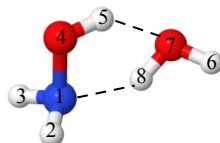


Table S2 Selected Z-matrices of the static and dynamic equilibrium structures of the intermediate complexes in the S_0 and S_1 states obtained from DFT/B3LYP/aug-cc-pVDZ geometry optimizations and sampled from NVT-BOMD simulations at the TD-DFT/B3LYP/aug-cc-pVDZ level, respectively. The Z-matrices of the remaining structures can be sent upon request.

G1-[1]

N						
H	1	B1				
H	1	B2	2	A1		
O	1	B3	2	A2	3	D1
H	4	B4	1	A3	2	D2
H	1	B5	4	A4	5	D3
O	1	B6	4	A5	5	D4
H	7	B7	1	A6	4	D5

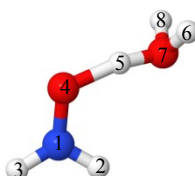
B1	1.02165601
B2	1.02172697
B3	1.43922688
B4	0.97358205
B5	3.38861506
B6	2.78941607
B7	0.97942585
A1	106.21155535
A2	104.50988309
A3	102.29914886
A4	83.81457446
A5	78.54715534
A6	26.87533992
D1	110.40315621
D2	126.56307384
D3	11.59623587
D4	-1.66968342
D5	172.18496761



E1-[1]

N						
H	1	B1				
H	1	B2	2	A1		
O	1	B3	2	A2	3	D1
H	4	B4	1	A3	2	D2
H	4	B5	1	A4	2	D3
O	4	B6	1	A5	2	D4
H	7	B7	4	A6	1	D5

B1	1.00611182
B2	1.05757127
B3	1.30261583
B4	1.34890474
B5	2.95563631
B6	2.40498212

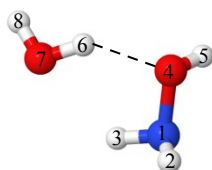


B7	1.08010786
A1	119.90991514
A2	114.44142409
A3	115.12885382
A4	118.56929576
A5	107.60394013
A6	113.80133926
D1	154.54582312
D2	20.65729013
D3	11.66237886
D4	26.43825912
D5	108.62664189

G1-[2]

N						
H	1	B1				
H	1	B2	2	A1		
O	1	B3	2	A2	3	D1
H	4	B4	1	A3	2	D2
O	4	B5	1	A4	2	D3
H	6	B6	4	A5	1	D4
H	6	B7	4	A6	1	D5

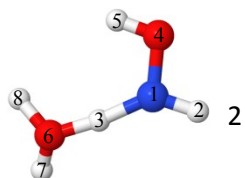
B1	1.02126637
B2	1.02283967
B3	1.45250852
B4	0.96489481
B5	2.81421854
B6	0.97341975
B7	0.96286396
A1	105.76382284
A2	103.26534016
A3	102.89001678
A4	87.61143531
A5	22.79069170
A6	127.04587158
D1	108.40069560
D2	126.75005207
D3	-104.72865818
D4	-173.35120157
D5	-149.64134385



E1-[2]

N						
H	1	B1				
H	1	B2	2	A1		
O	1	B3	2	A2	3	D1
H	4	B4	1	A3	2	D2
O	1	B5	4	A4	5	D3
H	6	B6	1	A5	4	D4
H	6	B7	1	A6	4	D5

B1	1.04437972
B2	1.32504490

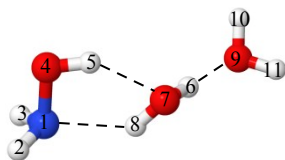


B3	1.34608952
B4	0.98513654
B5	2.46365156
B6	0.98946905
B7	1.13634898
A1	137.03450336
A2	102.94451621
A3	104.69053774
A4	116.09855113
A5	122.91878176
A6	111.55002689
D1	-171.80154414
D2	176.54791968
D3	0.74887120
D4	141.65717726
D5	15.39496187

G2-[2]

N						
H	1	B1				
H	1	B2	2	A1		
O	1	B3	3	A2	2	D1
H	4	B4	1	A3	3	D2
H	4	B5	1	A4	3	D3
O	4	B6	1	A5	3	D4
H	7	B7	4	A6	1	D5
O	7	B8	4	A7	1	D6
H	9	B9	7	A8	4	D7
H	9	B10	7	A9	4	D8

B1	1.02226269
B2	1.02083348
B3	1.44001562
B4	0.97813292
B5	3.43948412
B6	2.79528067
B7	0.97375254
B8	2.90614160
B9	0.96615216
B10	0.96590942
A1	105.99953660
A2	104.48048937
A3	101.64312320
A4	79.31148059
A5	77.47606030
A6	63.68829749
A7	126.80376057
A8	110.92341715
A9	109.42332095
D1	-110.19805097
D2	-126.79826224
D3	-114.00650351
D4	-127.64668610
D5	4.16503004
D6	102.25270443



D7 52.76810885
 D8 168.31804844

E2-[2]

N					
H	1	B1			
H	1	B2	2	A1	
O	1	B3	3	A2	D1
H	4	B4	1	A3	D2
H	4	B5	1	A4	D3
O	4	B6	1	A5	D4
H	7	B7	4	A6	D5
O	7	B8	4	A7	D6
H	9	B9	7	A8	D7
H	9	B10	7	A9	D8

B1	1.04526791
B2	1.02104456
B3	1.28519181
B4	1.22348233
B5	3.19239315
B6	2.36443841
B7	0.96547708
B8	2.48598069
B9	1.02587426
B10	0.97876351
A1	117.69650154
A2	113.11909711
A3	111.23014020
A4	109.13064042
A5	108.03597630
A6	122.07669802
A7	125.99781576
A8	127.54984326
A9	120.44476053
D1	-144.55777764
D2	169.60910954
D3	-171.03321524
D4	170.35695463
D5	-101.59855320
D6	97.04235481
D7	-105.62657339
D8	39.30238889

