

Electronic supplementary information

Atmospheric chemistry of CH₃O: its unimolecular reaction and reactions with H₂O, NH₃, and HF

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Table S1. The energy barriers of the CH₃O isomerization into CH₂OH, the CH₃O + H₂O, the CH₃O + NH₃, and CH₃O + HF reactions with zero-point energy involved for different theoretical methods at 0 K. (kcal/mol)

Methods	TS1	UE	TS2	UE	TS3	UE	TS4	UE
W3X-L//CCSD(T)-F12a/VDZ-F12	29.56	0.00	24.17	0.00	15.21	0.00	23.82	0.00
W2X//CCSD(T)-F12a/VDZ-F12	29.64	0.08	24.26	0.09	15.26	0.05	24.30	0.48
mPW2PLYP/maug-cc-pVTZ	31.03	1.47	23.77	0.40	15.39	0.18	22.33	1.49
M06-2X/maug-cc-pVTZ	30.37	0.81	23.23	0.94	15.94	0.73	22.71	1.11
B2PLYP/MG3S	30.49	0.93	23.44	0.73	15.02	0.19	22.07	1.75
M06-2X/aug-cc-pVTZ	30.24	0.68	22.88	1.29	15.78	0.57	22.37	1.45
mPW2PLYP/ma-TZVP	31.44	1.88	23.57	0.60	15.37	0.16	22.35	1.47
mPW2PLYP/aug-cc-pVTZ	30.83	1.27	23.39	0.78	15.04	0.17	21.91	1.91
M06-2X/ma-TZVP	30.60	1.04	22.74	1.43	15.69	0.48	22.58	1.24
B2PLYP/maug-cc-pVTZ	30.17	0.61	23.01	1.16	14.88	0.33	21.46	2.36
M11-L/aug-cc-pVTZ	32.75	3.19	23.82	0.35	15.44	0.23	24.59	0.77
G4	30.09	0.53	25.87	1.70	15.97	0.76	25.55	1.73
M11-L/ma-TZVP	33.30	3.74	23.62	0.55	15.21	0.00	24.36	0.54
M11-L/MG3S	33.11	3.55	23.89	0.28	15.09	0.12	24.9	1.08
B2PLYP/ma-TZVP	30.58	1.02	22.78	1.39	14.84	0.37	21.47	2.35
M11-L/maug-cc-pVTZ	32.95	3.39	24.13	0.04	15.96	0.75	24.83	1.01
CBS-QB3	29.74	0.18	25.24	1.07	15.06	0.15	27.62	3.80
M05-2X/MG3S	30.29	0.73	22.08	2.09	15.49	0.28	21.58	2.24
B2PLYP/aug-cc-pVTZ	29.96	0.40	22.61	1.56	14.52	0.69	21.03	2.79
B2PLYPD/MG3S	30.37	0.81	22.64	1.53	13.94	1.27	21.57	2.25
B3LYP/MG3S	31.48	1.92	24.09	0.08	16.06	0.85	20.69	3.13
B3LYP/maug-cc-pVTZ	31.25	1.69	23.84	0.33	15.93	0.72	20.39	3.43
B3LYP/aug-cc-pVTZ	31.12	1.56	23.78	0.39	15.83	0.62	20.21	3.61
B98/MG3S	31.25	1.69	23.01	1.16	14.90	0.31	20.77	3.05

