Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Theoretical Study on Proton Affinity of Sulfur Ylides

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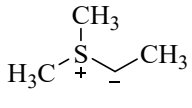
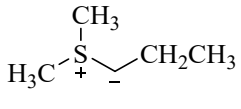
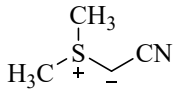
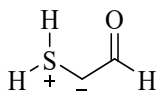
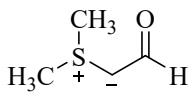
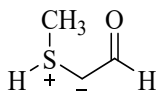
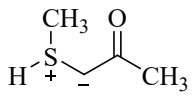
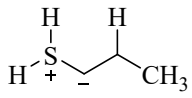
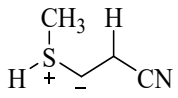
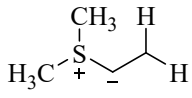
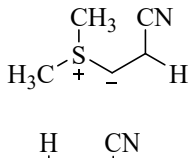
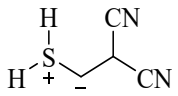
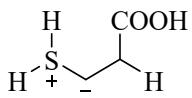
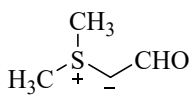
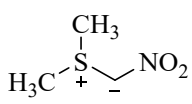
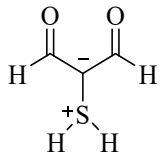
Table S1 The calculated PA of 23 sulfur ylides by using 26 kinds of DFTs (kJ/mol)

Entry	sulfur ylides	B3LYP	B3P86	M05-2X	M06	M06-2X	M06-HF	M06-L	ωB97XD
1		1118.48	1119.34	1126.16	1111.45	1116.67	1126.03	1120.06	1137.33
2		1120.75	1121.58	1128.00	1113.67	1118.74	1127.59	1123.12	1139.21
3		968.33	966.05	964.63	957.77	960.76	964.38	967.09	979.06
4		952.92	952.70	960.33	949.77	955.18	966.03	952.12	969.53
5		993.89	993.93	996.07	989.90	994.59	998.86	998.12	1011.18
6		971.34	971.57	974.37	968.39	973.13	978.07	975.34	988.83
7		999.73	1000.02	999.90	994.55	999.02	1000.86	1004.56	1016.21
8		1065.20	1064.69	1074.97	1058.58	1064.71	1078.55	1063.79	1082.59
9		936.90	934.32	933.91	927.73	929.98	934.98	935.30	947.91
10		1136.35	1138.60	1137.92	1123.47	1127.90	1133.22	1137.71	1149.76
11		968.33	966.05	964.11	957.77	960.76	964.38	967.09	979.06
12		808.38	803.19	800.80	798.59	799.62	799.06	806.01	816.54
13		943.08	942.65	939.26	937.63	937.34	935.40	947.03	956.18
14		993.89	993.93	996.07	989.90	994.59	998.86	998.12	1011.18
15		962.91	963.28	959.92	953.24	958.90	958.56	968.81	978.42
16		897.19	900.19	896.67	893.04	898.87	902.33	902.21	915.30

