Structures of Energetic Acetylene Derivatives $HC{\equiv}CCH_2ONO_2$, $(NO_2)_3CCH_2C{\equiv}CCH_2C(NO_2)_3$ and Trinitroethane, $(NO_2)_3CCH_3$

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SUPPORTING INFORMATION

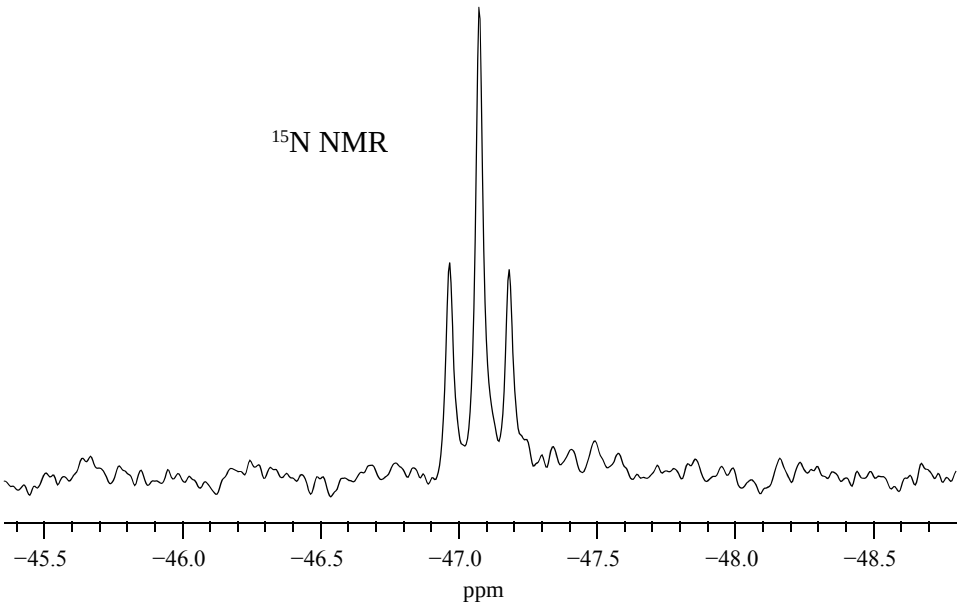

Fig. S1. ^{15}N NMR ($CDCl_3$) spectrum of propargyl nitrate (**1**).

