Supplementary Material for Hindered rotor tunneling splittings: an application of the two-dimensional non-separable method to benzyl alcohol and two of its fluorine derivatives

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TABLE S.1. Cartesian coordinates (in Å) of structure **3FBA-M1**

DF-LMP2-F12/cc-pVQZ energy (a.u.): -445.431996965447			
Cartesian coordinates			
Atomic Symbol	X	Y	Z
C	-0.3448315604	0.1853267189	-0.8633761800
C	0.7452393685	0.1883652653	0.0084459571
C	0.5181835601	0.0226819469	1.3620731335
C	-0.7514834137	-0.1468269210	1.8903866384
C	-1.8322084930	-0.1487116143	1.0155488766
C	-1.6305924524	0.0162262608	-0.3521504665
H	1.7526027277	0.3175086306	-0.3609936083
F	1.5715457114	0.0259366042	2.2015742064
H	-0.8769078000	-0.2724771734	2.9555629947
H	-2.8323653637	-0.2792526495	1.4039394123
H	-2.4769698601	0.0135723706	-1.0263296878
C	-0.1170888366	0.3645198528	-2.3420982516
O	0.9809513335	-0.3917648045	-2.8329049163
H	-1.0365723868	0.1254049550	-2.8810353715
H	0.1337088956	1.4008995687	-2.5613160826
H	0.8118604619	-1.3146123398	-2.6248518719

TABLE S.2. Cartesian coordinates (in Å) of structure **3FBA-M1***

DF-LMP2-F12/cc-pVQZ energy (a.u.): -445.431996965447			
Cartesian coordinates			
Atomic Symbol	X	Y	Z
C	-0.400806806	-0.920046591	-1.607258773
C	0.188431340	-2.108541359	-2.041558548
C	-0.082765083	-3.277895249	-1.355719052
C	-0.918372162	-3.318391231	-0.251172301
C	-1.501543959	-2.130404303	0.175335697
C	-1.244705743	-0.939104309	-0.497935036
H	0.846599400	-2.122307578	-2.898629044
F	0.486916553	-4.423633080	-1.776542203
H	-1.098877133	-4.257312478	0.250788632
H	-2.157091809	-2.136666303	1.034649225
H	-1.702480309	-0.018835795	-0.159663414
C	-0.117088837	0.364519853	-2.342098252
O	1.253801648	0.522553351	-2.680084306
H	-0.753742134	0.422515342	-3.227755214
H	-0.352234823	1.219261773	-1.710305967
H	1.759178415	0.479658666	-1.863824706

TABLE S.3. Cartesian coordinates (in Å) of structure **3FBA-M2**

DF-LMP2-F12/cc-pVQZ energy (a.u.): -445.431784564556			
Cartesian coordinates			
Atomic Symbol	X	Y	Z
C	0.2177342686	-0.1530369772	-0.8152996199
C	0.1138558561	-0.9410395974	0.3295811229
C	-0.0346527338	-0.3249488267	1.5610059751
C	-0.0842028156	1.0503642456	1.6997874119
C	0.0202703613	1.8310050205	0.5511133682
C	0.1700134494	1.2373649318	-0.6969611343
H	0.1468719786	-2.0208267819	0.2751133248
F	-0.1341781012	-1.0955666706	2.6615473521
H	-0.2011138731	1.4872025329	2.6804115500
H	-0.0159887461	2.9079642049	0.6362589165
H	0.2508285681	1.8459375073	-1.5866120081
C	0.3800858630	-0.7957783965	-2.1686686996
O	-0.4552102548	-0.2175411316	-3.1620494457
H	1.3952168501	-0.6510813354	-2.5339261765
H	0.2089205810	-1.8713967447	-2.0841427634
H	-1.3616988128	-0.2825994023	-2.8497519404

TABLE S.4. Cartesian coordinates (in Å) of structure **3FBA-M2***

DF-LMP2-F12/cc-pVQZ energy (a.u.): -445.431784564556			
Cartesian coordinates			
Atomic Symbol	X	Y	Z
C	1.438071676	-0.148534599	-1.312617343
C	1.118639732	0.939747098	-0.502619226
C	2.109806067	1.515977198	0.274283583
C	3.412371594	1.050667590	0.277683643
C	3.723767561	-0.037170474	-0.534355531
C	2.747269569	-0.633690003	-1.323746204
H	0.114967088	1.341640590	-0.469152605
F	1.790768666	2.567444269	1.053758161
H	4.152631267	1.531373877	0.899822428
H	4.735557159	-0.417328229	-0.547296274
H	2.992061715	-1.477832989	-1.952928026
C	0.380085863	-0.795778397	-2.168668700
O	0.409377478	-2.215123685	-2.109641596
H	-0.611163271	-0.518678703	-1.814434173
H	0.475480526	-0.439949577	-3.197105731
H	0.316041669	-2.467077355	-1.186986953

