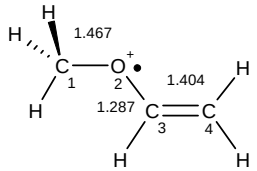
Supplementary Materials of

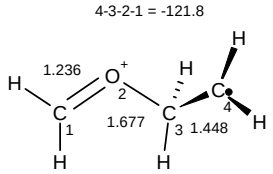
A G3(MP2) Study of the $C_3H_6O^{+\bullet}$ Isomers Fragmented from 1,4-Dioxane$^{+\bullet}$

by Chow-Shing Lam, Wai-Kee Li* and See-Wing Chiu*

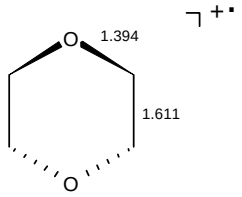
Figure S1



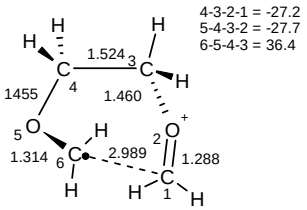
1 (C_s, ^{2}A")



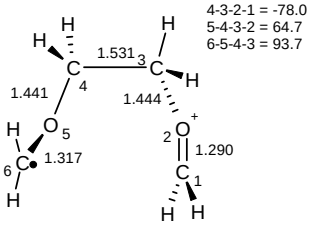
2 (C_1, ^{2}A)



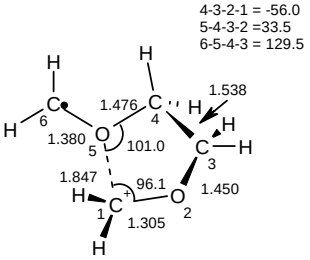
3 (C_{2h}, ^2A_g)



TS(3→4a) (C_1, ^{2}A)



4a (C_1, ^{2}A)



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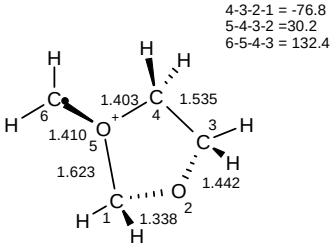
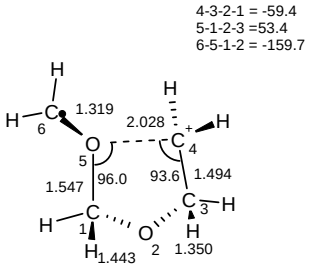
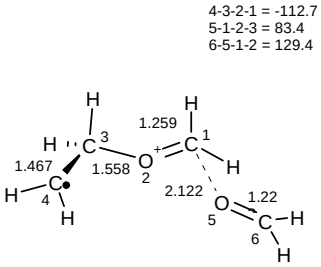


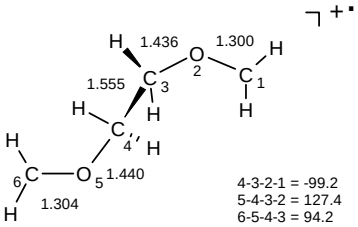
5 (C_1, ^{2}A)



TS(5→6a) (C_1, ^{2}A)



6a (C_1, ^{2}A)



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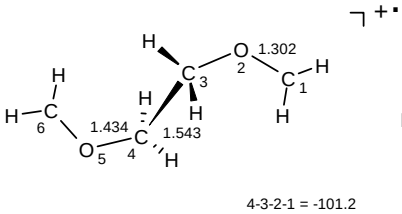
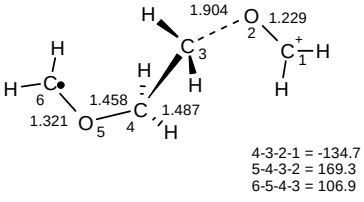
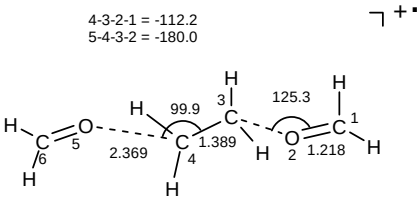


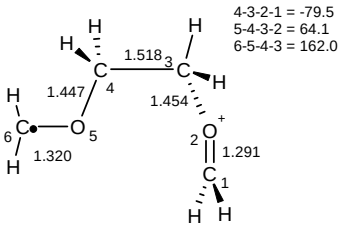
4b (C_i, ^2A_u)



