Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

p-Aminobenzoic Acid Polymorphs Under High Pressures

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Table S1 *Ab initio* calculated unit-cell parameters and atomic coordinates of α-PABA and β-PABA at 0 GPa, 7 GPa, and 13 GPa, respectively.

α-PABA	*a*	*b*	*c*	*V*	β
0 GPa	18.5351	5.4722	18.2145	1652.24	94.220
7 GPa	17.4913	3.4486	17.1378	965.40	95.829
13 GPa	17.0859	2.9521	16.5768	796.04	94.871

	α-PABA at 0 GPa			α-PABA at 7 GPa			α-PABA at 13 GPa		
Atom	X/a	Y/b	Z/c	X/a	Y/b	Z/c	X/a	Y/b	Z/c
C1	0.14916	-0.77084	-0.07572	0.15320	-0.70417	-0.06805	0.15324	-0.63507	-0.06640
C2	0.41937	0.74333	0.14239	0.43082	0.66098	0.15020	0.43166	0.59034	0.15174
C3	0.22251	-0.84754	-0.05243	0.22531	-0.80454	-0.02875	0.22425	-0.74266	-0.02610
C4	0.44469	0.80162	0.21830	0.46699	0.73863	0.22414	0.46822	0.67261	0.22733
C5	0.28440	-0.75394	-0.08572	0.28972	-0.73885	-0.06136	0.29192	-0.67888	-0.06049
C6	0.41197	0.70168	0.28029	0.43364	0.64019	0.28949	0.43317	0.57711	0.29493
C7	0.27545	-0.57752	-0.14425	0.28834	-0.56377	-0.13504	0.29112	-0.48811	-0.13576
C8	0.35194	0.53499	0.26894	0.36251	0.44967	0.28301	0.36118	0.37065	0.28933
C9	0.20156	-0.49999	-0.16765	0.21757	-0.45618	-0.17370	0.21951	-0.36744	-0.17450
C10	0.32622	0.47653	0.19238	0.32661	0.37087	0.20848	0.32553	0.28307	0.21300
C11	0.14020	-0.59571	-0.13389	0.15149	-0.52421	-0.14068	0.15172	-0.44032	-0.14065
C12	0.35945	0.57928	0.13708	0.36004	0.47553	0.14343	0.35965	0.39423	0.14553
C13	0.08336	-0.87218	-0.04014	0.08342	-0.80921	-0.03646	0.08232	-0.76146	-0.03551
C14	0.45627	0.85494	0.07798	0.46387	0.79428	0.08178	0.46385	0.75325	0.08200
H1	-0.02361	-0.88330	-0.04310	-0.02292	-0.83231	-0.04752	-0.02487	-0.83094	-0.04885
H2	0.45582	0.90234	-0.03024	0.45314	0.88754	-0.03129	0.45071	0.91108	-0.03268
H3	0.23077	-0.98602	-0.00777	0.22580	-0.91501	0.02806	0.22549	-0.89436	0.03206
H4	0.49099	0.93110	0.22773	0.52120	0.89526	0.22913	0.52275	0.84457	0.23183
H5	0.34107	-0.81910	-0.06747	0.34383	-0.82300	-0.03043	0.34668	-0.77510	-0.03000
H6	0.43228	0.75133	0.33907	0.46138	0.71773	0.34639	0.46000	0.67725	0.35244
H7	0.39006	-0.52799	-0.15720	0.40429	-0.60753	-0.14191	0.40877	-0.54694	-0.14482
H8	0.34346	0.46000	0.38554	0.35558	0.38978	0.40156	0.35187	0.32600	0.41107
H9	0.33046	-0.34742	-0.21684	0.35388	-0.33199	-0.21681	0.35852	-0.24199	-0.22045
H10	0.27867	0.30618	0.32235	0.28145	0.16847	0.34036	0.27808	0.07122	0.34905
H11	0.19309	-0.36028	-0.21206	0.21552	-0.31594	-0.23022	0.21842	-0.21597	-0.23207
H12	0.28082	0.34368	0.18208	0.27285	0.21104	0.202777	0.27103	0.11356	0.20797
H13	0.08338	-0.53282	-0.15232	0.09677	-0.44144	-0.17130	0.09600	-0.35308	-0.17161
H14	0.33918	0.53023	0.07196	0.33125	0.41886	0.08576	0.33056	0.33593	0.08645
N1	0.33655	-0.48893	-0.17908	0.35366	-0.50830	-0.16902	0.35774	-0.43248	-0.17177
N2	0.31905	0.43757	0.33506	0.32785	0.34985	0.34679	0.32482	0.26615	0.35514
O1	0.08985	-1.00802	0.01219	0.08421	-1.00207	0.02077	0.08331	-0.96595	0.02349
O2	0.51031	0.97732	0.08957	0.52440	0.95746	0.08895	0.52707	0.91030	0.08946
O3	0.42745	0.81300	0.01271	0.42853	0.74074	0.01918	0.42564	0.73770	0.01872
O4	0.02118	-0.80527	-0.06887	0.02366	-0.70227	-0.17197	0.02159	-0.66622	-0.07298

