

Molecular structure of 1,2,3-triethyldiaziridine: gas-phase electron diffraction and theoretical calculations

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S1. NMR experiment

(1*S**,2*S**)-1,2,3-Triethyldiaziridine (TEDA) was synthesized at the N.D. Zelinsky Institute of Organic Chemistry, RAS, according to the method given in literature.^{S1}

All the NMR spectra were recorded at 298 K on Bruker Avance III -400 instrument equipped with the Z-gradient broadband observe probe. 25 mg of the sample were dissolved in 0.6 ml of CDCl₃. The ¹H and ¹³C chemical shifts (δ), which values are reported in ppm, were calibrated to the residual protons (7.27 ppm) and carbon atoms (77.00 ppm) of the solvent. Coupling constants, *J*, are given in Hz. Multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet).

An analysis of the ¹H and ¹³C 1D NMR spectra of the (1*S**,2*S**)-1,2,3-Triethyldiaziridine (TEDA) registered at 298 K (Fig. S1-S4) has demonstrated that in solution the compound exists only in single conformation (there are clean peaks of only one compound).

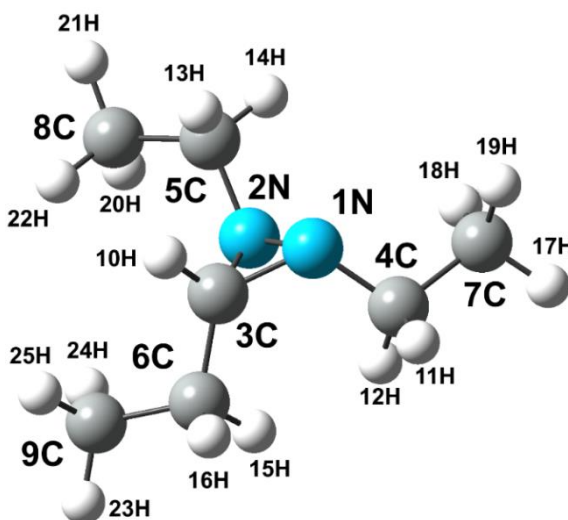


Figure S1. (1*S**,2*S**)-1,2,3-Triethyldiaziridine (conformer **1c**); *trans*-configuration of ethyl groups at diaziridine nitrogen atoms.

^1H NMR (400.16 MHz, CDCl_3) δ , ppm. J/Hz: 1.00 (t, $^3J_{\text{H,H}} = 7.2$ Hz, 3 H, CH_3), 1.06 (t, $^3J_{\text{H,H}} = 7.2$ Hz, 3 H, CH_3), 1.09 (t, $^3J_{\text{H,H}} = 7.1$ Hz, 3 H, CH_3), 1.47–1.63 (m, 2 H, $\text{CH}_2\text{-Cring}$), 2.23–2.32 (dq, $^2J_{\text{H,H}} = 11.8$ Hz, $^3J_{\text{H,H}} = 7.1$ Hz, 1 H, N-CH), 2.34–2.48 (m, 3H, CHring , N-CH, N-CH), 2.48–2.57 (dq, $^2J_{\text{H,H}} = 12.1$ Hz, $^3J_{\text{H,H}} = 7.3$ Hz, 1 H, N-CH). ^{13}C NMR (100.62 MHz, CDCl_3) δ , ppm.: 10.6 ($\text{CH}_3\text{-CH}_2\text{-Cring}$), 13.2 (CH_3), 13.8 (CH_3), 19.5 ($\text{-CH}_2\text{-Cring}$), 46.3 (N- $\text{CH}_2\text{-}$), 55.4 (N- $\text{CH}_2\text{-}$), 66.6 (Cring).

