

Supporting Information

Molecular Growth upon Ionization of Van der Waals Clusters Containing HCCH and HCN is a Pathway to Prebiotic Molecules.

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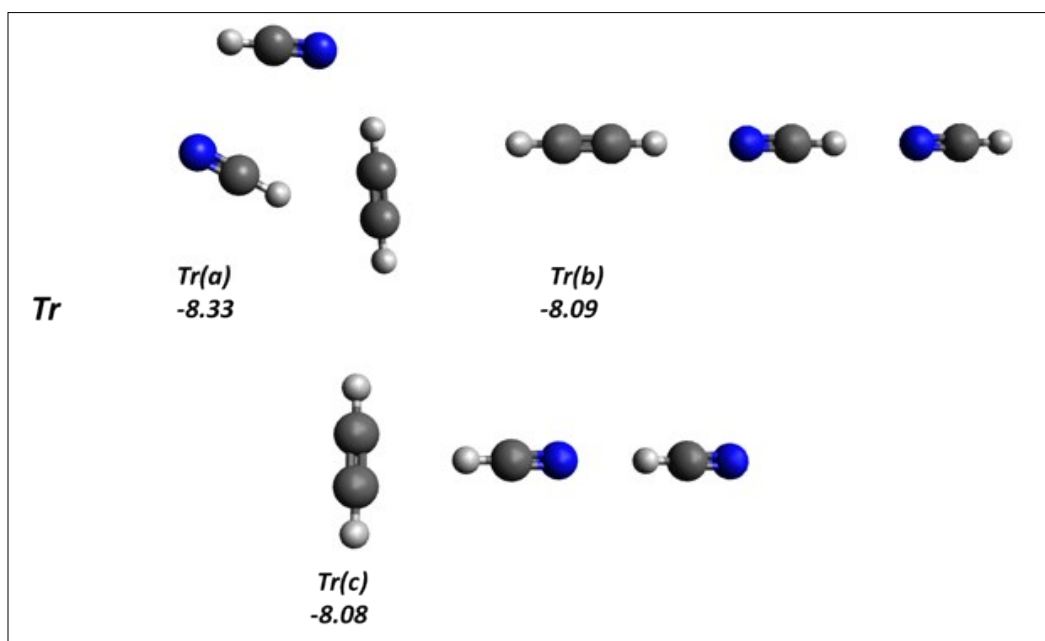
3 Space Science and Astrobiology Division, NASA Ames Research Center, Moffett Field, Mountain View, CA 94035, USA

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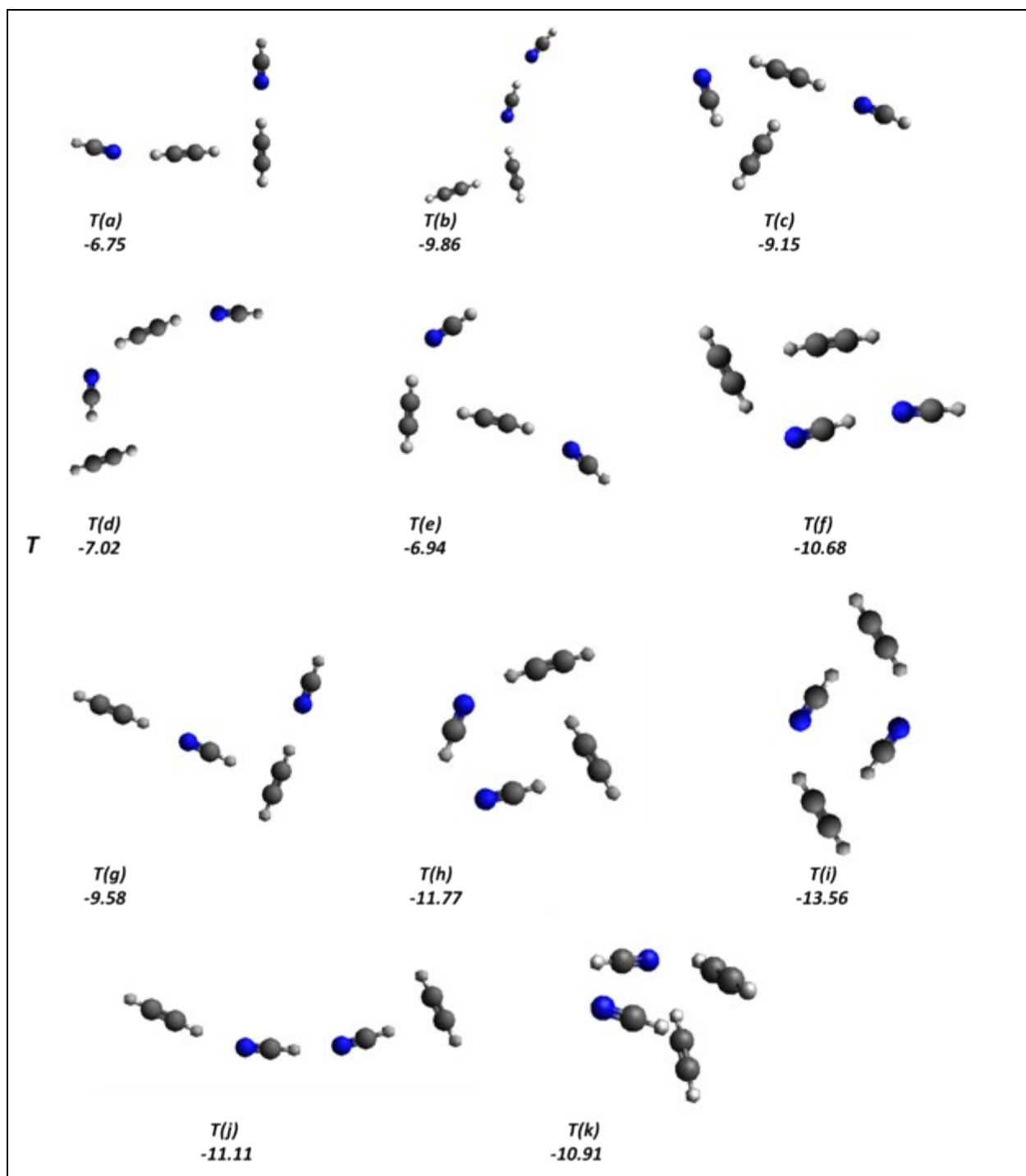
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@ These authors made equal contributions.

