

Conformational dimorphism in *o*-nitrobenzoic acid: alternative ways to avoid the O···O clash

A. Ibragimov, J. Ashurov, B. Ibragimov, A. Wang, H. Mouhib, and U. Englert

Figure S1: Experimental and simulated powder pattern for crystal form **1 α** .

Figure S2: Restrained internal degrees of freedom during PES calculation.

Table S1: Fourier coefficients of the PES shown in Figures 7 and 8 of the manuscript.

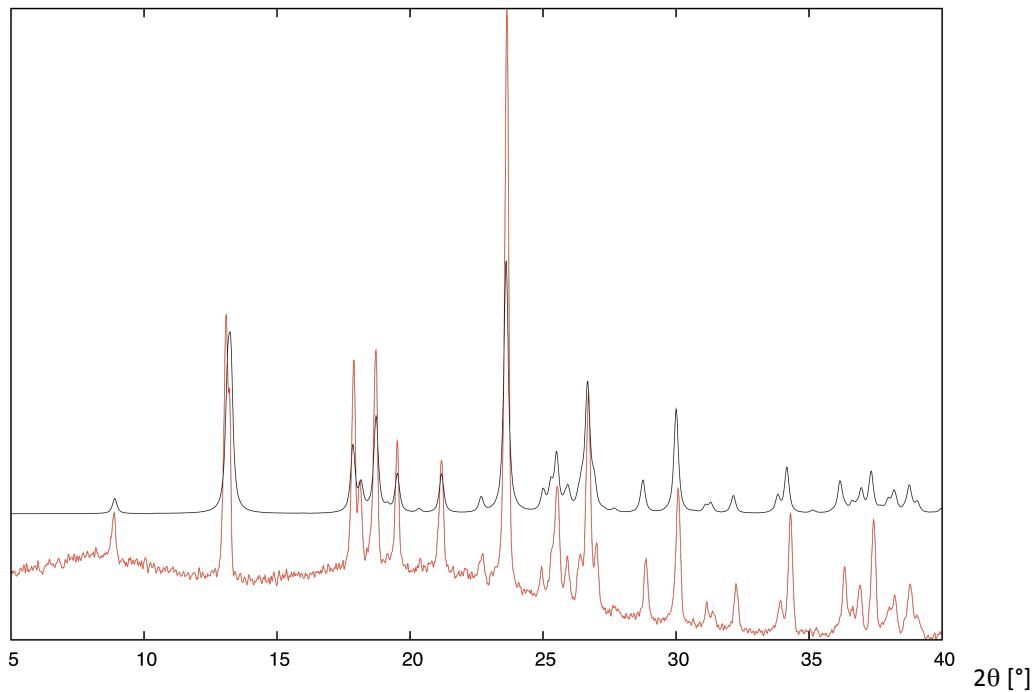


Figure S1: Experimental powder pattern (red) and simulated powder patterns for crystal form **1 α** (black).

Potential Energy Surface (PES)

In order to obtain a more complete overview over the conformational landscape, a two-dimensional potential energy surface (PES) was calculated at the MP2/6-311++G(d,p) level of theory. Calculations were carried out using the Gaussian09 program package; two degrees of freedom (F_1 and F_2 , see below) had to be restrained, while the rest of the molecule was allowed to optimize freely.

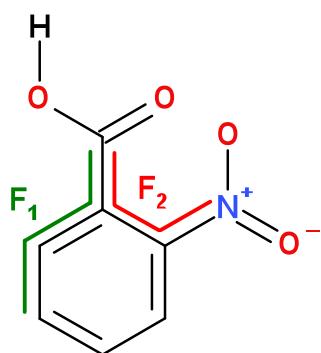


Figure S2. F_1 and F_2 symbolize the two dihedral angles which were restrained at -180° and 0° , respectively, during the computation of the PES for **1**.

Table S1: Fourier coefficients of the PES shown in Figures 7 and 8 of the manuscript. All 1184 *ab initio* data points are reproduced within 6.5%. The potential energy is obtained from $V(\theta_1, \theta_2) = \sum_{i=1}^{62} V_i f_i$

<i>i</i>	$V_i / \text{Hartree}$	f_i
1	-623.873622	1
2	-0.000047	$\cos(1\cdot02)$
3	-0.000087	$\sin(1\cdot02)$
4	0.002697	$\cos(2\cdot01)$
5	0.000172	$\sin(2\cdot01)$
6	0.001454	$\cos(2\cdot02)$
7	0.000154	$\cos(3\cdot02)$
8	-0.000016	$\sin(3\cdot02)$
9	0.001123	$\cos(4\cdot01)$
10	0.000096	$\sin(4\cdot01)$
11	0.000573	$\cos(4\cdot02)$
12	-0.000059	$\cos(5\cdot02)$
13	-0.000006	$\sin(5\cdot02)$
14	0.000064	$\cos(6\cdot01)$
15	0.000081	$\cos(6\cdot02)$
16	-0.000009	$\sin(6\cdot02)$
17	0.000298	$\cos(2\cdot01)\cos(1\cdot02)$
18	0.000024	$\cos(2\cdot01)\sin(1\cdot02)$
19	-0.000002	$\sin(2\cdot01)\cos(1\cdot02)$

