Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information for

A Vacuum Ultraviolet Photoionization Study on the Formation of Methanimine (CH_2NH) and Ethylenediamine ($NH_2CH_2CH_2NH_2$) in Low Temperature Interstellar Model Ices Exposed to Ionizing Radiation

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Table S1 Data applied to calculate the irradiation dose per molecule. * values from CASINO simulations, $ derived values based on 15 nA, 20 min irradiation of CH_3NH_2.

initial kinetic energy of the electrons, E_{init}	5 keV
irradiation current, I	20 ± 2 nA
total number of electrons	$(1.1 \pm 0.3)\times10^{14}$
average kinetic energy of backscattered electrons, E_{bs}^*	3.1 ± 0.3 keV
fraction of backscattered electrons, f_{bs}^*	0.3 ± 0.1
average kinetic energy of transmitted electrons, E_{trans}^*,	2.9 ± 0.3 keV
fraction of transmitted electrons, f_{trans}^*	0.5
average penetration depth, l^*	180 ± 80 nm
density of the ice, ρ	0.85 ± 0.05 g cm^{-3}
irradiated area, A	1.0 ± 0.1 cm^2
total number of molecules processed$	$(3 \pm 1)\times10^{17}$
dose per molecule, D$	1.0 ± 0.1 eV

Table S2 Theoretical values for the molecule geometry of CNH_3 and $C_2N_2H_8$ isomers and their ions.

Atom	X	Y	Z	Atom	X	Y	Z
H_2CNH				**H_2CNH^+**			
C	0.584348	0.028954	0.000407	C	0.598498	0.023834	-0.000021
H	-1.166258	0.735956	-0.000251	H	-1.561096	0.309440	-0.000069
H	1.075482	1.006604	-0.000763	H	1.071217	1.022722	0.000044
H	1.244023	-0.838535	-0.000968	H	1.245402	-0.864826	0.000009
N	-0.665619	-0.153964	-0.000066	N	-0.620931	-0.087191	0.000021
Atom	X	Y	Z	Atom	X	Y	Z
$^3CH_3N$				**$^3CH_3N^+$**			
C	0.000000	0.000000	-0.542736	C	0.000000	0.000000	-0.661067
H	0.000000	1.027837	-0.935418	H	0.000000	1.076160	-0.862293
H	-0.890133	-0.513918	-0.935418	H	-0.931982	-0.538080	-0.862293
H	0.890133	-0.513918	-0.935418	H	0.931982	-0.538080	-0.862293
N	0.000000	0.000000	0.866096	N	0.000000	0.000000	0.936183
Atom	X	Y	Z	Atom	X	Y	Z
$CHNH_2$				**$CHNH_2^+$**			
C	-0.763425	0.191020	-0.000052	C	-0.708468	0.155030	-0.000061
H	-1.247136	-0.803479	0.000169	H	-1.572427	-0.505327	0.000151
N	0.525142	-0.024423	0.000051	N	0.527230	-0.030424	0.000071
H	1.162890	0.760881	0.000002	H	1.183835	0.756126	-0.000072
H	0.988801	-0.932556	-0.000216	H	0.948786	-0.968009	-0.000209
Atom	X	Y	Z	Atom	X	Y	Z
$^3CHNH_2$				**$^3CHNH_2^+$**			
C	-0.768492	-0.000134	0.172029	C	-0.849378	0.000034	0.156575
H	-1.560245	0.000521	-0.576784	H	-1.468652	-0.000260	-0.741014
N	0.571054	-0.000018	-0.107523	N	0.616161	-0.000017	0.018755
H	1.086806	0.834059	0.148853	H	1.125711	0.875811	-0.164974
H	1.087013	-0.833653	0.148415	H	1.126085	-0.875639	-0.164752
Atom	X	Y	Z	Atom	X	Y	Z
$CH_3NHNHCH_3$				**$CH_3NHNHCH_3^+$**			
C	-0.016087	1.827841	0.099439	C	-0.057850	1.881992	0.132329
H	0.653402	2.003275	0.944607	H	0.649709	1.977094	0.954431
H	0.205281	2.581493	-0.656072	H	0.228114	2.564111	-0.663288
H	-1.048326	1.952461	0.449831	H	-1.065870	2.120303	0.477022
N	0.249943	0.509348	-0.466674	N	-0.002265	0.526287	-0.399047
H	-0.350222	0.404574	-1.280016	H	-0.296266	0.340675	-1.350792
N	-0.249943	-0.509348	0.466674	N	0.002265	-0.526287	0.399047
H	0.350222	-0.404574	1.280016	H	0.296266	-0.340675	1.350792

