

Supporting Information for: Alkynes as CH/ π Acceptors: Microwave Spectra and Structures of the CH₂F₂···Propyne and CH₂ClF···Propyne Dimers

Anthony A. Ernst, Cori L. Christenholz, Yasser J. Dhahir, Sean A. Peebles, Rebecca A. Peebles*

Department of Chemistry, Eastern Illinois University, 600 Lincoln Avenue,
Charleston, IL 61920, USA

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Full version of reference 26.

Table S1. Observed transition frequencies for the six measured isotopologues of DFM...propyne.

CH ₂ F ₂ ...H ₃ CCCH			CH ₂ F ₂ ...H ₃ CCCD			CH ₂ F ₂ ...H ₃ CC ¹³ CH			CH ₂ F ₂ ...H ₃ C ¹³ CCH			CH ₂ F ₂ ...H ₃ ¹³ CCCH			¹³ CH ₂ F ₂ ...H ₃ CCCH		
<i>J'</i>	<i>K_a'</i>	<i>K_c'</i>	<i>J''</i>	<i>K_a''</i>	<i>K_c''</i>	<i>ν</i> / MHz	<i>Δν</i> / MHz ^a	<i>ν</i> / MHz	<i>Δν</i> / MHz	<i>ν</i> / MHz	<i>Δν</i> / MHz	<i>ν</i> / MHz	<i>Δν</i> / MHz	<i>ν</i> / MHz	<i>Δν</i> / MHz	<i>ν</i> / MHz	<i>Δν</i> / MHz
2	1	1	1	1	0	5122.3590	0.0033										
3	1	3	2	1	2	6952.0528	-0.0012	6923.9418	-0.0010	6861.5434	-0.0034	6876.3723	-0.0015	6852.7132	-0.0031	6923.9418	-0.0010
3	0	3	2	0	2	7282.7254	0.0005	7252.4030	0.0025	7191.7948	0.0052	7200.6986	0.0084	7178.8511	0.0010	7252.4030	0.0025
3	2	2	2	2	1	7320.2740	-0.0026										
3	2	1	2	2	0	7358.3273	0.0014										
3	1	2	2	1	1	7677.3307	-0.0009	7643.8515	0.0001	7588.0758	0.0030	7586.1265	-0.0003	7568.0815	0.0019	7643.8515	0.0001
5	0	5	4	1	4	8510.6344	-0.0006										
2	1	2	1	0	1	9113.1039	-0.0050										
4	1	4	3	1	3	9258.6625	-0.0013	9221.3351	0.0030	9137.6589	-0.0063	9158.2071	-0.0066	9126.3585	-0.0010	9221.3351	0.0030
4	0	4	3	0	3	9666.3472	-0.0022	9626.5432	-0.0055	9543.7209	0.0042	9558.8653	-0.0004	9528.4335	0.0034	9626.5432	-0.0055
4	2	3	3	2	2	9752.7734	0.0002										
4	3	2	3	3	1	9777.6969	-0.0015										
4	3	1	3	3	0	9779.1078	0.0005										
4	2	2	3	2	1	9847.2509	0.0018										
4	1	3	3	1	2	10224.5351	0.0014	10180.0677	0.0003	10105.1240	-0.0042	10103.4547	-0.0017	10079.0218	-0.0023	10180.0677	0.0003
3	1	3	2	0	2	11194.1121	0.0002										
6	0	6	5	1	5	11275.7966	-0.0005										
5	1	5	4	1	4	11556.7488	-0.0002	11510.3091	-0.0016	11405.0319	0.0055	11431.8809	0.0047	11391.5967	0.0020	11510.3091	-0.0016
5	0	5	4	0	4	12014.3351	-0.0012	11965.5457	0.0023	11859.0063	-0.0033	11882.8547	-0.0016	11842.8437	-0.0020	11965.5457	0.0023
5	2	4	4	2	3	12178.7720	-0.0001										

5	3	3	4	3	2	12229.2254	-0.0004
5	3	2	4	3	1	12234.1463	0.0003
5	2	3	4	2	2	12365.1120	0.0018
5	1	4	4	1	3	12760.8115	-0.0008
4	1	4	3	0	3	13170.0531	0.0024
6	1	6	5	1	5	13844.9938	0.0003
7	0	7	6	1	6	14019.3743	0.0005
6	0	6	5	0	5	14321.9106	-0.0005
6	2	5	5	2	4	14596.6794	0.0009
6	3	4	5	3	3	14684.2770	-0.0001
6	3	3	5	3	2	14697.3455	-0.0003
6	2	4	5	2	3	14914.9747	0.0008
5	1	5	4	0	4	15060.4528	0.0024
6	1	5	5	1	4	15282.5369	0.0011
7	1	7	6	1	6	16122.5588	0.0016
7	0	7	6	0	6	16588.5673	-0.0031
7	2	6	6	2	5	17004.9407	0.0015
7	3	5	6	3	4	17142.4287	-0.0021

$$^a \Delta v = v_{\text{observed}} - v_{\text{calculated}}$$

Table S2. Observed transition frequencies for the ^{35}Cl and ^{37}Cl isotopologues of CFM...propyne.