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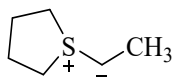
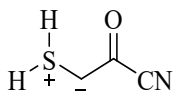
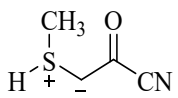
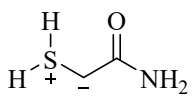
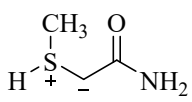
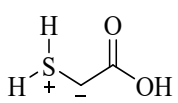
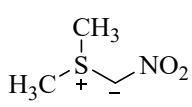
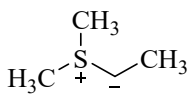
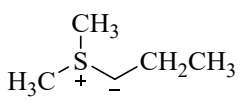
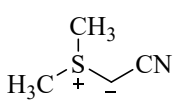
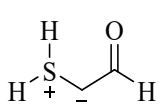
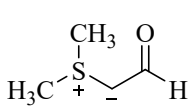
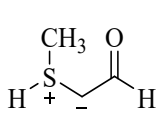
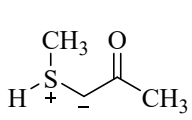
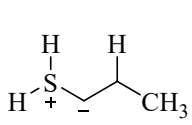
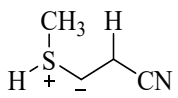
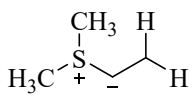
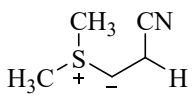
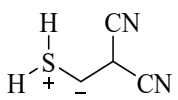
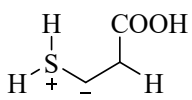
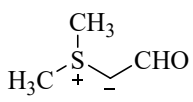
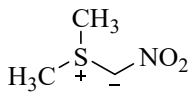
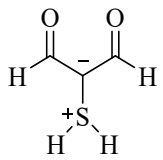
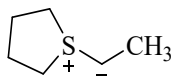
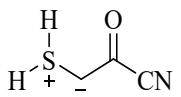
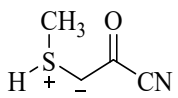
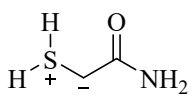
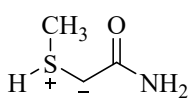
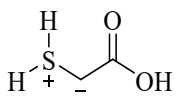
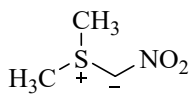
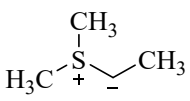
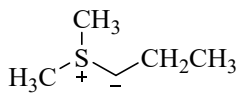
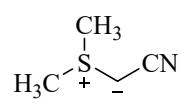
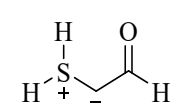
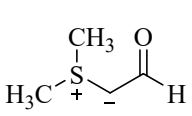
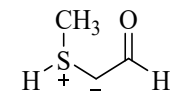
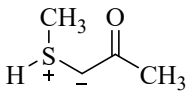
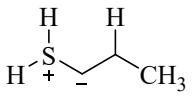
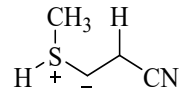
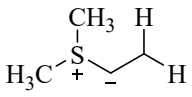
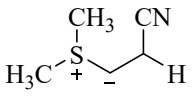
E-mail address: wrzheng@sues.edu.cn (W.R. Zheng).

17		1221.48	1128.30	1137.10	1122.91	1127.69	1139.07	1129.71	1148.77
18		868.54	865.26	861.92	861.04	862.50	863.58	867.68	880.16
19		913.46	910.62	906.37	906.46	905.80	905.28	913.11	924.18
20		1013.48	1014.90	1014.26	1006.78	1006.29	1013.06	1013.58	1026.49
21		1036.35	1037.48	1036.91	1030.16	1029.63	1034.52	1037.83	1049.45
22		957.17	958.09	956.52	952.43	952.86	953.41	959.67	971.66
23		962.91	963.28	959.92	953.24	958.90	958.56	968.81	978.42

Entry	sulfur ylides	BP86-D3	ωB97	KMLYP	MPW1P86	BMK	MPW3LYP	N12	N12-SX
1		1106.19	1136.89	1131.69	1116.65	1132.19	1115.59	1111.08	1125.05
2		1109.35	1137.98	1133.19	1118.67	1135.33	1117.69	1113.34	1127.42
3		958.19	977.25	963.64	962.73	975.49	965.05	960.74	966.77
4		939.71	972.73	960.04	951.17	969.34	950.28	941.38	953.52
5		985.88	1011.31	998.96	991.91	1007.02	991.16	986.27	996.88
6		961.54	990.83	977.87	969.72	985.81	968.42	962.49	974.57
7		990.80	1016.31	1004.48	997.59	1012.47	996.66	993.03	1003.39
8		1050.71	1083.55	1075.71	1062.16	1078.16	1062.56	1056.30	1069.03
9		926.64	946.44	931.13	930.96	945.50	933.50	928.29	934.10
10		1124.31	1146.99	1143.65	1132.93	1138.96	1132.78	1134.35	1144.97
11		958.19	977.25	963.64	962.73	975.49	965.05	960.74	966.77
12		804.87	812.76	790.08	800.14	812.42	805.64	799.59	798.98
13		936.76	953.54	940.08	939.55	954.98	939.94	937.00	941.77
14		985.88	1011.31	998.96	991.91	1007.02	991.16	986.27	996.88