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BMK/aug-cc-pVTZ	31.95	2.39	25.93	1.76	17.32	2.11	23.42	0.40
B2PLYPD/maug-cc-pVTZ	30.04	0.48	22.21	1.96	13.79	1.42	20.96	2.86
BMK/maug-cc-pVTZ	32.10	2.54	26.08	1.91	17.27	2.06	23.58	0.24
B98/maug-cc-pVTZ	30.92	1.36	22.64	1.53	14.72	0.49	20.44	3.38
B3LYP/ma-TZVP	31.54	1.98	23.51	0.66	15.86	0.65	20.20	3.62
B98/aug-cc-pVTZ	30.78	1.22	22.54	1.63	14.61	0.60	20.24	3.58
MPW3LYP/MG3S	31.57	2.01	23.06	1.11	14.97	0.24	19.85	3.97
B2PLYPD/ma-TZVP	30.46	0.90	21.98	2.19	13.74	1.47	20.97	2.85
BMK/ma-TZVP	32.59	3.03	26.03	1.86	17.71	2.50	23.78	0.04
B98/ma-TZVP	31.19	1.63	22.40	1.77	14.71	0.50	20.28	3.54
B2PLYPD/aug-cc-pVTZ	29.84	0.28	21.82	2.35	13.42	1.79	20.53	3.29
MPW3LYP/maug-cc-pVTZ	31.34	1.78	22.85	1.32	14.84	0.37	19.56	4.26
MPW3LYP/aug-cc-pVTZ	31.21	1.65	22.78	1.39	14.75	0.46	19.37	4.45
MPW3LYP/ma-TZVP	31.63	2.07	22.53	1.64	14.80	0.41	19.40	4.42
BMK/MG3S	32.39	2.83	26.72	2.55	17.79	2.58	24.81	0.99
HSEh1PBE/MG3S	30.63	1.07	21.57	2.60	13.51	1.70	19.53	4.29
HSEh1PBE/maug-cc-pVTZ	30.29	0.73	21.32	2.85	13.47	1.74	19.27	4.55
HSEh1PBE/aug-cc-pVTZ	30.14	0.58	21.05	3.12	13.35	1.86	19.06	4.76
HSEh1PBE/ma-TZVP	30.61	1.05	21.07	3.10	13.44	1.77	19.14	4.68
MN12-SX/aug-cc-pVTZ	33.75	4.19	27.09	2.92	17.06	1.85	26.01	2.19
M11/maug-cc-pVTZ	27.85	1.71	21.02	3.15	13.20	2.01	19.49	4.33
M06-HF/MG3S	28.64	0.92	19.44	4.73	13.69	1.52	19.78	4.04
M06-HF/maug-cc-pVTZ	28.05	1.51	19.42	4.75	13.81	1.40	19.76	4.06
M06-HF/ma-TZVP	28.14	1.42	19.25	4.92	13.39	1.82	20.23	3.59
MN12-SX/MG3S	33.95	4.39	27.35	3.18	17.10	1.89	26.44	2.62
MN12-SX/maug-cc-pVTZ	33.92	4.36	27.41	3.24	17.40	2.19	26.25	2.43
M11/aug-cc-pVTZ	27.72	1.84	20.71	3.46	12.81	2.40	19.09	4.73
M11/MG3S	28.01	1.55	20.37	3.80	12.45	2.76	19.25	4.57
M11/ma-TZVP	28.07	1.49	20.10	4.07	12.27	2.94	19.02	4.80
MPW1K/aug-cc-pVTZ	33.11	3.55	27.52	3.35	18.93	3.72	26.79	2.97
M06-HF/aug-cc-pVTZ	27.90	1.66	18.63	5.54	13.19	2.02	18.81	5.01
MPW1K/maug-cc-pVTZ	33.27	3.71	27.70	3.53	19.12	3.91	27.05	3.23
MPW1K/ma-TZVP	33.63	4.07	27.63	3.46	19.24	4.03	27.10	3.28
MPW1K/MG3S	33.54	3.98	27.94	3.77	19.12	3.91	27.47	3.65
BP86/MG3S	27.15	2.41	13.98	10.19	8.44	6.77	10.68	13.14
BP86/maug-cc-pVTZ	26.85	2.71	13.73	10.44	8.34	6.87	10.40	13.42
BP86/aug-cc-pVTZ	26.71	2.85	13.68	10.49	8.27	6.94	10.26	13.56
BP86/ma-TZVP	27.15	2.41	13.29	10.88	8.17	7.04	10.21	13.61

Table S2. Cartesian coordinates (Å) of optimized structures.

Species	Methods	Cartesian coordinates			
CH ₃ O	CCSD(T)-F12a/VDZ-F12	C	0.5789757603	0.0000000512	-0.0104858698
		H	0.8668628834	-0.0000250694	1.0545672683
		H	1.0005408686	0.9055115383	-0.4583370769
		H	1.0005392839	-0.9054918788	-0.4583783219
		O	-0.7938267962	0.0000003588	-0.0082589997
	QCISD/cc-pVTZ	C	-0.57989900	0.00000300	-0.01128100
		H	-0.87522400	-0.00017300	1.04965300
		H	-1.00227200	-0.90294700	-0.46197100
		H	-1.00228500	0.90308600	-0.46169800
		O	0.79489700	0.00000200	-0.00728700
	W1U	C	-0.57209800	0.00000100	-0.01424900
		H	-0.87281200	-0.00002700	1.05163900
		H	-1.00778800	-0.90750900	-0.45397500
		H	-1.00779000	0.90752900	-0.45393400
		O	0.79012200	0.00000000	-0.00727900
	W1BD	C	-0.57209800	0.00000100	-0.01424900
		H	-0.87281200	-0.00002700	1.05163900
		H	-1.00778800	-0.90750900	-0.45397500
		H	-1.00779000	0.90752900	-0.45393400
		O	0.79012200	0.00000000	-0.00727900
	mPW2PLYP/MG3S	C	0.57569500	0.00000000	-0.01244000
		H	0.86680800	-0.00001200	1.04926700
		H	0.99902100	0.90334500	-0.45736100
		H	0.99902000	-0.90333500	-0.45738000
		O	-0.78987700	0.00000000	-0.00748600
	M06-2X/MG3S	C	-0.57558700	0.00001100	-0.01242200
		H	-0.87025900	-0.00047600	1.05021600
		H	-0.99764900	-0.90507400	-0.45959400
		H	-0.99765200	0.90546300	-0.45884400
		O	0.78988500	0.00000200	-0.00715600
	G4	C	0.57118600	0.00001000	-0.01363300
		H	0.87219100	-0.00036200	1.05565400
		H	1.01386300	0.90879200	-0.45525000
		H	1.01383400	-0.90851800	-0.45581000
		O	-0.79087500	0.00000400	-0.00785000
	CBS-QB3	C	0.57287600	0.00000700	-0.01416300
H		0.87157100	-0.00024200	1.05450300	
H		1.01190900	0.90937700	-0.45389600	
H		1.01187900	-0.90920200	-0.45426600	
O		-0.79157700	0.00000300	-0.00767000	
M05-2X/aug-cc-pVTZ	C	-0.57972900	0.00002000	-0.01162600	
	H	-0.86661400	-0.00081000	1.04965700	
	H	-0.99467000	-0.90330100	-0.46105600	