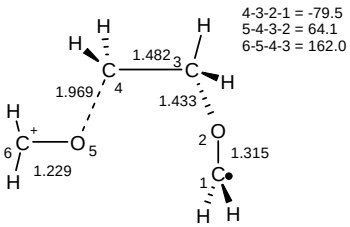
TS(4b→7) (C_1, ^{2}A)



7 (C_i, ^2A_u)

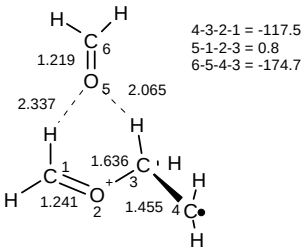


4c (C_1, ^{2}A)

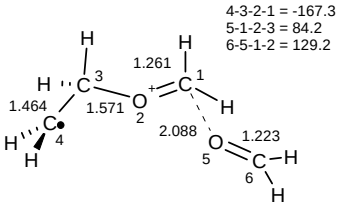


TS(4c→8) (C_1, ^{2}A)

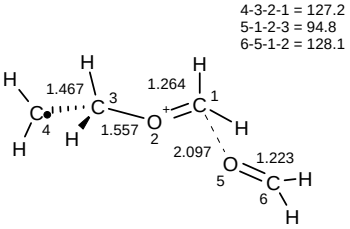
Figure S1 (continued)



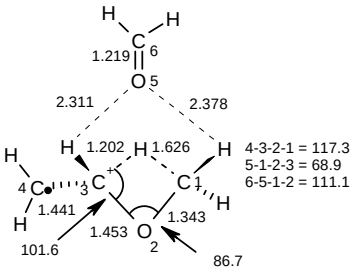
8 (C_1, ^{2}A)



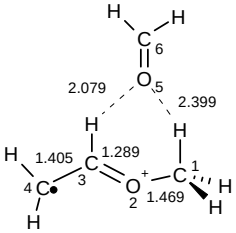
TS(6a→6b) (C_1, ^{2}A)



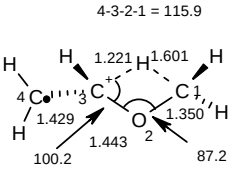
6b (C_1, ^{2}A)



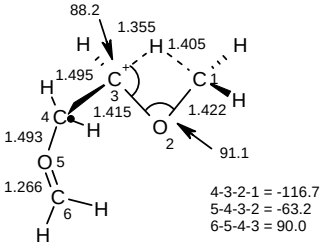
TS(6b→9) (C_1, ^{2}A)



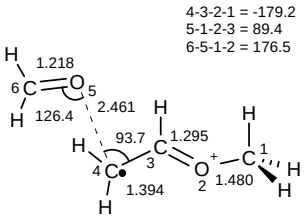
9 (C_s, ^{2}A')



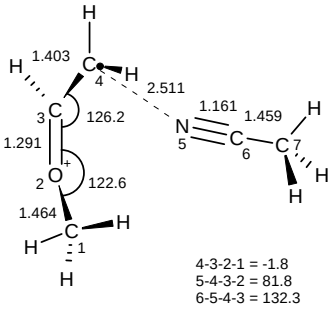
TS(2→1) (C_1, ^{2}A)



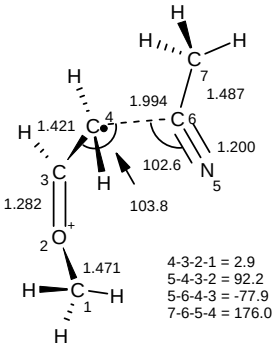
TS(4a→10) (C_1, ^{2}A)



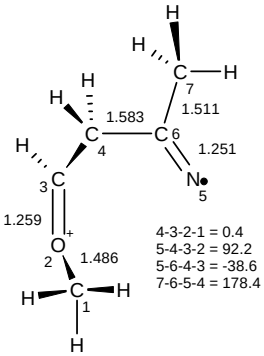
10 (C_1, ^{2}A)



11 (C_1, ^{2}A)

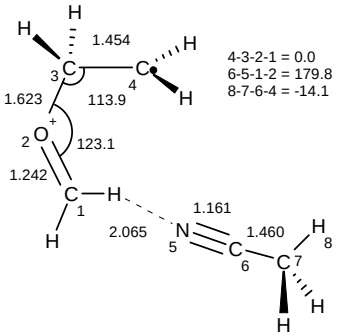


TS(11→12) (C_1, ^{2}A)

