

Supplementary Material:

Analysis of complexity measures and information planes of selected molecules in position and momentum spaces

Rodolfo O. Esquivel, Juan Carlos Angulo, Juan Antolín, Jesús S. Dehesa, and Sheila López-Rosa

5

Table S1. Chemical properties: energy (a.u.), dipole moment (debye), ionization potential (a.u.), hardness (a.u.) and electrophilicity (a.u.)

<i>Chemical Formula</i>	<i>Name</i>	<i>Number of Electrons</i>	<i>Energy</i>	<i>Dipole Moment</i>	<i>Ionization Potential</i>	<i>Hardness</i>	<i>Electrophilicity</i>
NH ₃	Ammonia	10	-56.420	1.7877	0.422	0.321	0.016
LiOH	Lithium Hydroxide	12	-83.165	4.576	0.364	0.190	0.080
Li ₂ O	Dilithium Oxide	14	-90.026	0.000	0.267	0.150	0.046
HBO	Boron Hydride Oxide	14	-100.468	2.840	0.510	0.339	0.043
HCO	Formyl Radical	15	-113.565	1.587	0.387	0.260	0.031
NO	Nitric Oxide	15	-129.534	2.003	0.421	0.259	0.050
H ₂ CO	Formaldehyde	16	-114.228	2.517	0.438	0.288	0.039
NHO	Nitrosyl Hydride	16	-130.178	1.786	0.425	0.259	0.053
O ₂	Oxygen	16	-149.948	0.000	0.552	0.491	0.004
CH ₃ O	Methoxy Radical	17	-114.797	3.355	0.387	0.363	0.001
CH ₃ NH ₂	Methyl Amine	18	-95.589	1.4985	0.387	0.307	0.011
CH ₃ OH	Methyl Alcohol	18	-115.435	1.945	0.444	0.334	0.018
NH ₂ OH	Hydroxylamine	18	-131.410	0.901	0.424	0.326	0.015
H ₂ O ₂	Hydrogen Peroxide	18	-151.216	1.751	0.474	0.346	0.024
NaOH	Sodium Hydroxide	20	-237.541	6.888	0.477	0.159	0.319
HCCO	Ketenyl Radical	21	-113.859	1.762	0.411	0.312	0.016

C_3H_3	Radical Propargyl	21	-115.643	0.181	0.351	0.282	0.009
BO_2	Boron Dioxide	21	-174.884	0.000	0.533	0.361	0.041
$MgOH$	Magnesium Hydroxide	21	-275.346	5.737	0.271	0.160	0.039
CH_2CCH_2	Allene	22	-116.289	0.000	0.371	0.275	0.017
CH_3CCH	Propyne	22	-116.292	0.733	0.346	0.300	0.004
C_3H_4	Cyclopropene	22	-116.292	0.733	0.346	0.264	0.013
CH_3CN	Acetonitrile	22	-132.221	4.629	0.457	0.331	0.024
CH_3NC	Methyl Isocyanide	22	-132.340	3.808	0.464	0.334	0.025
CH_2NN	Diazomethane	22	-148.326	4.502	0.391	0.231	0.056
NH_2CN	Cyanamide	22	-148.388	4.502	0.391	0.305	0.012
$HCCOH$	Ethynol	22	-152.141	1.747	0.371	0.282	0.014
CH_2CO	Ketene	22	-152.197	1.461	0.361	0.249	0.025
HN_3	Hydrogen Azide	22	-164.349	1.961	0.398	0.268	0.032
$HCNO$	Fulminic Acid	22	-168.134	3.248	0.403	0.294	0.020
$HOCN$	Cyanic Acid	22	-168.223	3.891	0.453	0.305	0.036
$HNCO$	Isocyanic Acid	22	-168.261	2.238	0.447	0.308	0.031
N_2O	Nitrous Oxide	22	-184.212	0.426	0.489	0.324	0.042