		H	-0.99472600	0.90393300	-0.45979100
		O	0.79179800	0.00000700	-0.00738200
	M05-2X/maug-cc-pVTZ	C	-0.57959500	0.00001900	-0.01164200
		H	-0.86730100	-0.00079000	1.04946700
		H	-0.99458400	-0.90327800	-0.46114200
		H	-0.99463800	0.90389500	-0.45990800
		O	0.79176200	0.00000700	-0.00732100
	CCSD(T)-F12a/VDZ-F12	O	0.000000000	0.000000000	0.1210648408
		H	0.000000000	0.7573423197	-0.4668634204
		H	0.000000000	-0.7573423197	-0.4668634204
	QCISD/cc-pVTZ	O	0.00000000	0.00000000	0.11806100
		H	0.00000000	0.75365100	-0.47224500
		H	0.00000000	-0.75365100	-0.47224500
	W1U	O	0.00000000	0.00000000	0.11767500
		H	0.00000000	0.76026200	-0.47070100
		H	0.00000000	-0.76026200	-0.47070100
	W1BD	O	0.00000000	0.00000000	0.11767500
		H	0.00000000	0.76026200	-0.47070100
		H	0.00000000	-0.76026200	-0.47070100
	mPW2PLYP/MG3S	O	0.00000000	0.00000000	0.11647500
		H	0.00000000	0.75974800	-0.46589900
		H	0.00000000	-0.75974800	-0.46589900
	M06-2X/MG3S	O	0.00000000	0.00000000	0.11633200
		H	0.00000000	0.76137700	-0.46532900
		H	0.00000000	-0.76137700	-0.46532900
	G4	O	0.00000000	0.00000000	0.11767500
		H	0.00000000	0.76026200	-0.47070100
		H	0.00000000	-0.76026200	-0.47070100
	CBS-QB3	O	0.00000000	0.00000000	0.11869700
		H	0.00000000	0.75707300	-0.47478600
		H	0.00000000	-0.75707300	-0.47478600
	M05-2X/aug-cc-pVTZ	O	0.00000000	0.00000000	0.11571800
		H	0.00000000	0.76311300	-0.46287200
		H	0.00000000	-0.76311300	-0.46287200
	M05-2X/maug-cc-pVTZ	O	0.00000000	0.00000000	0.11583200
		H	0.00000000	0.76267500	-0.46332900
		H	0.00000000	-0.76267500	-0.46332900
	CCSD(T)-F12a/VDZ-F12	N	0.000000000	-0.0000134653	0.1266037763
		H	0.000000000	0.9370892003	-0.2563940685
		H	-0.8115236102	-0.4685378675	-0.2563893539
		H	0.8115236102	-0.4685378675	-0.2563893539
	QCISD/cc-pVTZ	N	0.00000000	0.00000000	0.11773900
		H	0.00000000	0.93281400	-0.27472400
		H	-0.80784000	-0.46640700	-0.27472400
H ₂ O					
NH ₃					