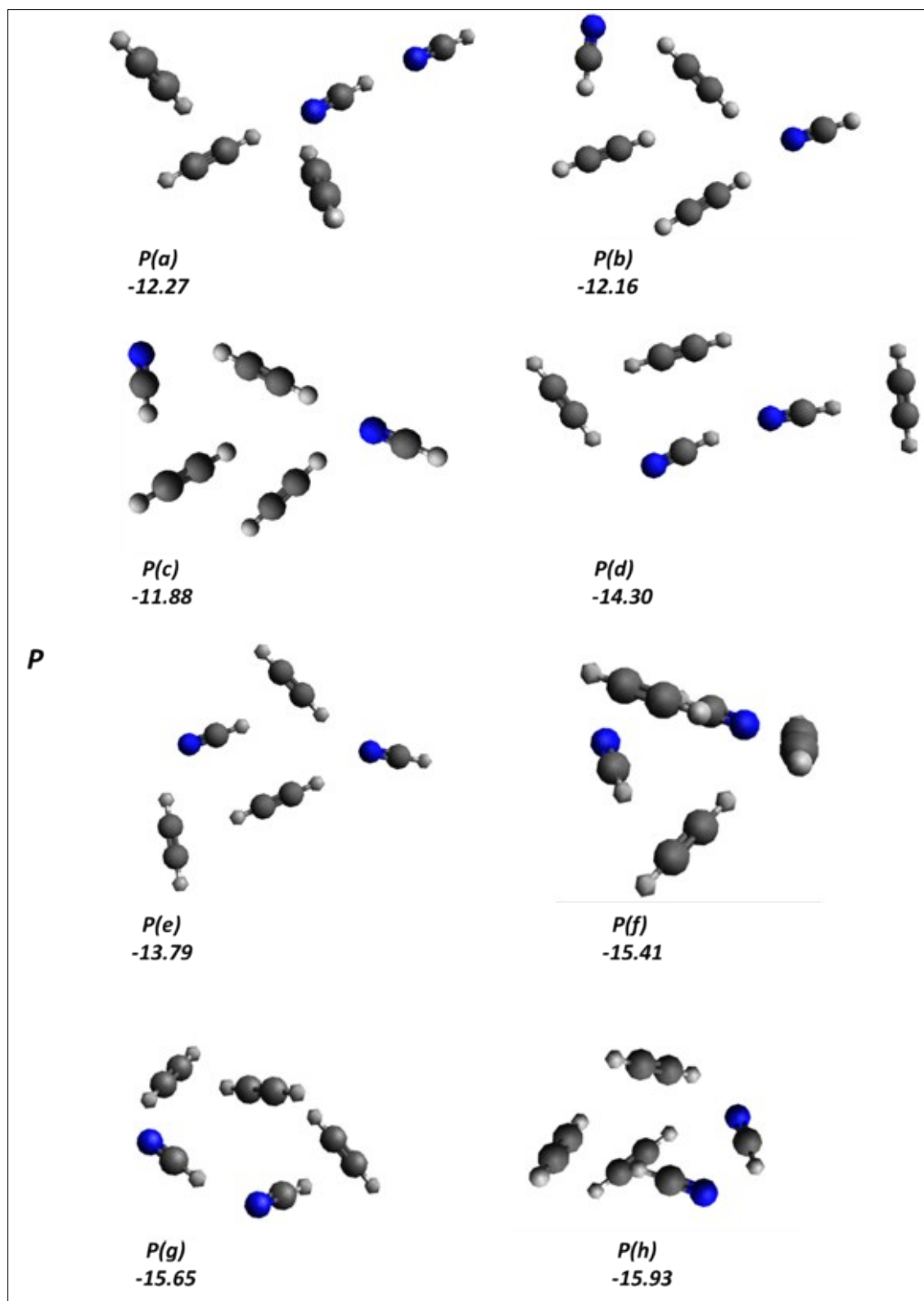
Present address: Fritz Haber Research Center for Molecular Dynamics, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel



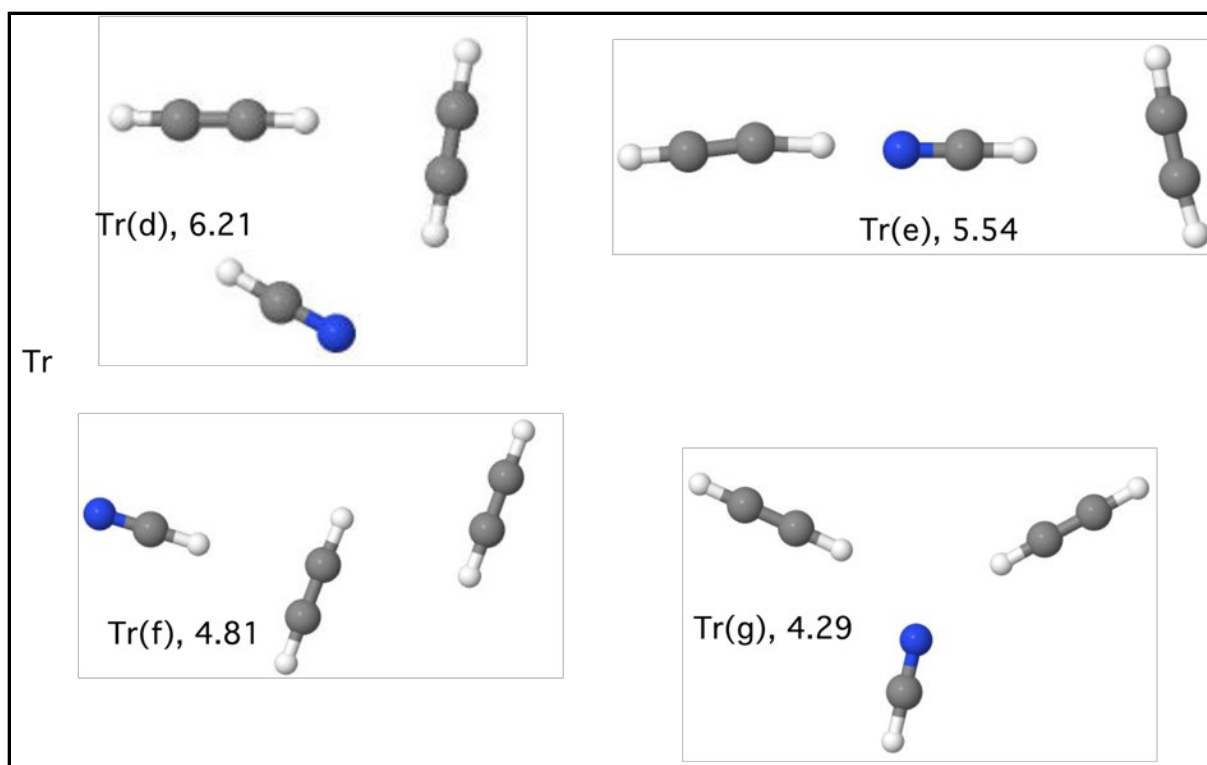
X 1: Trimer structures for 1:2 mixed clusters. BE are given in kcal/mol.