C	0.016087	-1.827841	-0.099439	C	0.057850	-1.881992	-0.132329
H	1.048326	-1.952461	-0.449831	H	1.065870	-2.120303	-0.477022
H	-0.205281	-2.581493	0.656072	H	-0.228114	-2.564111	0.663288
H	-0.653402	-2.003275	-0.944607	H	-0.649709	-1.977094	-0.954431
Atom	X	Y	Z	Atom	X	Y	Z
$H_2NCH_2CH_2NH_2$				**$H_2NCH_2CH_2NH_2^+$**			
N	1.467235	-0.558223	-0.238485	N	1.649073	-0.482818	-0.106493
H	2.352613	-0.666632	0.239672	H	2.163214	-0.404393	-0.970051
H	0.922827	-1.396268	-0.067161	H	1.692992	-1.372142	0.365271
C	0.725558	0.587047	0.284633	C	0.869475	0.527303	0.347502
H	1.237868	1.506806	-0.008397	H	1.159132	1.509213	-0.013010
H	0.648177	0.603502	1.384140	H	0.647637	0.483105	1.407339
C	-0.681973	0.600997	-0.297080	C	-0.869467	0.527333	-0.347489
H	-1.175813	1.543276	-0.025829	H	-1.159102	1.509233	0.013070
H	-0.603702	0.569982	-1.384980	H	-0.647638	0.483171	-1.407330
N	-1.419651	-0.594061	0.133800	N	-1.649103	-0.482808	0.106466
H	-1.724299	-0.496049	1.095300	H	-2.163045	-0.404507	0.970153
H	-2.252264	-0.726897	-0.425272	H	-1.693030	-1.372111	-0.365331
Atom	X	Y	Z	Atom	X	Y	Z
$H_2NCH_2NHCH_3$				**$H_2NCH_2NHCH_3^+$**			
N	-1.460052	-0.588360	-0.115897	N	-1.350176	-0.650407	-0.007934
H	-2.302382	-0.661056	0.440246	H	-1.612240	-1.020626	0.893078
H	-1.728228	-0.501483	-1.088763	H	-2.064393	-0.813112	-0.699780
C	-0.663079	0.563795	0.288990	C	-0.792651	0.639634	-0.008171
H	-0.568907	0.512536	1.386199	H	-1.060042	1.262483	0.862094
H	-1.121452	1.531975	0.046790	H	-1.077541	1.228444	-0.888505
N	0.617793	0.523231	-0.390331	N	0.681601	0.622304	0.007315
H	1.046401	1.438247	-0.364617	H	1.140402	1.522759	0.134171
C	1.536167	-0.490360	0.113919	C	1.497535	-0.547831	-0.033942
H	2.462071	-0.463399	-0.460416	H	2.431510	-0.319606	-0.547820
H	1.784731	-0.369104	1.179809	H	1.757270	-0.853577	0.992699
H	1.085060	-1.472425	-0.013101	H	0.935754	-1.360861	-0.488921
Atom	X	Y	Z	Atom	X	Y	Z
$(CH_3)_2NNH_2$				**$(CH_3)_2NNH_2^+$**			
N	-0.328929	0.239419	0.000000	N	-0.105641	0.050367	0.000000
C	-0.328929	-0.587433	1.196851	C	-0.105641	-0.670272	1.268283
H	-0.345336	0.048620	2.083676	H	-0.378963	0.006386	2.075107
H	-1.232089	-1.196438	1.205462	H	-0.833915	-1.473896	1.205842
H	0.552509	-1.243562	1.256237	H	0.885488	-1.089656	1.458005
C	-0.328929	-0.587433	-1.196851	C	-0.105641	-0.670272	-1.268283
H	-1.232089	-1.196438	-1.205462	H	-0.833915	-1.473896	-1.205842
H	-0.345336	0.048620	-2.083676	H	-0.378963	0.006386	-2.075107

