Annexure

Table 1 categorizes the 35 isomers of C_9H_{20} based on their branching. The corresponding chemical names (following IUPAC nomenclature) are given.

Table 1. Isomers of nonane

S.No	Number of carbons in spine	Isomers
1	9	n-nonane (N_1).
2	8	2-methyloctane(N_2), 3-methyloctane(N_3), 4-methyloctane(N_4).
3	7	(i) Dimethylheptanes 2,2-dimethylheptane(N_5), 2,3-dimethylheptane(N_6), 2,4-dimethylheptane(N_7), 2,5-dimethylheptane(N_8), 2,6-dimethylheptane(N_9), 3,3-dimethylheptane(N_{10}), 3,4-dimethylheptane(N_{11}), 3,5-dimethylheptane(N_{12}), 4,4-dimethylheptane(N_{13}). (ii) Ethylheptanes 3-ethylheptane(N_{14}), 4-ethylheptane(N_{15}).
4	6	(i) Trimethyl 2,2,3-trimethylhexane(N_{16}), 2,2,4-trimethylhexane(N_{17}), 2,2,5-trimethylhexane(N_{18}), 2,3,3-trimethylhexane(N_{19}), 2,3,4-trimethylhexane(N_{20}), 2,3,5-trimethylhexane(N_{21}), 2,4,4-trimethylhexane(N_{22}), 3,3,4-trimethylhexane(N_{23}). (ii) Methyl + Ethyl 3-ethyl-2-methylhexane(N_{24}), 4-ethyl-2-methylhexane(N_{25}), 3-ethyl-3-methylhexane(N_{26}), 3-ethyl-4-methylhexane(N_{27}).
5	5	(i) Tetramethyl 2,2,3,3-tetramethylpentane(N_{28}), 2,2,3,4-tetramethylpentane(N_{29}), 2,2,4,4-tetramethylpentane(N_{30}), 2,3,3,4-tetramethylpentane(N_{31}).

		(ii) Dimethyl + ethyl 3-Ethyl-2,2-dimethylpentane(N_{32}), 3-Ethyl-2,3-dimethylpentane(N_{33}), 3-Ethyl-2,4-dimethylpentane(N_{34}). (iii) Diethyl 3,3-diethylpentane(N_{35}).

IUPAC nomenclature of isomers tabulated are verified in [15]

By using MATLAB, the spectrum, spectral radius, spectral gap, second largest eigenvalue, graph energy and eigenvalue-based graph entropy of all the isomers have been calculated and the results are tabulated in Table 2.

Table 2. Spectral parameters of nonane

Nonane isomers	Density	Spectrum	Spectral gap	Graph energy	Eigenvalue based Graph Entropy
N_1	0.7180	$\left\{\begin{array}{c}\pm 1.90211^{(1)}, \pm 1.61803^{(1)}, \\ \pm 1.17557^{(1)}, \pm\ 0.61803^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.23917	10.6275	0.8716
N_2	0.7140	$\left\{\begin{array}{c}\pm 1.96157^{(1)}, \pm 1.66294^{(1)}, \\ \pm 1.11114^{(1)}, \pm 0.39018^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.29863	10.2516	0.8484
N_3	0.7210	$\left\{\begin{array}{c}\pm 2^{(1)}, \pm 1.61803^{(1)}, \pm 1^{(1)}, \\ \pm 0.61803^{(1)}, 0^{(1)}\end{array}\right\}$	0.38197	10.4721	0.8651
N_4	0.7200	$\left\{\begin{array}{c}\pm 2.01532^{(1)}, \pm 1.54801^{(1)}, \\ \pm 1.14288^{(1)}, \pm 0.48578^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.46731	10.3839	0.8582
N_5	0.7070	$\left\{\begin{array}{c}\pm 2.11688^{(1)}, \pm 1.63978^{(1)}, \\ \pm 0.91100^{(1)}, 0^{(1)}\end{array}\right\}$	0.4771	9.3353	0.7549
N_6	0.7260	$\left\{\begin{array}{c}\pm 2.08397^{(1)}, \pm 1.57184^{(1)}, \\ \pm\ 1^{(1)}, \pm 0.43173^{(1)}, 0^{(1)}\end{array}\right\}$	0.51213	10.1750	0.8472
N_7	0.7200	$\left\{\begin{array}{c}\pm 2.06082^{(1)}, \pm 1.59842^{(1)}, \\ \pm 1.09456^{(1)}, 0^{(1)}\end{array}\right\}$	0.4624	9.5076	0.7644
N_8	0.7200	$\left\{\begin{array}{c}\pm 2.03565^{(1)}, \pm 1.69069^{(1)}, \\ \pm 0.88413^{(1)}, \pm 0.46476^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.34496	10.1504	0.8465
N_9	0.7060	$\left\{\begin{array}{c}\pm 2^{(1)}, \pm 1.73205^{(1)}, \pm 1^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.2679	9.4641	0.7615
N_{10}	0.7200	$\left\{\begin{array}{c}\pm 2.16461^{(1)}, \pm 1.52804^{(1)}, \\ \pm 0.85362^{(1)}, \pm 0.50088^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.63657	10.0940	0.8459