20	-0.000075	$\sin(4\cdot\theta_1)\sin(1\cdot\theta_2)$
21	-0.000005	$\sin(4\cdot\theta_1)\cos(1\cdot\theta_2)$
22	0.000010	$\sin(6\cdot\theta_1)\sin(1\cdot\theta_2)$
23	-0.000003	$\sin(6\cdot\theta_1)\cos(1\cdot\theta_2)$
24	0.005643	$\cos(2\cdot\theta_1)\cos(2\cdot\theta_2)$
25	-0.004694	$\sin(2\cdot\theta_1)\sin(2\cdot\theta_2)$
26	0.000361	$\cos(2\cdot\theta_1)\sin(2\cdot\theta_2)$
27	0.000374	$\sin(2\cdot\theta_1)\cos(2\cdot\theta_2)$
28	0.000817	$\cos(4\cdot\theta_1)\cos(2\cdot\theta_2)$
29	-0.000832	$\sin(4\cdot\theta_1)\sin(2\cdot\theta_2)$
30	0.000096	$\cos(4\cdot\theta_1)\sin(2\cdot\theta_2)$
31	0.000081	$\sin(4\cdot\theta_1)\cos(2\cdot\theta_2)$
32	0.000236	$\cos(6\cdot\theta_1)\cos(2\cdot\theta_2)$
33	-0.000213	$\sin(6\cdot\theta_1)\sin(2\cdot\theta_2)$
34	0.000051	$\cos(2\cdot\theta_1)\cos(3\cdot\theta_2)$
35	-0.000187	$\sin(2\cdot\theta_1)\sin(3\cdot\theta_2)$
36	-0.000005	$\cos(2\cdot\theta_1)\sin(3\cdot\theta_2)$
37	-0.000003	$\sin(2\cdot\theta_1)\cos(3\cdot\theta_2)$
38	-0.000006	$\cos(4\cdot\theta_1)\sin(3\cdot\theta_2)$
39	-0.000007	$\sin(6\cdot\theta_1)\sin(3\cdot\theta_2)$
40	-0.000033	$\sin(2\cdot\theta_1)\sin(4\cdot\theta_2)$
41	-0.000022	$\cos(2\cdot\theta_1)\sin(4\cdot\theta_2)$
42	0.000218	$\cos(4\cdot\theta_1)\cos(4\cdot\theta_2)$
43	-0.000132	$\sin(4\cdot\theta_1)\sin(4\cdot\theta_2)$
44	0.000109	$\cos(6\cdot\theta_1)\cos(4\cdot\theta_2)$
45	-0.000082	$\sin(6\cdot\theta_1)\sin(4\cdot\theta_2)$
46	-0.000193	$\cos(2\cdot\theta_1)\cos(5\cdot\theta_2)$
47	0.000235	$\sin(2\cdot\theta_1)\sin(5\cdot\theta_2)$
48	-0.000024	$\cos(2\cdot\theta_1)\sin(5\cdot\theta_2)$
49	-0.000016	$\sin(2\cdot\theta_1)\cos(5\cdot\theta_2)$
50	-0.000073	$\cos(4\cdot\theta_1)\cos(5\cdot\theta_2)$
51	0.000077	$\sin(4\cdot\theta_1)\sin(5\cdot\theta_2)$
52	-0.000014	$\cos(4\cdot\theta_1)\sin(5\cdot\theta_2)$
53	-0.000012	$\sin(4\cdot\theta_1)\cos(5\cdot\theta_2)$
54	-0.000036	$\cos(6\cdot\theta_1)\cos(5\cdot\theta_2)$
55	-0.000006	$\cos(6\cdot\theta_1)\sin(5\cdot\theta_2)$
56	-0.000005	$\sin(6\cdot\theta_1)\cos(5\cdot\theta_2)$
57	0.000084	$\cos(2\cdot\theta_1)\cos(6\cdot\theta_2)$
58	-0.000127	$\sin(2\cdot\theta_1)\sin(6\cdot\theta_2)$
59	-0.000004	$\sin(2\cdot\theta_1)\cos(6\cdot\theta_2)$
60	0.000092	$\cos(4\cdot\theta_1)\cos(6\cdot\theta_2)$
61	-0.000094	$\sin(4\cdot\theta_1)\sin(6\cdot\theta_2)$
62	-0.000027	$\sin(6\cdot\theta_1)\sin(6\cdot\theta_2)$