15		960.22	979.70	957.93	960.40	963.09	959.62	956.15	962.19
16		893.92	919.26	900.05	898.62	912.34	894.68	894.31	899.94
17		1116.02	1148.27	1142.01	1126.11	1143.38	1124.94	1121.00	1134.56
18		859.58	879.62	861.42	862.56	875.90	865.48	859.23	864.55
19		899.20	924.36	910.21	907.70	919.09	910.12	904.41	911.30
20		1002.98	1024.62	1017.63	1011.55	1024.60	1010.57	1009.16	1016.57
21		1024.72	1047.56	1040.99	1033.99	1047.28	1033.20	1032.07	1040.12
22		949.13	969.54	959.21	955.40	970.21	954.07	950.14	957.23
23		960.22	979.70	957.93	960.40	963.09	959.62	956.15	962.19

Entry	sulfur ylides	M11-L	MN12-L	SOGGA11	SOGGA11-X	BP86	B97D	B97-D3	B3LYP-D3	CAM-B3LYP	TPSS
1		1091.69	1098.29	1094.61	1132.33	1100.71	1123.07	1123.83	1123.06	1120.85	1118.17
2		1092.68	1100.44	1095.74	1134.14	1103.26	1127.09	1126.81	1125.91	1122.67	1121.07
3		946.45	943.87	956.43	975.73	956.36	974.43	975.80	969.67	964.93	972.98
4		932.95	933.90	939.94	965.18	937.68	952.37	1008.24	954.77	955.83	953.73
5		975.67	978.67	981.47	1005.06	979.90	1000.52	1001.58	998.90	994.46	997.06
6		955.73	957.23	959.04	984.15	956.33	976.36	977.50	975.69	972.74	973.29
7		985.15	984.35	989.46	1011.51	985.75	1006.31	1006.87	1004.09	999.89	1001.59
8		1035.20	1039.17	1050.39	1077.14	1047.11	1067.15	1067.53	1068.28	1068.24	1063.04
9		913.30	911.61	924.99	944.12	925.06	942.46	943.81	938.15	933.64	941.26
10		1105.58	1107.64	1120.51	1144.25	1122.03	1141.14	1141.43	1138.15	1135.72	1138.01
11		946.45	943.87	956.43	975.73	956.36	974.43	975.80	969.67	964.93	972.98

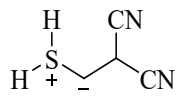
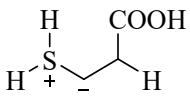
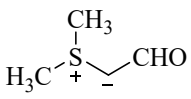
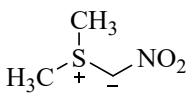
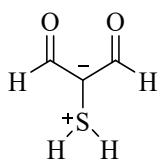
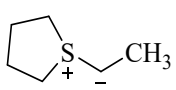
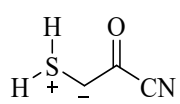
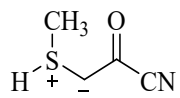
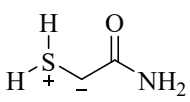
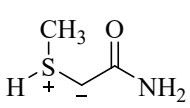
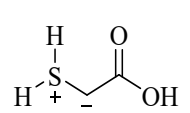
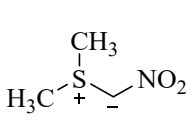
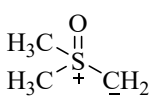
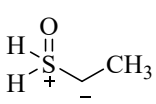
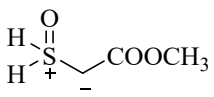
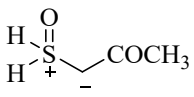
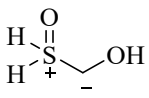
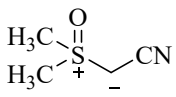
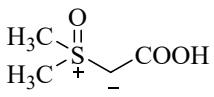
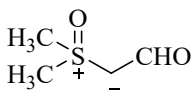
12		789.69	780.52	803.72	810.00	801.33	819.99	821.54	811.39	801.68	814.75
13		929.03	921.98	946.21	950.58	934.12	951.10	952.38	945.30	940.07	947.75
14		975.67	978.67	981.47	1005.06	979.90	1000.52	1001.58	998.90	994.46	997.06
15		947.42	939.83	965.52	973.10	955.06	978.00	977.32	967.37	960.10	971.70
16		886.03	878.41	902.48	908.92	890.60	902.70	907.36	900.21	899.13	903.01
17		1102.33	1110.64	1103.18	1142.71	1109.14	1133.71	1133.94	1133.52	1130.75	1127.91
18		848.49	844.21	866.15	874.67	857.17	875.54	876.21	870.74	865.62	871.64
19		893.05	890.42	905.58	920.39	899.90	914.77	915.73	913.00	911.91	915.97
20		995.31	991.30	1012.77	1020.70	1002.97	1015.22	1017.74	1013.44	1013.43	1018.24
21		1018.59	1015.45	1033.74	1043.78	1024.59	1037.78	1040.58	1036.38	1036.34	1040.70
22		945.38	937.31	960.47	966.79	946.99	963.05	964.70	959.08	955.80	960.70
23		947.42	939.83	965.54	973.10	954.97	978.00	977.32	967.37	960.10	971.70