								^{35}Cl	^{37}Cl			
J'	K_a'	K_c'	$2F'$	J''	K_a''	K_c''	$2F''$	ν / MHz	$\Delta\nu$ / MHz ^a	ν / MHz	$\Delta\nu$ / MHz	
2	1	1	1	1	0	1	2	7170.2236	-0.0050			
2	1	1	2	1	0	1	2	7178.9036	0.0034			
2	1	1	2	1	0	1	1	7191.9941	-0.0039	7105.3467	0.0028	
2	1	1	3	1	0	1	3	7193.1785	-0.0009			
2	1	1	4	1	0	1	3	7183.5336	0.0008	7098.7526	0.0003	
2	1	1	3	1	0	1	2	7185.9192	0.0008	7100.7347	0.0029	
3	1	2	3	2	0	2	3	9715.9520	-0.0011			
3	1	2	5	2	0	2	4	9717.1550	-0.0008	9602.6439	-0.0043	
3	1	2	2	2	0	2	1	9717.2530	-0.0015			
3	1	2	3	2	0	2	2	9721.0254	0.0012	9605.7539	0.0048	
3	1	2	4	2	0	2	3	9721.3046	0.0043	9606.0180	-0.0067	
3	1	2	4	2	0	2	4	9728.4389	0.0023			
5	0	5	6	4	1	3	5	9771.2974	-0.0016			
5	0	5	7	4	1	3	6	9776.8699	0.0012			
2	2	0	3	1	1	0	2	11464.3947	0.0004	11334.1121	0.0005	
2	2	0	2	1	1	0	2	11469.4758	0.0011			
2	2	0	2	1	1	0	1	11471.9764	-0.0040			
2	2	0	1	1	1	0	1	11479.1599	0.0038			
2	2	0	4	1	1	0	3			11341.9694	-0.0015	
2	2	1	2	1	1	1	1	11517.3518	0.0038			

2	2	1	3	1	1	1	3	11517.4727	0.0025		
2	2	1	4	1	1	1	3	11524.7223	-0.0007	11395.6327	-0.0016
2	2	1	3	1	1	1	2	11527.7681	-0.0058	11398.0210	0.0013
2	2	1	2	1	1	1	2	11532.9512	0.0006		
4	1	3	3	3	0	3	2	12277.9626	0.0005	12135.6009	-0.0015
4	1	3	6	3	0	3	5	12278.7574	-0.0042	12136.3205	0.0004
4	1	3	4	3	0	3	3	12282.7304	0.0030	12139.5219	0.0012
4	1	3	5	3	0	3	4	12283.7302	0.0008	12140.3566	0.0016
3	2	1	4	2	1	1	3	13869.6644	0.0042	13701.6401	0.0036
3	2	1	2	2	1	1	1	13884.8573	-0.0021		
3	2	1	5	2	1	1	4			13708.8910	-0.0034
3	2	2	5	2	1	2	4	14030.8367	0.0009		
3	2	2	4	2	1	2	3	14033.1982	-0.0005	13872.3990	0.0006
3	2	2	3	2	1	2	2	14031.3473	-0.0043		
3	2	2	2	2	1	2	1	14029.9558	0.0003		

$$^a \Delta V = v_{\text{observed}} - v_{\text{calculated}}$$

Table S3. Estimated A_r , B_r , C_r rigid rotational constants corrected for internal rotation effects, as described in text section III.B., for all isotopic species. Uncertainties are taken from the uncorrected constants (Table 3).

