Electronic Supplementary Material (ESI) for CrystEngComm

Growth and Dissolution Mechanism at the Opposite and Hemihedral Faces of Polar Crystals

Supplementary Information

(*2 pages*)

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Optimized fractional coordinates of α-resorcinol and urea crystals in asymmetric unit at using DFT-B3LYP-D level of theory using different basis sets

1. α-resorcinol Crystal

	Basis sets								
	6-21G			6-31G(d, p)			TZP		
Atom	X/*A*	Y/*B*	Z/*C*	X/*A*	Y/*B*	Z/*C*	X/*A*	Y/*B*	Z/*C*
C	-0.00258	0.22441	0.06344	0.00394	0.21717	0.06511	0.00761	0.2147	0.06333
C	0.05798	0.11688	0.22449	0.06098	0.11021	0.22148	0.06167	0.10851	0.21715
C	0.17145	0.0259	0.16658	0.17347	0.02551	0.1609	0.17225	0.02774	0.15706
C	0.22416	0.04409	-0.06067	0.22848	0.04947	-0.06365	0.22823	0.05476	-0.06353
C	0.16798	0.15511	-0.22185	0.17446	0.15706	-0.22216	0.17596	0.16037	-0.22037
C	0.05321	0.24251	-0.16152	0.06211	0.23968	-0.15704	0.06628	0.24024	-0.15531
H	-0.06678	0.42235	-0.26935	-0.05616	0.41169	-0.25869	-0.05224	0.40461	-0.25136
H	0.38947	-0.08788	-0.00935	0.38412	-0.08492	-0.01116	0.3797	-0.07637	-0.00962
H	-0.09278	0.28898	0.11346	-0.08393	0.28064	0.11467	-0.07835	0.27651	0.11224
H	0.01461	0.10419	0.39855	0.01676	0.09225	0.39386	0.01695	0.08806	0.38699
H	0.21535	-0.06005	0.29276	0.21502	-0.05924	0.28319	0.21239	-0.05597	0.27756
H	0.2121	0.16978	-0.39554	0.21794	0.17282	-0.39598	0.21923	0.17757	-0.39266
O	-7.27635E-4	0.34077	-0.33523	0.01234	0.34049	-0.32319	0.01937	0.34313	-0.31653
O	0.33215	-0.04388	-0.14015	0.33724	-0.02996	-0.14174	0.33628	-0.0204	-0.13933

2. Urea Crystal

	Basis sets								
	6-21G			6-31G(d, p)			TZP		
Atom	X/*A*	Y/*B*	Z/*C*	X/*A*	Y/*B*	Z/*C*	X/*A*	Y/*B*	Z/*C*
C	0	-0.5	0.3184	0	-0.5	0.3258	0	-0.5	0.3295
O	0	-0.5	-0.4031	0	-0.5	-0.4023	0	-0.5	-0.4024
N	0.1473	-0.3527	0.1661	0.1436	-0.3564	0.1758	0.1393	-0.3607	0.1797
H	0.2609	-0.2391	0.2751	0.2536	-0.2464	0.2826	0.2461	-0.2539	0.2849
H	0.1441	-0.3559	-0.0555	0.1421	-0.3579	-0.0411	0.1380	-0.3620	-0.0258