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Equilibrium structure of orotic acid from gas-phase electron diffraction data and quantum-chemical calculations

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Table S1 Conditions of the GED experiment for orotic acid.

Nozzle-to-film distance, mm	362.3 (LD)	193.9 (SD)
Beam current, μA	3.5	3.5
Exposure time, sec	45, 45, 45	60, 60, 50
Nozzle temperature, K	517	523
Residual gas pressure, mm Hg	$3.0 \cdot 10^{-5}$	$3.0 \cdot 10^{-5}$
Number of the diffraction patterns (substance)	3	3
Number of the diffraction patterns (standard CCl_4)	2	2
Wavelength of electrons (λ), Å	0.0496260	0.0498760
Interval of scattering variable (s), $Å^{-1}$	3.6 – 17.0 (Δs = 0.2)	8.8 – 30.0 (Δs = 0.2)

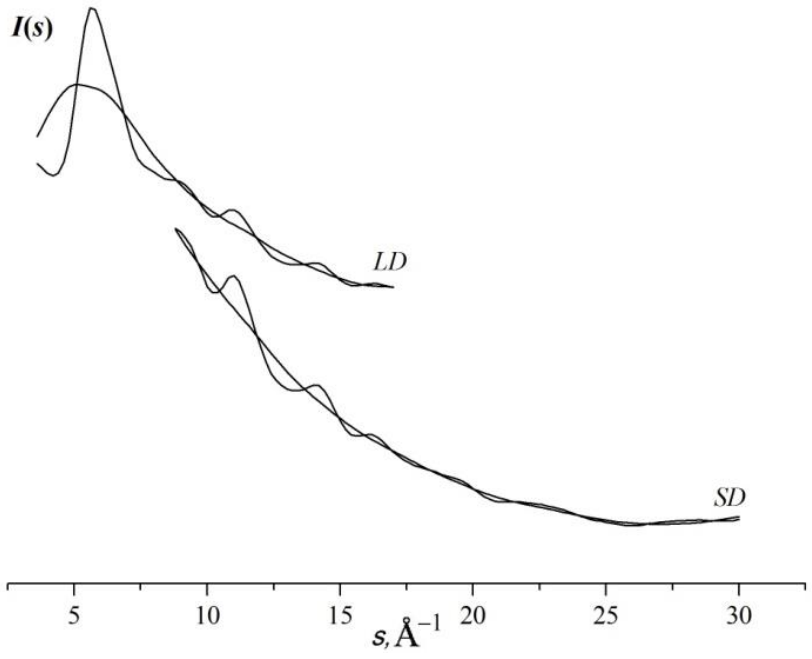

Figure S1 Experimental intensity curves *I(s)* of orotic acid with background lines for the long (LD) and short (SD) nozzle-to-film distances.

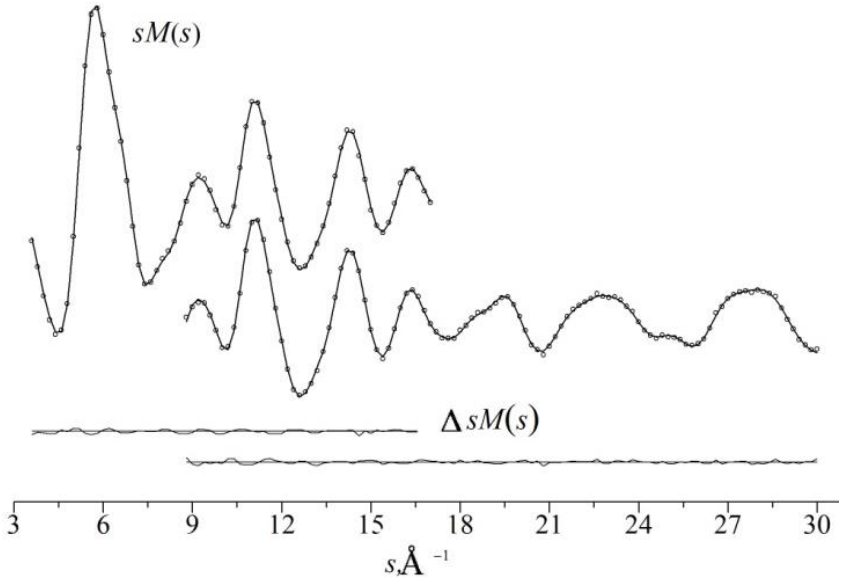

Figure S2 Experimental (circles) and theoretical (solid line) molecular intensity curves *sM(s)* with their difference curves *ΔsM(s)* for the long and short nozzle-to-film distances.