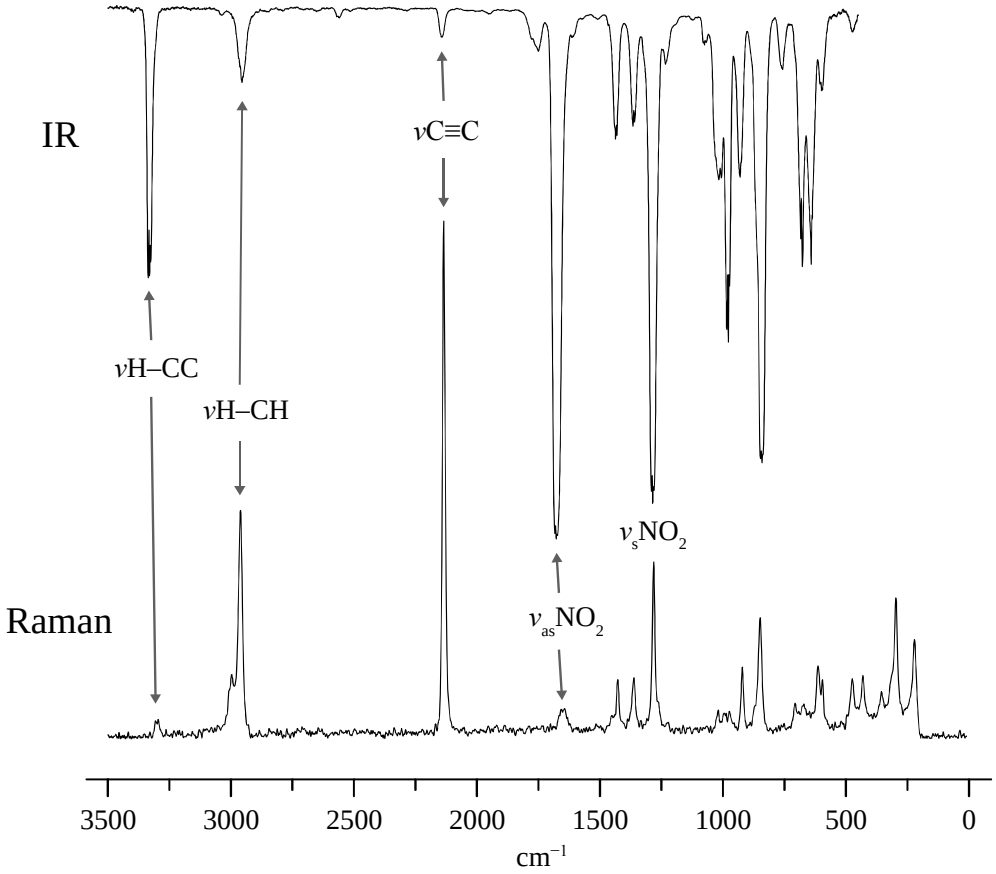

Fig. S2. IR and Raman spectrum of propargyl nitrate (**1**).

Table S1 and S2 show the full lists of inter-atomic distances, amplitudes of vibration and distance corrections for the $r_{a3,1}$ refinements, including details of which amplitudes were kept at fixed ratios and which were refined.

Table S1.

Name	Amplitude	(r_a)	e.s.d.	(r_e)	e.s.d.	u-Value	e.s.d.	Mult.	k-Value	Anharm.	Area	Orig. u-Value
u[1]	H(1)–C(2)	1.0943	0.0060	1.0808	0.0060	0.0724	Tied to u[46]	0.69	0.0135	2.0000	11.7	0.0723
u[46]	H(11)–C(12)	1.0943	0.0060	0.0060	0.0060	0.0724	0.0066	0.62	0.0135	2.0000	10.6	0.0723
u[51]	C(14)–H(20)	1.1217	0.0060	1.1083	0.0060	0.0761	Tied to u[46]	0.62	0.0134	2.0000	10.3	0.0760
u[5]	C(4)–H(9)	1.1217	0.0060	1.1083	0.0060	0.0761	Tied to u[46]	0.69	0.0134	2.0000	11.4	0.0760
u[6]	C(4)–H(10)	1.1217	0.0060	1.1083	0.0060	0.0761	Tied to u[46]	0.69	0.0134	2.0000	11.4	0.0760
u[50]	C(14)–H(19)	1.1217	0.0060	1.1083	0.0060	0.0761	Tied to u[46]	0.62	0.0134	2.0000	10.3	0.0760
u[53]	N(16)–O(17)	1.1945	0.0058	0.0058	0.0058	0.0304	0.0021	0.62	0.0036	2.0000	90.6	0.0369
u[8]	N(6)–O(7)	1.1945	0.0058	1.1909	0.0058	0.0304	Tied to u[53]	0.69	0.0036	2.0000	100.0	0.0369
u[47]	C(12)–C(13)	1.2057	0.0058	1.2009	0.0058	0.0286	Tied to u[53]	0.62	0.0048	2.0000	57.7	0.0347
u[2]	C(2)–C(3)	1.2057	0.0058	1.2009	0.0058	0.0286	Tied to u[53]	0.69	0.0048	2.0000	63.7	0.0347
u[9]	N(6)–O(8)	1.2130	0.0096	1.2108	0.0096	0.0311	Tied to u[53]	0.69	0.0022	2.0000	98.5	0.0377
u[54]	N(16)–O(18)	1.2170	0.0096	1.2148	0.0096	0.0311	Tied to u[53]	0.62	0.0022	2.0000	88.9	0.0377