H	0.552509	-1.243562	-1.256237	H	0.885488	-1.089656	-1.458005
N	0.937043	0.989579	0.000000	N	0.312886	1.308805	0.000000
H	0.870093	1.614486	-0.801011	H	0.235876	1.821698	-0.868229
H	0.870093	1.614486	0.801011	H	0.235876	1.821698	0.868229

Table S3 Theoretical infrared frequency modes for the CNH_3 and $C_2N_2H_8$ isomers and their ions.

H_2CNH			H_2CNH^+		
Normal modes	Frequency(cm^{-1})	IR Intensity	Normal modes	Frequency(cm^{-1})	IR Intensity
ν_1	1075.5062	37.0005	ν_1	582.8914	118.9476
ν_2	1101.4124	15.5365	ν_2	633.3062	132.9916
ν_3	1170.0398	45.5313	ν_3	987.4739	10.3758
ν_4	1373.3046	46.9702	ν_4	1058.5386	53.2054
ν_5	1492.8412	6.5260	ν_5	1341.6707	63.0830
ν_6	1713.0952	21.6437	ν_6	1730.4488	0.4752
ν_7	3010.4982	52.4169	ν_7	2914.2190	105.7087
ν_8	3103.8095	36.8335	ν_8	3028.5777	87.9035
ν_9	3425.8292	1.0857	ν_9	3507.1840	387.2770
$^3CH_3N$			$^3CH_3N^+$		
Normal modes	Frequency(cm^{-1})	IR Intensity	Normal modes	Frequency(cm^{-1})	IR Intensity
ν_1	963.5507	0.7019	ν_1	466.3037	8.6117
ν_2	963.5524	0.7019	ν_2	898.2116	7.7179
ν_3	1053.8599	4.9809	ν_3	898.2128	7.7178
ν_4	1379.2879	13.3115	ν_4	1320.4751	0.1288
ν_5	1419.7884	9.9782	ν_5	1352.6705	13.6947
ν_6	1419.7887	9.9775	ν_6	1352.672	13.6931
ν_7	2924.4886	2.4306	ν_7	2968.3363	63.0607
ν_8	2979.3148	14.2024	ν_8	3112.1254	89.7423
ν_9	2979.315	14.2047	ν_9	3112.1258	89.7373
$CHNH_2$			$CHNH_2^+$		
Normal modes	Frequency(cm^{-1})	IR Intensity	Normal modes	Frequency(cm^{-1})	IR Intensity
ν_1	801.4767	147.4518	ν_1	845.2991	35.7408
ν_2	1075.3634	25.535	ν_2	893.2671	182.5151
ν_3	1159.0683	12.2723	ν_3	965.3992	42.6828
ν_4	1387.5623	12.7364	ν_4	1177.4118	15.2562
ν_5	1438.5902	13.3644	ν_5	1565.7474	30.102
ν_6	1686.9227	11.4576	ν_6	1728.7476	91.2312
ν_7	2913.9804	110.6138	ν_7	3172.483	60.0396
ν_8	3369.3698	22.9474	ν_8	3337.5861	159.5816
ν_9	3534.9723	15.4043	ν_9	3439.4942	216.8281