CO ₂	Carbon Dioxide	22	-188.150	0.000	0.539	0.377	0.035
FCN	Cyanogen Fluoride	22	-192.205	2.147	0.498	0.360	0.026
HBS	Hydrogen Boron Sulfide	22	-423.039	1.397	0.401	0.250	0.046
C ₃ H ₅	Allyl Radical	23	-116.874	0.923	0.333	0.281	0.005
CH ₃ CO	Acetyl Radical	23	-152.755	2.428	0.360	0.258	0.020
NO ₂	Nitrogen Dioxide	23	-204.636	0.078	0.499	0.290	0.075
PO	Phosphorus Monoxide	23	-415.862	0.135	0.327	0.175	0.067
NS	Mononitrogen Monosulfide	23	-452.183	1.971	0.354	0.186	0.077
C ₃ H ₆	Cyclopropane	24	-117.518	0.000	0.417	0.331	0.011
C ₂ H ₅ N	Aziridine	24	-133.525	1.899	0.389	0.307	0.011
NHCHNH ₂	Aminomethanimine	24	-149.592	2.745	0.365	0.284	0.012
C ₂ H ₄ O	Ethylene Oxide	24	-153.372	2.200	0.446	0.347	0.014
CH ₃ CHO	Acetaldehyde	24	-153.416	2.628	0.422	0.289	0.031
CHONH ₂	Formamide	24	-169.461	3.761	0.415	0.308	0.018
CH ₂ O ₂	Dioxirane	24	-189.156	2.866	0.482	0.341	0.030

HCOOH	Formic Acid	24	-189.304	1.299	0.468	0.324	0.032
HNO ₂	Nitrous Acid	24	-205.223	2.084	0.471	0.287	0.060
O ₃	Ozone	24	-224.882	0.715	0.486	0.231	0.142
FNO	Nitrosyl Fluoride	24	-229.213	1.893	0.511	0.290	0.085
CF ₂	Difluoromethylene	24	-237.220	0.417	0.469	0.287	0.058
H ₂ CS	Thioformaldehyde	24	-436.815	1.678	0.349	0.202	0.054
SO	Sulfur Monoxide	24	-472.622	1.815	0.424	0.290	0.031
CH ₃ CHCH ₃	Isopropyl Radical	25	-118.042	1.378	0.328	0.287	0.003
CH ₂ CH ₂ CH ₃	Npropyl Radical	25	-118.050	4.976	0.349	0.272	0.011
CH ₃ CHOH	Ethoxy Radical	25	-153.397	1.131	0.464	0.353	0.018
CH ₃ OO	Methylperoxy Radical	25	-189.745	4.890	0.476	0.361	0.018
FO ₂	Dioxygen Monofluoride	25	-249.576	1.555	0.552	0.370	0.045
NF ₂	Difluoroamino Radical	25	-253.764	1.485	0.533	0.409	0.019
CH ₃ S	Thiomethoxy	25	-437.452	0.075	0.372	0.222	0.051
C ₃ H ₈	Propane	26	-118.750	0.076	0.467	0.350	0.019

CH ₃ NHCH ₃	Dimethylamine	26	-134.753	1.212	0.365	0.297	0.008
CH ₃ CH ₂ NH ₂	Ethylamine	26	-134.766	1.503	0.384	0.303	0.011
CH ₃ OCH ₃	Dimethyl Ether	26	-154.594	1.539	0.419	0.327	0.013
CH ₃ CH ₂ OH	Ethanol	26	-154.612	1.886	0.436	0.330	0.017
CH ₃ OOH	Methyl Peroxide	26	-190.380	1.521	0.444	0.333	0.018
F ₂ O	Difluorine Monoxide	26	-274.101	0.405	0.569	0.363	0.059
SiO ₂	Silicon Dioxide	30	-439.124	0.000	0.500	0.255	0.118
OCS	Carbonyl Sulfide	30	-510.726	0.774	0.418	0.270	0.041
ClCN	Chlorocyanogen	30	-551.636	5.950	0.465	0.315	0.036
PO ₂	Phosphorus Dioxide	31	-491.029	0.202	0.470	0.258	0.087
PS	Phosphorus Sulfide	31	-738.487	0.978	0.311	0.153	0.083
SO ₂	Sulfur Dioxide	32	-547.716	2.114	0.489	0.253	0.111
ClNO	Nitrosyl Chloride	32	-589.211	2.082	0.434	0.239	0.080
S ₂	Sulfur Diatomic	32	-795.264	0.000	0.384	0.257	0.032
OCIO	Chlorine Dioxide	33	-609.561	2.783	0.474	0.267	0.081
ClO ₂	Chlorine Dioxide	33	-609.586	1.016	0.474	0.267	0.081