Table S2 Experimental total intensity curves *I*(*s*) and background lines *B*(*s*).

a) Long nozzle-to-film distance *L* = 362.2 mm

s [Å^{-1}]	*I*(*s*)	*B*(*s*)
3.60	0.329573	0.350795
3.80	0.326132	0.358653
4.00	0.321885	0.366512
4.20	0.320061	0.373912
4.40	0.322126	0.380540
4.60	0.330968	0.385901
4.80	0.346932	0.389503
5.00	0.375842	0.391255
5.20	0.409230	0.391431
5.40	0.436819	0.390682
5.60	0.451623	0.389666
5.80	0.450229	0.388548
6.00	0.437994	0.386965
6.20	0.422075	0.384383
6.40	0.406369	0.380578
6.60	0.391114	0.375811
6.80	0.374693	0.370540
7.00	0.357396	0.365049
7.20	0.342552	0.359353
7.40	0.332888	0.353397
7.60	0.328106	0.347299
7.80	0.325481	0.341362
8.00	0.323091	0.335860

8.20	0.320060	0.330846
8.40	0.317639	0.326187
8.60	0.316805	0.321705
8.80	0.316405	0.317294
9.00	0.314977	0.312973
9.20	0.312331	0.308833
9.40	0.307687	0.304948
9.60	0.302241	0.301349
9.80	0.295994	0.298005
10.00	0.290712	0.294858
10.20	0.287645	0.291843
10.40	0.287572	0.288947
10.60	0.290005	0.286225
10.80	0.292709	0.283744
11.00	0.293357	0.281493
11.20	0.290755	0.279347
11.40	0.285821	0.277114
11.60	0.279174	0.274650
11.80	0.272689	0.271967
12.00	0.266666	0.269189
12.20	0.261561	0.266454
12.40	0.257109	0.263835
12.60	0.254070	0.261353
12.80	0.252094	0.258999
13.00	0.250911	0.256781
13.20	0.250241	0.254711
13.40	0.250010	0.252769
13.60	0.250250	0.250912
13.80	0.250870	0.249099
14.00	0.251507	0.247315
14.20	0.251156	0.245563
14.40	0.249223	0.243853
14.60	0.245479	0.242209
14.80	0.242004	0.240662
15.00	0.238120	0.239203
15.20	0.235619	0.237847
15.40	0.233892	0.236614
15.60	0.233610	0.235545
15.80	0.234142	0.234665
16.00	0.234922	0.233982
16.20	0.235277	0.233492
16.40	0.235073	0.233170
16.60	0.234251	0.232964
16.80	0.233165	0.232816
17.00	0.232259	0.232667