		H	0.80784000	-0.46640700	-0.27472400
	W1U	N	0.00000000	0.00000000	0.11542400
		H	0.00000000	0.93792800	-0.26932200
		H	-0.81227000	-0.46896400	-0.26932200
		H	0.81227000	-0.46896400	-0.26932200
	W1BD	N	0.00000000	0.00000000	0.11542300
		H	0.00000000	0.93792900	-0.26932100
		H	-0.81227100	-0.46896500	-0.26932100
		H	0.81227100	-0.46896500	-0.26932100
	mPW2PLYP/MG3S	N	0.00000000	0.00000000	0.11006500
		H	0.00000000	0.94025400	-0.25681900
		H	-0.81428400	-0.47012700	-0.25681900
		H	0.81428400	-0.47012700	-0.25681900
	M06-2X/MG3S	N	0.00000000	0.00000000	0.11154600
		H	0.00000000	0.94100500	-0.26027400
		H	-0.81493400	-0.47050200	-0.26027400
		H	0.81493400	-0.47050200	-0.26027400
	G4	N	0.00000000	0.00000000	0.12058500
		H	0.00000000	0.93425700	-0.28136600
		H	-0.80909000	-0.46712800	-0.28136600
		H	0.80909000	-0.46712800	-0.28136600
	CBS-QB3	N	0.00000000	0.00000000	0.11608700
		H	0.00000000	0.93921700	-0.27087000
		H	-0.81338600	-0.46960900	-0.27087000
		H	0.81338600	-0.46960900	-0.27087000
	M05-2X/aug-cc-pVTZ	N	0.00000000	0.00000000	0.10931700
		H	0.00000000	0.94015600	-0.25507300
		H	-0.81419900	-0.47007800	-0.25507300
		H	0.81419900	-0.47007800	-0.25507300
	M05-2X/maug-cc-pVTZ	N	0.00000000	0.00000000	0.10861700
		H	0.00000000	0.94090600	-0.25343900
		H	-0.81484800	-0.47045300	-0.25343900
		H	0.81484800	-0.47045300	-0.25343900
HF	CCSD(T)-F12a/VDZ-F12	F	0.0000000000	0.0000000000	0.0903331523
		H	0.0000000000	0.0000000000	-0.8276841523
	QCISD/cc-pVTZ	F	0.00000000	0.00000000	0.09157200
		H	0.00000000	0.00000000	-0.82414400
	W1U	F	0.00000000	0.00000000	0.09223100
		H	0.00000000	0.00000000	-0.83008200
	W1BD	F	0.00000000	0.00000000	0.09223100
		H	0.00000000	0.00000000	-0.83008200
	mPW2PLYP/MG3S	F	0.00000000	0.00000000	0.09177200
		H	0.00000000	0.00000000	-0.82594600
	M06-2X/MG3S	F	0.00000000	0.00000000	0.09177400

		H	0.00000000	0.00000000	-0.82596600
	G4	F	0.00000000	0.00000000	0.09195900
		H	0.00000000	0.00000000	-0.82762800
	CBS-QB3	F	0.00000000	0.00000000	0.09201700
		H	0.00000000	0.00000000	-0.82815200
	M05-2X/aug-cc-pVTZ	F	0.00000000	0.00000000	0.09213100
		H	0.00000000	0.00000000	-0.82917800
	M05-2X/maug-cc-pVTZ	F	0.00000000	0.00000000	0.09210500
		H	0.00000000	0.00000000	-0.82894400
TS1	CCSD(T)-F12a/VDZ-F12	C	-0.6321910990	-0.0001587060	0.0141199447
		H	0.1774326049	-0.0000810669	0.9794489665
		H	-1.1529995157	-0.9363049088	-0.1691491640
		H	-1.1526770924	0.9364448129	-0.1676456763
		O	0.7459211022	-0.0002611313	-0.0966800709
	QCISD/cc-pVTZ	C	-0.63499900	0.00003500	0.01410300
		H	0.17365800	-0.00313800	0.97742900
		H	-1.15598500	-0.93311000	-0.17914000
		H	-1.15604700	0.93386900	-0.17550700
		O	0.74354600	0.00027100	-0.08842500
	W1U	C	-0.03388600	0.63511400	0.00000000
		H	-0.25700500	1.14542500	0.93516100
		H	-0.25700500	1.14542500	-0.93516100
		H	0.98840900	-0.11654800	0.00000000
		O	-0.03388600	-0.74812300	0.00000000
	W1BD	C	-0.03388600	0.63511400	0.00000000
		H	-0.25700500	1.14542500	0.93516100
		H	-0.25700500	1.14542500	-0.93516100
		H	0.98840900	-0.11654800	0.00000000
		O	-0.03388600	-0.74812300	0.00000000
	mPW2PLYP/MG3S	C	-0.63347200	0.00000000	0.01191500
		H	0.17800300	0.00000000	0.97617400
		H	-1.15330000	-0.93322500	-0.17103100
		H	-1.15330000	0.93322500	-0.17103100
		O	0.74117900	0.00000000	-0.08820000
	M06-2X/MG3S	C	-0.62926800	0.00000000	0.01080100
		H	-1.15094100	-0.93574700	-0.16955900
		H	-1.15094100	0.93574800	-0.16955500
H		0.17492700	-0.00000300	0.98048100	
O		0.73782100	0.00000000	-0.08827200	
G4	C	-0.03293200	0.63451100	0.00000000	
	H	-0.26188500	1.14985100	0.93651300	
	H	-0.26188500	1.14985100	-0.93651300	
	H	0.98481900	-0.11627300	0.00000000	
	O	-0.03293200	-0.74881200	0.00000000	