CH ₃ SCH ₃	Dimethyl Sulfide	34	-477.214	1.635	0.334	0.265	0.009
CH ₃ CH ₂ SH	Ethanethiol	34	-477.218	1.682	0.353	0.264	0.015
SF ₂	Sulfur Difluoride	34	-596.892	1.658	0.396	0.247	0.045
H ₂ S ₂	Hydrogen Sulfide	34	-796.507	1.410	0.387	0.243	0.043
CS ₂	Carbon Disulfide	38	-833.302	0.000	0.372	0.214	0.059
SSO	Disulfur Monoxide	40	-870.246	1.431	0.404	0.186	0.128
CCl ₂	Dichloromethylene	40	-957.158	1.186	0.401	0.219	0.075
MgCl ₂	Magnesium Dichloride	46	-1119.088	0.000	0.450	0.235	0.098
S ₃	Sulfur Trimer	48	-1192.913	0.871	0.361	0.146	0.158
SiCl ₂	Dichlorosilylene	48	-1208.352	1.294	0.380	0.192	0.093
ClS ₂	Sulfur Chloride	49	-1254.976	0.960	0.343	0.175	0.080

Table S2. LMC and FS complexities in position (*r*), momentum (*p*) and product (*rp*) spaces.

<i>Chemical Formula</i>	<i>Name</i>	<i>C_r(LMC)</i>	<i>C_p(LMC)</i>	<i>C_{rp}(LMC)</i>	<i>C_r(FS)</i>	<i>C_p(FS)</i>	<i>C_{rp}(FS)</i>
NH ₃	Ammonia	18.329	4.890	89.633	22.098	6.275	138.665
LiOH	Lithium Hydroxide	15.817	4.839	76.545	22.569	6.115	137.998
Li ₂ O	Dilithium Oxide	14.707	4.843	71.226	24.406	6.323	154.319
HBO	Boron Hydride Oxide	15.921	5.710	90.901	26.266	6.750	177.287
HCO	Formyl Radical	20.482	7.614	155.955	32.700	8.300	271.396
NO	Nitric Oxide	18.222	7.168	130.609	30.542	7.988	243.978
H ₂ CO	Formaldehyde	16.159	5.408	87.391	28.659	6.678	191.377
NHO	Nitrosyl Hydride	15.386	5.329	81.996	28.056	6.753	189.456
O ₂	Oxygen	14.269	5.018	71.601	26.625	6.596	175.606
CH ₃ O	Methoxy Radical	21.197	6.553	138.900	35.209	7.551	265.849
CH ₃ NH ₂	Methyl Amine	16.455	4.717	77.619	31.372	6.233	195.534
CH ₃ OH	Methyl Alcohol	17.196	5.058	86.977	31.282	6.470	202.402
NH ₂ OH	Hydroxylamine	16.469	5.224	86.038	30.668	6.772	207.692
H ₂ O ₂	Hydrogen Peroxide	15.692	5.298	83.140	29.600	6.966	206.195
NaOH	Sodium Hydroxide	16.663	5.765	96.069	30.033	6.786	203.792
HCCO	Ketenyl Radical	18.736	5.848	109.576	32.104	7.482	240.193

C_3H_3	Radical Propargyl	14.619	5.307	77.576	34.925	6.691	233.679
BO_2	Boron Dioxide	14.240	5.258	74.872	32.142	6.613	212.558
$MgOH$	Magnesium Hydroxide	28.094	21.582	606.322	42.104	24.193	1018.634
CH_2CCH_2	Allene	14.887	5.254	78.209	36.060	6.722	242.410
CH_3CCH	Propyne	14.859	5.204	77.322	36.012	6.642	239.193
C_3H_4	Cyclopropene	14.859	5.204	77.322	36.012	6.642	239.193
CH_3CN	Acetonitrile	15.147	5.375	81.417	35.842	6.795	243.557
CH_3NC	Methyl Isocyanide	15.179	5.395	81.893	35.998	6.680	240.459
CH_2NN	Diazomethane	14.979	5.389	80.730	35.364	6.868	242.894
NH_2CN	Cyanamide	14.621	5.352	78.256	34.778	6.787	236.049
$HCCOH$	Ethynol	15.133	5.259	79.577	34.778	6.618	230.157
CH_2CO	Ketene	15.096	5.398	81.488	34.758	6.761	235.010
HN_3	Hydrogen Azide	14.139	5.206	73.603	33.966	6.807	231.193
$HCNO$	Fulminic Acid	14.556	5.252	76.453	33.987	6.747	229.303
$HOCN$	Cyanic Acid	14.422	5.264	75.922	33.817	6.673	225.656
$HNCO$	Isocyanic Acid	14.111	5.255	74.159	33.281	6.727	223.888
N_2O	Nitrous Oxide	13.642	4.935	67.319	32.764	6.542	214.329

