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Supporting information for article:

Accurate and efficient representation of intramolecular energy in *ab initio* generation of crystal structures. II. Smoothed intramolecular potentials

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Supplementary Information for article:

Accurate and efficient representation of intramolecular energy in *ab initio* generation of crystal structures. Part II: Smoothed Intramolecular potentials

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This document provides supplementary information regarding the cost of the computations reported in this paper. Further data can be accessed on Zenodo at https://zenodo.org/record/1290769, and used under the Creative Commons Attribution licence. This includes the structure files (.res format) for the final list of structures in all of the investigations, and input files for the calculations.

CrystalPredictor investigations were performed on Intel(R) Xeon(R) CPU E5-2650 v4 running at 2.20 GHz processors. LAM creation and CrystalOptimizer jobs were performed on the Imperial College HPC service, typically using Intel(R) Xeon(R) CPU E5-2620 running at 2.00 GHz processors.

ROY

	LAM model		**waLAM model**	
Step	**Number of calculations**	**CPU hours (approximate)**	**Number of calculations**	**CPU hours (approximate)**
Step 0: construction of LAMs	38	500	38	500
Step 1: CrystalPredictor minimizations	1,000,000	2,000	1,000,000	1,400
Step 2: CrystalOptimizer refinements*	6,539	280,000	2,277	98,000
TOTAL		**282,500**		**99,900**

*No CrystalOptimizer refinement calculations were actually performed in the context of the work reported in this paper. The CPU times reported here are estimated from the results of Vasileiadis *et al.* (2012) who considered an unusually large number (22) of independent conformational degrees of freedom, and performed all QM calculations at a relatively high level of theory (MP2 and B3LYP, for intramolecular variation and electrostatics respectively).

Molecule XXVI

	LAM model		waLAM model	
Step	**Number of calculations**	**CPU hours (approximate)**	**Number of calculations**	**CPU hours (approximate)**
Step 0: construction of LAMs	3,643	280,000	3,643	280,000
Step 1: CrystalPredictor minimizations	500,000	6,000	500,000	4,500
Step 2: CrystalOptimizer refinements	123	7,000	86	5,000
TOTAL		**293,000**		**289,500**

Glucose

	LAM model		waLAM model	
Step	**Number of calculations**	**CPU hours (approximate)**	**Number of calculations**	**CPU hours (approximate)**
Step 0: construction of LAMs	7776	6,900	7,776	6,900
Step 1: CrystalPredictor minimizations	500,000	220	500,000	230
Step 2: CrystalOptimizer refinements	1,160	2,450	408	860
TOTAL		**9,570**		**7,990**

Flufenamic acid

	waLAM model	
Step	**Number of calculations**	**CPU hours (approximate)**
Step 0: construction of LAMs	1,467	9,000
Step 1: CrystalPredictor minimizations	2,000,000	4,000
Step 2: CrystalOptimizer refinements	5,313	4,500
TOTAL		**17,500**