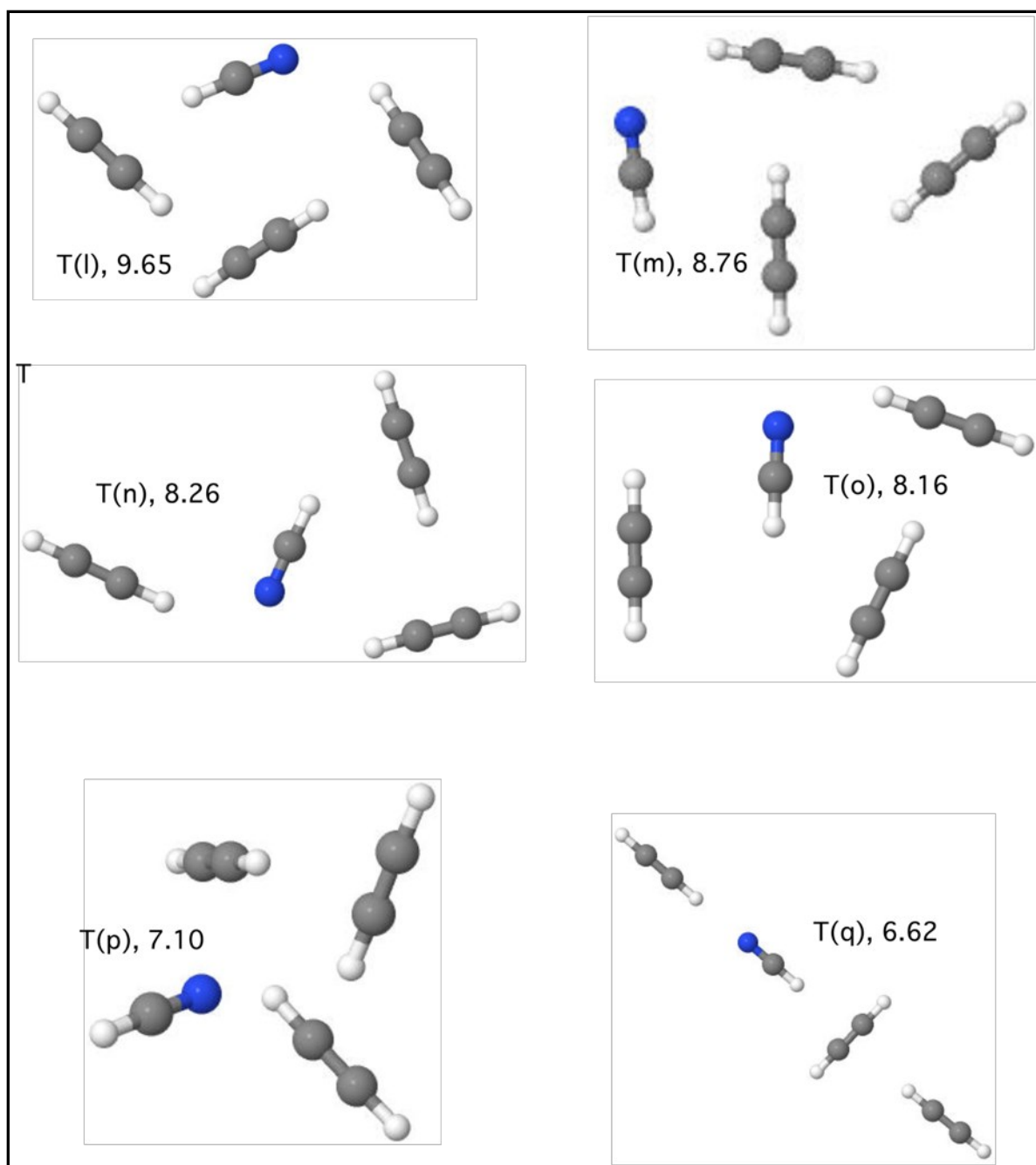
X 2: Tetramer structures for the (2:2) case. BE are given in kcal/mol.



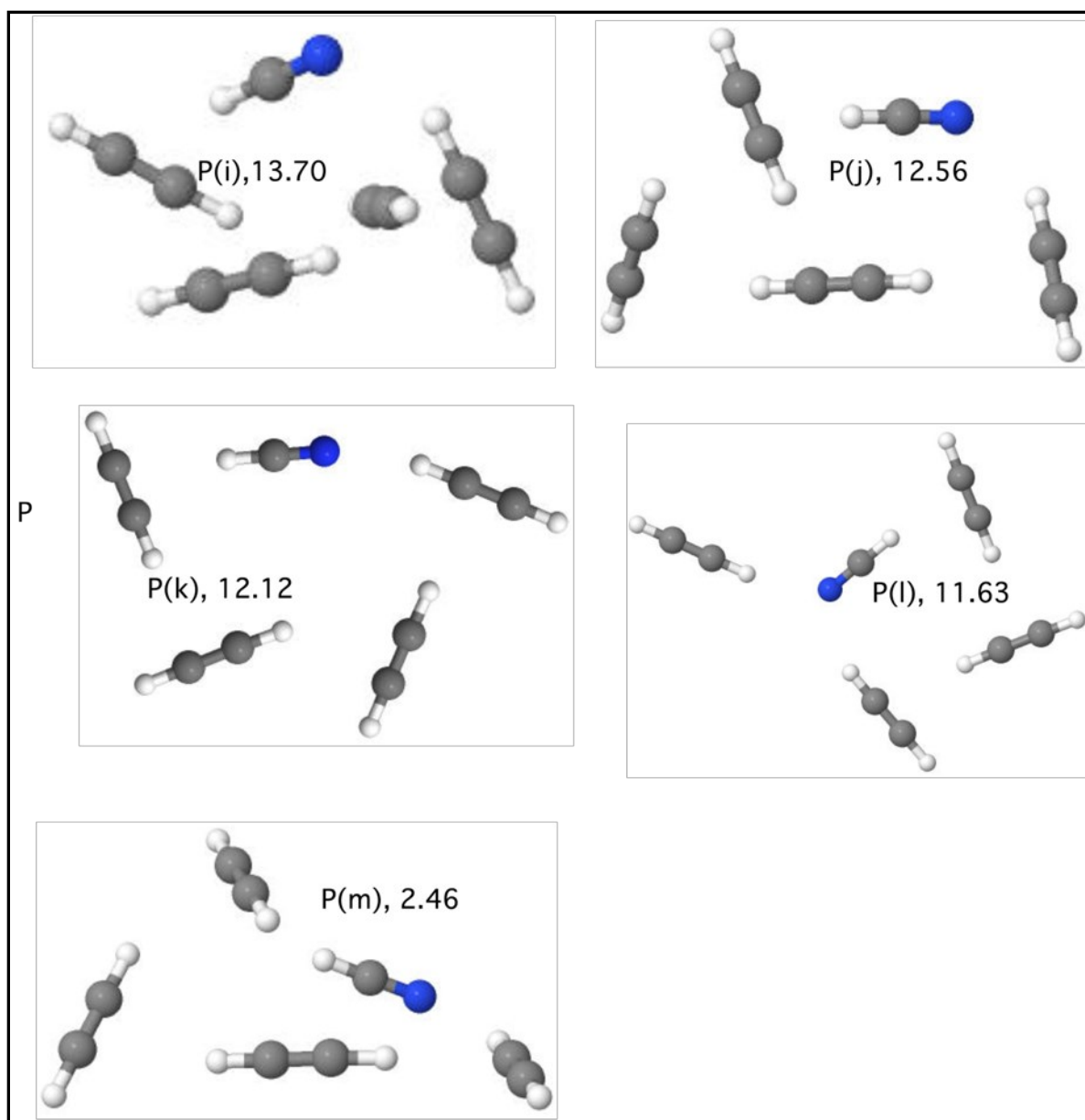
X 3: Pentamer structures for the (3:2) case. BE are given in kcal/mol.



X 4: Trimer (2HCCH and 1HCN) neutral starting geometries. BE are given in kcal/mol.



X 5: Tetramer (3HCCH and 1HCN) neutral cluster structures. BE are given in kcal/mol.



X 6: Pentamer (4HCCH and 1HCN) neutral cluster geometries. BE are given in kcal/mol.

Neutral clusters geometries

Pure HCN Clusters

2HCN

C	-7.2556743806	2.3721352200	0.0000000000
N	-6.1117332536	2.3548988813	0.0000000000
H	-8.3254178065	2.3891888854	0.0000000000
C	-2.8170379661	2.3723544079	0.0000000000
N	-1.6710759124	2.3969249386	0.0000000000
H	-3.8921103063	2.3518609551	0.0000000000

3HCN

C	-5.3565448798	0.4898586286	0.0000000000
N	-4.2142701307	0.4267699501	0.0000000000
H	-6.4247492911	0.5485021503	0.0000000000
C	-0.9777721680	0.3670349531	0.0000000000
N	0.1672149920	0.3663437880	0.0000000000
H	-2.0556336562	0.3697475883	0.0000000000

C	3.4115569987	0.4579996207	0.0000000000
N	4.5573018173	0.5046786145	0.0000000000
H	2.3353453179	0.4156007063	0.0000000000
C	-5.1668801480	0.5689662784	-0.1276272363
N	-4.0987742860	0.8355201433	-0.4408450504
H	-6.1664837660	0.3207342235	0.1642730314
C	-0.8105351866	0.2535875081	0.0259679171
N	0.2967286029	0.0247455374	0.2149647323
H	-1.8472785838	0.4664116427	-0.1500688192
C	-3.6385698017	3.1686478495	-2.8823402573
N	-3.8634291662	3.9460109560	-3.6941140524
H	-3.4433166647	2.4392538610	-2.1224862651
C	-5.2067169679	2.2533460595	0.0000000000
N	-4.5705242692	3.2067362008	0.0000000000