CO ₂	Carbon Dioxide	13.458	4.967	66.854	31.982	6.470	206.926
FCN	Cyanogen Fluoride	14.216	5.152	73.238	32.573	6.474	210.885
HBS	Hydrogen Boron Sulfide	39.219	12.909	506.268	45.008	13.545	609.627
C ₃ H ₅	Allyl Radical	18.363	5.750	105.581	42.281	7.095	299.994
CH ₃ CO	Acetyl Radical	19.461	6.781	131.961	41.942	8.218	344.662
NO ₂	Nitrogen Dioxide	15.622	6.023	94.086	36.221	7.105	257.364
PO	Phosphorus Monoxide	32.401	14.006	453.829	44.319	14.029	621.770
NS	Mononitrogen Monosulfide	37.529	13.892	521.334	46.670	13.788	643.470
C ₃ H ₆	Cyclopropane	14.573	4.700	68.496	36.814	6.216	228.832
C ₂ H ₅ N	Aziridine	15.076	4.854	73.171	37.026	6.357	235.383
NHCHNH ₂	Aminomethanimine	15.284	5.025	76.799	37.056	6.458	239.322
C ₂ H ₄ O	Ethylene Oxide	15.564	5.031	78.296	36.753	6.448	236.990
CH ₃ CHO	Acetaldehyde	15.986	5.219	83.430	37.453	6.557	245.587
CHONH ₂	Formamide	15.099	5.118	77.269	36.021	6.476	233.265
CH ₂ O ₂	Dioxirane	15.099	5.282	79.758	35.870	6.790	243.544

HCOOH	Formic Acid	14.796	5.204	77.001	35.225	6.528	229.965
HNO ₂	Nitrous Acid	14.424	5.168	74.547	35.028	6.611	231.566
O ₃	Ozone	14.057	5.075	71.342	34.472	6.660	229.580
FNO	Nitrosyl Fluoride	14.001	5.170	72.385	33.829	6.606	223.461
CF ₂	Difluoromethylene	14.085	5.253	73.983	33.166	6.476	214.793
H ₂ CS	Thioformaldehyde	38.934	11.926	464.325	47.354	12.728	602.734
SO	Sulfur Monoxide	28.632	9.671	276.908	40.560	10.750	436.024
CH ₃ CHCH ₃	Isopropyl Radical	18.342	5.215	95.647	43.754	6.616	289.479
CH ₂ CH ₂ CH ₃	Npropyl Radical	18.640	5.284	98.489	44.232	6.656	294.427
CH ₃ CHOH	Ethoxy Radical	15.947	5.118	81.609	37.328	6.479	241.853
CH ₃ OO	Methylperoxy Radical	18.130	6.056	109.797	41.062	7.142	293.257
FO ₂	Dioxygen Monofluoride	15.576	5.928	92.339	36.994	7.197	266.258
NF ₂	Difluoroamino Radical	15.602	6.039	94.216	36.560	7.173	262.231
CH ₃ S	Thiomethoxy	48.622	14.312	695.908	55.725	13.947	777.211
C ₃ H ₈	Propane	15.184	4.475	67.955	39.247	6.051	237.486

CH ₃ NHCH ₃	Dimethylamine	15.823	4.645	73.503	39.583	6.168	244.134
CH ₃ CH ₂ NH ₂	Ethylamine	15.794	4.632	73.166	39.522	6.169	243.825
CH ₃ OCH ₃	Dimethyl Ether	16.602	4.888	81.144	39.681	6.289	249.561
CH ₃ CH ₂ OH	Ethanol	16.492	4.847	79.941	39.477	6.311	249.153
CH ₃ OOH	Methyl Peroxide	16.305	5.139	83.786	38.912	6.599	256.795
F ₂ O	Difluorine Monoxide	13.780	5.021	69.189	34.504	6.686	230.701
SiO ₂	Silicon Dioxide	21.279	7.197	153.135	42.587	8.418	358.485
OCS	Carbonyl Sulfide	29.439	8.637	254.249	47.959	9.847	472.247
ClCN	Chlorocyanogen	34.096	9.156	312.185	50.455	10.743	542.020
PO ₂	Phosphorus Dioxide	26.608	9.562	254.412	48.502	10.036	486.758
PS	Phosphorus Sulfide	33.482	18.602	622.825	53.355	18.347	978.882
SO ₂	Sulfur Dioxide	25.582	8.033	205.489	46.479	9.105	423.187
ClNO	Nitrosyl Chloride	31.033	9.169	284.526	50.569	10.255	518.602
S ₂	Sulfur Diatomic	29.557	13.830	408.768	49.503	15.541	769.315
OCIO	Chlorine Dioxide	30.434	9.286	282.608	51.335	10.152	521.178
ClO ₂	Chlorine Dioxide	31.652	9.814	310.638	52.740	10.507	554.167