Table S2 The energies of highest occupied molecular orbital (E_{HOMO}) of sulfoxide ylides (ev).

Entry	sulfoxide ylides	E_{HOMO} (ev)
1		-6.93
2		-6.93
3		-7.79
4		-7.10
5		-7.13
6		-7.18
7		-7.31
8		-7.28

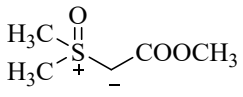
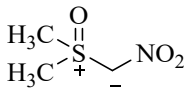
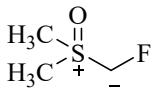
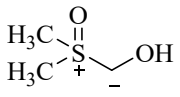
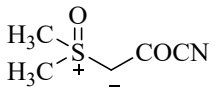
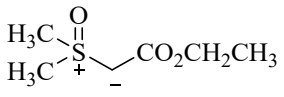
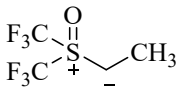
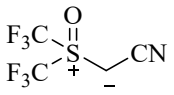
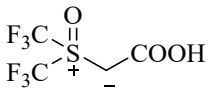
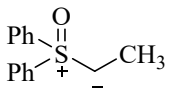
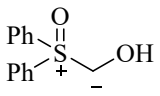
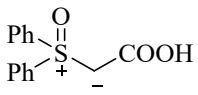
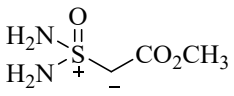
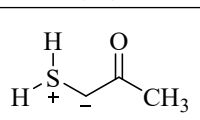
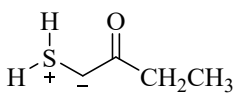
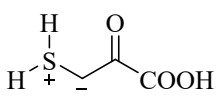
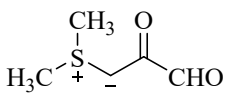
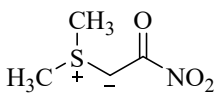
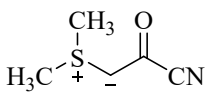
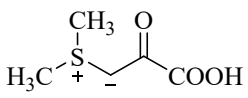
9		-7.14
10		-8.66
11		-7.59
12		-6.35
13		-8.64
14		-8.42
15		-8.47
16		-6.32
17		-6.41
18		-7.27
19		-7.52
20		-6.93
21		-6.93

Table S3 The energies of highest occupied molecular orbital (E_{HOMO}) of carbonyl ylides (ev).

Entry	carbonyl ylides	E_{HOMO} (ev)
1		-6.90
2		-6.90
3		-7.33
4		-6.97
5		-7.56
6		-7.37
7		-6.91