TABLE S.5. Cartesian coordinates (in Å) of structure **3FBA-M3**

DF-LMP2-F12/cc-pVQZ energy (a.u.): -445.430724510637			
	Cartesian coordinates		
Atomic Symbol	X	Y	Z
C	-0.4118645738	-0.0000001723	-0.8616326861
C	0.7183138758	-0.0000001677	-0.0502803090
C	0.5486129693	0.0000000085	1.3244427489
C	-0.6966751858	0.0000001801	1.9256874904
C	-1.8204429351	0.0000001737	1.1033210317
C	-1.6800346847	-0.0000000010	-0.2789574387
H	1.7087825274	-0.0000002982	-0.4779232097
F	1.6457333065	0.0000000124	2.1077499007
H	-0.7748274394	0.0000003136	3.0026088299
H	-2.8061342946	0.0000003057	1.5467601922
H	-2.5606372689	-0.0000000043	-0.9087316018
C	-0.2899245104	-0.0000003593	-2.3612900252
O	1.0808072868	-0.0000005168	-2.7241160595
H	-0.7973066786	-0.8832496826	-2.7583503721
H	-0.7973058886	0.8832493218	-2.7583499032
H	1.1318598710	0.0000120431	-3.6820512945

TABLE S.6. Cartesian coordinates (in Å) of structure **3FBA-M4**

DF-LMP2-F12/cc-pVQZ energy (a.u.): -445.430436355265			
Cartesian coordinates			
Atomic Symbol	X	Y	Z
C	-0.0000001298	-0.2274660686	-0.8029981832
C	-0.0000000778	-0.9621511722	0.3833801042
C	-0.0000000189	-0.2893123118	1.5903481231
C	-0.0000000095	1.0932219959	1.6695163790
C	-0.0000000616	1.8148916895	0.4813095802
C	-0.0000001215	1.1634226429	-0.7500931722
H	-0.0000000825	-2.0442654792	0.3797743173
F	0.0000000311	-1.0074042373	2.7316880978
H	0.0000000374	1.5765054282	2.6351264317
H	-0.0000000555	2.8952765813	0.5166544658
H	-0.0000001619	1.7264759726	-1.6702122744
C	-0.0000001936	-0.9718794463	-2.1108112253
O	-0.0000002395	-0.0444174781	-3.1833363813
H	0.8831800111	-1.6150308390	-2.1534085264
H	-0.8831689502	-1.6150511459	-2.1534116340
H	-0.0000002797	-0.5437601811	-4.0024519150

TABLE S.7. Cartesian coordinates (in Å) of structure **4FBA-M1**

DF-LMP2-F12/cc-pVQZ energy (a.u.): -445.431876253378			
Cartesian coordinates			
Atomic Symbol	X	Y	Z
C	-0.2188955006	0.2298701967	-0.9817902880
C	1.0472035951	0.2737976087	-0.3928611871
C	1.1989363825	0.1382155531	0.9813723984
C	0.0656553721	-0.0420434243	1.7587418878
C	-1.2037320381	-0.0907897515	1.2118304310
C	-1.3352622759	0.0470766248	-0.1676615375
H	1.9179590497	0.4153872261	-1.0187325145
H	2.1703679801	0.1698253867	1.4526185633
F	0.2067097645	-0.1740116802	3.0911303897
H	-2.0597563020	-0.2329789928	1.8548347103
H	-2.3213259088	0.0114059839	-0.6128263971
C	-0.3617397451	0.3786862188	-2.4715266661
O	0.4551772822	-0.5321158406	-3.1987284187
H	-1.4131818512	0.2740235295	-2.7493697827
H	-0.0321999148	1.3659925162	-2.7891517144
H	0.2431847450	-1.4168757334	-2.8891487876

TABLE S.8. Cartesian coordinates (in Å) of structure **4FBA-M1***

DF-LMP2-F12/cc-pVQZ energy (a.u.): -445.431876253378			
Cartesian coordinates			
Atomic Symbol	X	Y	Z
C	-0.402464336	-0.862094524	-1.622603927
C	-0.066097801	-2.099734583	-2.176570228
C	-0.097847856	-3.256645196	-1.408147788
C	-0.471037261	-3.158094053	-0.076930371
C	-0.810684534	-1.950930428	0.506360684
C	-0.772757126	-0.802429735	-0.280286061
H	0.222221750	-2.153344865	-3.217711609
H	0.159162517	-4.221236625	-1.820774159
F	-0.503585784	-4.276035180	0.672548990
H	-1.095658705	-1.919674004	1.547639984
H	-1.035472709	0.151021069	0.159802250
C	-0.361739745	0.378686219	-2.471526666
O	0.886791172	0.556047832	-3.131412731
H	-1.186913769	0.358126220	-3.187310639
H	-0.481224265	1.266841761	-1.854145844
H	1.571575545	0.541394607	-2.457293975