b) Nozzle-to-film distance L = 193.9 mm

s [Å^{-1}]	$I(s)$	$B(s)$
8.80	0.668523	0.667860
9.00	0.665808	0.661529

9.20	0.660855	0.655197
9.40	0.654455	0.649082
9.60	0.644378	0.643204
9.80	0.633851	0.637523
10.00	0.623035	0.631972
10.20	0.618177	0.626499
10.40	0.618629	0.621095
10.60	0.623089	0.615807
10.80	0.629632	0.610704
11.00	0.631748	0.605792
11.20	0.626869	0.600995
11.40	0.616448	0.596187
11.60	0.603034	0.591260
11.80	0.588770	0.586177
12.00	0.575801	0.580990
12.20	0.564163	0.575794
12.40	0.554773	0.570679
12.60	0.548946	0.565705
12.80	0.545231	0.560901
13.00	0.542767	0.556287
13.20	0.541309	0.551887
13.40	0.541189	0.547705
13.60	0.542005	0.543725
13.80	0.544039	0.539919
14.00	0.545752	0.536263
14.20	0.545302	0.532737
14.40	0.541160	0.529322
14.60	0.534468	0.525998
14.80	0.525970	0.522739
15.00	0.517751	0.519535
15.20	0.511238	0.516398
15.40	0.506863	0.513360
15.60	0.505772	0.510460
15.80	0.506144	0.507724
16.00	0.506851	0.505157
16.20	0.506620	0.502746
16.40	0.504771	0.500457
16.60	0.501516	0.498239
16.80	0.497258	0.496045
17.00	0.493170	0.493842
17.20	0.489813	0.491625
17.40	0.486758	0.489401
17.60	0.484570	0.487187
17.80	0.482396	0.484995
18.00	0.481387	0.482842
18.20	0.479892	0.480739
18.40	0.478799	0.478702
18.60	0.477518	0.476736
18.80	0.475676	0.474832
19.00	0.474270	0.472980

19.20	0.473052	0.471168
19.40	0.471913	0.469391
19.60	0.470241	0.467648
19.80	0.467621	0.465945
20.00	0.464563	0.464289
20.20	0.461407	0.462685
20.40	0.458267	0.461143
20.60	0.456324	0.459673
20.80	0.454429	0.458288
21.00	0.454093	0.457001
21.20	0.453929	0.455815
21.40	0.453998	0.454730
21.60	0.453984	0.453737
21.80	0.453791	0.452820
22.00	0.453306	0.451956
22.20	0.452820	0.451115
22.40	0.452294	0.450273
22.60	0.451878	0.449412
22.80	0.450694	0.448525
23.00	0.449660	0.447626
23.20	0.448812	0.446729
23.40	0.447621	0.445845
23.60	0.446144	0.444985
23.80	0.444849	0.444148
24.00	0.443068	0.443332
24.20	0.441518	0.442532
24.40	0.440301	0.441749
24.60	0.439290	0.440990
24.80	0.438851	0.440269
25.00	0.438050	0.439599
25.20	0.437409	0.438990
25.40	0.436706	0.438446
25.60	0.435826	0.437964
25.80	0.435360	0.437542
26.00	0.435143	0.437178
26.20	0.435252	0.436879
26.40	0.435892	0.436651
26.60	0.436966	0.436497
26.80	0.437387	0.436413
27.00	0.438016	0.436397
27.20	0.438382	0.436438
27.40	0.438636	0.436527
27.60	0.438831	0.436655
27.80	0.438870	0.436825
28.00	0.439242	0.437045
28.20	0.439379	0.437323
28.40	0.439602	0.437669
28.60	0.439768	0.438083
28.80	0.439379	0.438562
29.00	0.439081	0.439105

29.20	0.438977	0.439703
29.40	0.438841	0.440345
29.60	0.439121	0.441018
29.80	0.439471	0.441707
30.00	0.440220	0.442397