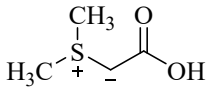
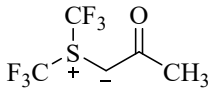
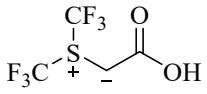
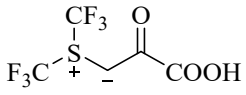
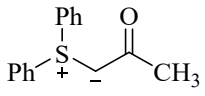
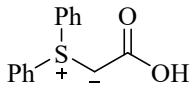
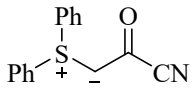
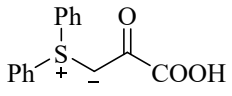
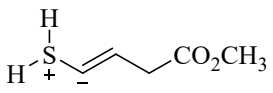
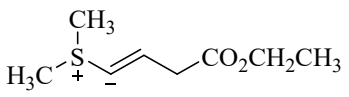
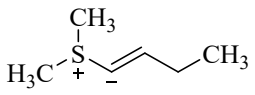
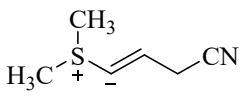
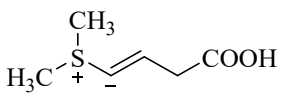
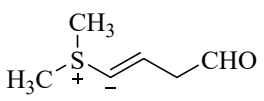
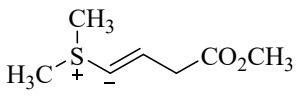
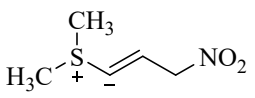
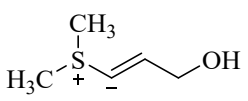
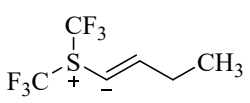
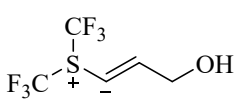
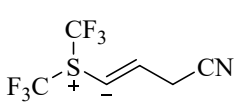
8		-6.62
9		-7.78
10		-7.97
11		-8.05
12		-6.60
13		-6.60
14		-7.09
15		-6.68

Table S4 The energies of highest occupied molecular orbital (E_{HOMO}) of allyl ylides (ev).

Entry	allyl ylides	E_{HOMO} (ev)
1		-7.14
2		-6.48
3		-6.26
4		-6.79
5		-6.41
6		-6.56
7		-6.51
8		-6.90
9		-6.47
10		-7.56
11		-7.69
12		-8.11

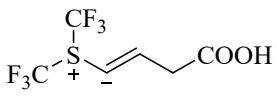
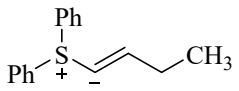
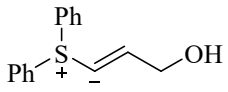
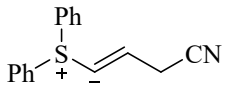
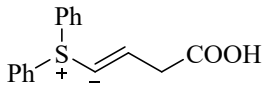
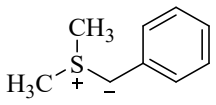
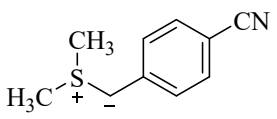
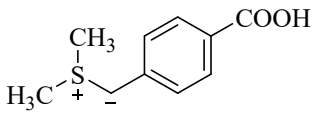
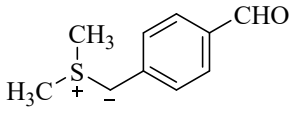
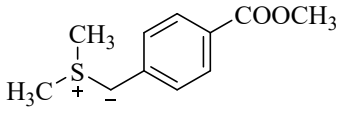
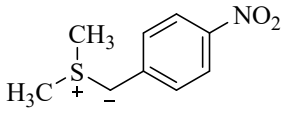
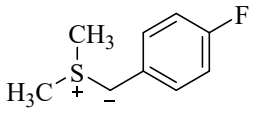
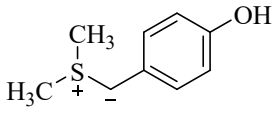
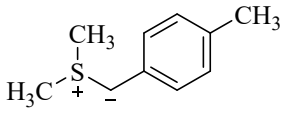
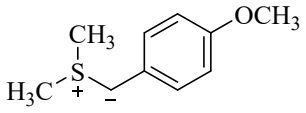
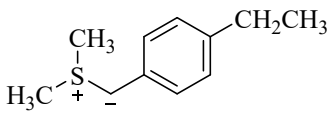
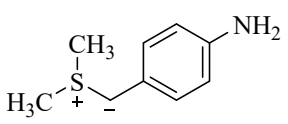
13		-7.82
14		-6.25
15		-6.45
16		-6.85
17		-6.60

Table S5 The energies of highest occupied molecular orbital (E_{HOMO}) of benzenyl ylides (ev).

Entry	benzenyl ylides	E_{HOMO} (ev)
1		-5.34
2		-5.91
3		-5.76
4		-5.81
5		-5.68
6		-6.09
7		-5.43
8		-5.12
9		-5.22
10		-5.08
11		-5.23
12		-4.91