	CBS-QB3	C	-0.03357300	0.63679400	0.00000000
		H	-0.25818700	1.14780700	0.93731000
		H	-0.25818700	1.14780700	-0.93731000
		H	0.98639300	-0.11599300	0.00000000
		O	-0.03357300	-0.75004800	0.00000000
	M05-2X/aug-cc-pVTZ	C	-0.63140800	0.00003800	0.00987000
		H	0.17019600	-0.00258100	0.98242800
		H	-1.14926000	-0.93349600	-0.17105400
		H	-1.14947600	0.93400100	-0.16807600
		O	0.73962400	0.00023100	-0.08781500
	M05-2X/maug-cc-pVTZ	C	-0.63163300	0.00000000	0.01032400
		H	-1.14914500	-0.93384300	-0.17042200
		H	-1.14914500	0.93384400	-0.17041900
		H	0.17050000	-0.00000300	0.98181300
		O	0.73969900	0.00000000	-0.08786500
TS2	CCSD(T)-F12a/VDZ-F12	C	-1.0071997687	-0.5164627632	0.0193782838
		H	0.4632796708	-0.7892170962	0.1503856359
		H	-1.0923990655	-1.0590293708	-0.9339082711
		H	-1.6304576097	-0.9005661880	0.8309251950
		O	-0.7459282413	0.7687712235	-0.0140650128
		O	1.4497341806	-0.1184515434	-0.0872667109
		H	0.6869656797	0.6251443639	-0.1822208154
		H	1.9117221542	0.0422363740	0.7439576955
	QCISD/cc-pVTZ	C	-1.00194800	-0.51726100	0.01915900
		H	0.46777500	-0.78558200	0.12062500
		H	-1.13129000	-1.05126700	-0.93288500
		H	-1.58787000	-0.91773500	0.85053000
		O	-0.74259000	0.76519500	-0.00652100
		O	1.45272900	-0.11437300	-0.08627400
		H	0.69343200	0.62267600	-0.17174200
H		1.88853000	0.02889800	0.76087700	
W1U	C	-0.99779100	-0.52527900	-0.00367800	
	H	0.45548300	-0.78925300	-0.23433500	
	H	-1.68889100	-0.89509600	-0.76583500	
	H	-1.02040800	-1.09001200	0.94328600	
	O	-0.74193300	0.76071300	0.03470200	
	O	1.45169300	-0.06583300	-0.12318000	
	H	1.92773200	-0.28029100	0.68907800	
	H	0.63475500	0.64728900	0.09770000	
W1BD	C	-0.99779100	-0.52527900	-0.00367800	
	H	0.45548300	-0.78925300	-0.23433500	
	H	-1.68889100	-0.89509600	-0.76583500	
	H	-1.02040800	-1.09001200	0.94328600	
	O	-0.74193300	0.76071300	0.03470200	

		O	1.45169300	-0.06583300	-0.12318000
		H	1.92773200	-0.28029100	0.68907800
		H	0.63475500	0.64728900	0.09770000
	mPW2PLYP/MG3S	C	-1.00375000	-0.52216800	0.00121300
		H	0.48004700	-0.78856400	-0.17960900
		H	-1.60515500	-0.91606400	-0.81842700
		H	-1.10897500	-1.05915300	0.95219500
		O	-0.74588800	0.75961700	0.02910900
		O	1.45098700	-0.07443100	-0.11890300
		H	1.93446600	-0.23737500	0.69743900
		H	0.68132200	0.65268000	0.05947100
	M06-2X/MG3S	C	-1.00059700	-0.52033300	-0.00059300
		H	0.45322300	-0.78478800	-0.20645500
		H	-1.65109800	-0.90254900	-0.78965800
		H	-1.05047300	-1.06895700	0.95186900
		O	-0.74383600	0.75645200	0.03212900
		O	1.44729300	-0.07100600	-0.12104400
		H	1.94844100	-0.25499700	0.68030200
		H	0.67583900	0.64971700	0.07882300
	G4	C	-0.98658300	-0.52726500	-0.00723300
		H	0.43218100	-0.78269900	-0.26242100
		H	-1.71878800	-0.88770200	-0.74025800
		H	-0.98502200	-1.10183200	0.94004400
		O	-0.73641100	0.76161400	0.03712000
		O	1.44657300	-0.06174000	-0.12466000
		H	1.90358000	-0.30586200	0.69117300
		H	0.60624800	0.64270100	0.11518300
	CBS-QB3	C	-0.99008200	-0.52881400	-0.00655400
		H	0.44845900	-0.78389000	-0.26760000
		H	-1.72482600	-0.88670800	-0.73582100
		H	-0.97898600	-1.10053500	0.94042700
		O	-0.73933700	0.76172700	0.03706900
		O	1.44671100	-0.06229000	-0.12368200
		H	1.91527900	-0.29915200	0.68716100
		H	0.62157700	0.64767300	0.10806600
	M05-2X/aug-cc-pVTZ	C	-1.00396100	-0.51496400	0.01915100
		H	0.42148800	-0.80343200	0.14937100
		H	-1.09626500	-1.04587800	-0.93472600
		H	-1.61238400	-0.90163600	0.83474900
		O	-0.73717700	0.76315500	-0.00705300
		O	1.45007900	-0.11505200	-0.08425500
		H	0.66199700	0.62677400	-0.16191300
		H	1.94571900	0.02912800	0.72807400
	M05-2X/maug-cc-pVTZ	C	-1.00067200	-0.52022100	0.00310800