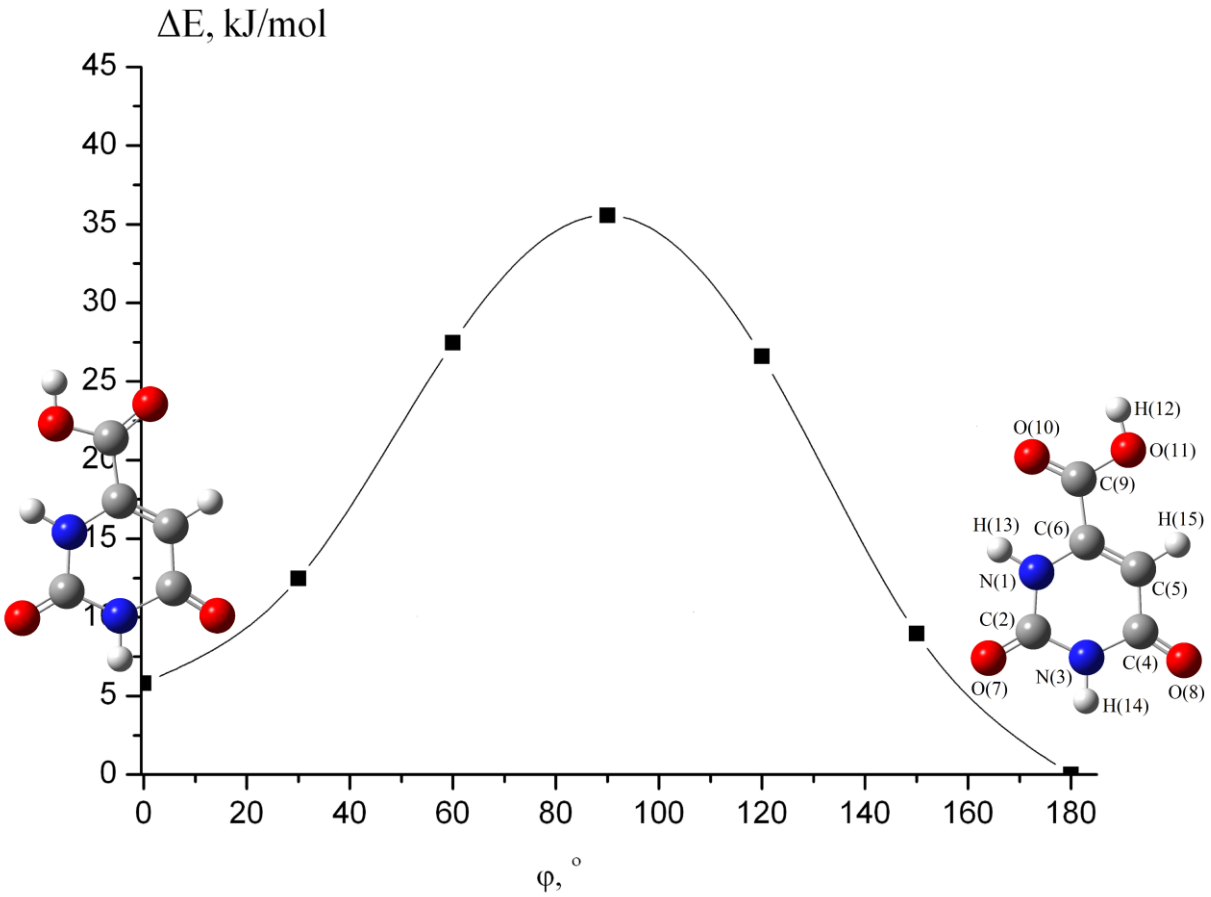

Figure S3 Potential energy of orotic acid as a function of the O(10)=C(9)–C(6)=C(5) torsional angle according to MP2/cc-pVTZ calculations.

Table S3 Vibrational corrections $\Delta(r_{ij,e} - r_{ij,a})$ to internuclear distances $r_{ij,a}$, theoretical $u_{ij,h1}$ and experimental $u_{ij,exp}$ vibrational amplitudes of orotic acid (*anti* conformer).

Term	r_a	$r_e - r_a$ [a]	u_{h1} [b]	u_{exp} [c,d]
O(11)–H(12)	0.986	-0.0145	0.0688	0.069 [e]
N(1)–H(13)	1.029	-0.0157	0.0704	0.070 [e]
N(3)–H(14)	1.030	-0.0154	0.0705	0.071 [e]
C(5)–H(15)	1.096	-0.0152	0.0742	0.074 [e]
C(9)–O(10)	1.209	-0.0041	0.0379	0.037(2)[1]
C(2)–O(7)	1.213	-0.0037	0.0378	0.037(2)[1]
C(4)–O(8)	1.215	-0.0036	0.0382	0.037(2)[1]
C(9)–O(11)	1.347	-0.0099	0.0458	0.045(5)[2]
C(5)–C(6)	1.355	-0.0071	0.0433	0.043(5)[2]
N(1)–C(6)	1.382	-0.0112	0.0454	0.045(5)[2]
N(1)–C(2)	1.389	-0.0117	0.0473	0.047(5)[2]
C(2)–N(3)	1.390	-0.0096	0.0474	0.047(5)[2]
N(3)–C(4)	1.404	-0.0108	0.0493	0.049(5)[2]
C(4)–C(5)	1.473	-0.0095	0.0501	0.050(5)[2]