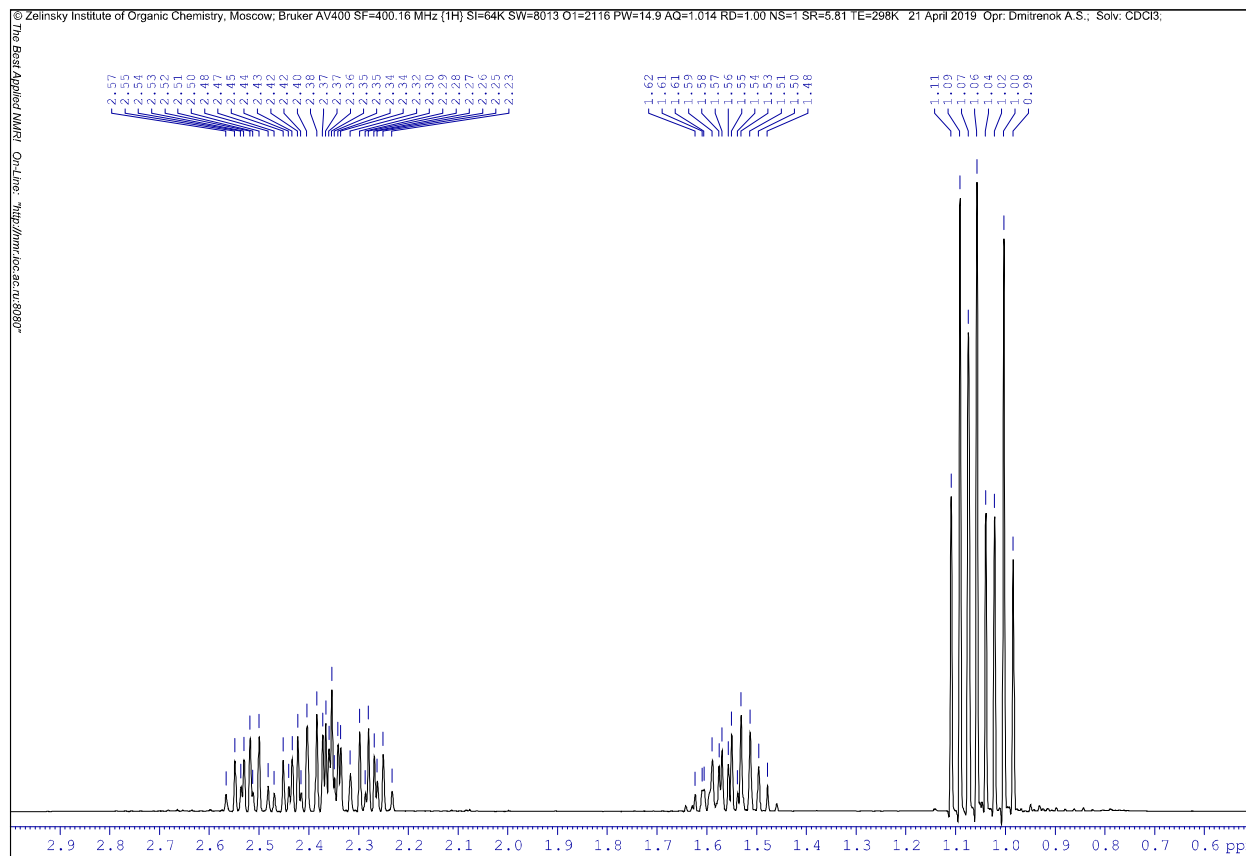


Figure S2. Fragment of the ^1H NMR spectrum for $(1S^*,2S^*)$ -1,2,3-Triethyldiaziridine (CDCl_3).

For further approval, set of 2D spectra $\{^1\text{H}\text{-}^{13}\text{C}\}$ HSQC (*Heteronuclear Spectroscopy Quantum Correlation*), $\{^1\text{H}\text{-}^{13}\text{C}\}$ HMBC (*Heteronuclear Multiple Bond Correlation*), and $\{^1\text{H}\text{-}^1\text{H}\}$ gNOESY (*Nuclear Overhauser Effect Spectroscopy*), was measured in the CDCl_3 solution at 298 K (Fig. S5-S7), that makes it possible to assign all the protons and carbon atoms and relations between them. The mixing time in NOESY was 0.7 s. All correlation NMR spectra were acquired with standard Bruker parameters.

The data of the heteronuclear correlation NMR spectra $\{^1\text{H}\text{-}^{13}\text{C}\}$ HSQC and $\{^1\text{H}\text{-}^{13}\text{C}\}$ HMBC are presented in Table S1. These spectra show how far away each proton is found from a particular carbon atom: respectively, through one or 2-3 bonds.