u[52]	O(15)–N(16)	1.4128	0.0067	0.0067	0.0067	0.0420	0.0022	0.62	0.0148	2.0000	76.6	0.0492
u[7]	O(5)–N(6)	1.4279	0.0060	1.4131	0.0060	0.0420	Tied to u[52]	0.69	0.0148	2.0000	83.7	0.0492
u[4]	C(4)–O(5)	1.4547	0.0051	1.4451	0.0051	0.0420	Tied to u[52]	0.69	0.0096	2.0000	70.4	0.0493
u[48]	C(13)–C(14)	1.4551	0.0071	1.4480	0.0071	0.0396	Tied to u[52]	0.62	0.0071	2.0000	47.8	0.0464
u[49]	C(14)–O(15)	1.4566	0.0088	1.4470	0.0088	0.0420	Tied to u[52]	0.62	0.0096	2.0000	63.7	0.0493
u[3]	C(3)–C(4)	1.4652	0.0106	1.4581	0.0106	0.0396	Tied to u[52]	0.69	0.0071	2.0000	52.4	0.0464
u[90]	H(19)···H(20)	1.8194	0.0097	0.0097	0.0097	0.1256	0.0080	0.62	0.0238	0.0000	1.1	0.1214
u[45]	H(9)···H(10)	1.8194	0.0097	1.7956	0.0097	0.1256	Tied to u[90]	0.69	0.0238	0.0000	1.2	0.1214
u[30]	C(3)···H(10)	1.9336	0.0098	1.9309	0.0098	0.1072	Tied to u[90]	0.69	0.0027	0.0000	6.6	0.1036
u[29]	C(3)···H(9)	2.0377	0.0103	2.0350	0.0103	0.1072	Tied to u[90]	0.69	0.0027	0.0000	6.3	0.1036
u[82]	O(15)···H(20)	2.1121	0.0100	2.0952	0.0100	0.1042	Tied to u[90]	0.62	0.0169	0.0000	7.3	0.1007
u[81]	O(15)···H(19)	2.1121	0.0100	2.0952	0.0100	0.1042	Tied to u[90]	0.62	0.0169	0.0000	7.3	0.1007
u[75]	C(13)···H(20)	2.1161	0.0084	2.1134	0.0084	0.1072	Tied to u[90]	0.62	0.0027	0.0000	5.5	0.1036
u[74]	C(13)···H(19)	2.1161	0.0084	2.1134	0.0084	0.1072	Tied to u[90]	0.62	0.0027	0.0000	5.5	0.1036
u[79]	O(15)···O(17)	2.1677	0.0072	0.0072	0.0072	0.0513	0.0019	0.62	0.0087	0.0000	57.1	0.0520
u[34]	O(5)···O(7)	2.1757	0.0077	2.1670	0.0077	0.0513	Tied to u[79]	0.69	0.0087	0.0000	62.7	0.0520
u[40]	O(7)···O(8)	2.1933	0.0059	2.1895	0.0059	0.0450	Tied to u[79]	0.69	0.0038	0.0000	62.2	0.0456