C(6)–C(9)	1.500	-0.0106	0.0508	0.050(5)[2]
C(9)…H(12)	1.878	-0.0138	0.1033	0.103[e]
C(2)…H(14)	2.040	-0.0099	0.1016	0.102
C(2)…H(13)	2.062	-0.0039	0.1016	0.102
C(6)…H(13)	2.071	-0.0096	0.0984	0.098
C(4)…H(14)	2.074	-0.0103	0.1025	0.103
C(6)…H(15)	2.137	-0.0128	0.0994	0.099
C(4)…H(15)	2.211	-0.0104	0.1041	0.104
O(10)…H(13)	2.246	-0.0208	0.195	0.195
O(10)…O(11)	2.258	-0.0080	0.0563	0.053(4)[3]
N(3)…O(8)	2.279	-0.0107	0.0597	0.056(4)[3]
N(3)…O(7)	2.282	-0.0093	0.0587	0.055(4)[3]
N(1)…O(7)	2.287	-0.0091	0.0585	0.055(4)[3]
O(10)…H(12)	2.311	-0.0120	0.1478	0.148
N(1)…N(3)	2.331	-0.0179	0.0586	0.055(4)[3]
N(1)…C(9)	2.373	-0.0167	0.0699	0.067(4)[3]
C(6)…O(11)	2.374	-0.0149	0.069	0.066(4)[3]
C(6)…O(10)	2.377	-0.0112	0.0634	0.060(4)[3]
C(5)…O(8)	2.388	-0.0076	0.0633	0.060(4)[3]
N(1)…C(5)	2.391	-0.0116	0.0572	0.054(4)[3]
N(3)…C(5)	2.407	-0.0153	0.0621	0.059(4)[3]
C(2)…C(6)	2.424	-0.0086	0.0596	0.056(4)[3]
C(4)…C(6)	2.438	-0.0092	0.0596	0.056(4)[3]
C(9)…H(13)	2.459	-0.0161	0.1503	0.15
O(7)…H(14)	2.472	-0.0079	0.1412	0.141
O(8)…H(14)	2.491	-0.0087	0.1428	0.143
C(2)…C(4)	2.493	-0.0020	0.0618	0.059(4)[3]
O(7)…H(13)	2.518	0.0035	0.1402	0.14
C(5)…C(9)	2.552	-0.0102	0.0706	0.067(4)[3]
O(11)…H(15)	2.589	-0.0097	0.1981	0.198
N(1)…O(10)	2.654	-0.0168	0.1114	0.105(9)[4]
O(8)…H(15)	2.694	-0.0044	0.1449	0.145
N(3)…C(6)	2.705	-0.0170	0.0695	0.063(9)[4]
N(1)…C(4)	2.807	-0.0090	0.0681	0.062(9)[4]
C(9)…H(15)	2.836	-0.0110	0.1492	0.149
C(2)…C(5)	2.842	-0.0051	0.0676	0.062(9)[4]
C(5)…O(11)	2.842	-0.0108	0.1162	0.110(9)[4]
C(6)…H(12)	3.196	-0.0124	0.0974	0.097
N(1)…H(14)	3.235	-0.0158	0.0946	0.095
N(3)…H(13)	3.247	-0.0096	0.0947	0.095
C(5)…H(13)	3.287	-0.0068	0.0943	0.094
C(5)…H(14)	3.330	-0.0127	0.0966	0.097
N(1)…H(15)	3.381	-0.0169	0.0955	0.096
N(3)…H(15)	3.395	-0.0148	0.098	0.098
C(6)…O(7)	3.531	-0.0037	0.064	0.070(4)[5]
H(12)…H(15)	3.532	-0.0001	0.2172	0.217
C(6)…O(8)	3.564	-0.0041	0.064	0.070(4)[5]
N(1)…O(11)	3.564	-0.0198	0.0716	0.078(4)[5]