N_{11}	0.7300	$\left\{\begin{array}{c}\pm 2.11199^{(1)}, \pm 1.49637^{(1)}, \\ \pm 1\ ^{(1)}, \pm 0.54806^{(1)}, 0^{(1)}\end{array}\right\}$	0.61562	10.3128	0.8574
N_{12}	0.7300	$\left\{\begin{array}{c}\pm 2.07431^{(1)}, \pm 1.61803^{(1)}, \\ \pm 0.83500^{(1)}, \pm 0.61803^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.45628	10.2907	0.8568
N_{13}	0.7210	$\left\{\begin{array}{c}\pm 2.17533^{(1)}, \pm 1.41421^{(1)}, \\ \pm 1.12603^{(1)}, 0^{(1)}\end{array}\right\}$	0.76112	9.4311	0.7614
N_{14}	0.7230	$\left\{\begin{array}{c}\pm 2.04208^{(1)}, \pm 1.52023^{(1)}, \\ \pm 1^{(1)}, \pm 0.72028^{(1)}, 0^{(1)}\end{array}\right\}$	0.52185	10.5651	0.8711
N_{15}	0.7300	$\left\{\begin{array}{c}\pm 2.05288^{(1)}, \pm 1.41421^{(1)}, \\ \pm 1.20864^{(1)}, \pm 0.56997^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.63867	10.4914	0.8656
N_{16}	0.7160	$\left\{\begin{array}{c}\pm 2.21635^{(1)}, \pm 1.51211^{(1)}, \\ \pm 0.89516^{(1)}, 0^{(1)}\end{array}\right\}$	0.70424	9.2472	0.7509
N_{17}	0.7160	$\left\{\begin{array}{c}\pm 2.16786^{(1)}, \pm 1.66159^{(1)}, \\ \pm 0.73450^{(1)}, 0^{(1)}\end{array}\right\}$	0.50627	9.1279	0.7420
N_{18}	0.7100	$\left\{\begin{array}{c}\pm 2.13578^{(1)}, \pm 1.73205^{(1)}, \\ \pm 0.66215^{(1)}, 0^{(1)}\end{array}\right\}$	0.40373	9.0599	0.7367
N_{19}	0.7340	$\left\{\begin{array}{c}\pm 2.23607^{(1)}, \pm 1.41421^{(1)}, \\ \pm 1^{(1)}, 0^{(1)}\end{array}\right\}$	0.82186	9.3005	0.7547
N_{20}	0.7350	$\left\{\begin{array}{c}\pm 2.16461^{(1)}, \pm 1.52804^{(1)}, \\ \pm 0.85362^{(1)}, \pm 0.50088^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.63657	10.0943	0.8459
N_{21}	0.7180	$\left\{\begin{array}{c}\pm 2.11688^{(1)}, \pm 1.63978^{(1)}, \\ \pm 0.91100^{(1)}, 0^{(1)}\end{array}\right\}$	0.4771	9.3353	0.7549
N_{22}	0.7200	$\left\{\begin{array}{c}\pm 2.19399^{(1)}, \pm 1.59038^{(1)}, \\ \pm 0.81060^{(1)}, 0^{(1)}\end{array}\right\}$	0.60361	9.1899	0.7467
N_{23}	0.7410	$\left\{\begin{array}{c}\pm 2.24698^{(1)}, \pm 1.41421^{(1)}, \\ \pm 0.80194^{(1)}, \pm 0.55496^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.83277	10.0361	0.8453
N_{24}	0.7290	$\left\{\begin{array}{c}\pm 2.11917^{(1)}, \pm 1.41421^{(1)}, \\ \pm 1.15904^{(1)}, \pm 0.40713^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.70496	10.1991	0.8479
N_{25}	0.7190	$\left\{\begin{array}{c}\pm 2.08397^{(1)}, \pm 1.57184^{(1)}, \\ \pm 1^{(1)}, \pm 0.43173^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.51213	10.1750	0.8472
N_{26}	0.7370	$\left\{\begin{array}{c}\pm 2.20595^{(1)}, \pm 1.33763^{(1)}, \\ \pm 1^{(1)}, \pm 0.58699^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.86832	10.2611	0.8570
N_{27}	0.7360	$\left\{\begin{array}{c}\pm 2.13578^{(1)}, \pm 1.41421^{(1)}, \\ \pm 1^{(1)}, \pm 0.66215^{(1)}, \\ 0^{(1)}\end{array}\right\}$	0.72157	10.4242	0.8649
N_{28}	0.7530	$\left\{\begin{array}{c}\pm 2.33441^{(1)}, \pm 1.41421^{(1)}, \\ \pm 0.74196^{(1)}, 0^{(1)}\end{array}\right\}$	0.9202	8.9811	0.7360
N_{29}	0.7350	$\left\{\begin{array}{c}\pm 2.25525^{(1)}, \pm 1.55821^{(1)}, \\ \pm 0.69704^{(1)}, 0^{(1)}\end{array}\right\}$	0.69704	9.0209	0.7367