TABLE S.9. Cartesian coordinates (in Å) of structure **4FBA-M2**

DF-LMP2-F12/cc-pVQZ energy (a.u.): -445.430278644345			
Cartesian coordinates			
Atomic Symbol	X	Y	Z
C	0.3085889755	-0.0000001937	-0.9759937757
C	1.3915881930	-0.0000002566	-0.0961094659
C	1.1962258597	-0.0000001748	1.2797501587
C	-0.1027889707	-0.0000000290	1.7603998080
C	-1.1976817266	0.0000000367	0.9163099613
C	-0.9843904112	-0.0000000469	-0.4603976310
H	2.4021836486	-0.0000003708	-0.4857725754
H	2.0251970744	-0.0000002221	1.9720208316
F	-0.3027154941	0.0000000512	3.0933453745
H	-2.1940894171	0.0000001508	1.3333560873
H	-1.8241771231	0.0000000021	-1.1381673239
C	0.5682418811	-0.0000002865	-2.4577279663
O	-0.6679710705	-0.0000002006	-3.1534900464
H	1.1582679371	0.8831356089	-2.7174253683
H	1.1582763758	-0.8831213582	-2.7174438961
H	-0.4756594229	-0.0000002620	-4.0933393946

TABLE S.10. Cartesian coordinates (in Å) of structure **BA-M1**

DF-LMP2-F12/cc-pVQZ energy (a.u.): -346.251756752780			
Cartesian coordinates			
Atomic Symbol	X	Y	Z
C	-0.2109793671	0.2167041383	-0.4484175670
C	1.0886553962	0.2235577749	0.0633279992
C	1.3110355121	0.0384462319	1.4228148072
C	0.2360088107	-0.1558745504	2.2875972647
C	-1.0612752791	-0.1641170344	1.7863447924
C	-1.2808699833	0.0216239294	0.4237574699
H	1.9208736742	0.3747618295	-0.6114108933
H	2.3209113537	0.0454039139	1.8093209038
H	0.4097040958	-0.2997924701	3.3448967647
H	-1.8993393166	-0.3144725245	2.4527774895
H	-2.2911191590	0.0151693665	0.0336557020
C	-0.4415761188	0.4178953801	-1.9212254915
O	0.3340552494	-0.4616952970	-2.7284111875
H	-1.5071248168	0.3170360211	-2.1410376123
H	-0.1347510623	1.4182992841	-2.2207993791
H	0.1562582576	-1.3565555259	-2.4265211152

TABLE S.11. Cartesian coordinates (in Å) of structure **BA-M1***

DF-LMP2-F12/cc-pVQZ energy (a.u.): -346.251756752780			
Cartesian coordinates			
Atomic Symbol	X	Y	Z
C	0.2109793671	-0.2167041383	0.4484175670
C	-1.0886553962	-0.2235577749	-0.0633279992
C	-1.3110355121	-0.0384462319	-1.4228148072
C	-0.2360088107	0.1558745504	-2.2875972647
C	1.0612752791	0.1641170344	-1.7863447924
C	1.2808699833	-0.0216239294	-0.4237574699
H	-1.9208736742	-0.3747618295	0.6114108933
H	-2.3209113537	-0.0454039139	-1.8093209038
H	-0.4097040958	0.2997924701	-3.3448967647
H	1.8993393166	0.3144725245	-2.4527774895
H	2.2911191590	-0.0151693665	-0.0336557020
C	0.4415761188	-0.4178953801	1.9212254915
O	-0.3340552494	0.4616952970	2.7284111875
H	1.5071248168	-0.3170360211	2.1410376123
H	0.1347510623	-1.4182992841	2.2207993791
H	-0.1562582576	1.3565555259	2.4265211152

TABLE S.12. Cartesian coordinates (in Å) of structure **BA-M2**

DF-LMP2-F12/cc-pVQZ energy (a.u.): -346.249920738367			
Cartesian coordinates			
Atomic Symbol	X	Y	Z
C	-0.2939057238	0.0000939468	-0.4377422521
C	1.0378868083	0.0001255282	-0.0321388682
C	1.3557174619	0.0000482955	1.3242479129
C	0.3490685400	-0.0000607694	2.2835608093
C	-0.9842165567	-0.0000926588	1.8815542007
C	-1.3008851471	-0.0000155829	0.5282612175
H	1.8168178821	0.0002102634	-0.7795279544
H	2.3930097181	0.0000735728	1.6300635665
H	0.5992795206	-0.0001204868	3.3352678440
H	-1.7744293485	-0.0001772661	2.6196327215
H	-2.3397142969	-0.0000407485	0.2197760517
C	-0.6782745727	0.0001748487	-1.8923586796
O	0.4914146895	-0.0002901039	-2.6946756303
H	-1.2898467848	-0.8826178735	-2.0986267622
H	-1.2891957081	0.8833989467	-2.0987048115
H	0.2159547261	0.0006180967	-3.6132726783