β-PABA	*a*	*b*	*c*	*V*	β
0 GPa	6.5399	10.1441	12.8568	831.195	97.1401
7 GPa	5.7362	7.9205	11.7896	663.009	100.653
13 GPa	5.5262	7.4112	10.9888	596.631	100.429

	β-PABA at 0 GPa			β-PABA at 7 GPa			β-PABA at 13 GPa		
Atom	X/a	Y/b	Z/c	X/a	Y/b	Z/c	X/a	Y/b	Z/c
C1	0.20176	0.31223	0.52382	0.18611	0.30908	0.49000	0.18781	0.31835	0.47967
C2	-0.10174	0.06682	0.73443	-0.13420	0.00217	0.71632	-0.12861	-0.01350	0.71040
C3	0.09220	0.22791	0.59456	0.07120	0.20600	0.56808	0.07265	0.20851	0.56054
C4	-0.10687	0.17780	0.56364	-0.15769	0.14657	0.53272	-0.16044	0.15266	0.52275
C5	0.09681	0.11783	0.76615	0.09198	0.06619	0.75378	0.10009	0.04860	0.75106
C6	-0.20268	0.09839	0.63258	-0.25919	0.04407	0.60614	-0.26017	0.04124	0.59836
C7	0.19165	0.19678	0.69681	0.19483	0.16471	0.67881	0.20131	0.15711	0.67469

H1	0.17631	0.40134	0.38810	0.13410	0.45939	0.35614	0.13257	0.49289	0.34727
H2	-0.09836	-0.05949	0.86143	-0.12342	-0.14043	0.86392	-0.11747	-0.16422	0.86482
H3	-0.31116	-0.07079	0.77105	-0.36089	-0.17970	0.75618	-0.34812	-0.21202	0.74602
H4	-0.18655	0.20151	0.48506	-0.25434	0.18199	0.44745	-0.26077	0.19817	0.43527
H5	0.17518	0.09455	0.84525	0.18328	0.03969	0.84135	0.19339	0.01455	0.84206
H6	-0.35772	0.06086	0.60788	-0.43746	-0.00181	0.58119	-0.44234	-0.00155	0.57622
H7	0.34541	0.23597	0.72144	0.37089	0.21288	0.70737	0.38028	0.20343	0.70503
N1	-0.20034	-0.00887	0.80709	-0.24070	-0.09151	0.79416	-0.23563	-0.11759	0.78939
O1	0.09237	0.33947	0.42915	0.04078	0.37129	0.39914	0.03943	0.39585	0.39162
O2	0.37791	0.35412	0.54874	0.39877	0.33555	0.50634	0.40509	0.33488	0.49208