Table S1. The $\{^1\text{H}-^{13}\text{C}\}$ HSQC and $\{^1\text{H}-^{13}\text{C}\}$ HMBC data for the $(1S^*,2S^*)$ -1,2,3-triethyldiaziridine. Atom numeration is given in Fig. S1.

Atoms numbers	^{13}C NMR chemical shift, ppm	$^1\text{H}-^{13}\text{C}$ HSQC interactions	$^1\text{H}-^{13}\text{C}$ HMBC interactions
3C	66.6	10H	Not registered
4C	46.3	11H, 12H	10H, 17H, 18H, 19H
5C	55.4	13H, 14H	10H, 20H, 21H, 22H
6C	19.5	15H, 16H	10H, 23H, 34H, 25H
7C	13,8	17H, 18H, 19H	11H, 12H
8C	13.2	20H, 21H, 22H	13H, 14H
9C	10,6	23H, 24H, 25H	15H, 16H

The 2D NMR spectrum $\{^1\text{H}-^1\text{H}\}$ gNOESY shows the spatial arrangement of the protons relative to each other (Table S2 and Fig. S7). Proton 10H has cross-peaks with protons 23H, 24H, and 25H; proton 11H has cross-peaks with protons 15H and 16H. The mixing time in the NOESY spectrum was 0.7 s.

Table S2. The $\{^1\text{H}-^1\text{H}\}$ NOESY data of $(1S^*,2S^*)$ -1,2,3-triethyldiaziridine. Atom numeration is given in Fig. S1.

Atoms numbers	^1H NMR chemical shift, ppm	Coupling constant, (J Hz)	$^1\text{H}-^1\text{H}$ NOESY interactions
10H	2.35. t, 1H	7.2 ($^3J_{10\text{H}-15\text{H}} = ^3J_{10\text{H}-16\text{H}}$)	23H, 24H, 25H
11H	2.34-2.43, dq, 1H	-	12H, 15H, 16H, 17H, 18H, 19H
12H	2.48-2.57, dq, 1H	12.1 ($^2J_{12\text{H}-11\text{H}}$) 7.3 ($^3J_{11\text{H}-17\text{H}} = ^3J_{11\text{H}-18\text{H}} = ^3J_{11\text{H}-19\text{H}}$)	11H, 17H, 18H, 19H
13H	2.23-2.32, dq, 1H	11.8 ($^2J_{13\text{H}-14\text{H}}$) 7.3 ($^3J_{13\text{H}-20\text{H}} = ^3J_{13\text{H}-21\text{H}} = ^3J_{13\text{H}-22\text{H}}$)	14H, 20H, 21H, 22H
14H	2.38-2.47	11.8 ($^2J_{14\text{H}-13\text{H}}$) 7.3 ($^3J_{14\text{H}-20\text{H}} = ^3J_{14\text{H}-21\text{H}} = ^3J_{14\text{H}-22\text{H}}$)	13H, 20H, 21H, 22H
15H,16H	1.46-1.64, m, 2H	-	11H, 23H, 24H, 25H
17H, 18H, 19H	1.09, t, 3H	7.1 ($^3J_{\text{H-H}}$)	11H, 12H
20H, 21H, 22H	1.06, t, 3H	7.2 ($^3J_{\text{H-H}}$)	13H, 14H
23H, 24H, 25H	1.00, t, 3H	7.2 ($^3J_{\text{H-H}}$)	10H, 15H, 16H