TABLE S.13. Parameters (in 100/amu·Å^2) used to fit by Fourier series the one-dimensional parameters of $d_{\tau\varsigma}$ elements of the inverse of **D** matrix for system **3FBA**

Parameter	τ=1,ς=1	τ=1,ς=2	τ=2,ς=2
$a_0^{\tau\varsigma}$	5.6091	-2.5027	127.3530
$a_1^{\tau\varsigma}$	0.3477	-0.2082	-0.0659
$a_2^{\tau\varsigma}$	0.5095	-0.4828	0.8277
$a_3^{\tau\varsigma}$	0.0280	-0.0085	-0.0117
$a_4^{\tau\varsigma}$	0.0399	-0.0375	0.0153
$a_5^{\tau\varsigma}$	-0.0002	0.0011	-0.0008
$a_6^{\tau\varsigma}$	0.0004	0.0008	-0.0122
$b_1^{\tau\varsigma}$	0.2335	-6.1262	4.3689
$b_2^{\tau\varsigma}$	0.1511	-0.0761	3.8746
$b_3^{\tau\varsigma}$	0.0005	-0.1265	0.7214
$b_4^{\tau\varsigma}$	0.0098	-0.0237	0.1290
$b_5^{\tau\varsigma}$	0.0004	-0.0055	0.0282
$b_6^{\tau\varsigma}$	0.0001	-0.0004	0.0152

TABLE S.14. Parameters (in 100/amu·Å^2) used to fit by Fourier series the cross-term parameters of $d_{\tau\varsigma}$ elements of the inverse of **D** matrix for system **3FBA**