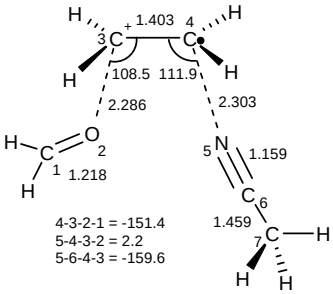


12 (C_1, ^{2}A)

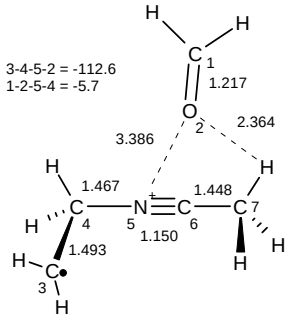
Figure S1 (continued)



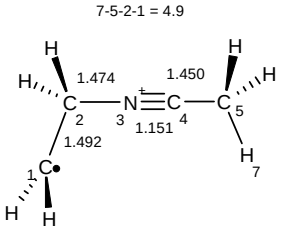
13 (C_1, ^{2}A)



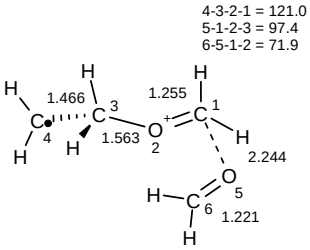
TS(13→14) (C_1, ^{2}A)



14 (C_1, ^{2}A)



15 (C_1, ^{2}A)



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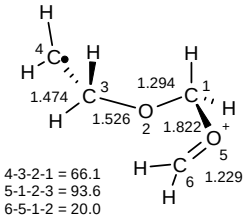
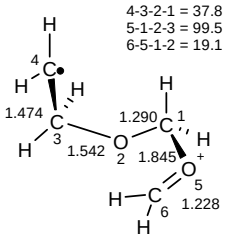
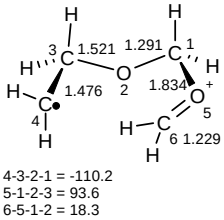


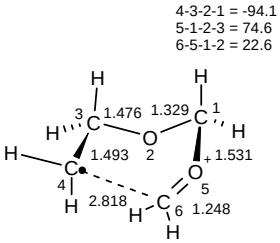
16a (C_1, ^{2}A)



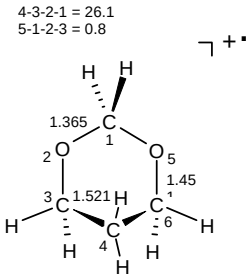
TS(16a→16b) (C_1, ^{2}A)



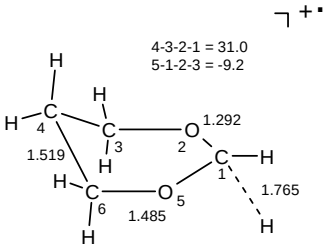
16b (C_1, ^{2}A)



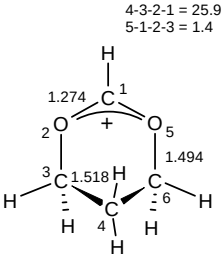
TS(16b→17) (C_1, ^{2}A)



17 (C_s, ^{2}A')

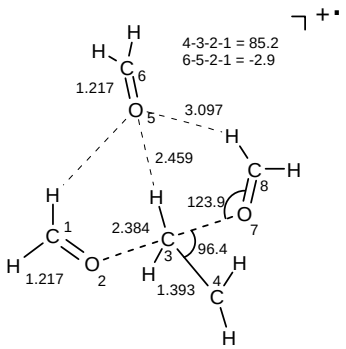


TS(17→18) (C_s, ^{2}A')

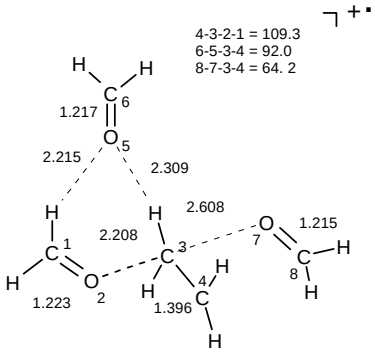


18a (C_s, ^{1}A")