CH ₃ SCH ₃	Dimethyl Sulfide	43.179	8.841	381.755	62.193	10.184	633.383
CH ₃ CH ₂ SH	Ethanethiol	43.193	9.148	395.128	62.192	10.349	643.612
SF ₂	Sulfur Difluoride	23.088	7.614	175.794	45.869	8.693	398.764
H ₂ S ₂	Hydrogen Sulfide	33.365	14.977	499.718	54.844	15.983	876.593
CS ₂	Carbon Disulfide	31.540	11.615	366.320	57.500	13.232	760.837
SSO	Disulfur Monoxide	28.568	11.232	320.885	56.396	12.275	692.232
CCl ₂	Dichloromethylene	33.193	12.496	414.800	59.796	13.525	808.719
MgCl ₂	Magnesium Dichloride	27.977	11.443	320.138	60.209	12.364	744.450
S ₃	Sulfur Trimer	29.189	13.970	407.786	64.165	15.508	995.053
SiCl ₂	Dichlorosilylene	29.108	13.964	406.462	63.384	14.697	931.524
ClS ₂	Sulfur Chloride	31.640	15.477	489.713	68.048	15.910	1082.619

Table S3. Information measures I , J , D and L in position (r) and momentum (p) spaces.

<i>Chemical Formula</i>	<i>Name</i>	I_r	I_p	J_r	J_p	D_r	D_p	L_r	L_p
NH ₃	Ammonia	35.359	3.951	0.625	1.588	0.526	0.035	34.873	141.252
LiOH	Lithium Hydroxide	42.817	2.871	0.527	2.130	0.586	0.022	27.011	219.366
Li ₂ O	Dilithium Oxide	40.522	3.028	0.602	2.088	0.446	0.023	32.993	212.967
HBO	Boron Hydride Oxide	44.908	3.083	0.585	2.189	0.504	0.025	31.573	228.637
HCO	Formyl Radical	47.148	3.727	0.694	2.227	0.502	0.032	40.769	234.576
NO	Nitric Oxide	53.282	3.066	0.573	2.605	0.595	0.024	30.633	296.801
H ₂ CO	Formaldehyde	44.410	3.103	0.645	2.152	0.442	0.024	36.591	222.885
NHO	Nitrosyl Hydride	50.288	2.734	0.558	2.470	0.523	0.019	29.415	273.967
O ₂	Oxygen	57.172	2.309	0.466	2.856	0.636	0.015	22.433	340.759
CH ₃ O	Methoxy Radical	41.945	3.951	0.839	1.911	0.390	0.035	54.285	186.471
CH ₃ NH ₂	Methyl Amine	33.729	4.042	0.930	1.542	0.260	0.035	63.319	135.176
CH ₃ OH	Methyl Alcohol	39.736	3.451	0.787	1.875	0.349	0.028	49.302	181.200
NH ₂ OH	Hydroxylamine	44.865	3.073	0.684	2.204	0.413	0.023	39.892	230.958
H ₂ O ₂	Hydrogen Peroxide	50.972	2.671	0.581	2.608	0.502	0.018	31.235	297.351
NaOH	Sodium Hydroxide	67.031	1.867	0.448	3.635	0.787	0.012	21.169	489.255
HCCO	Ketenyl Radical	45.164	3.759	0.711	1.990	0.443	0.030	42.302	198.209