Parameter	τ=1,ς=1	τ=1,ς=2	τ=2,ς=2
$c_{11}^{\tau\varsigma}$,$d_{11}^{\tau\varsigma}$	0.0245, -0.0039	-0.0153, -0.4117	0.0584, 0.2311
$c_{12}^{\tau\varsigma}$,$d_{12}^{\tau\varsigma}$	0.0013, 0.0227	-0.0015, -0.0048	0.1942, -0.0266
$c_{13}^{\tau\varsigma}$,$d_{13}^{\tau\varsigma}$	0.0013, -0.0004	-0.0076, -0.0057	0.0200, -0.0235
$c_{14}^{\tau\varsigma}$,$d_{14}^{\tau\varsigma}$	0.0008, 0.0004	-0.0010, 0.0001	0.0088, -0.0009
$c_{15}^{\tau\varsigma}$,$d_{15}^{\tau\varsigma}$	0.0001, 0.0000	-0.0002, -0.0002	0.0013, -0.0013
$c_{16}^{\tau\varsigma}$,$d_{16}^{\tau\varsigma}$	0.0002, 0.0000	0.0001, 0.0001	-0.0002, -0.0013
$c_{21}^{\tau\varsigma}$,$d_{21}^{\tau\varsigma}$	0.0937, -0.0720	-0.2166, -0.2465	1.0097, -0.1383
$c_{22}^{\tau\varsigma}$,$d_{22}^{\tau\varsigma}$	0.0410, -0.0054	-0.0786, 0.0534	0.7274, -0.6456
$c_{23}^{\tau\varsigma}$,$d_{23}^{\tau\varsigma}$	0.0130, -0.0152	-0.0429, 0.0358	0.2680, -0.2639
$c_{24}^{\tau\varsigma}$,$d_{24}^{\tau\varsigma}$	0.0037, -0.0032	-0.0135, 0.0129	0.0986, -0.1211
$c_{25}^{\tau\varsigma}$,$d_{25}^{\tau\varsigma}$	0.0009, -0.0011	-0.0039, 0.0045	0.0304, -0.0339
$c_{26}^{\tau\varsigma}$,$d_{26}^{\tau\varsigma}$	0.0000, -0.0002	-0.0009, 0.0011	0.0066, -0.0080
$c_{31}^{\tau\varsigma}$,$d_{31}^{\tau\varsigma}$	0.0029, -0.0046	-0.0007, -0.0174	-0.0043, 0.0269
$c_{32}^{\tau\varsigma}$,$d_{32}^{\tau\varsigma}$	0.0036, -0.0019	-0.0003, -0.0001	0.0161, -0.0055
$c_{33}^{\tau\varsigma}$,$d_{33}^{\tau\varsigma}$	0.0008, -0.0015	-0.0005, -0.0001	0.0024, -0.0044
$c_{34}^{\tau\varsigma}$,$d_{34}^{\tau\varsigma}$	0.0000, -0.0002	0.0001, 0.0000	0.0021, -0.0003
$c_{35}^{\tau\varsigma}$,$d_{35}^{\tau\varsigma}$	-0.0001, 0.0000	0.0000, -0.0001	-0.0001, 0.0007
$c_{36}^{\tau\varsigma}$,$d_{36}^{\tau\varsigma}$	-0.0003, 0.0000	0.0001, -0.0001	-0.0006, 0.0009
$c_{41}^{\tau\varsigma}$,$d_{41}^{\tau\varsigma}$	0.0117, -0.0184	-0.0228, 0.0114	0.1012, -0.1265
$c_{42}^{\tau\varsigma}$,$d_{42}^{\tau\varsigma}$	0.0177, -0.0160	-0.0273, 0.0295	0.2055, -0.2350
$c_{43}^{\tau\varsigma}$,$d_{43}^{\tau\varsigma}$	0.0090, -0.0099	-0.0206, 0.0217	0.1953, -0.2049
$c_{44}^{\tau\varsigma}$,$d_{44}^{\tau\varsigma}$	0.0036, -0.0038	-0.0118, 0.0119	0.1130, -0.1133
$c_{45}^{\tau\varsigma}$,$d_{45}^{\tau\varsigma}$	0.0012, -0.0012	-0.0052, 0.0050	0.0516, -0.0495
$c_{46}^{\tau\varsigma}$,$d_{46}^{\tau\varsigma}$	0.0001, -0.0003	-0.0019, 0.0019	0.0169, -0.0166
$c_{51}^{\tau\varsigma}$,$d_{51}^{\tau\varsigma}$	-0.0006, 0.0004	0.0007, 0.0002	-0.0002, -0.0008
$c_{52}^{\tau\varsigma}$,$d_{52}^{\tau\varsigma}$	0.0001, -0.0003	0.0001, -0.0001	-0.0011, 0.0003
$c_{53}^{\tau\varsigma}$,$d_{53}^{\tau\varsigma}$	0.0003, -0.0003	0.0001, 0.0000	-0.0009, -0.0012
$c_{54}^{\tau\varsigma}$,$d_{54}^{\tau\varsigma}$	0.0002, -0.0001	0.0000, 0.0000	0.0010, -0.0002
$c_{55}^{\tau\varsigma}$,$d_{55}^{\tau\varsigma}$	0.0000, 0.0000	-0.0001, 0.0000	0.0005, -0.0005
$c_{56}^{\tau\varsigma}$,$d_{56}^{\tau\varsigma}$	0.0001, 0.0000	-0.0001, 0.0000	0.0009, -0.0007
$c_{61}^{\tau\varsigma}$,$d_{61}^{\tau\varsigma}$	-0.0004, -0.0004	0.0011, -0.0005	-0.0216, 0.0116
$c_{62}^{\tau\varsigma}$,$d_{62}^{\tau\varsigma}$	0.0019, -0.0018	-0.0017, 0.0019	0.0075, -0.0027
$c_{63}^{\tau\varsigma}$,$d_{63}^{\tau\varsigma}$	0.0023, -0.0021	-0.0032, 0.0026	0.0240, -0.0209
$c_{64}^{\tau\varsigma}$,$d_{64}^{\tau\varsigma}$	0.0011, -0.0010	-0.0023, 0.0019	0.0218, -0.0201
$c_{65}^{\tau\varsigma}$,$d_{65}^{\tau\varsigma}$	0.0003, -0.0003	-0.0012, 0.0009	0.0132, -0.0113
$c_{66}^{\tau\varsigma}$,$d_{66}^{\tau\varsigma}$	0.0001, 0.0000	-0.0006, 0.0003	0.0058, -0.0042

TABLE S.15. Parameters (in 100/amu·Å^2) used to fit by Fourier series the one-dimensional parameters of $d_{\tau\varsigma}$ elements of the inverse of **D** matrix for system **4FBA**

Parameter	τ=1,ς=1	τ=1,ς=2	τ=2,ς=2
$a_0^{\tau\varsigma}$	5.9708	-2.3557	127.0170
$a_2^{\tau\varsigma}$	0.2385	-0.2530	0.7348
$a_4^{\tau\varsigma}$	0.0127	-0.0142	0.0094
$a_6^{\tau\varsigma}$	-0.0011	0.0022	-0.0135
$b_1^{\tau\varsigma}$	0.2146	-6.0986	4.2882
$b_2^{\tau\varsigma}$	0.1474	-0.0672	3.9607
$b_3^{\tau\varsigma}$	-0.0013	-0.1269	0.7125
$b_4^{\tau\varsigma}$	0.0092	-0.0225	0.1307
$b_5^{\tau\varsigma}$	0.0002	-0.0053	0.0288
$b_6^{\tau\varsigma}$	-0.0002	-0.0001	0.0154

TABLE S.16. Parameters (in 100/amu·Å^2) used to fit by Fourier series the cross-term parameters of $d_{\tau\varsigma}$ elements of the inverse of **D** matrix for system **4FBA**