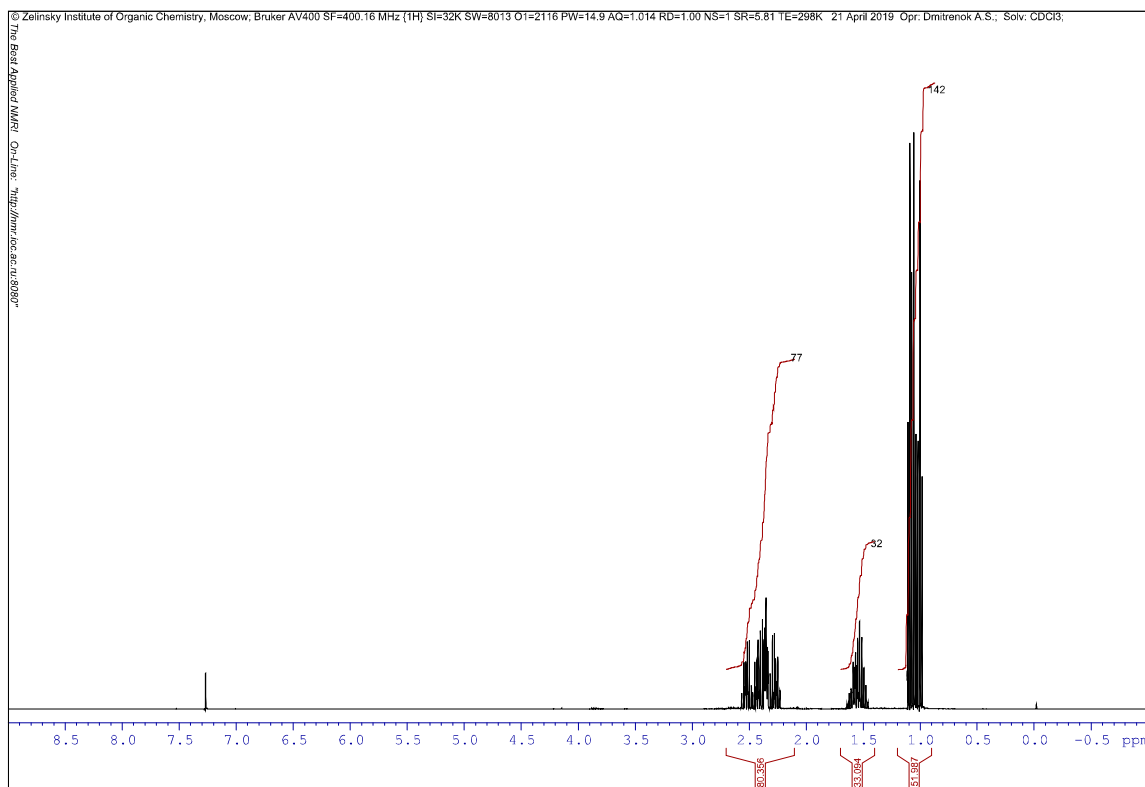


Figure S3. ^1H NMR spectrum of $(1S^*,2S^*)$ -1,2,3-Triethyldiaziridine (CDCl_3).