	CH ₂ F ₂ ··· CH ₃ CCH	CH ₂ F ₂ ··· CH ₃ CCD	CH ₂ F ₂ ··· CH ₃ C ¹³ CH	CH ₂ F ₂ ··· CH ₃ ¹³ CCH	CH ₂ F ₂ ··· ¹³ CH ₃ CCH	¹³ CH ₂ F ₂ ··· CH ₃ CCH
A / MHz	5814.3278(15)	5411.674(3)	5668.305(24)	5808.350(24)	5732.183(13)	5809.045(15)
B / MHz	1331.3493(5)	1317.7862(8)	1316.8117(11)	1315.0416(11)	1312.6609(6)	1325.3981(6)
C / MHz	1099.2040(4)	1074.9320(8)	1084.0441(14)	1087.8428(14)	1083.4602(7)	1094.9527(8)
P_{cc} / u Å ²	3.37527(16)	3.3716(3)	3.3754(6)	3.3728(6)	3.3675(3)	3.3745(4)

Table S4. Principal axis coordinates in Å for all *ab initio* structures included in Table 1 and for the inertial fit structure included in Table 6.

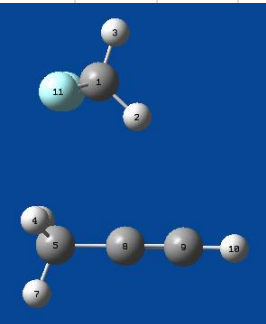
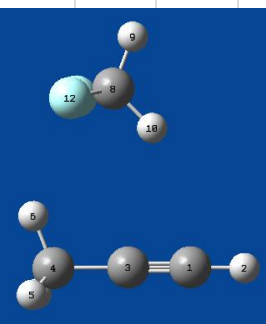
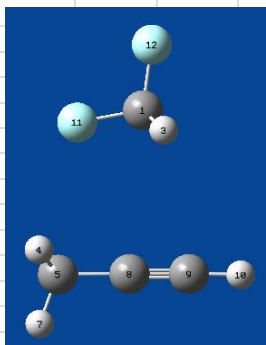
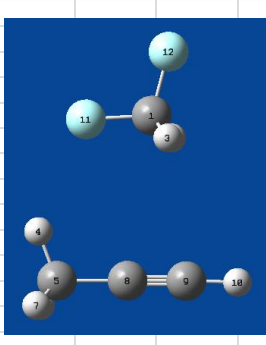
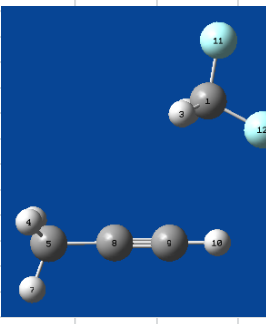
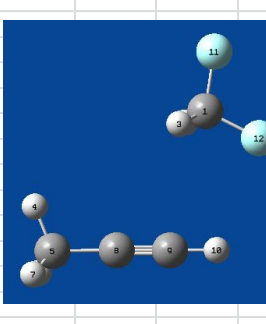
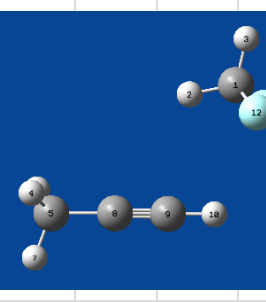
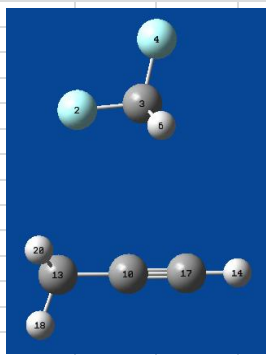
1-1a					1-1b				
	a	b	c			a	b	c	
C1	-1.42594	0.67070	0.00000		C1	-2.27688	1.23124	0.00000	
H2	-0.46305	1.16504	0.00000		C2	-2.55564	2.25473	0.00000	
H3	-2.27540	1.34291	0.00000		C3	-1.97865	0.05334	0.00000	
H4	0.84134	-1.53627	0.87909		C4	-1.62581	-1.36654	0.00000	
C5	1.45565	-1.36335	0.00000		H5	-2.02883	-1.85775	-0.88148	
H6	0.84134	-1.53627	-0.87909		H6	-0.54739	-1.49464	0.00000	
H7	2.27017	-2.08257	0.00000		H7	-2.02883	-1.85775	0.88148	
C8	1.98154	0.00218	0.00000		C8	1.47174	0.63925	0.00000	
C9	2.41725	1.13640	0.00000		H9	2.35797	1.26218	0.00000	
H10	2.81405	2.12014	0.00000		H10	0.53783	1.18603	0.00000	
F11	-1.50544	-0.12685	1.10603		F11	1.50575	-0.16255	1.10535	
F12	-1.50544	-0.12685	-1.10603		F12	1.50575	-0.16255	-1.10535	
1-1Ia					1-1Ib				
	a	b	c			a	b	c	
C1	1.27919	-0.31927	0.00000		C1	-1.30119	-0.28455	0.00000	
H2	0.90276	-0.77701	-0.90551		H2	-0.90407	-0.72385	0.90569	
H3	0.90276	-0.77701	0.90551		H3	-0.90407	-0.72385	-0.90569	