H	-5.7630079947	1.3363875453	0.0000000000
C	-1.6193553554	2.0933067185	0.0000000000
N	-1.1560795740	1.0450468335	0.0000000000
H	-2.0930364828	3.0551066360	0.0000000000
C	-3.5813311724	-0.9572864563	0.0000000000
N	-4.7239960780	-0.8686415338	0.0000000000
H	-2.5095453461	-0.9930174984	0.0000000000

4HCN

C	-5.0666078237	-0.1701571996	0.7967086248
N	-4.2317088474	0.1302551458	1.5215640132
H	-5.8247197495	-0.4317710585	0.0792939607
C	-1.6881304229	1.6209844296	0.4316278550
N	-1.0994721292	2.0739786834	-0.4410357994
H	-2.2762529959	1.1827588057	1.2192338739
C	-2.3052158440	2.0027958245	-3.3426499569
N	-3.1461589132	1.7103247072	-4.0638689695
H	-1.5416258410	2.2577796844	-2.6284894779

C	-5.6850226611	0.2110740775	-2.9777830551
N	-6.2691010544	-0.2490101238	-2.1059176706
H	-5.1008957177	0.6553160239	-3.7648963984
C	-5.2183569746	0.9433768664	0.5037999792
N	-4.5537932316	1.3025495264	1.3655545920
H	-5.8107541533	0.5980738327	-0.3191615505
C	-1.6756563907	0.5981217118	0.4646664637
N	-1.1270830817	0.0945677216	-0.4075003263
H	-2.2404184354	1.0588947745	1.2541831559
C	-3.3820664122	1.1538888376	-2.6150603484
N	-4.4902332459	1.4441711112	-2.5802880931
H	-2.3473901760	0.8785115636	-2.6171110851
C	-3.4527985224	-2.1441520851	-0.8667893377
N	-4.5592596588	-1.8463012900	-0.8640773064
H	-2.4131437175	-2.3963535706	-0.8660261435

C	-5.4512202550	0.2679931161	0.1621409378
N	-4.3073865038	0.2709445641	0.1826164580
H	-6.5211006424	0.2659305043	0.1427351645
C	-1.0941190273	0.4216808083	0.0190405161
N	0.0430503148	0.5077416347	-0.0804060000
H	-2.1661982060	0.3445539839	0.1083601883
C	3.1822972431	0.9117934330	-0.4336148624
N	4.3070400387	1.0801663816	-0.5680430011
H	2.1207237679	0.7557587591	-0.3078513749
C	7.4680067306	1.5945685849	-0.9965082195
N	8.5876688652	1.7828553875	-1.1569628215
H	6.4154256742	1.4186598425	-0.8467029853

5HCN

C	-5.3507966035	1.1868361063	0.1652023210
N	-5.0411784105	0.5945245279	1.0952872140
H	-5.6009670269	1.7465110223	-0.7166631584

C	-2.0551142679	0.1226953415	-0.4559618635
N	-1.4849016823	0.6045348903	-1.3253566364
H	-2.6102969274	-0.3116300267	0.3506389166
C	-3.3195760781	2.9818139453	-2.3052656245
N	-4.4044475219	3.2803780817	-2.0879428043
H	-2.3099537441	2.6695713410	-2.4825125500
C	-4.3006408600	-0.8080381041	-3.4150627027
N	-4.8582731110	-0.2189755802	-2.6063401534
H	-3.7778384102	-1.3575529734	-4.1691417856
C	-4.3022319251	-1.1202374647	3.7384401668
N	-3.8834722466	-1.7793553416	4.5784131293
H	-4.6806111845	-0.5054837656	2.9395875312
C	-6.2332226052	0.0706718018	0.3666991689
N	-5.1478562948	0.0684877744	-0.0003557002
H	-7.2485810691	0.0783424785	0.7025282392
C	-2.0227673023	0.9769416292	-0.6848932230

N	-1.6529086305	0.0570452102	-1.2598785467
H	-2.3990381879	1.8449658599	-0.1725797975
C	-7.0477733323	1.3450872430	-2.7984093286
N	-7.3826753882	2.2453009349	-2.1725252935
H	-6.6890929276	0.4937185854	-3.3544096395
C	-4.0956857054	-1.0171747363	-2.9950437028
N	-5.0950946271	-0.9617646230	-3.5527471967
H	-3.1599018393	-1.0288307053	-2.4621204533
C	-4.9627853696	3.5179698405	-0.4960618900
N	-3.9108236744	3.4932741617	-0.0424472151
H	-5.9444270482	3.5029805462	-0.9346344241
C	-6.3901212435	1.5170339152	2.2899954200
N	-5.2989454622	1.1757667947	2.3619378302
H	-7.4179499584	1.8240532924	2.1775082174
C	-9.5255753141	1.8212718406	-0.1485130847

N	-9.1657914784	2.0222900476	0.9203511243
H	-9.8228726933	1.6157282729	-1.1647104743
C	-8.4698112682	0.4273424768	-3.7263144151
N	-9.3428752561	0.8755623659	-3.1353845860
H	-7.6210478248	0.0081243557	-4.2434300839
C	-4.6589665628	-0.7076817944	-3.5156411681
N	-5.5592338483	-0.6347196165	-4.2202748004
H	-3.8379143776	-0.7598167980	-2.8184123390
C	-3.3843591247	-0.0472814877	0.2009986310
N	-3.0659976808	-0.4337715898	-0.8294752042
H	-3.7262289069	0.3256189246	1.1536309330
C	-8.4947318222	1.2186466484	4.1651134238
N	-8.3382364205	1.2061985710	3.0124227427
H	-8.1905638700	1.1966962831	2.0098713993
C	-7.5603155482	1.2001665680	-1.0031764774
N	-7.8275308065	1.1885583655	0.1093600861

H	-7.3156291266	1.2046385227	-2.0553275143
C	-6.7745959767	1.1931340743	-5.2479231162
N	-7.0248493121	1.0893305824	-4.1352502841
H	-6.5634127052	1.2698018155	-6.3040556429
C	-9.3419530963	-1.2425041812	-5.6561638016
N	-9.3855100145	-1.2825589363	-6.8001406833
H	-9.2929138826	-1.1998698073	-4.5883184630
C	-7.6143356352	0.1166056847	-8.8435385511
N	-6.8483523714	0.8135264287	-8.3550549481
H	-8.3390134130	-0.5412266185	-9.2761901698
C	-5.5037113964	1.5710242289	2.3313821451
N	-4.4274700343	1.3869695298	2.6808905353
H	-6.5074910421	1.7383356880	1.9911460205
C	-8.5757963669	1.4571284546	-0.3301710274
N	-8.4185747917	1.8765396395	0.7242976731
H	-8.7201873864	1.0585560147	-1.3271951766

C	-8.9927262495	-0.1674322498	-4.2687662841
N	-8.9282965547	0.2787048283	-3.2167543118
H	-9.0518064476	-0.5883728443	-5.2609589172
C	-9.1275804542	-1.8830580521	-8.2654265027
N	-9.1194384159	-1.4289253809	-7.2156324583
H	-9.1355915136	-2.3095503261	-9.2468280154
C	-9.8769140997	3.6741670375	3.0963359892
N	-10.4265818237	4.3087160200	3.8771785858
H	-9.3636094238	3.0802194120	2.3628097449
C	-5.3202302773	-0.1430901037	0.6373075020
N	-4.1901008588	-0.0359592555	0.4904372063
H	-6.3857425111	-0.2420019704	0.7768063620
C	-1.0698983363	0.3412151024	0.0777019146
N	0.0551379015	0.4909245443	-0.0736648911
H	-2.1328467469	0.2018450253	0.2197874690
C	3.1609797304	0.9485920201	-0.5145385459

