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Supporting information for article:

Role of weak C—H···O and strong N—H···O intermolecular interactions on the high-symmetry molecular packing of *trans*-cyclohexane-1,4-dicarboxamide

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Supplementary Information

Table S1. Topological analysis of selected contacts calculated at PBE/6-31G** theory level for clusters **I** and **II**.

Contact	**Comp**	**ρ (eA^{-3})**	**∇^2 (eA^{-5})**	**λ_3 (eA^{-5})**	**G(kcal/mol)**	**V(kcal/mol)**	**H(kcal/mol)**
N–H_s···O	**1**	0.2247	2.2884	4.5124	15.5	-16.1	-0.6
	2	0.2314	2.4308	4.7490	16.3	-16.7	-0.4
N–H_a···O	**1**	0.1566	1.7486	3.1217	11.6	-11.9	-0.3
	2	0.1718	1.8356	3.3832	12.4	-12.9	-0.5
C–H_{in}···O	**1**	0.0469	0.5597	0.8408	3.2	-2.8	0.4
	2	0.0803	0.8597	1.4336	5.6	-5.5	0.1
C–H_{out}···O	**1**	0.0453	0.5792	0.8289	3.3	-2.7	0.6
	2	0.0455	0.5647	0.8433	3.2	-2.7	0.5

Table S2. Experimental wavenumbers (cm^{-1}) of the FTIR and Raman spectra of solid trans-1,4-dicarboxamidecliclohexane, calculated frequencies and IR and Raman intensities and tentative assignment.

Experimental		MP2/6-311++G(d,p)			Tentative Assignment
IR	Raman	ν (cm^{-1})^{a}	I_{IR}	I_{Ra}	
3345		3560	77	2	ν_{as} NH_2 *in-phase*
	3336	3560	2	90	ν_{as} NH_2 *out-of-phase*
3170		3424	88	< 1	ν_{s} NH_2 *out-of-phase*
	3147	3424	< 1	351	ν_{s} NH_2 *in-phase*
2958		2966	53	0	ν CH_2
	2957	2962	0	68	
	2940	2954	0	130	
2938		2951	36	0	
	2909	2908	0	296	
2902		2907	46	< 1	
		2903	39	< 1	
	2901	2902	< 1	83	
	2860	2894	0	158	ν CH *in-phase*
2860		2893	29	0	ν CH *out-of-phase*
2728					overtones and/or combination modes
2677					
2611					
1689		1679	552	< 1	ν C=O *out-of-phase*
	1678	1679	< 1	34	ν C=O *in-phase*
	1647	1546	0	5	$\delta_{(scissor)}$ NH_2 *in-phase*
1644 sh		1545	206	0	$\delta_{(scissor)}$ NH_2 *out-of-phase*
	1463	1433	0	5	δ CH_2
1455		1424	18	0	
1448		1419	6	0	
	1444	1415	0	13	
		1361	0	3	ν C–C (C=O) *in-phase*
1427		1356	205	0	ν C–C (C=O) *out-of-phase*
1361		1318	53	0	ν C–N *out-of-phase*

Experimental		MP2/6-311++G(d,p)			Tentative Assignment
IR	Raman				
1321		1302	< 1	0	δ CH_2
	1312	1301	0	3	ν C–N *in-phase*
	1299	1298	0	7	
	1265	1265	0	5	δ CH_2
1264		1249	1	0	
	1255	1246	0	4	ν C–C (cycle)
1201		1238	110	0	δ CH_2
	1159	1201	0	14	δ CCH *in-phase*
		1184	3	0	ν C–C (cycle)
1145		1174	71	0	δ CCH *out-of-phase*
	1130	1109	0	5	ν C–C (cycle)
	1109	1093	0	20	ν C–C (cycle)
1043		1070	< 1	0	
1027		1039	22	0	δ CNH *out-of-phase*
	1058	1028	0	10	δ CNH *in-phase*
	1053 sh	1021	0	2	δ CH_2
	1034	1009	0	10	ν C–C (cycle)
976		995	3	0	δ CH_2
		947	< 1	0	δ CCH
	943	902	0	2	
915		895	8	0	δ cycle
897		870	4	0	
874		835	3	0	δ CH_2
	796 sh	763	0	1	δ cycle
	790	759	0	18	
	729	733	0	< 1	δ C=O *out-of-plane*
720		705	12	0	δ C=O *out-of-plane*
685		624	28	0	δ NCO *out-of-phase*
	651	598	0	8	δ NCO *out-of-phase*
	640	544	0	< 1	δ(twisting) NH_2
523		536	69	0	δ(twisting) NH_2
		487	3	0	

Experimental		MP2/6-311++G(d,p)			Tentative Assignment
IR	Raman				
	516	475	0	1	δ cycle
	457	430	0	1	
441		402	15	0	δ NCC *out-of-phase*
	368	358	< 1	2	δ NH_2 *out-of-plane*
347/330		352	388	0	δ NH_2 *out-of-plane*
	292	339	< 1	< 1	τ
241		281	17	0	τ
	237	230	0	3	δ cycle
		219	< 1	0	τ cycle
	207	198	0	1	τ
	95	163	0	1	τ
		124	6	0	τ
		55	7	0	τ
		23	19	0	τ
		21	0	3	τ

[a] scaled by the 0.9483 factor.