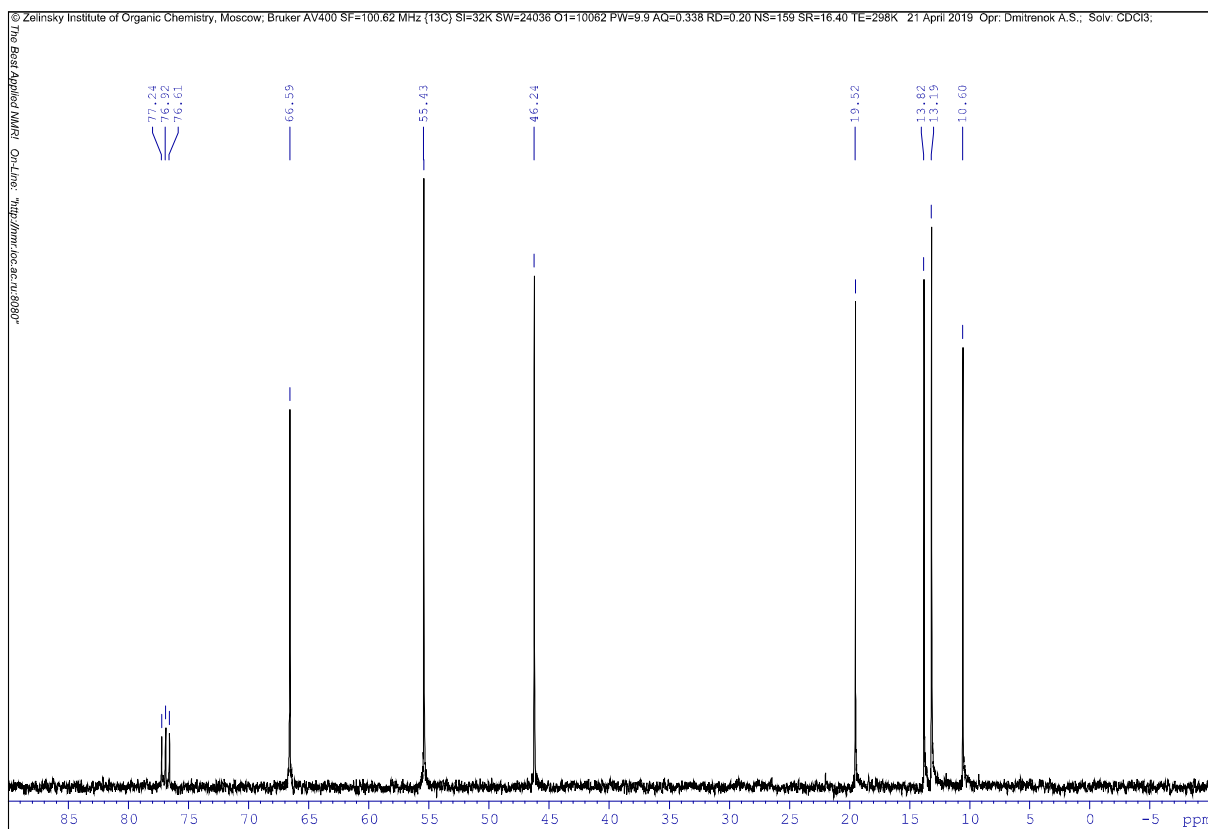


Figure S4. ^{13}C NMR spectrum of $(1S^*,2S^*)$ -1,2,3-Triethyldiaziridine (CDCl_3).

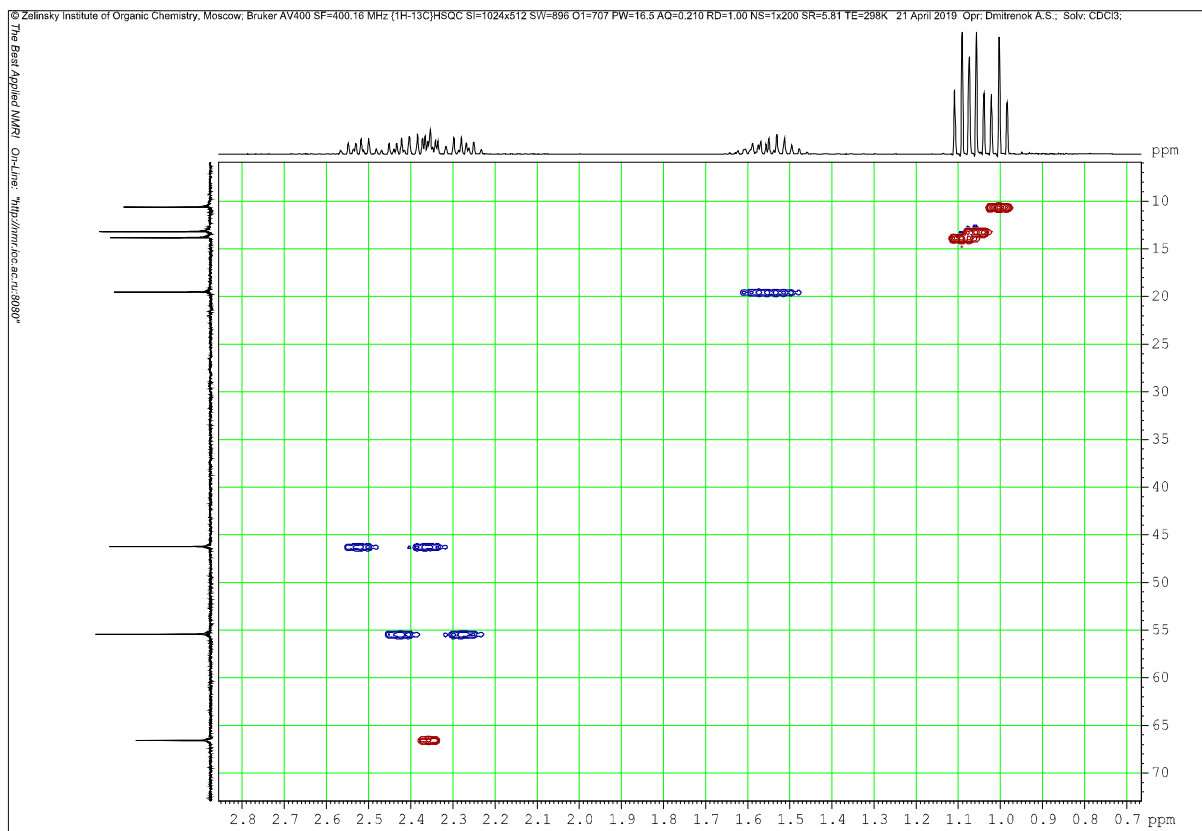


Figure S5. $\{^1\text{H}-^{13}\text{C}\}$ HSQC spectrum of $(1S^*,2S^*)$ -1,2,3-Triethyldiaziridine (CDCl_3).