C ₃ H ₃	Radical Propargyl	35.850	3.973	0.974	1.684	0.215	0.034	67.870	154.263
BO ₂	Boron Dioxide	51.429	2.501	0.625	2.644	0.408	0.017	34.874	303.534
MgOH	Magnesium Hydroxide	72.165	6.982	0.583	3.465	0.893	0.047	31.457	455.310
CH ₂ CCH ₂	Allene	34.380	4.181	1.049	1.608	0.196	0.037	75.823	143.893
CH ₃ CCH	Propyne	34.372	4.154	1.048	1.599	0.196	0.036	75.698	142.733
C ₃ H ₄	Cyclopropene	34.372	4.154	1.048	1.599	0.196	0.036	75.698	142.733
CH ₃ CN	Acetonitrile	38.577	3.710	0.929	1.831	0.240	0.031	63.212	174.949
CH ₃ NC	Methyl Isocyanide	38.665	3.655	0.931	1.828	0.239	0.031	63.408	174.421
CH ₂ NN	Diazomethane	42.763	3.341	0.827	2.056	0.282	0.026	53.081	208.023
NH ₂ CN	Cyanamide	42.721	3.243	0.814	2.093	0.282	0.025	51.843	213.709
HCCOH	Ethynol	43.351	3.159	0.802	2.095	0.298	0.025	50.718	214.029
CH ₂ CO	Ketene	43.450	3.188	0.800	2.121	0.299	0.025	50.501	217.992
HN ₃	Hydrogen Azide	46.920	2.946	0.724	2.311	0.325	0.021	43.476	247.947
HCNO	Fulminic Acid	47.560	2.860	0.715	2.359	0.341	0.021	42.641	255.808
HOCN	Cyanic Acid	47.639	2.807	0.710	2.377	0.342	0.020	42.216	258.724
HNCO	Isocyanic Acid	47.582	2.792	0.699	2.409	0.342	0.020	41.290	263.993
N ₂ O	Nitrous Oxide	51.862	2.551	0.632	2.565	0.385	0.017	35.444	289.908

CO ₂	Carbon Dioxide	52.542	2.408	0.609	2.687	0.401	0.016	33.521	310.842
FCN	Cyanogen Fluoride	53.291	2.381	0.611	2.719	0.421	0.016	33.730	316.488
HBS	Hydrogen Boron Sulfide	95.653	3.402	0.471	3.982	1.721	0.023	22.782	560.801
C ₃ H ₅	Allyl Radical	33.000	4.950	1.281	1.433	0.179	0.047	102.365	121.145
CH ₃ CO	Acetyl Radical	41.737	4.253	1.005	1.932	0.274	0.036	71.105	189.554
NO ₂	Nitrogen Dioxide	54.331	2.580	0.667	2.754	0.407	0.019	38.422	322.651
PO	Phosphorus Monoxide	93.118	3.147	0.476	4.458	1.398	0.021	23.176	664.281
NS	Mononitrogen Monosulfide	98.935	3.131	0.472	4.403	1.641	0.021	22.869	652.189
C ₃ H ₆	Cyclopropane	31.688	4.197	1.162	1.481	0.165	0.037	88.384	127.209
C ₂ H ₅ N	Aziridine	35.547	3.795	1.042	1.675	0.201	0.032	75.036	153.063
NHCHNH ₂	Aminomethanimine	39.358	3.440	0.942	1.877	0.237	0.028	64.484	181.539
C ₂ H ₄ O	Ethylene Oxide	40.077	3.343	0.917	1.929	0.251	0.027	61.989	189.055
CH ₃ CHO	Acetaldehyde	40.139	3.418	0.933	1.919	0.251	0.028	63.621	187.575
CHONH ₂	Formamide	43.829	2.985	0.822	2.169	0.287	0.023	52.590	225.540
CH ₂ O ₂	Dioxirane	48.619	2.763	0.738	2.457	0.338	0.019	44.730	271.863