		H	0.42591000	-0.79807500	-0.16568800
		H	-1.58232900	-0.91734300	-0.82769100
		H	-1.12072300	-1.04635000	0.95676900
		O	-0.74233400	0.75924900	0.02745600
		O	1.45058800	-0.07739300	-0.11781200
		H	1.95201300	-0.22085000	0.69114200
		H	0.66312900	0.64909200	0.04966300
TS3	CCSD(T)-F12a/VDZ-F12	N	1.5180406323	-0.0687038889	-0.0043179261
		H	2.1007511400	-0.1656606568	-0.8256919043
		H	2.0663383556	-0.1500765223	0.8422202726
		H	0.9589285393	0.8030650925	-0.0183853262
		C	-1.0615664067	-0.5348896878	0.0018879918
		H	0.5080198190	-0.7293829118	-0.0097347558
		H	-1.4002518313	-1.0281545103	-0.9227180466
		H	-1.3800401362	-1.0455990913	0.9243774503
		O	-0.9082671119	0.7555611768	0.0123612443
	QCISD/cc-pVTZ	N	-1.51833700	-0.06420500	0.00000100
		H	-2.08486100	-0.14028600	0.83350000
		H	-2.08487100	-0.14030900	-0.83348900
		H	-0.93113800	0.78980500	-0.00001300
		C	1.05242900	-0.53834600	0.00000200
		H	-0.52352300	-0.73421300	0.00000600
		H	1.38345300	-1.04403200	0.92035200
		H	1.38344400	-1.04404200	-0.92034500
		O	0.89641000	0.74907300	-0.00000400
	W1U	N	-1.52277600	-0.07188000	0.00000400
		H	-2.09159700	-0.12628600	0.83622300
H		-2.09160100	-0.12630100	-0.83621000	
H		-0.87166200	0.75375000	-0.00000400	
C		1.07749300	-0.52788300	0.00000200	
H		-0.56578400	-0.78369800	0.00000800	
H		1.41670600	-1.02758200	0.92286000	
H		1.41670200	-1.02759800	-0.92284900	
O		0.87271400	0.75102200	-0.00000900	
W1BD	N	-1.52277600	-0.07188000	0.00000400	
	H	-2.09159700	-0.12628600	0.83622300	
	H	-2.09160100	-0.12630100	-0.83621000	
	H	-0.87166200	0.75375000	-0.00000400	
	C	1.07749300	-0.52788300	0.00000200	
	H	-0.56578400	-0.78369800	0.00000800	
	H	1.41670600	-1.02758200	0.92286000	
	H	1.41670200	-1.02759800	-0.92284900	
	O	0.87271400	0.75102200	-0.00000900	
mPW2PLYP/MG3S	N	-1.52764700	-0.06378600	0.00000400	