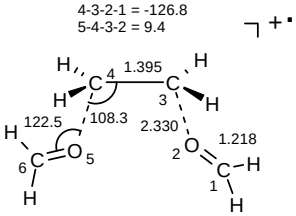
Figure S1 (continued)



TS(19→19) (C_s, ^{2}A")



19 (C_1, ^{2}A)



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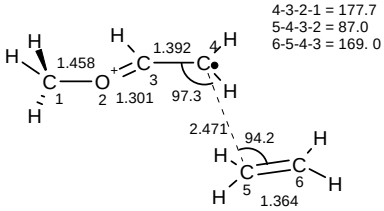
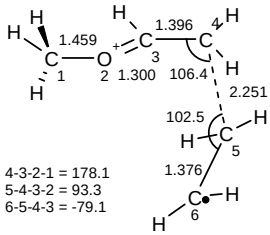
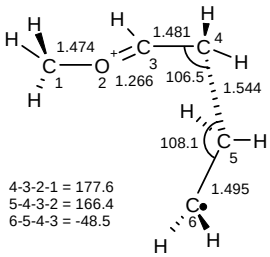


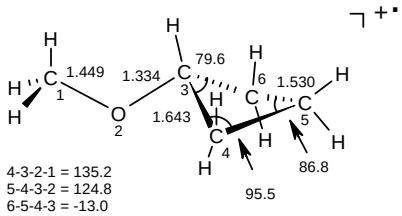
20 (C_1, ^{2}A)



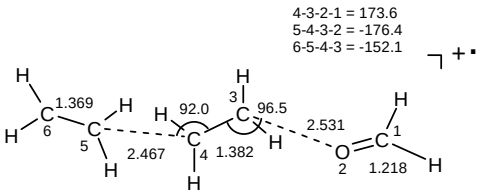
TS(20→21) (C_1, ^{2}A)



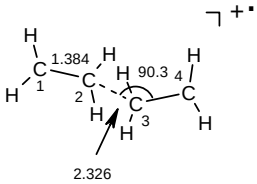
21 (C_1, ^{2}A)



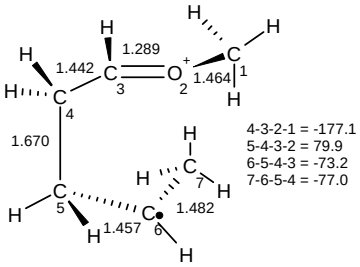
TS(21→21) (C_s, ^{2}A")



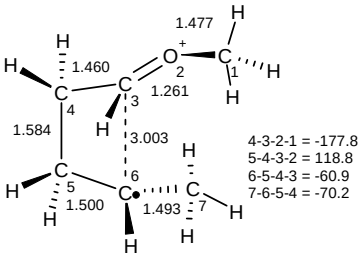
22 (C_1, ^{2}A)



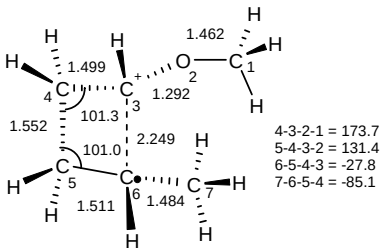
23 (C_2, ^{2}B)



24 (C_1, ^{2}A)

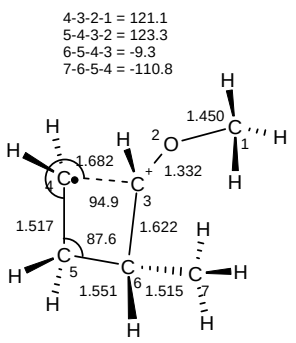


TS(24→25) (C_1, ^{2}A)

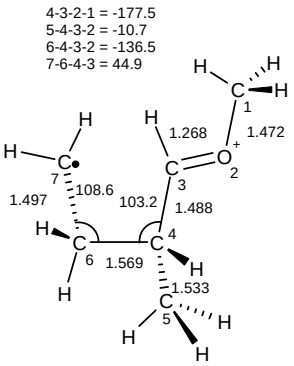


25 (C_1, ^{2}A)

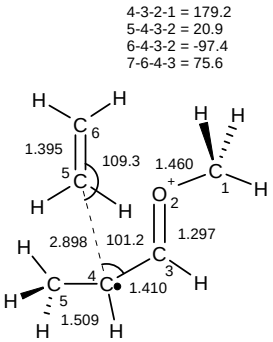
Figure S1 (continued)