C5	-2.23021	1.14839	0.00000		C5	2.37943	1.11268	0.00000	
H6	-1.75320	1.57411	-0.87798		H6	2.94406	1.40683	0.88061	
H7	-3.27777	1.43710	0.00000		H7	2.94406	1.40683	-0.88061	
C8	-2.10351	-0.30917	0.00000		C8	2.14676	-0.33175	0.00000	
C9	-2.00822	-1.52046	0.00000		C9	1.96107	-1.53254	0.00000	
H10	-1.94316	-2.57937	0.00000		H10	1.81995	-2.58405	0.00000	
F11	0.92369	1.00044	0.00000		F11	-1.00649	1.05088	0.00000	
F12	2.64130	-0.39246	0.00000		F12	-2.65833	-0.41933	0.00000	
1-1IIa						1-1IIb			
	a	b	c			a	b	c	
C1	-1.38398	0.28511	0.00000		C1	-1.37302	0.28196	0.00000	
H2	-0.83737	0.51513	0.90549		H2	-0.82482	0.50797	0.90556	
H3	-0.83737	0.51513	-0.90549		H3	-0.82482	0.50797	-0.90556	
H4	3.20201	1.52707	-0.88083		H4	2.78382	1.86819	0.00000	
C5	3.32750	0.90309	0.00000		C5	3.30263	0.91314	0.00000	
H6	3.20201	1.52707	0.88083		H6	3.93803	0.87211	0.88052	
H7	4.34304	0.51653	0.00000		H7	3.93803	0.87211	-0.88052	
C8	2.36090	-0.19559	0.00000		C8	2.35060	-0.19814	0.00000	
C9	1.57068	-1.11812	0.00000		C9	1.57172	-1.13026	0.00000	
H10	0.87353	-1.91858	0.00000		H10	0.88414	-1.93895	0.00000	
F11	-2.55433	0.98507	0.00000		F11	-2.53832	0.99046	0.00000	
F12	-1.68418	-1.04809	0.00000		F12	-1.68282	-1.04893	0.00000	
1-IVa					Table 6 Inertial Fit				
	a	b	c			a	b	c	
C1	1.70937	0.00000	-0.67829		F2	1.06036	1.04895	0.00000	
H2	0.70578	0.00000	-1.08385		C3	1.31375	-0.28459	0.00000	
H3	2.49316	0.00000	-1.42613		F4	2.65935	-0.46314	0.00000	
H4	-3.49161	0.88089	-1.19345		H5	0.90275	-0.71921	0.91527	
C5	-3.44768	0.00000	-0.55851		H6	0.90275	-0.71921	-0.91527	
H6	-3.49161	-0.88089	-1.19345		C10	-2.18813	-0.31360	0.00000	
H7	-4.32545	0.00000	0.08217		C13	-2.33883	1.13821	0.00000	
C8	-2.22517	0.00000	0.24565		H14	-1.95404	-2.56878	0.00000	
C9	-1.21755	0.00000	0.92380		C17	-2.06348	-1.51444	0.00000	
H10	-0.33606	0.00000	1.51505		H18	-3.40051	1.41030	0.00000	
F11	1.86027	-1.10453	0.10879		H19	-1.87116	1.57806	-0.88827	
F12	1.86027	1.10453	0.10879		H20	-1.87116	1.57806	0.88827	