		H	-2.09242400	-0.14887200	0.83301500
		H	-2.09242800	-0.14888700	-0.83300300
		H	-0.95595800	0.79894500	-0.00000500
		C	1.06582000	-0.53714900	0.00000200
		H	-0.54979700	-0.73624200	0.00000800
		H	1.39428500	-1.03748500	0.92055700
		H	1.39428100	-1.03750200	-0.92054500
		O	0.90008200	0.74743000	-0.00000900
	M06-2X/MG3S	N	-1.52439900	-0.07413600	0.00000400
		H	-2.09028100	-0.15116200	0.83593800
		H	-2.09028500	-0.15117800	-0.83592600
		H	-0.92233700	0.77830500	-0.00000500
		C	1.09125000	-0.52480800	0.00000200
		H	-0.58386600	-0.75795600	0.00000800
		H	1.43165000	-1.01309400	0.92401400
		H	1.43164500	-1.01311000	-0.92400300
		O	0.86834600	0.74700000	-0.00000900
	G4	N	-1.50363600	-0.07982100	0.00000400
		H	-2.07569100	-0.11612400	0.83713700
		H	-2.07569500	-0.11613900	-0.83712500
		H	-0.78947400	0.71982900	-0.00000400
		C	1.07299900	-0.52108000	0.00000200
		H	-0.55239800	-0.80526100	0.00000800
		H	1.43267800	-1.01492400	0.92370600
		H	1.43267200	-1.01494000	-0.92369500
		O	0.83942100	0.75409800	-0.00000900
	CBS-QB3	N	-1.51801300	-0.07767500	0.00000400
		H	-2.08767400	-0.12429000	0.83884400
		H	-2.08767800	-0.12430600	-0.83883200
		H	-0.84482000	0.74073400	-0.00000500
		C	1.08288600	-0.52424400	0.00000200
		H	-0.57205700	-0.79944600	0.00000900
		H	1.43943700	-1.01665200	0.92441500
		H	1.43943200	-1.01666900	-0.92440500
		O	0.85526700	0.75372700	-0.00000800
	M05-2X/aug-cc-pVTZ	N	-1.52255700	-0.06647400	0.00000400
		H	-2.08469400	-0.14706800	0.83440500
		H	-2.08469900	-0.14708400	-0.83439200
		H	-0.92600700	0.78424900	-0.00000500
		C	1.07028100	-0.53382000	0.00000200
		H	-0.54552200	-0.74218500	0.00000800
		H	1.39422600	-1.02931700	0.92225200
		H	1.39422200	-1.02933400	-0.92224000
		O	0.88608600	0.74737200	-0.00000900

	M05-2X/maug-cc-pVTZ	N	-1.52078800	-0.06731900	0.00000400
		H	-2.08328300	-0.14518200	0.83449400
		H	-2.08328700	-0.14519800	-0.83448200
		H	-0.91680400	0.77962600	-0.00000500
		C	1.07011000	-0.53323600	0.00000200
		H	-0.54645200	-0.74660200	0.00000800
		H	1.39741700	-1.02679900	0.92211000
		H	1.39741300	-1.02681500	-0.92209800
		O	0.88248200	0.74770300	-0.00000900
TS4	CCSD(T)-F12a/VDZ-F12	F	1.4310451570	-0.1052987409	-0.0067636560
		H	0.4977591632	0.6412415145	0.1668805472
		C	-0.9369688768	-0.5217701387	-0.0169040758
		H	0.2750653903	-0.8314701895	-0.3320883167
		H	-1.7990790451	-0.8267327775	-0.6006543263
		H	-0.7774887038	-1.0699820753	0.9273492950
		O	-0.6544630848	0.7702004073	-0.0015354673
		QCISD/cc-pVTZ	F	1.41409300	-0.09929200
	H		0.44174300	0.66894400	0.17327000
	C		-0.92130900	-0.54268700	-0.01181700
	H		0.28434800	-0.80401100	-0.33924700
	H		-1.79141600	-0.84003800	-0.58433000
	H		-0.78205900	-1.06372800	0.94483700
	O		-0.66895000	0.77357300	0.01070800
	W1U		F	1.43669500	-0.10061900
		H	0.43237100	0.68771500	0.16770500
		C	-0.92978300	-0.53789400	-0.01048700
		H	0.22729200	-0.86750000	-0.33104300
		H	-1.79063500	-0.83564500	-0.60140900
		H	-0.83453700	-1.05369200	0.95968200
		O	-0.67325500	0.77525800	0.00842000
		W1BD	F	1.43669500	-0.10061900
	H		0.43237100	0.68771500	0.16770500
	C		-0.92978300	-0.53789400	-0.01048700
H	0.22729200		-0.86750000	-0.33104300	
H	-1.79063500		-0.83564500	-0.60140900	
H	-0.83453700		-1.05369200	0.95968200	
O	-0.67325500		0.77525800	0.00842000	
mPW2PLYP/MG3S	F		1.42769000	-0.10274000	-0.02335300
	H	0.46448800	0.66038300	0.16238300	
	C	-0.94039000	-0.52531800	-0.00919000	
	H	0.23382300	-0.85858300	-0.33775800	
	H	-1.80466000	-0.82231700	-0.58799000	
	H	-0.79845800	-1.06295100	0.94022700	
	O	-0.66275700	0.77000400	0.01105700	