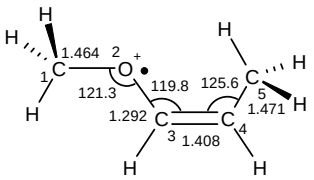
TS(25→26) (C_1, ^{2}A)



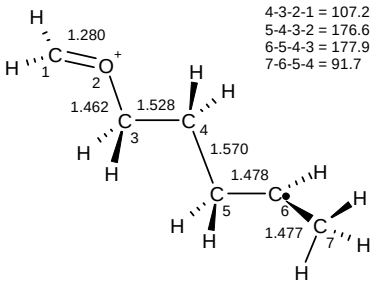
26 (C_1, ^{2}A)



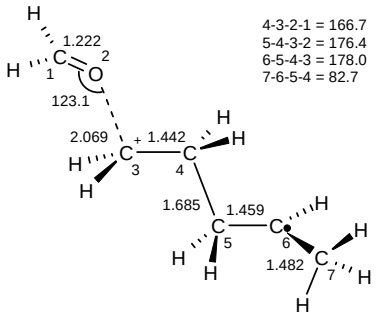
TS(26→27) (C_1, ^{2}A)



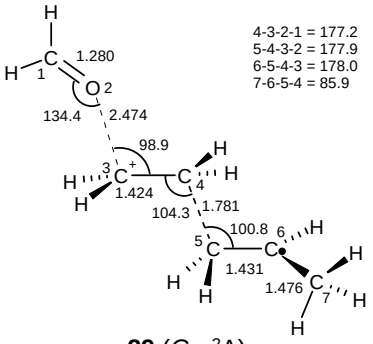
27a (C_s, ^{2}A")



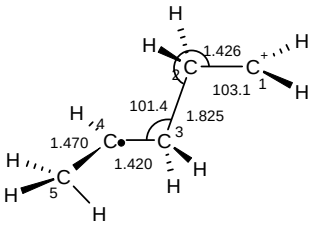
28 (C_1, ^{2}A)



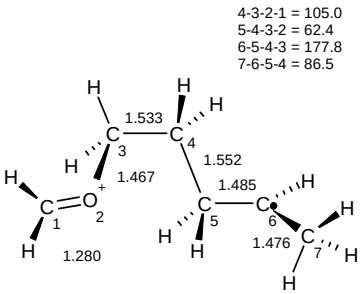
TS(28→29) (C_1, ^{2}A)



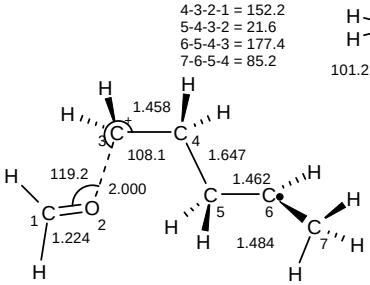
29 (C_1, ^{2}A)



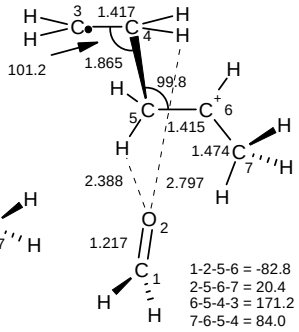
30 (C_1, ^{2}A)



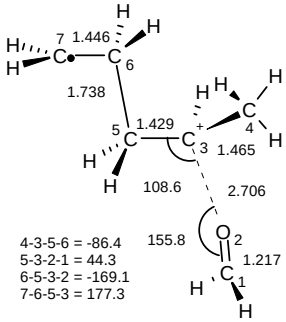
31 (C_1, ^{2}A)



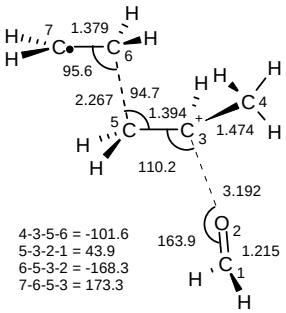
TS(31→32) (C_1, ^{2}A)