Table S4, Continued. Principal axis coordinates in Å for all *ab initio* structures included in Table 1 and for the inertial fit structure included in Table 6.

Table 6 Inertial Fit Using Corrected Constants

	a	b	c
F2	1.026844	1.023722	0.000000
C3	1.328906	-0.299642	0.000000
F4	2.680149	-0.428784	0.000000
H5	0.934107	-0.749020	0.915270
H6	0.934107	-0.749020	-0.915270
C10	-2.188601	-0.311954	0.000000
C13	-2.335722	1.140213	0.000000
H14	-1.960066	-2.567707	0.000000
C17	-2.066910	-1.513105	0.000000
H18	-3.396735	1.414926	0.000000
H19	-1.866970	1.578917	-0.888271
H20	-1.866970	1.578917	0.888271

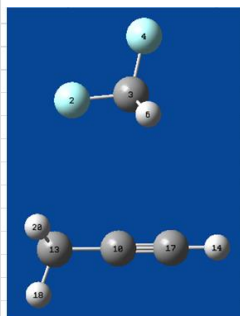
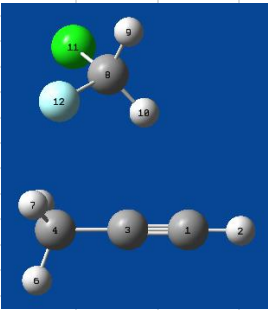
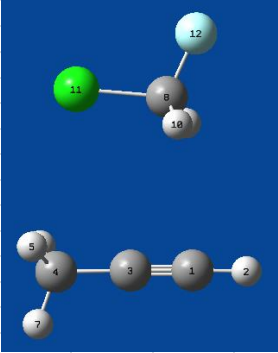
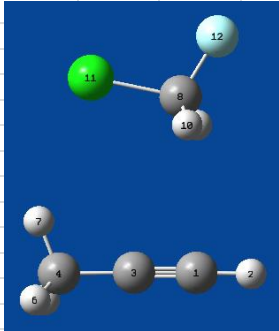
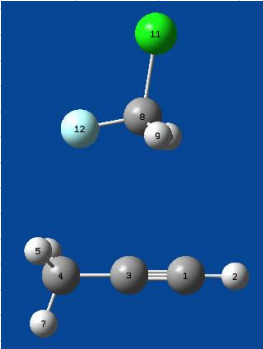


Table S5. Principal axis coordinates in Å for all *ab initio* structures included in Table 2.

2-Ia				
	a	b	c	
C1	2.56985	0.14104	1.19979	
H2	2.88329	0.16133	2.21308	
C3	2.22683	0.12738	0.03407	
C4	1.82408	0.10596	-1.37236	
H5	1.41759	1.06943	-1.66691	
H6	2.67775	-0.11795	-2.00656	
H7	1.06117	-0.64898	-1.54148	
C8	-1.08650	-0.60218	0.70115	
H9	-1.86448	-0.86655	1.40324	
H10	-0.11207	-0.49298	1.15493	
Cl11	-1.52106	0.95939	-0.03621	
F12	-1.01757	-1.57448	-0.26520	

2-IIa				
	a	b	c	
C1	-2.17858	-1.62322	0.00000	
H2	-2.04293	-2.67552	0.00000	
C3	-2.35696	-0.42120	0.00000	
C4	-2.59462	1.02236	0.00000	
H5	-2.15258	1.48314	0.87878	
H6	-2.15258	1.48314	-0.87878	
H7	-3.66147	1.22943	0.00000	
C8	1.10985	-0.63877	0.00000	
H9	0.63116	-0.99947	-0.89818	
H10	0.63116	-0.99947	0.89818	
Cl11	1.00179	1.14169	0.00000	
F12	2.42274	-1.02698	0.00000	

2-IIb				
	a	b	c	
C1	-2.19478	-1.59829	0.00000	
H2	-2.01080	-2.64323	0.00000	
C3	-2.42871	-0.40582	0.00000	
C4	-2.73155	1.02543	0.00000	
H5	-3.30946	1.29165	-0.88093	
H6	-3.30946	1.29165	0.88093	
H7	-1.81552	1.60923	0.00000	
C8	1.10225	-0.62511	0.00000	
H9	0.60026	-0.95250	-0.89826	
H10	0.60026	-0.95250	0.89826	
Cl11	1.11596	1.15880	0.00000	
F12	2.38581	-1.10103	0.00000	

2-IIIa				
	a	b	c	
C1	-2.43883	-1.58576	0.00000	
H2	-2.31309	-2.63922	0.00000	
C3	-2.60267	-0.38173	0.00000	
C4	-2.81548	1.06577	0.00000	
H5	-2.36483	1.51910	0.87807	
H6	-2.36483	1.51910	-0.87807	
H7	-3.87854	1.29135	0.00000	
C8	0.76713	-0.19644	0.00000	
H9	0.41724	-0.68348	0.89801	
H10	0.41724	-0.68348	-0.89801	
Cl11	2.54755	-0.23114	0.00000	
F12	0.32419	1.10193	0.00000	