Parameter	τ=1,ς=1	τ=1,ς=2	τ=2,ς=2
$c_{21}^{\tau\varsigma}$,$d_{21}^{\tau\varsigma}$	0.0645, -0.0520	-0.1827, -0.0393	0.9801, -0.4901
$c_{22}^{\tau\varsigma}$,$d_{22}^{\tau\varsigma}$	0.0322, -0.0164	-0.0787, 0.0644	0.6530, -0.7048
$c_{23}^{\tau\varsigma}$,$d_{23}^{\tau\varsigma}$	0.0105, -0.0140	-0.0353, 0.0398	0.2770, -0.2886
$c_{24}^{\tau\varsigma}$,$d_{24}^{\tau\varsigma}$	0.0026, -0.0029	-0.0120, 0.0137	0.1014, -0.1288
$c_{25}^{\tau\varsigma}$,$d_{25}^{\tau\varsigma}$	0.0007, -0.0009	-0.0036, 0.0046	0.0312, -0.0369
$c_{26}^{\tau\varsigma}$,$d_{26}^{\tau\varsigma}$	-0.0001, -0.0002	-0.0007, 0.0012	0.0065, -0.0091
$c_{41}^{\tau\varsigma}$,$d_{41}^{\tau\varsigma}$	0.0054, -0.0103	-0.0170, 0.0281	0.1018, -0.1541
$c_{42}^{\tau\varsigma}$,$d_{42}^{\tau\varsigma}$	0.0119, -0.0123	-0.0250, 0.0276	0.1918, -0.2291
$c_{43}^{\tau\varsigma}$,$d_{43}^{\tau\varsigma}$	0.0068, -0.0072	-0.0192, 0.0211	0.1907, -0.2024
$c_{44}^{\tau\varsigma}$,$d_{44}^{\tau\varsigma}$	0.0031, -0.0031	-0.0116, 0.0115	0.1092, -0.1095
$c_{45}^{\tau\varsigma}$,$d_{45}^{\tau\varsigma}$	0.0012, -0.0009	-0.0051, 0.0047	0.0497, -0.0465
$c_{46}^{\tau\varsigma}$,$d_{46}^{\tau\varsigma}$	0.0003, -0.0003	-0.0021, 0.0017	0.0162, -0.0148
$c_{61}^{\tau\varsigma}$,$d_{61}^{\tau\varsigma}$	-0.0007, 0.0007	0.0017, -0.0006	-0.0236, 0.0127
$c_{62}^{\tau\varsigma}$,$d_{62}^{\tau\varsigma}$	0.0007, -0.0007	-0.0008, 0.0009	0.0063, -0.0012
$c_{63}^{\tau\varsigma}$,$d_{63}^{\tau\varsigma}$	0.0014, -0.0012	-0.0029, 0.0022	0.0253, -0.0244
$c_{64}^{\tau\varsigma}$,$d_{64}^{\tau\varsigma}$	0.0009, -0.0006	-0.0025, 0.0022	0.0234, -0.0207
$c_{65}^{\tau\varsigma}$,$d_{65}^{\tau\varsigma}$	0.0003, -0.0002	-0.0014, 0.0011	0.0133, -0.0124
$c_{66}^{\tau\varsigma}$,$d_{66}^{\tau\varsigma}$	0.0003, -0.0001	-0.0008, 0.0005	0.0067, -0.0053

TABLE S.17. Parameters (in 100/amu·Å^2) used to fit by Fourier series the one-dimensional parameters of $d_{\tau\varsigma}$ elements of the inverse of **D** matrix for system **BA**

Parameter	τ=1,ς=1	τ=1,ς=2	τ=2,ς=2
$a_0^{\tau\varsigma}$	6.2942	-2.6735	127.4790
$a_2^{\tau\varsigma}$	0.3952	-0.3970	0.8124
$a_4^{\tau\varsigma}$	0.0278	-0.0261	0.0140
$a_6^{\tau\varsigma}$	-0.0007	0.0019	-0.0135
$b_1^{\tau\varsigma}$	0.2382	-6.1209	4.2365
$b_2^{\tau\varsigma}$	0.1486	-0.0648	3.6205
$b_3^{\tau\varsigma}$	-0.0001	-0.1200	0.7007
$b_4^{\tau\varsigma}$	0.0099	-0.0235	0.1196
$b_5^{\tau\varsigma}$	0.0003	-0.0051	0.0271
$b_6^{\tau\varsigma}$	0.0000	-0.0002	0.0147

TABLE S.18. Parameters (in 100/amu·Å^2) used to fit by Fourier series the cross-term parameters of $d_{\tau\varsigma}$ elements of the inverse of **D** matrix for system **BA**