C(2)…O(8)	3.567	0.0008	0.0671	0.073(4)[5]
C(4)…O(7)	3.580	0.0008	0.0685	0.075(4)[5]
C(5)…O(10)	3.626	-0.0093	0.0685	0.075(4)[5]
C(2)…C(9)	3.688	-0.0115	0.0748	0.081(4)[5]
C(6)…H(14)	3.716	-0.0138	0.0968	0.097[e]
O(11)…H(13)	3.787	-0.0192	0.1486	0.149[e]
C(5)…H(12)	3.796	-0.0028	0.1305	0.131[e]
C(4)…H(13)	3.814	-0.0020	0.0962	0.096[e]
C(4)…C(9)	3.866	-0.0113	0.0733	0.069(29)[6]
C(2)…H(15)	3.925	-0.0071	0.0975	0.098[e]
N(1)…O(8)	4.012	-0.0034	0.0699	0.067(12)[7]
C(2)…O(10)	4.018	-0.0099	0.1221	0.119(12)[7]
O(10)…H(15)	4.027	-0.0093	0.1462	0.146[e]
C(5)…O(7)	4.046	0.0002	0.0698	0.067(12)[7]
H(13)…H(14)	4.066	-0.0045	0.1291	0.129[e]
N(3)…C(9)	4.181	-0.0176	0.0774	0.074(12)[7]
H(13)…H(15)	4.190	-0.0116	0.1314	0.131[e]
N(1)…H(12)	4.236	-0.0177	0.1162	0.116[e]
H(14)…H(15)	4.238	-0.0090	0.1314	0.131[e]
H(12)…H(13)	4.264	-0.0217	0.1959	0.196[e]
C(4)…O(11)	4.301	-0.0090	0.1212	0.118(12)[7]
O(7)…O(8)	4.536	0.0047	0.0821	0.082[e]
O(7)…C(9)	4.632	-0.0037	0.0899	0.090[e]
O(7)…O(10)	4.718	-0.0014	0.1517	0.152[e]
C(2)…O(11)	4.773	-0.0132	0.0799	0.080[e]
C(4)…O(10)	4.802	-0.0099	0.079	0.079[e]
N(3)…O(10)	4.833	-0.0151	0.1035	0.104[e]
O(8)…C(9)	4.913	-0.0034	0.0849	0.085[e]
N(3)…O(11)	4.976	-0.0169	0.1029	0.103[e]
O(8)…H(13)	5.016	0.0062	0.0983	0.098[e]
O(7)…H(15)	5.126	0.0012	0.10	0.10[e]
O(8)…O(11)	5.131	0.0016	0.1473	0.147
C(9)…H(14)	5.187	-0.0115	0.1032	0.103[e]
C(4)…H(12)	5.246	0.0022	0.1336	0.134[e]
C(2)…H(12)	5.522	-0.0063	0.1136	0.114[e]
O(10)…H(14)	5.800	-0.0082	0.1291	0.129[e]
O(7)…O(11)	5.818	-0.0051	0.0848	0.085[e]
N(3)…H(12)	5.852	-0.0063	0.1177	0.118[e]
O(8)…O(10)	5.923	-0.0016	0.0817	0.082[e]
O(11)…H(14)	5.972	-0.0091	0.1268	0.127[e]
O(8)…H(12)	6.088	0.0160	0.1642	0.164[e]
O(7)…H(12)	6.490	0.0024	0.1303	0.130[e]
H(12)…H(14)	6.853	0.0041	0.1383	0.138[e]

[a] Calculated with MP2/cc-pVTZ cubic force field.
[b] Calculated value (from MP2/cc-pVTZ quadratic force field) .
[c] Amplitudes with equal superscripts were refined in one group. Differences between amplitudes in each group were fixed at the corresponding calculated values (from MP2/cc-pVTZ harmonic force field). [d] Estimated errors given in parentheses are 2.5σ. [e] Fixed at the calculated u_{h1} value.