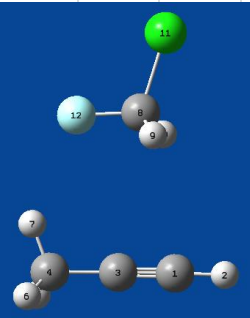
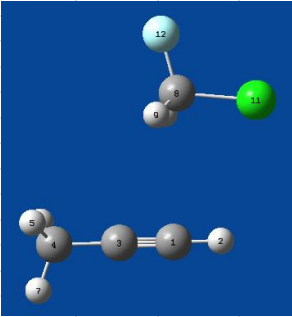
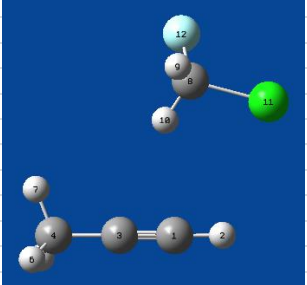
2-IIIb				
	a	b	c	
C1	-2.39635	-1.60241	0.00000	
H2	-2.19520	-2.64413	0.00000	
C3	-2.64800	-0.41362	0.00000	
C4	-2.96122	1.01561	0.00000	
H5	-3.54137	1.27773	-0.88066	
H6	-3.54137	1.27773	0.88066	
H7	-2.04877	1.60487	0.00000	
C8	0.78050	-0.12681	0.00000	
H9	0.39980	-0.59004	0.89799	
H10	0.39980	-0.59004	-0.89799	
Cl11	2.55443	-0.27373	0.00000	
F12	0.42029	1.19801	0.00000	

Table S5, Continued. Principal axis coordinates in Å for all *ab initio* structures included in Table 2.

2-IVa			
	a	b	c
C1	1.84106	-1.30102	0.00000
H2	1.19020	-2.13931	0.00000
C3	2.58060	-0.33717	0.00000
C4	3.48053	0.81680	0.00000
H5	3.31827	1.43261	-0.88068
H6	3.31827	1.43261	0.88068
H7	4.51726	0.49127	0.00000
C8	-0.87699	0.60714	0.00000
H9	-0.27713	0.62763	-0.89788
H10	-0.27713	0.62763	0.89788
Cl11	-1.81205	-0.91078	0.00000
F12	-1.72746	1.68056	0.00000



2-Vb			
	a	b	c
C1	-1.80544	-1.24377	-0.26494
H2	-1.09186	-2.01131	-0.43364
C3	-2.61427	-0.35764	-0.07352
C4	-3.59617	0.70394	0.15005
H5	-4.30524	0.74671	-0.67219
H6	-4.14926	0.52753	1.06859
H7	-3.10815	1.67221	0.22667
C8	1.06801	0.65248	0.45042
H9	1.29711	0.87605	1.48282
H10	0.01050	0.53093	0.26425
Cl11	1.86733	-0.88636	0.03781
F12	1.55338	1.66195	-0.33781



2-VIa			
	a	b	c
C1	2.19071	-1.06780	0.00000
H2	1.58722	-1.94109	0.00000
C3	2.87369	-0.06318	0.00000
C4	3.71097	1.13693	0.00000
H5	3.51617	1.74292	-0.88080
H6	3.51617	1.74292	0.88080
H7	4.76350	0.86684	0.00000
C8	-0.89940	-0.05282	0.00000
H9	-0.38143	0.25012	0.89798
H10	-0.38143	0.25012	-0.89798
Cl11	-2.51080	0.70323	0.00000
F12	-1.02275	-1.41925	0.00000

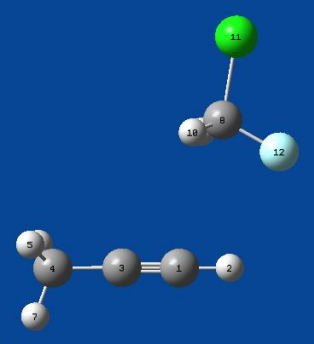


Table S6. Summary of dipole moment data for DFM···propyne, including transitions measured and number of points fitted (corresponding to individual Stark effect voltages) for each transition.

	$ M' $	$ M'' $	number of fields
$3_{13} \leftarrow 2_{12}$	0	0	9
$3_{03} \leftarrow 2_{02}$	0	0	1
	1	1	6
	3	2	9
$3_{12} \leftarrow 2_{11}$	0	0	9
	1	1	5
$4_{14} \leftarrow 3_{13}$	0	0	7
	1	1	7
	2	2	5
$4_{04} \leftarrow 3_{03}$	0	0	8
	1	1	8
	2	2	8
	3	3	4
			$\Delta V_{\text{rms}} = 4.1 \text{ kHz}$
$\mu_a = 1.568(2) \text{ D}$ $\mu_b = 0.587(2) \text{ D}$ $\mu_{\text{ot}} = 1.674(3) \text{ D}^a$			

^a μ_c was fixed to zero, assuming C_s symmetry for the complex. Attempts to include μ_c in the fit were unsuccessful.