N	4.2825006403	1.1184120011	-0.6722199618
H	2.1022049164	0.7889803746	-0.3648201681
C	7.4285543261	1.7059871650	-1.0780153180
N	8.5444249418	1.9309818400	-1.2170296554
H	6.3792635307	1.4966289759	-0.9470898536
C	-9.6181585087	-0.4962188649	1.2648726677
N	-8.4921859881	-0.4134077091	1.0808406751
H	-10.6714707746	-0.5738731467	1.4370605980

Mixed Clusters

1HCCH:1HCN

C	-5.4183825730	3.3410506134	0.4259096918
C	-4.2299471511	3.4820532854	0.4429306265
H	-6.4787303389	3.2270097472	0.4146845270
N	-4.2916722655	-1.1332147558	-0.8988177226
C	-4.4163433713	-0.0389049594	-0.5815245835
H	-3.1724003881	3.6191108099	0.4617045399

H	-4.5332064003	0.9857482730	-0.2848379522
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C	-5.5518728464	3.6248015116	-0.2108758888
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C	-4.4382661061	3.5552773091	0.2229896573
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H	-6.5434709184	3.6862341688	-0.5961693869
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H	-3.4430724728	3.4935561696	0.6088723392
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N	-1.1952961570	3.3535808062	1.3759717915
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C	-0.0914681816	3.2646652451	1.6654818393
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H	0.9399516559	3.1818055930	1.9354732708
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2HCCH:1HCN

C	4.368455	-0.797427	-0.009124
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C	4.169373	0.387834	0.032532
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H	4.613848	-1.839654	-0.049672
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H	4.045896	1.447899	0.072396
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H	1.479725	-0.124321	-0.006251
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C	0.378205	-0.071794	0.011453
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N	-0.774414	-0.016891	0.056828
H	-2.271322	0.144864	-0.104277
C	-3.494616	0.241610	-0.070137
C	-4.749390	0.147704	-0.037890
H	-5.832432	0.098355	-0.063634
C	2.2131983	0.3632655	0.0111116
C	2.3849906	1.5481280	0.0251004
H	2.0530044	-0.6933975	-0.0004832
H	2.5515849	2.6008634	0.0370799
C	-1.4343977	1.2836221	-0.0220289
C	-2.6317858	1.2725907	-0.0382313
H	-3.6976432	1.2836570	-0.0534327
H	-0.3642688	1.2905834	-0.0075192
N	0.3206868	-2.5219094	-0.0060962
C	-0.7002176	-2.0010140	-0.0042420

H -1.6353408 -1.4792365 -0.0027431

N -0.0117431 -1.4781973 0.0106068

C -0.2674762 -2.5937584 0.0385988

H -0.5064223 -3.6359855 0.0648744

C -3.6698179 1.3909000 -0.0102354

C -2.5816790 0.8932876 -0.0105928

H -4.6373481 1.8366904 -0.0100200

H -1.6127775 0.4447784 -0.0109079

H 1.8062122 0.1453702 -0.0052517

C 2.7389039 0.6665466 0.0017373

C 3.7860197 1.2459507 0.0100533

H 4.7172074 1.7635281 0.0174682

C	-0.1851492	-0.5660279	-0.0131336
H	-0.6590900	0.3891729	-0.0177567
C	0.3189950	-1.6560708	-0.0067671
H	0.7584565	-2.6270097	-0.0023259
C	-4.2544215	1.0445718	-0.0068722
C	-3.7664014	-0.0517641	0.0182731
H	-4.6961091	2.0135046	-0.0285603
H	-3.3319170	-1.0241292	0.0429789
N	4.5559482	0.8459997	0.0051269
C	3.4799612	0.4410053	0.0033327
H	2.4791177	0.0561773	0.0007782

3HCCH:1HCN

C	0.4899019	-1.7935888	-0.4022802
C	-0.4008672	-2.4865530	-0.8038457
H	1.2982222	-1.1822292	-0.0584504
H	-1.1864002	-3.1073535	-1.1702980
C	-2.9048719	-0.4709806	0.8177422

C	-3.8188535	0.2905373	0.6811361
H	-4.6418680	0.9594999	0.5716513
H	-2.0818315	-1.1440110	0.9249858
N	0.4026340	2.1070229	-0.9801877
C	-0.6219157	1.6370699	-0.7741874
H	-1.5743418	1.1887584	-0.5616343
C	3.1742272	0.6848961	0.2016540
C	3.8061618	-0.1796902	0.7377192
H	2.5935425	1.4453844	-0.2765547
H	4.3782622	-0.9424065	1.2140428

C	2.100176	-0.640406	-0.038248
C	2.153402	0.557303	-0.065641
H	2.067820	-1.706359	-0.018712
H	2.206076	1.622361	-0.089550
H	-0.448232	0.107830	0.097108

C	-1.521094	0.100668	0.101867
N	-2.666743	0.089184	0.103963
H	-4.991163	0.023764	-0.013436
C	-6.060455	0.006688	-0.042102
C	-7.259077	-0.011365	-0.073546
H	-8.323438	-0.025107	-0.096813
H	4.880163	-0.105133	-0.003590
C	5.945880	-0.058166	-0.006448
C	7.142906	-0.000608	-0.011377
H	8.207183	0.045206	-0.015774

C	3.2320950	-0.5582128	0.0012917
C	4.1471246	0.2131866	0.0076530
H	2.4142631	-1.2447278	-0.0047135
H	4.9679327	0.8929667	0.0138824
C	0.6236917	2.0367383	-0.0124401

C	-0.5575831	2.2357188	-0.0146752
H	-1.6140294	2.3943813	-0.0167938
H	1.6742287	1.8455723	-0.0101876
C	-0.3411405	-2.6687978	-0.0051792
C	-0.3359773	-1.4708787	-0.0056912
H	-0.3233088	-0.3995092	-0.0062594
H	-0.3385639	-3.7348054	-0.0044206
C	-3.4820140	-0.3316953	-0.0224544
H	-3.3281140	-1.3902444	-0.0269979
N	-3.6197497	0.8058004	-0.0171807

C	-0.492012	-1.534669	1.562549
C	-1.553372	-1.894426	1.988609
H	0.446605	-1.197881	1.179362
H	-2.491466	-2.223645	2.371520
C	-1.486080	1.656877	0.059517

C	-1.408583	2.852935	0.021431
H	-1.356180	3.916502	-0.002694
H	-1.529866	0.590324	0.093540
C	3.030882	0.281230	0.777381
C	2.055959	0.783887	0.293046
H	1.175582	1.219330	-0.126867
H	3.903975	-0.154898	1.205023
N	-0.147101	-0.835561	-1.756329
C	-0.119778	-1.283455	-2.810495
H	-0.099163	-1.697874	-3.795291

C	3.1861509	-1.2389826	0.0369941
C	4.1455520	-0.5267580	0.1145388
H	2.3238784	-1.8669606	-0.0323354
H	5.0073780	0.0966049	0.1840525
C	1.2226134	1.9589564	-0.0280304

C	0.3734510	2.8025528	-0.0628003
H	-0.3689365	3.5667585	-0.0931524
H	1.9806639	1.2041141	0.0033223
N	-0.1628570	-1.9361203	-0.1580556
C	-0.5817302	-0.8691280	-0.1484587
H	-0.9576542	0.1331086	-0.1358633
C	-3.8813470	-0.7979574	0.0785912
C	-4.2359504	0.3447619	0.0933639
H	-4.5659931	1.3580302	0.1079676
H	-3.5611260	-1.8154985	0.0653748