	M06-2X/MG3S	F	1.41662500	-0.10210100	-0.02420200
		H	0.48693700	0.65004900	0.16050500
		C	-0.94078500	-0.52218800	-0.00930300
		H	0.28433900	-0.82941100	-0.32948100
		H	-1.80140500	-0.82736900	-0.59433000
		H	-0.78257500	-1.06999500	0.93412000
		O	-0.66152600	0.76609500	0.01285300
	G4	F	1.42161000	-0.10053400	-0.02219700
		H	0.46483100	0.66388900	0.16347000
		C	-0.92558600	-0.53545000	-0.01032800
		H	0.26945400	-0.83379300	-0.33276900
		H	-1.78390900	-0.84375700	-0.60831200
		H	-0.82552100	-1.06705000	0.95436800
		O	-0.67072900	0.77477700	0.01062300
	CBS-QB3	F	1.44200200	-0.10017500	-0.02054200
		H	0.40913100	0.70429300	0.17075500
		C	-0.92420000	-0.54383900	-0.00936300
		H	0.19678500	-0.88797100	-0.35597300
		H	-1.79634200	-0.83379500	-0.59159800
		H	-0.84040500	-1.04371600	0.97195100
		O	-0.67524900	0.77822400	0.00574100
M05-2X/aug-cc-pVTZ	F	1.42016200	-0.10286100	-0.02388800	
	H	0.51802300	0.63599300	0.15494100	
	C	-0.94760800	-0.52035100	-0.00641600	
	H	0.28735000	-0.82272700	-0.32540200	
	H	-1.78773400	-0.83225800	-0.61249800	
	H	-0.79754100	-1.06832300	0.93340700	
	O	-0.66448800	0.76689600	0.01288000	
M05-2X/maug-cc-pVTZ	F	1.41952600	-0.10303500	-0.02390000	
	H	0.51807800	0.63548800	0.15480300	
	C	-0.94729800	-0.52031700	-0.00661400	
	H	0.28792800	-0.82227900	-0.32416300	
	H	-1.78727700	-0.83145700	-0.61332000	
	H	-0.79942100	-1.06833900	0.93357000	
	O	-0.66390700	0.76697500	0.01298600	
CH ₂ OH	CCSD(T)-F12a/VDZ-F12	H	-1.0913611686	0.7287946128	-0.0539640877
		C	0.6822604414	0.0275089642	-0.0707914385
		H	1.1078570924	0.9945801009	0.1579117032
		H	1.2346263555	-0.8817930676	0.0992503517
		O	-0.6717327208	-0.1304226103	0.0236974713
	QCISD/cc-pVTZ	H	-1.08070000	0.73659500	-0.06192700
		C	0.68437600	0.02699600	-0.06773700
		H	1.11525700	0.98754200	0.17798900
		H	1.23179400	-0.88414100	0.10913000

		O	-0.67157600	-0.12524700	0.02265400
	W1U	H	-1.09662400	0.73329400	-0.05319200
		C	0.68393400	0.02742400	-0.06139300
		H	1.11926800	0.99244300	0.15939400
		H	1.23403900	-0.88534200	0.10023400
		O	-0.67003600	-0.12561800	0.02024100
	W1BD	H	-1.09662400	0.73329400	-0.05319200
		C	0.68393400	0.02742400	-0.06139300
		H	1.11926800	0.99244300	0.15939400
		H	1.23403900	-0.88534200	0.10023400
		O	-0.67003600	-0.12561800	0.02024100
	mPW2PLYP/MG3S	H	-1.09783600	0.72713900	-0.05429300
		C	0.68269200	0.02750600	-0.06035900
		H	1.11220200	0.99147400	0.15724500
		H	1.23195800	-0.88170300	0.09782500
		O	-0.66781000	-0.12524400	0.02017200
	M06-2X/MG3S	H	-1.10206700	0.72479000	-0.05621900
		C	0.68085500	0.02801400	-0.06364000
		H	1.11110700	0.99212600	0.16509400
		H	1.23359700	-0.88093200	0.10337400
		O	-0.66597100	-0.12550900	0.02119800
	G4	H	-1.09050300	0.73481900	-0.06871300
		C	0.68320300	0.02814400	-0.07333000
		H	1.12065400	0.98665800	0.19336100
		H	1.22944300	-0.88769800	0.11593600
		O	-0.66985200	-0.12533100	0.02492400
	CBS-QB3	H	-1.09138300	0.73533000	-0.06766000
		C	0.68460000	0.02759200	-0.06638500
		H	1.12315700	0.98976100	0.17682300
		H	1.23074600	-0.88936800	0.10217200
		O	-0.67126500	-0.12515900	0.02337200
	M05-2X/aug-cc-pVTZ	H	-1.10167400	0.72494300	-0.05664600
		C	0.68273800	0.02769300	-0.05892600
		H	1.10941900	0.99275600	0.15459900
		H	1.23572800	-0.87936800	0.09356500
		O	-0.66748800	-0.12556100	0.02025400
	M05-2X/maug-cc-pVTZ	H	-1.10129700	0.72521000	-0.05726200
		C	0.68273300	0.02769100	-0.05894200
		H	1.10915500	0.99298000	0.15488500
		H	1.23559600	-0.87957200	0.09326600
		O	-0.66748200	-0.12559600	0.02034600