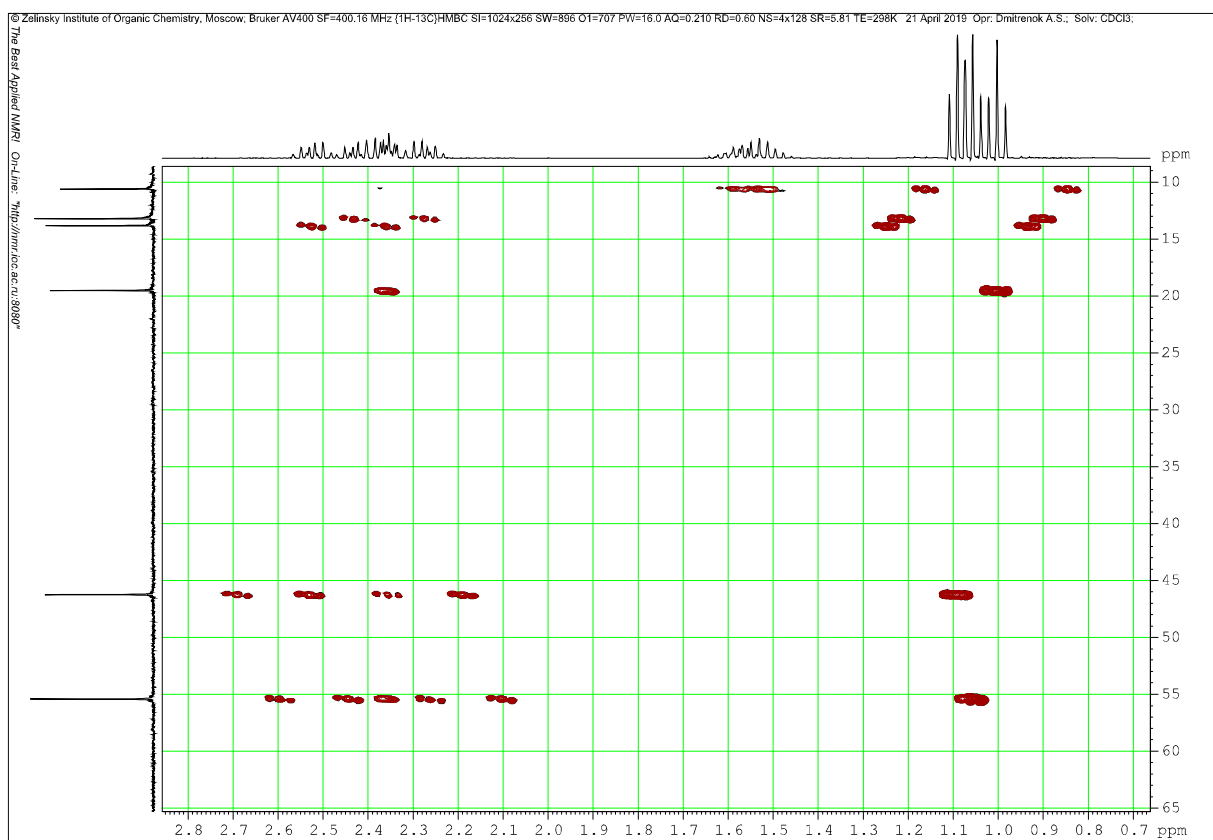


Figure S6. $\{^1\text{H}-^{13}\text{C}\}$ HMBC spectrum of $(1S^*,2S^*)$ -1,2,3-Triethyldiaziridine (CDCl_3).