Parameter	τ=1,ς=1	τ=1,ς=2	τ=2,ς=2
$c_{21}^{\tau\varsigma}$,$d_{21}^{\tau\varsigma}$	0.0853,232.4840	-0.2020, -0.1402	0.9854, -0.2897
$c_{22}^{\tau\varsigma}$,$d_{22}^{\tau\varsigma}$	0.0388,132.4760	-0.0786, 0.0579	0.6369, -0.6237
$c_{23}^{\tau\varsigma}$,$d_{23}^{\tau\varsigma}$	0.0126, 25.1012	-0.0375, 0.0368	0.2517, -0.2607
$c_{24}^{\tau\varsigma}$,$d_{24}^{\tau\varsigma}$	0.0033, 6.4150	-0.0123, 0.0131	0.0902, -0.1150
$c_{25}^{\tau\varsigma}$,$d_{25}^{\tau\varsigma}$	0.0009, 0.7867	-0.0035, 0.0044	0.0276, -0.0332
$c_{26}^{\tau\varsigma}$,$d_{26}^{\tau\varsigma}$	0.0000, -0.2078	-0.0007, 0.0012	0.0059, -0.0090
$c_{41}^{\tau\varsigma}$,$d_{41}^{\tau\varsigma}$	0.0090, 20.5502	-0.0195, 0.0216	0.0995, -0.1433
$c_{42}^{\tau\varsigma}$,$d_{42}^{\tau\varsigma}$	0.0158, 36.5011	-0.0264, 0.0291	0.1908, -0.2234
$c_{43}^{\tau\varsigma}$,$d_{43}^{\tau\varsigma}$	0.0086, 21.9533	-0.0198, 0.0215	0.1856, -0.1953
$c_{44}^{\tau\varsigma}$,$d_{44}^{\tau\varsigma}$	0.0035, 10.0673	-0.0116, 0.0115	0.1052, -0.1056
$c_{45}^{\tau\varsigma}$,$d_{45}^{\tau\varsigma}$	0.0012, 2.7850	-0.0049, 0.0047	0.0479, -0.0436
$c_{46}^{\tau\varsigma}$,$d_{46}^{\tau\varsigma}$	0.0001, 0.3223	-0.0019, 0.0016	0.0147, -0.0136
$c_{61}^{\tau\varsigma}$,$d_{61}^{\tau\varsigma}$	-0.0007, -0.4765	0.0016, -0.0006	-0.0258, 0.0127
$c_{62}^{\tau\varsigma}$,$d_{62}^{\tau\varsigma}$	0.0014, 3.5145	-0.0011, 0.0015	0.0052, -0.0018
$c_{63}^{\tau\varsigma}$,$d_{63}^{\tau\varsigma}$	0.0020, 4.3241	-0.0031, 0.0025	0.0236, -0.0245
$c_{64}^{\tau\varsigma}$,$d_{64}^{\tau\varsigma}$	0.0011, 1.5230	-0.0024, 0.0022	0.0228, -0.0197
$c_{65}^{\tau\varsigma}$,$d_{65}^{\tau\varsigma}$	0.0004, 0.3095	-0.0015, 0.0011	0.0134, -0.0124
$c_{66}^{\tau\varsigma}$,$d_{66}^{\tau\varsigma}$	0.0003, -0.2564	-0.0008, 0.0005	0.0072, -0.0046

TABLE S.19. Parameters (in cm^{-1}) for the one-dimensional potentials of the three systems.

Parameter	3FBA	4FBA	BA
a_0	557.84	548.16	521.13
a_1	-22.67	-	-
a_2	19.79	77.53	79.50
a_3	4.18	-	-
a_4	-6.96	-5.53	-10.04
a_5	0.30	-	-
a_6	-2.65	-2.59	-7.64
b_1	3.16	11.35	-39.49
b_2	56.83	46.97	22.30
b_3	193.75	194.43	187.20
b_4	-2.45	-2.12	-2.43
b_5	0.02	0.06	0.12
b_6	1.50	1.52	1.32

TABLE S.20. Coupling parameters (in cm^{-1}) for the three systems.

