.353	-0.294	0.195	1.310
SOBFEU	1.746	0.205	-0.319	-0.270	0.216	1.204
VEPMAF	1.702	0.223	-0.354	-0.291	0.183	1.335
WURYAL	1.736	0.209	-0.329	-0.276	0.210	1.233
XAKBET	1.728	0.213	-0.341	-0.280	0.227	1.290
	2.067	0.150	-0.196	-0.157	0.220	1.185
	1.644	0.226	-0.229	-0.218	0.369	1.694
XOTJAR	1.706	0.222	-0.353	-0.282	0.186	1.350
	1.742	0.209	-0.337	-0.266	0.203	1.174

YILWEV	1.623	0.235	-0.246	-0.230	0.481	1.828
	1.729	0.215	-0.345	-0.283	0.212	1.273
	1.770	0.202	-0.330	-0.280	0.246	1.092
	1.637	0.226	-0.229	-0.213	0.480	1.698
YILWIZ	1.625	0.234	-0.246	-0.228	0.468	1.825
	1.731	0.213	-0.341	-0.284	0.221	1.269
	1.791	0.192	-0.302	-0.261	0.253	1.047
	1.740	0.209	-0.332	-0.265	0.183	1.188
YUFPOE	1.852	0.171	-0.256	-0.242	0.257	0.976
	1.653	0.222	-0.223	-0.206	0.383	1.630
	1.760	0.205	-0.333	-0.271	0.230	1.153
ZIKVUK	1.806	0.186	-0.280	-0.261	0.245	1.074
	1.757	0.205	-0.332	-0.271	0.225	1.151
	1.825	0.180	-0.272	-0.252	0.251	1.036
ZUGFAK	1.647	0.225	-0.227	-0.211	0.414	1.655
	1.740	0.214	-0.358	-0.281	0.226	1.180
	1.641	0.224	-0.222	-0.208	0.466	1.679

Table S04. The topological characteristics of electron density at the bond critical points (a.u.), equilibrium interatomic distances (\AA) and electron delocalization indices $\text{DI}(\text{S-N})$ for S-N bonds

Refcode in the Cambridge Structural Database (CSD)	R_{AB}	$\rho(r_b)$	$\lambda_1(r_b)$	$\lambda_2(r_b)$	$\lambda_3(r_b)$	$\text{DI}(\text{S-N})$
CLMTDZ	1.577	0.255	-0.365	-0.295	0.746	1.430
	1.569	0.258	-0.374	-0.300	0.819	1.462
DASWAV	1.625	0.232	-0.315	-0.249	0.503	1.327
DESFEP	1.652	0.225	-0.317	-0.233	0.305	1.251
FUWMIT	1.592	0.249	-0.373	-0.272	0.610	1.394
	1.639	0.229	-0.322	-0.241	0.392	1.288
HEHQUG	1.622	0.240	-0.344	-0.261	0.381	1.280
HIDFAB	1.591	0.248	-0.364	-0.272	0.657	1.371
HIMRUT	1.644	0.229	-0.324	-0.239	0.325	1.280
ISEBIR	1.700	0.218	-0.336	-0.276	0.197	1.244
LAXZAM	1.664	0.227	-0.330	-0.252	0.167	1.248
	1.624	0.236	-0.338	-0.246	0.447	1.325
LAXZEQ	1.615	0.239	-0.346	-0.251	0.504	1.346
LAXZIU	1.616	0.239	-0.345	-0.251	0.495	1.340
LEFHOU	1.634	0.225	-0.323	-0.235	0.493	1.254
	1.643	0.229	-0.324	-0.241	0.324	1.260
LOKBIW	1.642	0.227	-0.322	-0.232	0.368	1.269
MALJAL	1.583	0.253	-0.375	-0.280	0.708	1.414
MALJAL	1.617	0.241	-0.347	-0.260	0.427	1.284
MAVQEG	1.634	0.232	-0.331	-0.243	0.381	1.295
MTDZDT	1.706	0.205	-0.290	-0.212	0.184	1.070
PIHQUS	1.639	0.228	-0.322	-0.235	0.391	1.261
	1.639	0.228	-0.322	-0.235	0.391	1.261
PIZDOR	1.629	0.236	-0.327	-0.259	0.375	1.316
PUZXAJ	1.634	0.230	-0.324	-0.239	0.417	1.291
QACYOI	1.590	0.249	-0.365	-0.275	0.661	1.368
QOBFUI	1.710	0.214	-0.325	-0.265	0.168	1.208
QOBGAP	1.690	0.222	-0.340	-0.277	0.169	1.254
	1.698	0.219	-0.338	-0.277	0.195	1.251
QUDWUH	1.640	0.228	-0.324	-0.234	0.378	1.277
REHMIA	1.637	0.232	-0.331	-0.243	0.355	1.300
RIHHUN	1.575	0.256	-0.382	-0.284	0.768	1.451
SOBFEU	1.634	0.234	-0.333	-0.247	0.356	1.301
VEPMAF	1.568	0.259	-0.389	-0.293	0.814	1.459
WURYAL	1.620	0.237	-0.341	-0.249	0.474	1.324

	1.621	0.245	-0.375	-0.272	0.489	1.286
	1.617	0.244	-0.372	-0.269	0.464	1.286
XAKBET	1.632	0.233	-0.330	-0.247	0.400	1.281
XOTJAR	1.594	0.247	-0.360	-0.271	0.652	1.353
	1.621	0.240	-0.357	-0.259	0.470	1.293
ZALXUF	1.578	0.255	-0.366	-0.295	0.726	1.454
ZUGFAK	1.674	0.222	-0.315	-0.247	0.165	1.220

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