Supplementary Material for PCCP

Conformational preferences of chiral molecules: free jet rotational spectrum of 1-phenyl-1-propanol

Barbara M. Giuliano, Paolo Ottaviani, Laura B. Favero, Walther Caminati,* Jens-Uwe Grabow,

Anna Giardini and Mauro Satta

Supplementary Informatio

Table 1: Theoretical structures (B3LYP 6-311++G**, Z-matrices) of the three most stable conformers (T, GE, GZ, see Table 1 of the paper) of 1-phenyl-1-propanol (1PP).

3) 1PP-T

1	6	12						
2	6	12	1			1.39997		
3	6	12	2	1		1.39270	120.570	
4	6	12	3	2	1	1.39526	120.251	0.247
5	6	12	4	3	2	1.39317	119.614	-0.27
6	6	12	5	4	3	1.39473	120.010	0.00
7	1	1	2	1	3	1.08417	119.272	180.808
8	1	1	3	2	4	1.08457	119.774	179.958
9	1	1	4	3	5	1.08424	120.187	180.288
10	1	1	5	4	3	1.08445	120.121	180.441
11	1	1	6	5	4	1.08595	119.662	180.510
12	6	12	1	6	5	1.51923	120.500	178.395
13	6	12	12	1	2	1.53256	112.421	75.518
14	6	12	13	12	1	1.53055	113.417	175.385
15	8	16	12	13	1	1.43536	106.738	123.007
16	1	1	15	12	14	0.96293	108.422	152.094
17	1	1	12	13	1	1.09991	108.322	240.514
18	1	1	14	13	15	1.09490	111.148	-90.98
19	1	1	13	14	12	1.09482	110.267	121.156
20	1	1	13	14	12	1.09538	110.256	238.732
21	1	1	14	13	15	1.09124	110.963	29.150
22	1	1	14	13	15	1.09337	110.732	149.405

2) 1PP-GE

1	6	12						
2	6	12	1			1.40064		
3	6	12	2	1		1.39219	120.591	
4	6	12	3	2	1	1.39586	120.237	0.120
5	6	12	4	3	2	1.39259	119.630	-0.27
6	6	12	5	4	3	1.39528	119.996	0.061
7	1	1	2	1	3	1.08431	119.318	180.705
8	1	1	3	2	4	1.08455	119.795	180.045
9	1	1	4	3	5	1.08425	120.166	180.278
10	1	1	5	4	3	1.08444	120.135	180.392

11	1	1	6	5	4	1.08568	119.683	180.369
12	6	12	1	6	5	1.51945	120.779	179.077
13	6	12	12	1	2	1.53294	113.677	70.483
14	6	12	13	12	1	1.53003	113.998	64.333
15	8	16	12	13	1	1.43630	105.844	122.748
16	1	1	15	12	14	0.96323	108.425	178.035
17	1	1	12	13	1	1.09966	108.284	239.834
18	1	1	14	13	15	1.09303	111.748	-69.71
19	1	1	13	14	12	1.09486	110.341	122.176
20	1	1	13	14	12	1.09444	110.144	239.702
21	1	1	14	13	15	1.09479	111.381	50.900
22	1	1	14	13	15	1.09285	110.528	170.308

3) 1PP-GZ

1	6	12						
2	6	12	1			1.39923		
3	6	12	2	1		1.39298	120.947	
4	6	12	3	2	1	1.39440	120.033	-0.64
5	6	12	4	3	2	1.39351	119.511	0.032
6	6	12	5	4	3	1.39458	120.328	0.366
7	1	1	2	1	3	1.08617	119.500	180.118
8	1	1	3	2	4	1.08448	119.849	180.643
9	1	1	4	3	5	1.08421	120.221	180.356
10	1	1	5	4	3	1.08461	119.995	180.273
11	1	1	6	5	4	1.08360	120.073	179.881
12	6	12	1	6	5	1.52224	121.686	178.598
13	6	12	12	1	2	1.53836	113.641	87.201
14	6	12	13	12	1	1.53027	115.212	62.695
15	8	16	12	13	1	1.43232	106.800	235.422
16	1	1	15	12	14	0.96300	108.501	153.924
17	1	1	12	13	1	1.09910	107.051	118.645
18	1	1	14	13	15	1.09187	110.990	26.681
19	1	1	13	14	12	1.09515	110.077	122.124
20	1	1	13	14	12	1.09503	109.666	239.403
21	1	1	14	13	15	1.09333	110.176	146.190
22	1	1	14	13	15	1.09273	111.669	265.820