u[85]	O(17)···O(18)	2.1943	0.0059	2.1905	0.0059	0.0450	Tied to u[79]	0.62	0.0038	0.0000	56.4	0.0456
u[36]	O(5)···H(9)	2.2032	0.0074	2.1863	0.0074	0.0993	Tied to u[79]	0.69	0.0169	0.0000	7.7	0.1007
u[37]	O(5)···H(10)	2.2050	0.0072	2.1881	0.0072	0.0993	Tied to u[79]	0.69	0.0169	0.0000	7.7	0.1007
u[80]	O(15)···O(18)	2.2382	0.0040	2.2188	0.0040	0.0515	Tied to u[79]	0.62	0.0194	0.0000	55.3	0.0522
u[35]	O(5)···O(8)	2.2493	0.0064	2.2299	0.0064	0.0515	Tied to u[79]	0.69	0.0194	0.0000	60.7	0.0522
u[55]	H(11)···C(13)	2.2865	0.0086	2.2817	0.0086	0.0765	Tied to u[79]	0.62	0.0048	0.0000	5.1	0.0776
u[10]	H(1)···C(3)	2.2865	0.0086	2.2817	0.0086	0.0765	Tied to u[79]	0.69	0.0048	0.0000	5.6	0.0776
u[44]	O(8)···H(10)	2.3216	0.0123	2.2446	0.0123	0.2218	Tied to u[79]	0.69	0.0770	0.0000	7.4	0.2248
u[70]	C(13)···O(15)	2.3575	0.0059	2.3433	0.0059	0.0663	Tied to u[79]	0.62	0.0142	0.0000	39.3	0.0672
u[76]	C(14)···N(16)	2.4012	0.0104	2.3643	0.0104	0.0595	Tied to u[79]	0.62	0.0369	0.0000	33.8	0.0603
u[25]	C(3)···O(5)	2.4022	0.0098	2.3880	0.0098	0.0663	Tied to u[79]	0.69	0.0142	0.0000	42.6	0.0672
u[31]	C(4)···N(6)	2.4120	0.0067	2.3751	0.0067	0.0595	Tied to u[79]	0.69	0.0369	0.0000	37.1	0.0603
u[88]	O(18)···H(19)	2.5197	0.0106	0.0106	0.0106	0.2304	0.0121	0.62	0.0770	0.0000	6.1	0.2248
u[89]	O(18)···H(20)	2.5197	0.0106	2.4427	0.0106	0.2304	Tied to u[88]	0.62	0.0770	0.0000	6.1	0.2248
u[78]	C(14)···O(18)	2.5611	0.0084	2.4956	0.0084	0.0836	Tied to u[88]	0.62	0.0655	0.0000	36.2	0.0816
u[33]	C(4)···O(8)	2.5886	0.0080	2.5231	0.0080	0.0836	Tied to u[88]	0.69	0.0655	0.0000	39.6	0.0816
u[39]	N(6)···H(10)	2.6066	0.0115	2.5573	0.0115	0.1629	Tied to u[88]	0.69	0.0493	0.0000	5.7	0.1589
u[63]	C(12)···C(14)	2.6503	0.0062	2.6489	0.0062	0.0524	Tied to u[88]	0.62	0.0014	0.0000	26.2	0.0511
u[18]	C(2)···C(4)	2.6604	0.0088	2.6590	0.0088	0.0524	Tied to u[88]	0.69	0.0014	0.0000	28.9	0.0511
u[83]	N(16)···H(19)	2.6754	0.0126	2.6261	0.0126	0.1629	Tied to u[88]	0.62	0.0493	0.0000	5.1	0.1589
u[84]	N(16)···H(20)	2.6754	0.0126	2.6261	0.0126	0.1629	Tied to u[88]	0.62	0.0493	0.0000	5.1	0.1589
u[24]	C(2)···H(10)	2.9847	0.0084	2.9968	0.0084	0.1328	Tied to u[88]	0.69	−0.0121	0.0000	4.3	0.1296
u[28]	C(3)···O(8)	2.9858	0.0066	2.9395	0.0066	0.0768	Tied to u[26]	0.69	0.0463	0.0000	34.3	0.0818
u[23]	C(2)···H(9)	3.1077	0.0087	3.1198	0.0087	0.1215	Tied to u[26]	0.69	−0.0121	0.0000	4.1	0.1293
u[26]	C(3)···N(6)	3.1093	0.0048	0.0048	0.0048	0.0627	0.0022	0.69	0.0222	0.0000	28.8	0.0668
u[69]	C(12)···H(20)	3.2024	0.0074	3.2145	0.0074	0.1217	Tied to u[26]	0.62	−0.0121	0.0000	3.6	0.1296
u[68]	C(12)···H(19)	3.2024	0.0074	3.2145	0.0074	0.1215	Tied to u[26]	0.62	−0.0121	0.0000	3.6	0.1293
u[38]	N(6)···H(9)	3.3990	0.0101	3.3497	0.0101	0.1493	Tied to u[26]	0.69	0.0493	0.0000	4.4	0.1589
u[64]	C(12)···O(15)	3.4044	0.0095	3.3896	0.0095	0.1124	Tied to u[26]	0.62	0.0148	0.0000	27.2	0.1197
u[32]	C(4)···O(7)	3.4444	0.0063	3.4230	0.0063	0.0560	Tied to u[26]	0.69	0.0214	0.0000	29.7	0.0596
u[77]	C(14)···O(17)	3.4482	0.0100	3.4268	0.0100	0.0560	Tied to u[26]	0.62	0.0214	0.0000	26.9	0.0596
u[19]	C(2)···O(5)	3.4604	0.0119	3.4456	0.0119	0.1124	Tied to u[26]	0.69	0.0148	0.0000	29.6	0.1197
u[71]	C(13)···N(16)	3.6312	0.0084	0.0084	0.0084	0.0816	0.0039	0.62	0.0222	0.0000	22.4	0.0668
u[43]	O(8)···H(9)	3.6763	0.0112	3.5993	0.0112	0.2745	Tied to u[71]	0.69	0.0770	0.0000	4.6	0.2248
u[42]	O(7)···H(10)	3.7254	0.0116	3.6883	0.0116	0.1944	Tied to u[71]	0.69	0.0371	0.0000	4.6	0.1592

