Supporting Information Available

Table S1. Comparison between Vibrational Frequencies[a] of Tetrahydrobiopterin Calculated by Density Functional Theory and Molecular Mechanics (using the OPLS Force Field).

Normal mode	QM[b]	MM[c]	D[d]	%[e]	Normal mode	QM	MM	D	%
1	33	41	-7	23.7	46	1058	981	77	7.2
2	50	54	-4	8.3	47	1077	1013	64	6.0
3	83	90	-7	8.8	48	1083	1019	64	5.9
4	97	103	-6	6.5	49	1114	1055	59	5.3
5	123	110	13	10.7	50	1146	1080	66	5.7
6	149	136	13	8.9	51	1179	1166	12	1.0
7	166	157	9	5.5	52	1209	1185	24	2.0
8	180	192	-12	6.7	53	1215	1200	15	1.2
9	203	222	-18	9.1	54	1246	1209	37	2.9
10	232	243	-11	4.7	55	1255	1220	34	2.7
11	237	255	-18	7.6	56	1270	1230	40	3.1
12	253	272	-19	7.5	57	1273	1254	19	1.5
13	282	283	-1	0.3	58	1298	1290	8	0.6
14	288	293	-5	2.0	59	1306	1307	-1	0.1
15	301	300	1	0.4	60	1315	1324	-9	0.7
16	328	318	10	3.3	61	1322	1352	-30	2.3
17	338	337	1	0.3	62	1328	1366	-37	2.8
18	391	359	32	8.2	63	1349	1379	-30	2.2
19	404	386	18	4.6	64	1359	1403	-44	3.2
20	415	406	9	2.3	65	1404	1404	0	0
21	462	420	42	9.2	66	1432	1444	-12	.8
22	486	435	50	10.4	67	1438	1467	-29	2.0

23	498	442	56	11.4	68	1448	1481	-33	2.3
24	511	465	46	8.9	69	1450	1504	-54	3.7
25	526	501	25	4.8	70	1462	1528	-66	4.5
26	545	529	16	3.1	71	1510	1548	-38	2.5
27	554	544	10	1.8	72	1557	1597	-39	2.5
28	559	556	3	0.6	73	1591	1607	-16	1.0
29	611	606	5	0.8	74	1607	1705	-97	6.0
30	645	619	26	4.0	75	1668	1799	-131	7.9
31	660	634	26	4.0	76	2850	2873	-23	.8
32	685	676	9	1.2	77	2892	2921	-29	1.0
33	686	702	-17	2.5	78	2912	2943	-31	1.1
34	706	733	-27	3.8	79	2916	2948	-32	1.1
35	737	773	-36	4.7	80	2924	2950	-26	.9
36	811	791	-20	2.5	81	2981	2972	9	.3
37	849	828	21	2.5	82	2989	2977	12	.4
38	862	845	16	1.9	83	3016	2979	37	1.2
39	900	874	26	2.9	84	3380	3380	0	0
40	948	897	51	5.4	85	3437	3455	-18	0.5
41	988	917	71	7.2	86	3468	3504	-37	1.1
42	1019	921	98	9.6	87	3507	3507	0	0
43	1024	956	68	6.6	88	3548	3578	-30	0.8
44	1034	963	71	6.8	89	3552	3582	-30	0.8
45	1055	980	75	7.1	90	3686	3677	-8	0.2
RMSD[f]			38						
MAX[g]			131						

[a] In cm^{-1}.

[b] Calculated by the density functional theory (B3LYP/6-31+G(d,p)) with the Gaussian98 program [1].

[c] Calculated by molecular mechanics using the OPLS force field parameters determined in this work. The calculations were performed with the Gromacs program [2].

[d] Difference between the same normal mode calculated by quantum mechanics and molecular mechanics (in cm^{-1}).

[e] The percent difference of the same normal mode calculated by quantum mechanics and molecular mechanics (in cm^{-1}).

[f] Root-mean square deviation.

[g] Maximum difference.