Table S7. Transition frequencies, electric fields and ($\nu_{\text{observed}} - \nu_{\text{calculated}}$) frequencies for Stark effect measurements on DFM···propyne. Frequency shifts ($\nu_{\text{field}} - \nu_0$) were fitted, rather than fitting absolute frequencies at each field.

J	K_a'	K_c'	M'	J	K_a''	K_c''	M''	$E / (\text{V cm}^{-1})$	$\nu_{\text{obs}} / \text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}} / \text{MHz}$
3	1	3	0	2	1	2	0	69.7	6952.0412	-0.0059
3	1	3	0	2	1	2	0	102.2	6952.0335	-0.0057
3	1	3	0	2	1	2	0	134.6	6952.0230	-0.0054
3	1	3	0	2	1	2	0	167.0	6952.0111	-0.0035
3	1	3	0	2	1	2	0	199.5	6951.9946	-0.0033
3	1	3	0	2	1	2	0	231.9	6951.9771	-0.0012
3	1	3	0	2	1	2	0	264.3	6951.9525	-0.0032
3	1	3	0	2	1	2	0	296.7	6951.9295	-0.0007
3	1	3	0	2	1	2	0	329.2	6951.8978	-0.0041
3	0	3	0	2	0	2	0	69.7	7282.6290	-0.0022
3	0	3	1	2	0	2	1	37.1	7282.7105	-0.0001
3	0	3	1	2	0	2	1	69.7	7282.6707	-0.0034
3	0	3	1	2	0	2	1	102.2	7282.6167	0.0029
3	0	3	1	2	0	2	1	134.6	7282.5274	0.0004
3	0	3	1	2	0	2	1	167.0	7282.4114	0.0016
3	0	3	1	2	0	2	1	199.5	7282.2588	0.0020
3	0	3	3	2	0	2	2	69.7	7282.7530	0.0023
3	0	3	3	2	0	2	2	102.2	7282.7775	-0.0029
3	0	3	3	2	0	2	2	134.6	7282.8174	-0.0039
3	0	3	3	2	0	2	2	167.0	7282.8715	-0.0019
3	0	3	3	2	0	2	2	199.5	7282.9362	-0.0004
3	0	3	3	2	0	2	2	231.9	7283.0123	0.0013
3	0	3	3	2	0	2	2	264.3	7283.0992	0.0025
3	0	3	3	2	0	2	2	296.7	7283.1965	0.0030
3	0	3	3	2	0	2	2	329.2	7283.3060	0.0046
3	1	2	0	2	1	1	0	69.7	7677.3183	-0.0044
3	1	2	0	2	1	1	0	102.2	7677.3104	-0.0020
3	1	2	0	2	1	1	0	134.6	7677.2991	0.0007
3	1	2	0	2	1	1	0	167.0	7677.2802	-0.0003
3	1	2	0	2	1	1	0	199.5	7677.2595	0.0008
3	1	2	0	2	1	1	0	231.9	7677.2345	0.0013
3	1	2	0	2	1	1	0	264.3	7677.2044	0.0006
3	1	2	0	2	1	1	0	296.7	7677.1707	0.0001
3	1	2	0	2	1	1	0	329.2	7677.1346	0.0009
3	1	2	1	2	1	1	1	37.1	7677.3009	-0.0023
3	1	2	1	2	1	1	1	69.7	7677.2422	0.0105
3	1	2	1	2	1	1	1	102.2	7677.1316	0.0147
3	1	2	1	2	1	1	1	134.6	7676.9684	0.0094
3	1	2	1	2	1	1	1	199.5	7676.5153	0.0014

Table S7, continued. Transition frequencies, electric fields and ($\nu_{\text{observed}} - \nu_{\text{calculated}}$) frequencies for Stark effect measurements on DFM···propyne. Frequency shifts ($\nu_{\text{field}} - \nu_0$) were fitted, rather than fitting absolute frequencies at each field.