$^3CHNH_2$			$^3CHNH_2^+$		
Normal modes	Frequency(cm^{-1})	IR Intensity	Normal modes	Frequency(cm^{-1})	IR Intensity
ν_1	520.137	30.9842	ν_1	569.0733	17.2517
ν_2	610.4615	219.6403	ν_2	715.1091	116.3377
ν_3	1070.3104	17.7116	ν_3	955.8706	34.4621
ν_4	1099.6283	1.1623	ν_4	972.5576	8.0127
ν_5	1267.8758	18.2884	ν_5	1110.2469	3.7313
ν_6	1625.8034	22.7909	ν_6	1555.383	42.3441
ν_7	3063.6355	30.2464	ν_7	3104.1286	49.0516
ν_8	3464.8578	3.4299	ν_8	3316.4336	80.4391
ν_9	3531.5805	14.6469	ν_9	3421.6898	194.3654
$CH_3NHNHCH_3$			$CH_3NHNHCH_3^+$		
Normal modes	Frequency(cm^{-1})	IR Intensity	Normal modes	Frequency(cm^{-1})	IR Intensity
ν_1	49.7107	6.3924	ν_1	112.8545	0.0751
ν_2	234.2774	0.9594	ν_2	148.8191	3.1889
ν_3	285.3485	0.0000	ν_3	155.5647	0.0000
ν_4	292.0175	5.1310	ν_4	294.0692	1.9831
ν_5	474.4309	0.0000	ν_5	402.9769	0.0000
ν_6	815.9057	0.0000	ν_6	511.8491	0.0000
ν_7	892.8219	132.1914	ν_7	590.0594	168.2007
ν_8	960.6316	0.0000	ν_8	922.7047	0.0000
ν_9	1044.4290	25.9933	ν_9	1026.3576	14.7526
ν_{10}	1106.7215	0.0000	ν_{10}	1121.8020	24.6704
ν_{11}	1108.4551	14.1059	ν_{11}	1123.8278	0.0000
ν_{12}	1151.7854	12.4246	ν_{12}	1128.0659	1.6143
ν_{13}	1181.2046	0.0000	ν_{13}	1220.7657	0.0000
ν_{14}	1292.2594	0.0000	ν_{14}	1402.7582	0.0000
ν_{15}	1431.1926	5.1148	ν_{15}	1432.3455	12.6587
ν_{16}	1446.5412	4.7441	ν_{16}	1464.1766	5.2859
ν_{17}	1446.7211	0.0000	ν_{17}	1468.4634	0.0000
ν_{18}	1479.2835	0.0000	ν_{18}	1476.7806	29.2365
ν_{19}	1483.8601	13.7356	ν_{19}	1479.2059	0.0000
ν_{20}	1515.4655	22.3501	ν_{20}	1500.0455	0.0000
ν_{21}	1517.1866	0.0000	ν_{21}	1505.3241	65.2002
ν_{22}	1538.4557	0.0000	ν_{22}	1612.1145	0.0000
ν_{23}	2973.5900	160.9774	ν_{23}	3038.1648	0.0000
ν_{24}	2976.7763	0.0000	ν_{24}	3038.5829	2.2985