HCOOH	Formic Acid	48.366	2.641	0.728	2.472	0.337	0.019	43.871	274.330
HNO ₂	Nitrous Acid	52.388	2.476	0.669	2.670	0.374	0.017	38.591	307.969
O ₃	Ozone	57.042	2.273	0.604	2.930	0.424	0.014	33.161	354.055
FNO	Nitrosyl Fluoride	57.622	2.179	0.587	3.032	0.441	0.014	31.752	372.608
CF ₂	Difluoromethylene	58.849	2.027	0.564	3.196	0.472	0.013	29.864	403.204
H ₂ CS	Thioformaldehyde	91.074	3.216	0.520	3.958	1.471	0.021	26.464	555.725
SO	Sulfur Monoxide	99.453	2.257	0.408	4.762	1.557	0.013	18.384	733.511
CH ₃ CHCH ₃	Isopropyl Radical	30.608	4.986	1.430	1.327	0.152	0.048	120.639	107.892
CH ₂ CH ₂ CH ₃	Npropyl Radical	30.608	5.061	1.445	1.315	0.152	0.050	122.622	106.476
CH ₃ CHOH	Ethoxy Radical	40.048	3.403	0.932	1.904	0.251	0.028	63.517	185.402
CH ₃ OO	Methylperoxy Radical	46.628	3.180	0.881	2.246	0.311	0.025	58.331	237.541
FO ₂	Dioxygen Monofluoride	59.692	2.315	0.620	3.109	0.452	0.015	34.438	386.854
NF ₂	Difluoroamino Radical	60.253	2.234	0.607	3.211	0.468	0.015	33.362	406.065
CH ₃ S	Thiomethoxy	87.510	3.862	0.637	3.612	1.356	0.030	35.868	484.462
C ₃ H ₈	Propane	29.589	4.508	1.326	1.342	0.141	0.041	107.825	109.781

CH ₃ NHCH ₃	Dimethylamine	33.093	4.072	1.196	1.515	0.171	0.035	92.334	131.596
CH ₃ CH ₂ NH ₂	Ethylamine	33.089	4.080	1.194	1.512	0.171	0.035	92.142	131.252
CH ₃ OCH ₃	Dimethyl Ether	37.259	3.626	1.065	1.734	0.214	0.030	77.576	161.232
CH ₃ CH ₂ OH	Ethanol	37.242	3.639	1.060	1.734	0.214	0.030	77.032	161.232
CH ₃ OOH	Methyl Peroxide	45.030	3.016	0.864	2.188	0.288	0.022	56.702	228.464
F ₂ O	Difluorine Monoxide	62.458	1.983	0.552	3.372	0.475	0.011	28.982	437.147
SiO ₂	Silicon Dioxide	78.996	2.080	0.539	4.048	0.762	0.013	27.939	574.802
OCS	Carbonyl Sulfide	87.733	2.483	0.547	3.966	1.032	0.015	28.528	557.507
ClCN	Chlorocyanogen	92.739	2.670	0.544	4.024	1.204	0.016	28.325	569.800
PO ₂	Phosphorus Dioxide	83.663	2.406	0.580	4.172	0.854	0.016	31.157	601.416
PS	Phosphorus Sulfide	116.668	3.329	0.457	5.512	1.534	0.020	21.829	913.419
SO ₂	Sulfur Dioxide	88.687	2.040	0.524	4.464	0.955	0.012	26.780	665.719
ClNO	Nitrosyl Chloride	93.484	2.329	0.541	4.403	1.105	0.014	28.082	652.087
S ₂	Sulfur Diatomic	120.651	2.681	0.410	5.796	1.593	0.014	18.551	984.958
OClO	Chlorine Dioxide	93.811	2.236	0.547	4.541	1.065	0.014	28.573	683.123
ClO ₂	Chlorine Dioxide	93.908	2.337	0.562	4.497	1.065	0.015	29.708	673.077

CH ₃ SCH ₃	Dimethyl Sulfide	71.901	3.629	0.865	2.806	0.760	0.027	56.783	331.815
CH ₃ CH ₂ SH	Ethanethiol	71.886	3.604	0.865	2.872	0.760	0.027	56.799	343.484
SF ₂	Sulfur Difluoride	90.936	1.799	0.504	4.832	0.913	0.010	25.287	749.769
H ₂ S ₂	Hydrogen Sulfide	113.715	2.896	0.482	5.519	1.411	0.016	23.642	915.087
CS ₂	Carbon Disulfide	108.093	2.762	0.532	4.790	1.152	0.016	27.385	740.069
SSO	Disulfur Monoxide	107.860	2.281	0.523	5.382	1.071	0.013	26.687	881.223
CCl ₂	Dichloromethylene	115.767	2.464	0.517	5.490	1.267	0.014	26.202	907.920
MgCl ₂	Magnesium Dichloride	118.212	2.129	0.509	5.808	1.090	0.012	25.658	987.999
S ₃	Sulfur Trimer	120.348	2.613	0.533	5.935	1.062	0.014	27.479	1020.606
SiCl ₂	Dichlorosilylene	121.417	2.349	0.522	6.257	1.093	0.013	26.623	1104.761
ClS ₂	Sulfur Chloride	123.420	2.643	0.551	6.020	1.095	0.015	28.897	1042.597