N_{30}	0.7200	$\left\{ \begin{array}{c} \pm 2.23607^{(1)}, \pm 1.73205^{(1)}, \\ 0^{(1)} \end{array} \right\}$	0.50402	7.9362	0.5985
N_{31}	0.7350	$\left\{ \begin{array}{c} \pm 2.28825^{(1)}, \pm 1.41421^{(1)}, \\ 0.87403^{(1)}, 0^{(1)} \end{array} \right\}$	0.87404	9.1529	0.7465
N_{32}	0.7310	$\left\{ \begin{array}{c} \pm 2.23607^{(1)}, \pm 1.41421^{(1)}, \\ \pm 1^{(1)}, 0^{(1)} \end{array} \right\}$	0.82186	9.3005	0.7547
N_{33}	0.7510	$\left\{ \begin{array}{c} \pm 2.26382^{(1)}, \pm 1.27932^{(1)}, \\ \pm 1^{(1)}, \pm 0.48831^{(1)}, \\ 0^{(1)} \end{array} \right\}$	0.9845	10.0629	0.8461
N_{34}	0.7340	$\left\{ \begin{array}{c} \pm 2.17533^{(1)}, \pm 1.41421^{(1)}, \\ \pm 1.12603^{(1)}, 0^{(1)} \end{array} \right\}$	0.76112	9.43115	0.7614
N_{35}	0.7500	$\left\{ \begin{array}{c} \pm 2.23607^{(1)}, \pm 1^{(1)}, \pm 1^{(1)}, \\ \pm 1^{(1)}, 0^{(1)} \end{array} \right\}$	1.23607	10.4721	0.8708

Density of nonane in column 2 are taken from [20]