u[56]	H(11)···C(14)	3.7273	0.0088	3.7297	0.0088	0.1054	Tied to u[71]	0.62	−0.0024	0.0000	3.1	0.0863
u[22]	C(2)···O(8)	3.7308	0.0110	3.7023	0.0110	0.1062	Tied to u[71]	0.69	0.0285	0.0000	27.4	0.0870
u[11]	H(1)···C(4)	3.7374	0.0106	3.7398	0.0106	0.1054	Tied to u[71]	0.69	−0.0024	0.0000	3.4	0.0863
u[86]	O(17)···H(19)	3.7680	0.0120	3.7309	0.0120	0.1944	Tied to u[71]	0.62	0.0371	0.0000	4.1	0.1592
u[87]	O(17)···H(20)	3.7680	0.0120	3.7309	0.0120	0.1944	Tied to u[71]	0.62	0.0371	0.0000	4.1	0.1592
u[73]	C(13)···O(18)	3.9760	0.0078	3.9297	0.0078	0.0879	Tied to u[20]	0.62	0.0463	0.0000	23.3	0.0818
u[17]	H(1)···H(10)	3.9994	0.0116	4.0217	0.0116	0.1749	Tied to u[20]	0.69	−0.0223	0.0000	0.5	0.1627
u[20]	C(2)···N(6)	4.0020	0.0089	0.0089	0.0089	0.1132	0.0065	0.69	0.0112	0.0000	22.4	0.1053
u[16]	H(1)···H(9)	4.1289	0.0121	0.0121	0.0121	0.1710	0.0157	0.69	−0.0223	0.0000	0.5	0.1621
u[27]	C(3)···O(7)	4.1756	0.0085	4.1755	0.0085	0.0854	Tied to u[20]	0.69	0.0001	0.0000	24.5	0.0794
u[62]	H(11)···H(20)	4.2296	0.0116	4.2519	0.0116	0.1716	Tied to u[16]	0.62	−0.0223	0.0000	0.5	0.1627
u[61]	H(11)···H(19)	4.2296	0.0116	4.2519	0.0116	0.1710	Tied to u[16]	0.62	−0.0223	0.0000	0.5	0.1621
u[41]	O(7)···H(9)	4.3155	0.0123	4.2784	0.0123	0.1679	Tied to u[16]	0.69	0.0371	0.0000	4.0	0.1592
u[57]	H(11)···O(15)	4.4172	0.0113	4.3994	0.0113	0.1760	Tied to u[16]	0.62	0.0178	0.0000	3.5	0.1669
u[12]	H(1)···O(5)	4.4778	0.0136	4.4600	0.0136	0.1760	Tied to u[16]	0.69	0.0178	0.0000	3.8	0.1669
u[72]	C(13)···O(17)	4.5022	0.0109	0.0109	0.0109	0.0902	0.0056	0.62	0.0001	0.0000	20.6	0.0794
u[15]	H(1)···O(8)	4.5697	0.0137	4.5534	0.0137	0.1317	Tied to u[72]	0.69	0.0163	0.0000	3.7	0.1159
u[65]	C(12)···N(16)	4.7410	0.0124	4.7298	0.0124	0.1197	Tied to u[72]	0.62	0.0112	0.0000	17.1	0.1053
u[13]	H(1)···N(6)	4.9203	0.0120	4.9142	0.0120	0.1746	Tied to u[72]	0.69	0.0061	0.0000	3.0	0.1536
u[21]	C(2)···O(7)	5.0212	0.0175	5.0337	0.0175	0.1707	Tied to u[72]	0.69	−0.0125	0.0000	20.4	0.1502
u[67]	C(12)···O(18)	5.1535	0.0075	0.0075	0.0075	0.0954	0.0065	0.62	0.0285	0.0000	18.0	0.0870
u[66]	C(12)···O(17)	5.5121	0.0149	5.5246	0.0149	0.1648	Tied to u[67]	0.62	−0.0125	0.0000	16.8	0.1502
u[58]	H(11)···N(16)	5.7724	0.0145	5.7663	0.0145	0.1685	Tied to u[67]	0.62	0.0061	0.0000	2.3	0.1536
u[14]	H(1)···O(7)	5.8917	0.0229	5.9090	0.0229	0.2418	Tied to u[67]	0.69	−0.0173	0.0000	2.9	0.2205
u[60]	H(11)···O(18)	6.2189	0.0096	6.2026	0.0096	0.1271	Tied to u[67]	0.62	0.0163	0.0000	2.5	0.1159
u[59]	H(11)···O(17)	6.4799	0.0173	6.4972	0.0173	0.2418	Tied to u[67]	0.62	−0.0173	0.0000	2.4	0.2200

Table S2.

Name	Type	Value	Calculated	Difference	Uncertainty
u46	Amplitude	0.07230	0.07239	−0.00009	0.01000
u53	Amplitude	0.03690	0.03043	0.00647	0.00400
u52	Amplitude	0.04920	0.04196	0.00724	0.00500
u90	Amplitude	0.12140	0.12558	−0.00418	0.01000
u79	Amplitude	0.05200	0.05130	0.00070	0.00500
u88	Amplitude	0.22480	0.23040	−0.00560	0.02000
u26	Amplitude	0.06680	0.06275	0.00405	0.00700
u71	Amplitude	0.06680	0.08157	−0.01477	0.00700
u16	Amplitude	0.16210	0.17098	−0.00888	0.02000
u72	Amplitude	0.07940	0.09024	−0.01084	0.00800
u67	Amplitude	0.08700	0.09543	−0.00843	0.01000
u20	Amplitude	0.10530	0.11321	−0.00791	0.01000