C	2.700108	-1.693196	0.027294
C	3.836791	-1.311527	0.030831
H	1.690498	-2.039746	0.024980
H	4.848504	-0.976318	0.034119
C	2.327450	2.116510	-0.036205

C	1.856980	3.219728	-0.037232
H	1.462106	4.209661	-0.038502
H	2.734814	1.127911	-0.035151
N	-0.861215	-0.908176	0.014130
C	-0.468049	0.168837	0.012840
H	-0.076043	1.167436	0.011250
C	-4.307320	-0.957821	0.009520
C	-5.426420	-0.527929	0.007948
H	-3.308213	-1.335168	0.011058
H	-6.420841	-0.146366	0.006628

4HCCH:1HCN

C	0.1465491	-1.6705097	-0.0178406
C	-1.0150832	-1.3988314	-0.1323080
H	1.1826548	-1.9237369	0.0674885
H	-2.0504444	-1.1558280	-0.2379648
C	-0.9824426	2.9160650	1.1526383
H	-1.1046852	3.9507607	0.9246359

C	-0.8425963	1.7583282	1.4272221
H	-0.7126209	0.7217540	1.6533292
C	-4.7412140	-0.2236721	-0.3986791
H	-5.3540470	-1.0022640	-0.7920058
C	-4.0612047	0.6565473	0.0434724
H	-3.4472953	1.4356710	0.4385121
N	2.7060531	0.9467415	-1.4182814
C	1.6880607	1.2993659	-1.0279770
H	0.7413365	1.6241411	-0.6426139
C	3.7592025	-3.0772860	0.2026418
H	3.7183949	-4.0121566	0.7127704
C	3.8181862	-2.0300360	-0.3751779
H	3.8532259	-1.0914321	-0.8873124
C	0.1465491	-1.6705097	-0.0178405
C	-1.0150832	-1.3988314	-0.1323080
H	1.1826548	-1.9237369	0.0674882

H	-2.0504444	-1.1558280	-0.2379640
C	-0.9824426	2.9160650	1.1526382
H	-1.1046852	3.9507607	0.9246352
C	-0.8425963	1.7583282	1.4272220
H	-0.7126209	0.7217540	1.6533292
C	-4.7412140	-0.2236721	-0.3986798
H	-5.3540470	-1.0022640	-0.7920051
C	-4.0612047	0.6565473	0.0434720
H	-3.4472953	1.4356710	0.4385123
N	2.7060531	0.9467415	-1.4182813
C	1.6880607	1.2993659	-1.0279773
H	0.7413365	1.6241411	-0.6426139
C	3.7592025	-3.0772860	0.2026418
H	3.7183949	-4.0121566	0.7127704
C	3.8181862	-2.0300360	-0.3751779
H	3.8532259	-1.0914321	-0.8873124

C	4.407533	-1.811617	0.000000
C	3.916317	-0.706283	0.000000
H	4.852926	-2.788012	0.000000
H	3.472543	0.275420	0.000000
C	-2.010954	2.952179	0.000000
H	-1.616536	3.950194	0.000000
C	-2.455832	1.827569	0.000000
H	-2.871659	0.833715	0.000000
C	2.562746	2.721227	0.000000
H	3.543066	3.156445	0.000000
C	1.454643	2.236844	0.000000
H	0.454285	1.838993	0.000000
C	-3.612419	-1.664119	0.000000
H	-2.601277	-2.041958	0.000000
C	-4.736347	-1.217084	0.000000
H	-5.736086	-0.828744	0.000000
C	0.755087	-2.162609	0.000000

H	1.831251	-2.032588	0.000000
N	-0.391518	-2.290522	0.000000
C	3.5332715	-0.6858663	0.0068587
C	4.5133833	0.0222124	0.0088909
H	2.6710318	-1.3322414	0.0043980
H	5.3913319	0.6396246	0.0099402
C	2.0400752	2.7603521	0.0030198
C	1.3371547	3.7445141	0.0017267
H	0.7317623	4.6312195	0.0007844
H	2.6615087	1.8790568	0.0042222
N	-1.4994437	-0.1657902	-0.0228563
C	-0.8233222	0.7702909	-0.0168081
H	-0.1747333	1.6396964	-0.0110265
C	0.4453069	-2.9704264	-0.0047857
C	1.4160318	-3.6910532	0.0025877
H	-0.4177246	-2.3264237	-0.0093639

H	2.2729990	-4.3371248	0.0118532
C	-6.1213547	0.1587222	0.0192545
H	-7.1728930	0.3691503	0.0306385
C	-4.9362868	-0.0756686	0.0019149
H	-3.8790410	-0.2763345	-0.0156969
C	1.2558679	-1.1784742	1.4552424
C	0.8721448	-2.1360098	2.0632619
H	1.6171769	-0.3304593	0.9143497
H	0.5414073	-2.9931782	2.6042499
C	-2.4588162	-1.5276348	0.6966568
C	-3.4153287	-1.7613677	0.0147190
H	-4.2734827	-1.9765164	-0.5802760
H	-1.5928252	-1.3172927	1.2883494
N	0.6892063	-0.4193644	-2.4406076
C	-0.2954899	-0.6830528	-1.9169479
H	-1.2110507	-0.9267480	-1.4114292

C 2.8941857 1.3911500 -0.8218325

C 3.2516646 1.9576784 0.1712583

H 2.5543510 0.8746801 -1.6949368

H 3.5846280 2.4625874 1.0493538

C -0.6104403 2.0258874 0.2228229

H 0.4070547 2.2054633 -0.0492580

C -1.7500095 1.8236822 0.5290301

H -2.7641991 1.6380806 0.799390

1HCCH:2HCN

C 1.6338874974 0.0000000000 -0.6233062437

H 1.4913158293 0.0000000000 0.4378830948

C 1.7794361193 0.0000000000 -1.8124212018

H 1.9331746804 0.0000000000 -2.8674207699

N 0.0190557315 0.0000000000 2.3367471532

C -1.1255714145 0.0000000000 2.3863498898

H -2.1957351004 0.0000000000 2.4024124926

H -0.8455537570 0.0000000000 -1.2902426481

C	-1.8270670004	0.0000000000	-0.8531132464
N	-2.8555454987	0.0000000000	-0.3464875084
N	-0.4853662238	0.5697058996	6.1961724732
C	-0.3412508315	0.3415462751	5.0828597468
N	0.0449057598	-0.3083442034	1.9084169331
C	0.1553000856	-0.5289334181	0.7911994720
H	0.2583368692	-0.7349802891	-0.2534988831
H	-0.7748506970	1.0396115177	8.4723578978
C	-0.9020196985	1.2522933393	9.5140432417
C	-1.0435691956	1.4901060274	10.6788888037
H	-1.1693954063	1.7013673204	11.7152883703
H	-0.2064385850	0.1271532398	4.0364124305
C	-3.3804686424	1.6751993988	-0.0005385839
N	-2.7857620268	2.6533752402	-0.0011003007

H	-3.9394452867	0.7566699215	-0.0000485735
C	-1.0924748646	5.4503616383	-0.0010105451
N	-0.5017130918	6.4331164691	-0.0008827196
H	-1.6471789444	4.5283044862	-0.0011254225
C	-4.7324686768	-1.6885121329	0.0019357725
C	-5.7560921601	-1.0679167775	0.0004087788
H	-3.8293826229	-2.2562790955	0.0033014396
H	-6.6769728429	-0.5294696433	-0.0009398458