ν_{25}	3046.5231	78.8358	ν_{25}	3116.4385	0.2815
ν_{26}	3046.6431	0.0000	ν_{26}	3117.2818	0.0000
ν_{27}	3095.6242	50.5520	ν_{27}	3156.6600	1.2636
ν_{28}	3095.7023	0.0000	ν_{28}	3157.0660	0.0000
ν_{29}	3450.0833	0.0000	ν_{29}	3548.2904	0.0000
ν_{30}	3471.0086	0.0657	ν_{30}	3557.5745	168.3875
	$(CH_3)_2NNH_2$			$(CH_3)_2NNH_2^+$	
Normal modes	Frequency(cm^{-1})	IR Intensity	Normal modes	Frequency(cm^{-1})	IR Intensity
ν_1	164.5265	36.2334	ν_1	100.5343	0.0109
ν_2	262.6485	7.0780	ν_2	137.5117	0.3196
ν_3	274.4501	0.0136	ν_3	291.3740	11.5028
ν_4	408.7494	4.3265	ν_4	404.9324	10.2624
ν_5	436.2408	1.8204	ν_5	409.7203	3.1825
ν_6	439.5743	16.7883	ν_6	468.9608	0.0372
ν_7	811.4670	14.3654	ν_7	527.4746	191.1342
ν_8	982.7986	20.2362	ν_8	798.0330	1.1307
ν_9	1039.6479	14.8111	ν_9	1027.9332	13.9603
ν_{10}	1107.2052	0.6997	ν_{10}	1086.7726	4.0227
ν_{11}	1116.1826	60.2056	ν_{11}	1111.9567	0.9131
ν_{12}	1132.4435	10.5313	ν_{12}	1137.1129	2.2901
ν_{13}	1199.1632	4.5031	ν_{13}	1159.6141	3.3527
ν_{14}	1256.8760	0.2674	ν_{14}	1389.1960	0.8233
ν_{15}	1396.6579	5.0630	ν_{15}	1425.1564	14.3774
ν_{16}	1433.1014	0.9195	ν_{16}	1448.8353	1.2036
ν_{17}	1460.5832	2.7575	ν_{17}	1465.7927	14.8286
ν_{18}	1477.4936	9.1040	ν_{18}	1468.5245	0.0053
ν_{19}	1487.7995	8.9362	ν_{19}	1487.3965	9.4913
ν_{20}	1497.8457	0.2099	ν_{20}	1488.6399	23.4394
ν_{21}	1511.7046	11.5259	ν_{21}	1526.7873	14.2940
ν_{22}	1650.6901	34.0909	ν_{22}	1659.5838	79.5095
ν_{23}	2942.0905	46.2139	ν_{23}	3031.4526	0.3176
ν_{24}	2950.5747	105.9159	ν_{24}	3035.2911	1.5530
ν_{25}	3051.9818	43.5185	ν_{25}	3117.8989	0.2308
ν_{26}	3054.6447	30.7283	ν_{26}	3118.8408	0.0931
ν_{27}	3097.9984	6.0858	ν_{27}	3156.4993	0.0642
ν_{28}	3103.3640	44.1226	ν_{28}	3161.0826	0.6534
ν_{29}	3421.1784	1.7475	ν_{29}	3513.6341	121.0814
ν_{30}	3498.3215	0.0350	ν_{30}	3645.6045	106.4104

$NH_2CH_2CH_2NH_2$			$NH_2CH_2CH_2NH_2^+$		
Normal modes	Frequency(cm^{-1})	IR Intensity	Normal modes	Frequency(cm^{-1})	IR Intensity
ν_1	179.9656	4.2047	ν_1	118.9283	0.4519
ν_2	235.6987	20.7799	ν_2	173.5474	0.0577
ν_3	290.2833	44.0429	ν_3	334.9658	0.2470
ν_4	348.0012	22.5367	ν_4	375.9995	3.6233
ν_5	504.1945	12.0775	ν_5	417.6388	88.9136
ν_6	812.9440	91.1544	ν_6	472.3067	13.0408
ν_7	853.7207	75.6127	ν_7	516.2050	260.7918
ν_8	878.8733	79.2875	ν_8	518.9747	19.2435
ν_9	927.4051	34.2551	ν_9	826.9022	12.9578
ν_{10}	1007.0535	12.4586	ν_{10}	865.4095	4.4735
ν_{11}	1050.4762	8.4471	ν_{11}	1030.8206	9.5415
ν_{12}	1111.8972	5.2103	ν_{12}	1073.0899	0.2365
ν_{13}	1182.9452	4.0095	ν_{13}	1116.1998	0.1456
ν_{14}	1219.1725	4.7418	ν_{14}	1219.8789	1.0774
ν_{15}	1325.2989	3.0479	ν_{15}	1282.5953	69.0741
ν_{16}	1342.2669	2.1699	ν_{16}	1290.7199	7.8323
ν_{17}	1408.0343	8.9275	ν_{17}	1351.8296	3.2982
ν_{18}	1431.9029	6.5813	ν_{18}	1355.1309	2.5404
ν_{19}	1498.5561	4.4343	ν_{19}	1498.4649	10.5689
ν_{20}	1511.8609	3.3838	ν_{20}	1500.7886	3.6261
ν_{21}	1643.5125	35.9144	ν_{21}	1669.0592	61.4084
ν_{22}	1655.7046	25.0305	ν_{22}	1673.0249	61.3540
ν_{23}	2913.0618	90.1722	ν_{23}	3094.1370	6.9372
ν_{24}	2963.3322	84.6318	ν_{24}	3100.5815	0.0027
ν_{25}	3036.8892	48.2593	ν_{25}	3192.4228	0.3734
ν_{26}	3064.3194	31.7873	ν_{26}	3196.4396	0.1725
ν_{27}	3487.5711	4.5441	ν_{27}	3555.6620	303.5859
ν_{28}	3492.3403	0.2313	ν_{28}	3566.9258	70.1105
ν_{29}	3568.3256	3.0076	ν_{29}	3674.4148	121.0612
ν_{30}	3573.3657	0.9236	ν_{30}	3674.6780	59.1663
$H_2NCH_2NHCH_3$			$H_2NCH_2NHCH_3^+$		
Normal modes	Frequency(cm^{-1})	IR Intensity	Normal modes	Frequency(cm^{-1})	IR Intensity
ν_1	155.5951	3.0447	ν_1	110.8234	9.5533
ν_2	199.3598	3.9098	ν_2	136.7661	3.8321
ν_3	256.3639	43.6882	ν_3	229.1249	21.1248

