

Free Radicals Formed by H Atom Addition to Allenenes as Determined by Muon Spin Spectroscopy

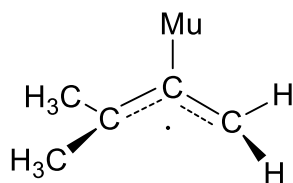
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Supporting Information:

Computational Details, Optimized Geometries and Isotropic Hyperfine Constants

Muonium addition to 1,1-dimethylallene – radical 1a



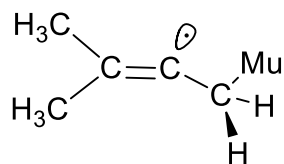
SCF Energy -195.9546009 Hartree

Reaction Energy -276 kJ mol⁻¹

Reference geometry for the protiated isomer from DFT at the UB3LYP/6-311G(d,p) level, and isotropic hyperfine constants from a single-point calculation with the EPR-III basis set.

	Cartesian coordinates /Å			hfc /MHz
C(13)	-0.39759	-0.03281	-0.00001	56.1
C(13)	0.84527	-0.66554	0.00000	-44.5
C(13)	2.09761	-0.08422	0.00000	48.8
C(13)	-1.66408	-0.83761	0.00000	-21.7
C(13)	-0.56767	1.45756	0.00000	-19.6
CH₃	-1.46702	-1.91155	0.00001	1.8
CH₃	-2.28284	-0.60658	-0.87756	66.1
CH₃	-2.28284	-0.60657	0.87757	66.1
CH₃	0.37900	1.99698	-0.00007	1.7
CH₃	-1.13980	1.78396	0.87806	53.5
CH₃	-1.13993	1.78395	-0.87798	53.5
H	2.98867	-0.69870	0.00000	-40.6
H	2.24496	0.98848	0.00001	-38.3
H(Mu)	0.81865	-1.75417	0.00000	11.2

Muonium addition to 1,1-dimethylallene – radical 1b



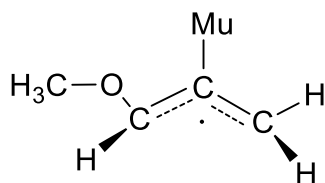
SCF Energy -195.9192838 Hartree

Reaction Energy -183 kJ mol⁻¹

Reference geometry for the protiated isomer from DFT at the UB3LYP/6-311G(d,p) level, and isotropic hyperfine constants from a single-point calculation with the EPR-III basis set.

	Cartesian coordinates /Å			hfc /MHz
C(13)	0.44504	-0.06195	0.00000	1.4
C(13)	-0.76929	-0.56525	-0.00001	276.6
C(13)	-2.18456	-0.16705	0.00001	22.9
C(13)	1.67748	-0.94169	-0.00001	54.7
C(13)	0.71553	1.43465	0.00001	59.1
CH₃	1.41161	-1.99915	-0.00002	-2.6
CH₃	2.29816	-0.74024	0.88099	-6.0
CH₃	2.29817	-0.74021	-0.88099	-6.0
CH₃	-0.20308	2.02324	0.00002	-3.8
CH₃	1.30214	1.71797	-0.88132	-4.8
CH₃	1.30216	1.71796	0.88133	-4.8
CH₂	-2.70837	-0.55010	-0.88210	23.8
CH₂	-2.70835	-0.55009	0.88212	23.8
H(Mu)	-2.29763	0.92837	0.00000	134.1

Muonium addition to 1-methoxyallene – radical 2a



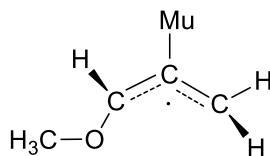
SCF Energy -231.8520414 Hartree

Reaction Energy -302 kJ mol⁻¹

Reference geometry for the protiated isomer from DFT at the UB3LYP/6-311G(d,p) level, and isotropic hyperfine constants from a single-point calculation with the EPR-III basis set.