2HCCH:2HCN

C	-1.9350788835	5.1232701573	0.0510548598
C	-0.8148617037	4.7005429151	0.0294551583
H	-2.9311753951	5.4987958978	0.0703810841
H	0.1861947987	4.3221699507	0.0109244519
C	-2.6125594786	1.3277079132	-0.0636433274
C	-3.0775186165	0.2259972788	-0.0833700103
H	-2.2045060165	2.3129908826	-0.0466895575
C	-4.2466753254	-4.2358500508	0.0421323058

N	-4.1273474182	-3.1017721340	-0.0532765916
H	-4.3589122982	-5.2951994084	0.1309820457
N	2.4029226265	3.5480242532	-0.0088469513
C	3.4872781557	3.1804128100	0.0045805858
H	4.4966038461	2.8261630373	0.0157798049
H	-3.4892547954	-0.7606268498	-0.0994640098
C	-0.9270674788	6.8649557251	0.0184494300
C	-0.4189539189	5.7799748902	0.0230564223
H	-1.3807289374	7.8302991022	0.0160604589
H	0.0345054955	4.8115690961	0.0247941440
N	-1.9106901238	0.1750953106	-0.0450247735
C	-2.5079484635	-0.8019693378	-0.0615562182
C	-3.9174951682	-4.9222919085	0.0401457014
N	-3.7921482930	-3.7874065915	-0.0309873946
H	-4.0391273216	-5.9814757693	0.1037732812

C	0.8039709192	2.1921941654	-0.0071951872
C	1.8533178582	2.7636304537	0.0016299522
H	2.7880117683	3.2685110137	0.0086270330
H	-3.0568087291	-1.7278058432	-0.0742147609
H	-0.1272464784	1.6573127787	-0.0175581912
N	-1.3831537146	5.3119204895	-0.0182646782
C	-0.4750049395	4.6122149680	-0.0208135724
H	0.3530255776	3.9295785924	-0.0223737441
C	-3.0103631411	2.0360334219	0.0200805600
C	-3.0031310174	0.8377304910	0.0234085448
C	-2.7327013616	-3.7211434975	-0.0136122007
N	-2.7920245801	-2.5781637164	0.0098792147
H	-2.6773541773	-4.7886870524	-0.0357732811
C	0.6876156828	1.3941495579	0.0069223819
C	1.8589309525	1.6441666670	0.0003640536

H	2.9053365208	1.8471505070	-0.0051097871
H	-3.0002580990	-0.2326080014	0.0258993536
H	-0.3626163482	1.1870727498	0.0125666911
H	-3.0182256721	3.1038117533	0.0168262699
C	-1.5488542786	4.0186913737	0.0000000000
C	-0.3594347238	4.1711713393	0.0000000000
H	0.7048164429	4.2988527744	0.0000000000
N	-4.9398994171	0.7480817386	0.0000000000
C	-4.4428116459	-0.2835919299	0.0000000000
C	-3.9909604384	-3.9188366780	0.0000000000
C	-2.8226424111	-3.6600531858	0.0000000000
H	-5.0311160241	-4.1562611728	0.0000000000
N	3.1103450219	4.5081394978	0.0000000000
C	4.2562570288	4.5269610700	0.0000000000
H	5.3247052213	4.5593768629	0.0000000000

H	-3.9852565364	-1.2534886209	0.0000000000
H	-1.7774967907	-3.4457074082	0.0000000000
H	-2.6024744053	3.8636745319	0.0000000000
C	-2.2286629269	5.0469056397	0.0000000000
C	-1.0317918580	4.9879183135	0.0000000000
H	0.0346766869	4.9094967011	0.0000000000
C	-1.8134356211	1.2517783076	0.0000000000
C	-2.1017978184	0.0890323584	0.0000000000
C	-4.1982767560	-3.9761683339	0.0000000000
N	-3.4436120741	-3.1147538617	0.0000000000
H	-4.9084595910	-4.7770107476	0.0000000000
N	2.1036023464	3.7431138344	0.0000000000
C	2.8117041274	2.8423923098	0.0000000000
H	3.4811516185	2.0104813015	0.0000000000
H	-2.3740810752	-0.9454407653	0.0000000000
H	-3.2919651317	5.1059911396	0.0000000000

H	-1.5713701943	2.2941530978	0.0000000000
N	-4.8298132978	3.7668311372	-1.5520935886
C	-5.6903208618	4.3620438252	-2.0173191846
H	-6.4949102570	4.9215701060	-2.4472785367
N	-2.5601840932	1.7641917409	1.6671799465
C	-3.0244512824	2.2870335157	0.7570329021
H	-3.4729326894	2.7845164761	-0.0856597023
C	-2.0443826775	5.5528033797	0.9877582733
C	-2.2668775329	5.8359401532	-0.1542467195
H	-1.8431578349	5.2901581838	2.0037301412
H	-2.4608172557	6.0856558427	-1.1732907026
C	-1.3202681711	3.6962435711	4.1030165285
C	-1.0426283629	4.7183652681	4.6625268003
H	-0.7899503432	5.6215351541	5.1697538653
H	-1.5763974943	2.7944730413	3.5863236863

C	-0.4173048162	7.5281253467	0.0000000000
C	-0.8822786946	6.4251284649	0.0000000000
H	-0.0051047821	8.5103146970	0.0000000000
H	-1.2962829634	5.4381152484	0.0000000000
C	-4.7355311616	-0.7863364675	0.0000000000
C	-3.6146243578	-1.2099556115	0.0000000000
H	-2.6155852008	-1.5953173751	0.0000000000
N	-0.4134183358	-2.2511330002	0.0000000000
C	0.6660189695	-2.6375632935	0.0000000000
H	1.6732694319	-3.0036391067	0.0000000000
N	-2.2114971983	3.2730602570	0.0000000000
C	-2.6851693673	2.2299939907	0.0000000000
H	-3.1330360902	1.2519526102	0.0000000000
H	-5.7393377550	-0.4272296955	0.0000000000

C	3.5293530907	6.7705972746	-0.1076265088
C	3.9399564275	5.6455016401	-0.0761843781
H	3.1838941273	7.7790369948	-0.1367167159
H	4.3203313741	4.6444954182	-0.0484307948
N	1.9860220573	0.7349054160	-0.0943143333
C	0.9118929893	1.1329895669	-0.0803788623
H	-0.0776774823	1.5441617272	-0.0656490991
C	5.0945606223	2.0206661198	0.0488660941
C	6.0991717950	2.6681211560	0.1307055037
H	4.1986740848	1.4375081897	-0.0222989797
H	7.0002365818	3.2329945611	0.2035963216
N	-0.3725709865	3.9980206257	-0.0040769818
C	0.5436623520	4.6862996192	-0.0134416079
H	1.4205792193	5.3095821025	-0.0237517444

N	2.8844911739	5.4645596747	-0.0830336247
C	3.7766443197	4.7458197994	-0.0056317678
H	4.6010171211	4.0559651892	0.0609571697
N	2.4275010150	1.5500222985	0.0746646947
C	1.4219531133	2.0991486391	0.0649650629
H	0.4955813286	2.6402333950	0.0522239417
C	5.7209320836	1.8815994147	0.0722103303
C	6.7560175827	2.4863758446	0.0523685211
H	4.7783365534	1.3697836354	0.0888632308
H	7.6885612109	3.0052661295	0.0338590045
C	-1.4996311153	4.5208931879	0.0051640305
C	-0.4033375164	5.0006764595	-0.0575233740
H	-2.4887167426	4.1209524362	0.0583620786
H	0.5761858541	5.4303279041	-0.1047222734
C	-0.9384831581	8.4886462009	0.0000000000