ν_4	354.2506	2.7450	ν_4	298.3746	1.4209
ν_5	517.6992	6.6231	ν_5	520.0678	99.4510
ν_6	742.3573	133.3957	ν_6	627.0610	60.7215
ν_7	832.5152	105.1208	ν_7	641.4707	76.2000
ν_8	905.6845	8.3208	ν_8	786.4589	3.2459
ν_9	999.4335	10.5407	ν_9	832.3506	14.4057
ν_{10}	1041.1852	13.1506	ν_{10}	1017.4395	41.2582
ν_{11}	1139.8032	3.4008	ν_{11}	1057.1552	6.1410
ν_{12}	1169.3373	64.2341	ν_{12}	1120.2903	26.2495
ν_{13}	1182.3384	10.8405	ν_{13}	1170.1044	9.7959
ν_{14}	1249.0761	8.9192	ν_{14}	1195.4672	7.1864
ν_{15}	1338.5552	2.4211	ν_{15}	1306.6047	9.4839
ν_{16}	1426.8185	24.4433	ν_{16}	1367.2696	0.9236
ν_{17}	1455.9869	13.7573	ν_{17}	1383.2562	31.6166
ν_{18}	1487.4081	12.6813	ν_{18}	1423.0346	10.0826
ν_{19}	1496.4614	0.8865	ν_{19}	1427.8173	31.8465
ν_{20}	1517.9698	3.0244	ν_{20}	1461.8472	28.6748
ν_{21}	1523.9726	6.8419	ν_{21}	1494.9044	12.1352
ν_{22}	1639.8778	30.8845	ν_{22}	1672.7270	48.4770
ν_{23}	2913.6289	97.5123	ν_{23}	2927.5904	60.8846
ν_{24}	2933.2343	115.6178	ν_{24}	2945.0094	24.0464
ν_{25}	2958.2492	91.4081	ν_{25}	3009.4568	4.5659
ν_{26}	3068.2083	37.6601	ν_{26}	3068.4715	5.5108
ν_{27}	3113.2954	14.8337	ν_{27}	3143.3810	20.4867
ν_{28}	3494.2785	0.3165	ν_{28}	3494.4745	99.8736
ν_{29}	3541.8180	0.3031	ν_{29}	3562.3324	83.0464
ν_{30}	3582.3946	0.8282	ν_{30}	3653.6543	68.2966