	Cartesian coordinates /Å			hfc /MHz
C (13)	-2.36353	-0.19324	0.00000	51.3
C (13)	-0.98490	-0.33945	0.00000	-42.3
C (13)	-0.09510	0.71935	-0.00001	43.7
O (17)	1.25765	0.65968	0.00000	-15.2
C (13)	1.87645	-0.62058	-0.00001	-3.3
H	-3.01600	-1.05546	0.00001	-43.3
H	-2.82849	0.78586	-0.00001	-40.1
H	-0.43165	1.74917	-0.00001	-36.3
OCH ₃	1.60451	-1.19290	0.89366	9.1
OCH ₃	2.94917	-0.43568	-0.00002	-1.0
OCH ₃	1.60450	-1.19290	-0.89367	9.1
H (Mu)	-0.58693	-1.34951	0.00001	10.1

Muonium addition to 1-methoxyallene – radical 2b



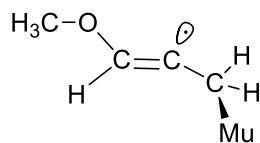
SCF Energy -231.8530766 Hartree

Reaction Energy -305 kJ mol⁻¹

Reference geometry for the protiated isomer from DFT at the UB3LYP/6-311G(d,p) level, and isotropic hyperfine constants from a single-point calculation with the EPR-III basis set.

	Cartesian coordinates /Å			hfc /MHz
C(13)	-2.08988	-0.63150	0.00000	46.6
C(13)	-1.38842	0.55370	0.00000	-41.7
C(13)	-0.00693	0.68544	0.00000	48.0
O(17)	0.78963	-0.41050	0.00000	-13.2
C(13)	2.18923	-0.15842	0.00000	-2.9
H	-3.17172	-0.63750	0.00000	-39.0
H	-1.57821	-1.58502	0.00000	-37.7
H	0.48637	1.65215	0.00000	-42.1
OCH₃	2.48963	0.39907	-0.89452	7.4
OCH₃	2.68114	-1.12967	0.00000	-1.2
OCH₃	2.48963	0.39907	0.89452	7.4
H(Mu)	-1.93794	1.49063	0.00000	9.7

Muonium addition to 1-methoxyallene – radical 2c



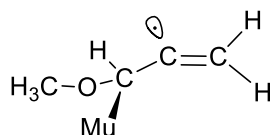
SCF Energy -231.8157955 Hartree

Reaction Energy -207 kJ mol⁻¹

Reference geometry for the protiated isomer from DFT at the UB3LYP/6-311G(d,p) level, and isotropic hyperfine constants from a single-point calculation with the EPR-III basis set.

	Cartesian coordinates /Å			hfc /MHz
C(13)	2.36299	-0.29040	0.00000	8.3
C(13)	0.90071	-0.16139	0.00000	245.1
C(13)	-0.02772	0.77057	0.00000	-25.9
O(17)	-1.38158	0.60956	0.00000	-29.6
C(13)	-1.83339	-0.73995	0.00000	3.7
OCH₃	-1.47937	-1.27081	-0.89090	2.1
OCH₃	-2.92173	-0.69844	0.00000	2.3
OCH₃	-1.47938	-1.27081	0.89090	2.1
H	0.22403	1.83317	0.00000	119.7
CH₂	2.72866	-0.82347	0.88392	25.4
CH₂	2.72866	-0.82346	-0.88392	25.4
H(Mu)	2.83627	0.70432	0.00000	138.9

Muonium addition to 1-methoxyallene – radical 2d



SCF Energy -231. 8028982 Hartree

Reaction Energy -173 kJ mol⁻¹

Reference geometry for the protiated isomer from DFT at the UB3LYP/6-311G(d,p) level, and isotropic hyperfine constants from a single-point calculation with the EPR-III basis set.

	Cartesian coordinates /Å			hfc /MHz
C(13)	-2.53622	-0.05651	0.20040	1.9
C(13)	-1.34144	-0.17852	-0.31574	294.1
C(13)	-0.01785	0.45200	-0.19767	6.7
O(17)	0.97785	-0.52742	0.03814	-7.9
C(13)	2.27193	0.03428	0.12371	-1.3
OCH₃	2.96563	-0.78852	0.29610	-0.3
OCH₃	2.35226	0.74857	0.95638	0.7
OCH₃	2.55320	0.54994	-0.80635	-0.1
CH₂	-2.74203	0.65431	1.00705	162.4
CH₂	-3.37936	-0.65499	-0.13410	98.5
H(Mu)	-0.03957	1.18889	0.63111	112.0
H(Mu)	0.20858	1.01370	-1.11945	21.6

Full listing of reference 29

Gaussian 16, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.