Parameter	3FBA	4FBA	BA
a_0	557.84	548.16	521.13
a_1	-22.67	-	-
c_{11}, d_{11}	19.80, -0.46	- , -	- , -
c_{12}, d_{12}	7.63, -7.44	- , -	- , -
c_{11}, d_{11}	19.80, -0.46	- , -	- , -
c_{12}, d_{12}	7.63, -7.44	- , -	- , -
c_{13}, d_{13}	1.58, -2.19	- , -	- , -
c_{14}, d_{14}	0.31, -0.32	- , -	- , -
c_{15}, d_{15}	-0.02, 0.02	- , -	- , -
c_{16}, d_{16}	-0.01, 0.05	- , -	- , -
c_{21}, d_{21}	249.57, -195.93	250.87, -210.77	232.48, -190.44
c_{22}, d_{22}	146.34, -232.31	153.82, -241.96	132.48, -213.06
c_{23}, d_{23}	28.60, -27.16	30.29, -28.71	25.10, -22.34
c_{24}, d_{24}	8.53, -9.56	9.46, -10.41	6.41, -7.99
c_{25}, d_{25}	1.19, -2.28	1.31, -2.48	0.79, -2.01
c_{26}, d_{26}	0.24, -0.17	0.29, -0.31	-0.21, 0.25
c_{31}, d_{31}	1.24, -2.61	- , -	- , -
c_{32}, d_{32}	1.10, -1.43	- , -	- , -
c_{33}, d_{33}	0.02, 0.19	- , -	- , -
c_{34}, d_{34}	-0.06, 0.10	- , -	- , -
c_{35}, d_{35}	-0.08, 0.08	- , -	- , -
c_{36}, d_{36}	-0.15, 0.15	- , -	- , -
c_{41}, d_{41}	24.33, -30.76	22.22, -29.55	20.55, -25.92
c_{42}, d_{42}	44.36, -44.61	41.28, -41.75	36.50, -40.15
c_{43}, d_{43}	23.87, -25.69	23.36, -25.33	21.95, -23.96
c_{44}, d_{44}	10.95, -11.08	10.45, -10.59	10.07, -9.66
c_{45}, d_{45}	3.44, -3.41	3.38, -3.28	2.78, -3.21
c_{46}, d_{46}	0.66, -0.78	0.72, -0.87	0.32, -0.31
c_{51}, d_{51}	0.14, -0.13	- , -	- , -
c_{52}, d_{52}	-0.01, -0.01	- , -	- , -
c_{53}, d_{53}	-0.23, 0.06	- , -	- , -
c_{54}, d_{54}	-0.04, 0.07	- , -	- , -
c_{55}, d_{55}	-0.11, 0.10	- , -	- , -
c_{56}, d_{56}	-0.04, 0.11	- , -	- , -
c_{61}, d_{61}	0.03, -0.29	-0.09, -0.42	-0.48, 1.39
c_{62}, d_{62}	3.19, -4.01	3.48, -4.30	3.51, -4.10
c_{63}, d_{63}	5.11, -4.75	5.38, -4.94	4.32, -4.72
c_{64}, d_{64}	2.24, -2.04	2.31, -2.12	1.52, -1.83
c_{65}, d_{65}	0.76, -0.81	0.91, -0.92	0.31, -0.72
c_{66}, d_{66}	0.15, -0.24	0.22, -0.28	-0.26, 0.15

TABLE S.21. Parameters (in cm^{-1}) to fit the linear reaction path potentials of the three systems.

Parameter	3FBA	4FBA	BA
a_0	310.65	315.76	340.07
a_1	-43.54	-	-
a_2	90.40	193.81	249.48
a_3	-6.35	-	-
a_4	188.30	119.15	61.92
a_5	29.57	-	-
a_6	-102.67	-191.88	-223.91
a_7	12.63	-	-
a_8	-115.65	-91.28	-51.77
a_9	-6.80	-	-
a_{10}	-62.29	-10.60	3. 77
a_{11}	-13.32	-	-
a_{12}	-10.95	9.23	2.72
a_{13}	-6.20	-	-
a_{14}	8.15	0.38	-0.46
a_{15}	2.20	-	-
a_{16}	3.66	-2.23	-0.25
a_{17}	2.61	-	-
a_{18}	-2.07	1.18	2.56
a_{19}	-1.10	-	-
a_{20}	-1.42	0.42	-1.77
a_{21}	-1.70	-	-
a_{22}	0.23	-1.21	0.66
a_{23}	0.14	-	-
a_{24}	0.63	0.30	0.12
a_{25}	1.38	-	-
a_{26}	-0.53	-0.04	0.31
a_{27}		-	-
a_{28}		0.19	-0.41
a_{29}		-	-
a_{30}		-0.39	-0.38
a_{31}		-	-
a_{32}		0.17	0.06
a_{33}		-	-
a_{34}		0.36	-0.41
a_{35}		-	-
a_{36}		-0.23	-0.17
a_{37}		-	-
a_{38}		-0.26	-0.24
a_{39}		-	-
a_{40}		-0.22	-0.26
a_{41}		-	-
a_{42}		-0.57	0.09

TABLE S.22. Tunneling splittings (in MHz) of the three systems.

	LRP
3FBA	0.26
4FBA	2.75
BA	44.75

TABLE S.23. Energy levels along the LRP potential for 3FBA.

Level	Energy / (cm^{-1})
0^-	48.937544421292
0^+	48.937553289914
1^-	97.120247363121
1^+	97.120255746611

TABLE S.24. Energy levels along the LRP potential for 4FBA.

Level	Energy / (cm^{-1})
0^+0^+	48.629386253060
0^+0^-	48.629386840881
0^-0^-	48.629478109963
0^-0^+	48.629478751194

TABLE S.25. Energy levels along the LRP potential for BA.

Level	Energy / (cm^{-1})
0^+0^+	45.474093162051
0^+0^-	45.474095860494
0^-0^+	45.475586311217
0^-0^-	45.475589934062