J	K_a'	K_c'	M'	J	K_a''	K_c''	M''	$E / (\text{V cm}^{-1})$	$\nu_{\text{obs}} / \text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}} / \text{MHz}$
4	1	4	0	3	1	3	0	134.6	9258.6346	-0.0031
4	1	4	0	3	1	3	0	167.0	9258.6200	-0.0037
4	1	4	0	3	1	3	0	199.5	9258.6046	-0.0021
4	1	4	0	3	1	3	0	231.9	9258.5825	-0.0042
4	1	4	0	3	1	3	0	264.3	9258.5602	-0.0034
4	1	4	0	3	1	3	0	296.7	9258.5333	-0.0043
4	1	4	0	3	1	3	0	329.2	9258.5039	-0.0046
4	1	4	1	3	1	3	1	134.6	9258.6960	0.0004
4	1	4	1	3	1	3	1	167.0	9258.7122	-0.0006
4	1	4	1	3	1	3	1	199.5	9258.7325	-0.0012
4	1	4	1	3	1	3	1	231.9	9258.7566	-0.0017
4	1	4	1	3	1	3	1	264.3	9258.7846	-0.0020
4	1	4	1	3	1	3	1	296.7	9258.8161	-0.0024
4	1	4	1	3	1	3	1	329.2	9258.8522	-0.0020
4	1	4	2	3	1	3	2	37.1	9258.6723	-0.0070
4	1	4	2	3	1	3	2	69.7	9258.7116	-0.0071
4	1	4	2	3	1	3	2	102.2	9258.7735	-0.0085
4	1	4	2	3	1	3	2	134.6	9258.8618	-0.0072
4	1	4	2	3	1	3	2	167.0	9258.9734	-0.0064
4	0	4	0	3	0	3	0	102.2	9666.3090	-0.0061
4	0	4	0	3	0	3	0	134.6	9666.2876	-0.0024
4	0	4	0	3	0	3	0	167.0	9666.2586	0.0007
4	0	4	0	3	0	3	0	199.5	9666.2190	0.0001
4	0	4	0	3	0	3	0	231.9	9666.1733	0.0003
4	0	4	0	3	0	3	0	264.3	9666.1163	-0.0040
4	0	4	0	3	0	3	0	296.7	9666.0537	-0.0069
4	0	4	0	3	0	3	0	329.2	9665.9888	-0.0053
4	0	4	1	3	0	3	1	102.2	9666.3243	-0.0055
4	0	4	1	3	0	3	1	134.6	9666.3127	-0.0027
4	0	4	1	3	0	3	1	167.0	9666.2924	-0.0046
4	0	4	1	3	0	3	1	199.5	9666.2708	-0.0039
4	0	4	1	3	0	3	1	231.9	9666.2448	-0.0036
4	0	4	1	3	0	3	1	264.3	9666.2145	-0.0037
4	0	4	1	3	0	3	1	296.7	9666.1797	-0.0043
4	0	4	1	3	0	3	1	329.2	9666.1414	-0.0045

Table S7, continued. Transition frequencies, electric fields and ($\nu_{\text{observed}} - \nu_{\text{calculated}}$) frequencies for Stark effect measurements on DFM···propyne. Frequency shifts ($\nu_{\text{field}} - \nu_0$) were fitted, rather than fitting absolute frequencies at each field.

J	K_a'	K_c'	M'	J	K_a''	K_c''	M''	$E / (\text{V cm}^{-1})$	$\nu_{\text{obs}} / \text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}} / \text{MHz}$
4	0	4	2	3	0	3	2	102.2	9666.3767	0.0030
4	0	4	2	3	0	3	2	134.6	9666.3935	0.0020
4	0	4	2	3	0	3	2	167.0	9666.4143	0.0000
4	0	4	2	3	0	3	2	199.5	9666.4409	-0.0011
4	0	4	2	3	0	3	2	231.9	9666.4762	0.0017
4	0	4	2	3	0	3	2	264.3	9666.5124	0.0005
4	0	4	2	3	0	3	2	296.7	9666.5551	0.0009
4	0	4	2	3	0	3	2	329.2	9666.6036	0.0022
4	0	4	3	3	0	3	3	134.6	9666.5146	-0.0039
4	0	4	3	3	0	3	3	167.0	9666.6055	-0.0044
4	0	4	3	3	0	3	3	199.5	9666.7198	-0.0010
4	0	4	3	3	0	3	3	231.9	9666.8546	0.0032

Full version of reference 26:

Gaussian 09, Revision **C.01**, Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G.A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H.P.; Izmaylov, A.F.; Bloino, J.; Zheng, G.; Sonnenberg, J.L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J.A., Jr.; Peralta, J.E.; Ogliaro, F.; Bearpark, M.; Heyd, J.J.; Brothers, E.; Kudin, K.N.; Staroverov, V.N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J.C.; Iyengar, S.S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N.J.; Klene, M.; Knox, J.E.; Cross, J.B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R.E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R.L.; Morokuma, K.; Zakrzewski, V.G.; Voth, G.A.; Salvador, P.; Dannenberg, J.J.; Dapprich, S.; Daniels, A.D.; Farkas, Ö.; Foresman, J.B.; Ortiz, J.V.; Cioslowski, J.; Fox, D.J. Gaussian, Inc., Wallingford CT, 2009.