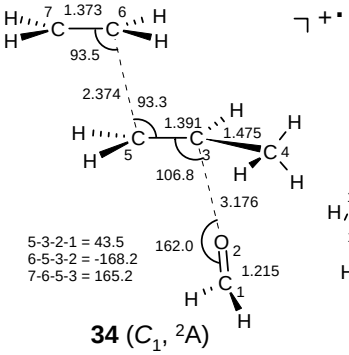
32 (C_1, ^{2}A)



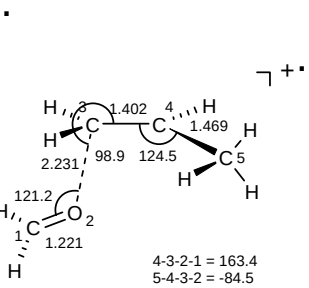
33 (C_1, ^{2}A)



TS(33→34) (C_1, ^{2}A)



34 (C_1, ^{2}A)



35 (C_1, ^{2}A)

TABLE S1. The G3(MP2) Energies E_0 and H_{298} (both in hartrees) of Various Species Involved in the Fragmentation reaction of 1,4-Dioxane$^{+\bullet}$ and the Reactions between $C_3H_6O^{+\bullet}$ Fragment Ions with Selected Reactants.

Species	E_0	H_{298}	Species	E_0	H_{298}
1	-192.47801	-192.47175	**16b**	-306.82220	-306.81260
2	-192.44453	-192.43762	**TS(16b→17)**	-306.82016	-306.81240
1,4-dioxane	-307.18951	-307.18322	**17**	-306.83945	-306.83247
3	-306.85483	-306.84845	**TS(17→18)**	-306.82956	-306.82272
TS(3→4a)	-306.80423	-306.79698	**18a**	-306.33911	-306.33285
4a	-306.80939	-306.80106	hydrogen	-0.50184	-0.50184
TS(4a→5)	-306.81662	-306.80919	**TS(6a→6a)**	-306.80319	-306.79257
5	-306.81870	-306.81108	**19**	-421.17639	-421.15970
TS(5→6a)	-306.79498	-306.78780	**TS(19→19)**	-421.17444	-421.15866
6a	-306.82166	-306.81143	ethylene	-78.43439	-78.43037
formaldehyde	-114.35347	-114.34965	**20**	-270.92242	-270.91198
TS(4a→4b)	-306.79407	-306.78627	**TS(20→21)**	-270.92233	-270.91288
4b	-306.79810	-306.78947	**21**	-270.93793	-270.92878
TS(4b→7)	-306.78586	-306.77661	**TS(21→21)**	-270.92407	-270.91609
7	-306.80417	-306.79230	**22**	-270.88629	-270.87412
4c	-306.81049	-306.80219	**23**	-156.52110	-156.51352
TS(4c→8)	-306.78119	-306.77211	propene	-117.67204	-117.66694
8	-306.81946	-306.80829	**24**	-310.17795	-310.16701
TS(6a→6b)	-306.82092	-306.81146	**TS(24→25)**	-310.17908	-310.16869
6b	-306.82144	-306.81116	**25**	-310.18109	-310.17081
TS(6b→9)	-306.76065	-306.75035	**TS(25→26)**	-310.16806	-310.15868
9	-306.85132	-306.84059	**26**	-310.17749	-310.16683
TS(2→1)	-192.38486	-192.37910	**TS(26→27)**	-310.16617	-310.15545
TS(4a→10)	-306.75378	-306.74573	**27a**	-231.73134	-231.72352
10	-306.84796	-306.83755	**28**	-310.15259	-310.14194
acetonitrile	-132.54642	-132.54181	**TS(28→29)**	-310.13742	-310.12597
11	-325.04669	-325.03517	**29**	-310.13852	-310.12557
TS(11→12)	-325.01236	-325.00240	**30**	-195.77390	-195.76526
12	-325.02438	-325.01435	**31**	-310.15207	-310.14131
13	-325.01874	-325.00659	**TS(31→32)**	-310.13171	-310.12051
TS(13→14)	-325.00385	-324.99182	**32**	-310.14502	-310.13154
14	-325.03638	-325.02330	**33**	-310.14337	-310.13028
15	-210.66647	-210.65819	**TS(33→34)**	-310.14050	-310.12738
TS(6b→16a)	-306.81897	-306.80929	**34**	-310.13965	-310.12565
16a	-306.82272	-306.81313	**35**	-231.69048	-231.67635
TS(16a→16b)	-306.82153	-306.81277			