

The Barnes Update Applied in the Gauss-Newton Method: an Improved Algorithm to Locate Bond Breaking Points

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Molecular Cartesian coordinates (in Å) of chorismate, TS, prephenate, initial point in BBP searches, and BBP (the BBP structure corresponds to the MNVAR=20 run)

Chorismate

C	-1.2503768	-0.2316883	-0.5425449
C	0.1060268	-0.8811373	-0.4023541
C	0.6537095	-0.7967968	1.0213833
C	-0.4373158	-1.1531512	2.0024042
C	-1.7261202	-0.8841976	1.7439952
C	-2.1392939	-0.2800144	0.4641530
C	-3.6065986	0.2094527	0.3010390
O	-3.8935246	0.7199220	-0.7954745
O	-4.3347297	0.0155194	1.2969339
O	1.7675238	-1.6178641	1.1857330
H	2.4867078	-1.1907777	0.6319205
H	0.9220352	0.2729470	1.1996198
H	-1.5786904	0.1647643	-1.5070157
O	1.0816092	-0.4776191	-1.3578834
H	-0.0148414	-1.9646031	-0.6029896
C	1.0374667	1.8937861	-1.5682305
C	1.6709683	0.7549833	-1.2701457
C	3.1543211	0.7662098	-0.8155964
H	1.6187658	2.8140359	-1.5175229
H	-0.0183463	1.9149203	-1.8420918
H	-0.1026024	-1.5671974	2.9590076
H	-2.5289419	-1.0632625	2.4617608
O	3.5238376	-0.2420594	-0.1602175
O	3.8167493	1.7663161	-1.1135602

TS

C	-1.1668246	-1.1365631	-0.6120612
C	0.0925055	-1.7336628	-0.5778086
C	0.9258988	-1.7405181	0.6945108
C	0.4292666	-0.7426393	1.6946334
C	-0.5894076	0.0858363	1.4304370
C	-1.3685204	-0.0103604	0.1822209
C	-2.7246975	0.7563966	0.0833754
O	-3.3287348	0.6300330	-0.9989379
O	-3.0519060	1.3928200	1.1015122
O	0.9387513	-3.0511722	1.2904270
H	1.5716764	-3.5576089	0.7729027
H	1.9513338	-1.4352357	0.4201725
H	-1.8519604	-1.2827520	-1.4495977
O	1.1045546	-0.4798516	-1.5923516
H	0.3021432	-2.5789021	-1.2427512
C	-0.1748307	1.4123575	-1.1460139
C	1.0140869	0.6921450	-1.0672555
C	2.1868262	1.2341695	-0.1781557
H	-0.2041733	2.3854352	-0.6539114
H	-0.9523964	1.1711284	-1.8695185
H	0.9947433	-0.6747478	2.6278416
H	-0.9130286	0.8650914	2.1222540
O	3.0642120	0.4035518	0.1392255
O	2.1290330	2.4484223	0.0874519

Prephenate

C	-1.0884011	-1.1536404	-0.7037139
C	-0.2330367	-2.1123031	-0.3427850
C	0.7829339	-1.9217279	0.7550193
C	0.3581003	-0.8270110	1.6895487
C	-0.4914200	0.1335247	1.3197960
C	-1.1309392	0.1916373	-0.0390361
C	-2.6340821	0.7367142	0.0298369
O	-3.3399037	0.4454257	-0.9533759
O	-2.9129704	1.4269111	1.0237816
O	0.9775711	-3.1332527	1.5046119
H	1.4524950	-3.7240013	0.9130901
H	1.7532183	-1.6034246	0.3187014
H	-1.8005199	-1.2803997	-1.5220188
O	1.3189665	0.2231401	-2.2667868
H	-0.2099981	-3.0745113	-0.8709169
C	-0.3702754	1.2324963	-0.9253096
C	1.0594317	0.8141878	-1.2369824
C	2.1816128	1.2214254	-0.2267799
H	-0.3614266	2.1943610	-0.3942631
H	-0.9272979	1.3167626	-1.8710619
H	0.8477512	-0.8168899	2.6675833
H	-0.7546319	0.9589881	1.9831049
O	3.0514671	0.3637580	0.0111405
O	2.0753221	2.3945336	0.1792107

Initial point in BBP searches

C	-1.1383260	-1.1503640	-0.6628870
C	-0.0212400	-1.8781990	-0.5248970
C	0.9121940	-1.7677510	0.6559480
C	0.4262960	-0.7592160	1.6565930
C	-0.5666990	0.0959440	1.3845440
C	-1.2586180	0.1259970	0.0570200
C	-2.7004930	0.7675110	0.0438150
O	-3.3228570	0.6179270	-1.0256740
O	-3.0399790	1.3803890	1.0720110
O	0.9667320	-3.0669460	1.2805530
H	1.5710320	-3.5791040	0.7356980
H	1.9240240	-1.4606270	0.3376230
H	-1.8391010	-1.2978510	-1.4876880
O	1.1949760	-0.3857720	-1.7165790
H	0.2028940	-2.7002870	-1.2144400
C	-0.2972770	1.2848690	-1.0441430
C	1.0422840	0.6610390	-1.1003760
C	2.2027070	1.2273800	-0.2064520
H	-0.3067370	2.2786650	-0.5854130
H	-0.9012770	1.1979830	-1.9534720
H	0.9668420	-0.7239340	2.6071070
H	-0.8963990	0.8573860	2.0944790
O	3.0771950	0.3990690	0.1105070
O	2.1278590	2.4419400	0.0511730

BBP

C	-1.1512148	-1.1720091	-0.6329713
C	-0.0448643	-1.9184003	-0.4808128
C	0.8891383	-1.8133369	0.6975068
C	0.4132448	-0.7834754	1.6848439
C	-0.5869774	0.0682722	1.4072144
C	-1.2698066	0.1323174	0.0752438
C	-2.7193515	0.7550754	0.0443313
O	-3.3149489	0.6077215	-1.0413734
O	-3.0940925	1.3453242	1.0723852
O	0.9716938	-3.1240344	1.3133532
H	1.5192959	-3.6287077	0.7018751
H	1.9037479	-1.5191607	0.3802546
H	-1.8891600	-1.3879256	-1.4112414
O	1.2145787	-0.3199892	-1.7759182
H	0.3065042	-2.5771436	-1.2857193
C	-0.3056251	1.3318410	-1.0317687
C	1.0328204	0.6862836	-1.1115845
C	2.2065078	1.2335513	-0.2104774
H	-0.1453707	2.4046721	-0.7623180
H	-0.9430616	1.2549346	-1.9252632
H	1.0215277	-0.6424000	2.5866643
H	-0.9300903	0.8147494	2.1264805
O	3.0707228	0.3878293	0.0845488
O	2.1549012	2.4472509	0.0611895