C	-1.4566521378	7.4095717918	0.0000000000
H	-0.4782677306	9.4490169907	0.0000000000
H	-1.9162541541	6.4427734700	0.0000000000
N	-2.5905320575	-0.1600316624	0.0000000000
C	-2.2604686058	-1.2561411177	0.0000000000
H	-1.9461296940	-2.2841641009	0.0000000000
C	-1.4311353631	-4.8331138487	0.0000000000
C	-0.3678679089	-4.2837597132	0.0000000000
H	-2.3704046104	-5.3383181669	0.0000000000
H	0.5876936662	-3.8097969660	0.0000000000
N	-2.6677608765	4.2205940705	0.0000000000
C	-2.7299374021	3.0768978563	0.0000000000
H	-2.7776690611	2.0010427097	0.0000000000
C	-5.0068368666	4.7698414815	0.9565657151
C	-5.5926802923	4.5031521146	-0.0529242966

H	-6.1294416672	4.2771790790	-0.9455281816
N	-2.2197738266	1.4735175020	1.0117197088
C	-2.5435766441	2.3434739974	0.3382520472
H	-2.8478840307	3.1789683285	-0.2597921263
C	-1.4003761096	5.6359456159	0.4226398150
C	-1.1753124653	5.7224504703	-0.7497262166
H	-1.6011873117	5.5566689500	1.4690722825
H	-0.9683912639	5.8102724790	-1.7915264209
C	-2.3265918845	3.3277161797	3.5305752369
N	-2.6133281464	4.4380350071	3.4777839343
H	-2.0644326380	2.2880112941	3.5402330041
H	-4.4825099000	4.9979683015	1.8590383725

3HCCH:2HCN

C	-1.6484561506	6.2290463357	0.4852339721
C	-1.0982163825	5.2129783090	0.1732672892
H	-2.1395094005	7.1331928657	0.7617690471
H	-0.6008595413	4.3086424846	-0.1050028956

N	-1.4493696676	-0.5104664881	-0.1693790061
C	-2.0851190378	-1.4041907389	0.1609994710
C	-4.5625683458	-4.8625815043	1.1942026062
N	-3.9008720675	-3.9530849079	0.9850706402
H	-5.1815106299	-5.7129791183	1.3896092199
C	0.8506854707	1.9691411825	-0.5972953166
C	1.5946461355	2.8714832057	-0.8550049059
H	2.2568136744	3.6739572613	-1.0860834337
H	-2.6844356092	-2.2463870091	0.4670880859
H	0.1850179966	1.1616969145	-0.3728879627
C	-2.0469843082	0.9529588407	-3.3229713649
C	-2.3952358694	1.2468658759	-4.4294738908
H	-1.7395730328	0.6862994620	-2.3355500807
H	-2.7021715306	1.5124008105	-5.4143659324
N	-2.0417949552	5.2977278078	0.2645183522
C	-1.0079729112	4.8109782331	0.1690966370

H	-0.0550865088	4.3233900686	0.0802431320
C	-2.7510652250	1.6977148091	0.2504213036
C	-2.5260991245	0.5226265528	0.1923384793
C	-3.6559717159	-3.7259906651	-0.0664760363
N	-2.7561906383	-3.0184404578	-0.0422201719
H	-4.4983002791	-4.3849014875	-0.0893595587
C	1.1058561775	2.0695252815	-0.0557279380
C	2.0662167420	2.7848901542	-0.0928828083
H	2.9308772289	3.4077927258	-0.1256241418
H	-2.3459339764	-0.5285899305	0.1418555348
H	0.2483018364	1.4307552309	-0.0237449477
H	-2.9564860693	2.7443563821	0.3015238491
C	1.5147681748	-1.3001668695	-0.6733308350
C	0.4556266144	-1.8297057967	-0.4980143554
H	2.4532854021	-0.8189403425	-0.8255464196
H	-0.4905271034	-2.3013706573	-0.3433182485

N	-1.5312988867	5.3192640943	0.1646550102
C	-0.6457891379	4.6132761241	-0.0152222611
H	0.1625163740	3.9257268625	-0.1815772545
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H	-3.0120480365	-0.3196662442	-0.3084331299
H	-0.0581711530	1.0564872645	0.0078122021
H	-2.9880645074	2.9795626448	0.1746425256
C	0.4782630834	-1.0388152435	2.0847887002
C	-0.6535811923	-1.3560664612	1.8591254198

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C	-1.7697412454	-1.1187057432	0.0000000000
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C	-2.1922922302	2.1468034861	-0.2483247196
C	-2.3184387031	0.9647917933	-0.1008635304
C	-3.0181276922	-3.4576035414	0.0037100441
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H	-3.6337377273	-4.3149534385	-0.1720216538
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C	1.8320210436	-0.8451749182	1.3362347337
C	0.7243369636	-1.1734503187	1.0205544037
H	2.8190085275	-0.5600222889	1.6224691867
H	-0.2604236777	-1.4862784403	0.7446804385
C	-4.1506444256	4.5252430892	0.1740170997
C	-4.8797141209	4.1187614274	-0.6848883660
H	-5.5318989376	3.7778963526	-1.4564029283
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C	-3.6007112120	1.2747275873	1.2888448231
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C	-1.0328677934	6.6189635060	0.5517166020

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H	-1.0331810187	6.3333974558	1.5818447266
H	-1.0709782128	7.1896569004	-1.6382392743
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H	-1.6346480725	2.2751895088	3.2730064392
H	-3.4983703009	4.8895339145	0.9385116657
C	-0.6801062198	1.8267617612	-0.2420970307
C	-0.7659855884	3.0175558251	-0.3341863168
H	-0.6073480351	0.7666661815	-0.1568736289
H	-0.8416788643	4.0809476663	-0.4148047461
N	-4.3943377791	2.8927390970	-1.7235079138
C	-4.9602404316	3.8513201720	-1.4527564006
H	-5.4764606419	4.7563772470	-1.1870566148
N	-1.5837128884	1.5777017050	1.2552784115

C	-2.1825807841	1.7281558677	0.2899153372
H	-2.7625424304	1.8866737455	-0.6017542107
C	-2.1486616149	5.4146784953	0.7332936172
C	-2.1691182384	5.8127218509	-0.3964233880
H	-2.1079405104	5.0541301080	1.7402666186
H	-2.1739736584	6.1622890771	-1.4038321815
C	-1.5185836298	3.6298909533	3.8674330016
C	-1.7247781953	4.6222953284	4.5055640112
H	-1.8999770676	5.4989092571	5.0863973259
H	-1.3431867356	2.7517617340	3.2802998583
C	-5.5740794367	6.9614039060	-0.0049009050
C	-6.6646115892	7.0084918357	-0.4976687548
H	-4.5961276738	6.9077500373	0.4236481065
H	-7.6387425985	7.0716863535	-0.9271645237
C	-5.0179590255	4.8975770383	1.4101236190

C	-5.6951947797	4.6816063519	0.4464116727
H	-6.2971282257	4.4910155627	-0.4127748962
N	-2.3794650251	1.6452830759	1.1390135218
C	-2.7625572488	2.2605603921	0.2510721421
H	-3.1201838659	2.8416692640	-0.5786537157
C	-1.3168733245	5.5976065395	0.4633247536
C	-0.8962701661	5.4404032420	-0.6467264998
H	-1.6769265054	5.7268401699	1.4608729508
H	-0.5185410027	5.3032284308	-1.6344008721
C	-2.1324770135	3.5632798936	3.5391031125
N	-2.3786188221	4.6729240583	3.6886988456
H	-1.9198048938	2.5299600020	3.3479561052
H	-4.4187457169	5.0830842355	2.2754365105
C	-3.9377284416	3.6215607997	-3.0547589878
C	-3.7692322970	4.5713755468	-2.3446245744
H	-4.0939162861	2.7854566099	-3.6983753171
H	-3.6103260945	5.4071859739	-1.6987206816