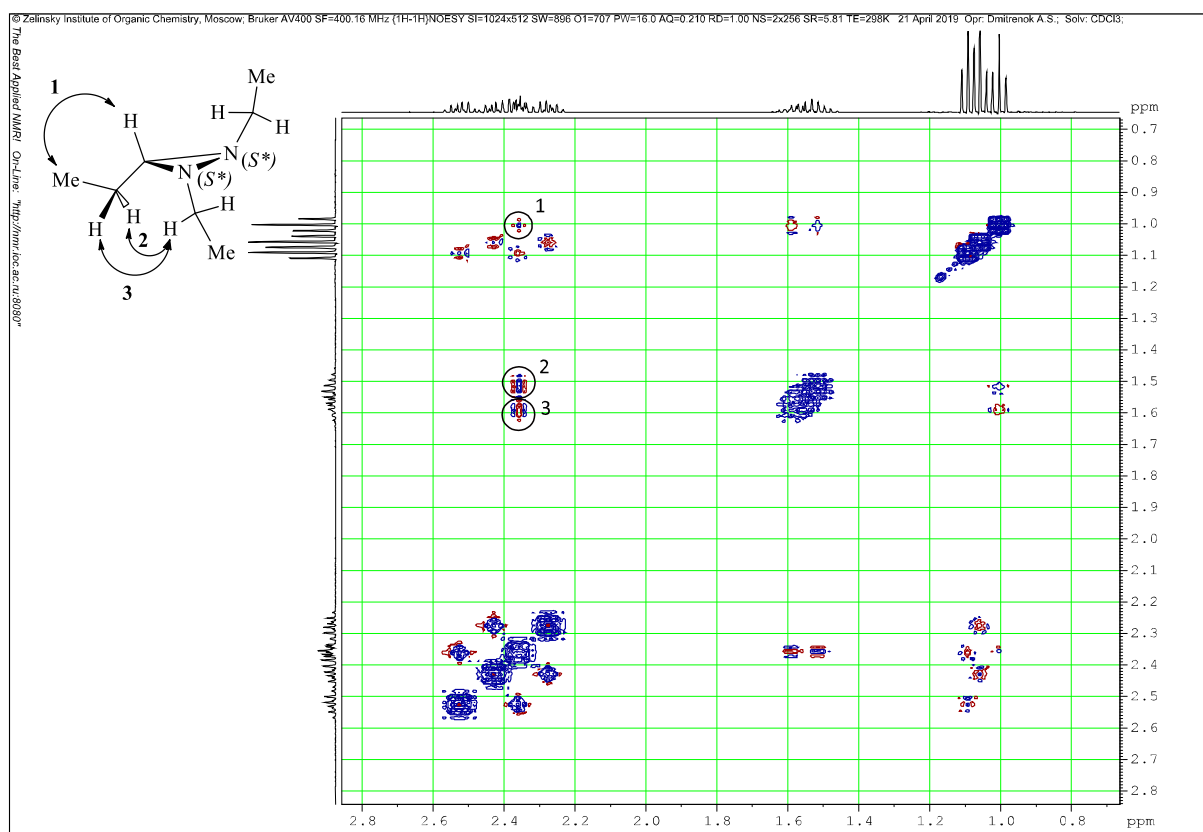


Figure S7. $\{^1\text{H}$ - $^1\text{H}\}$ NOESY spectrum of $(1S^*,2S^*)$ -1,2,3-Triethyldiaziridine (CDCl_3).

S2. IR spectrum

The IR spectrum was recorded on Bruker “Alpha” spectrometer in the range 400-4000 cm^{-1} (resolution 2 cm^{-1}) in a thin layer (Fig. S8). The substance at the tip of the spatula was applied to a KBr plate and pressed against another KBr plate. The plates were placed in a metal mandrel and compressed with 4 screws. After that, the whole construction was placed in the socket of the IR spectrometer. The images were taken out at room temperature ($\sim 20^\circ\text{C}$).

IR (thin layer): $\nu = 3897, 3869, 3852, 3832, 3733, 3699, 3475, 3443, 2972, 2936, 2877, 2360, 2342, 2180, 1822, 1728, 1633, 1463, 1448, 1410, 1377, 1345, 1288, 1180, 1118, 1096, 1041, 993, 888, 840, 682, 633, 591, 558, 465 \text{ cm}^{-1}$.

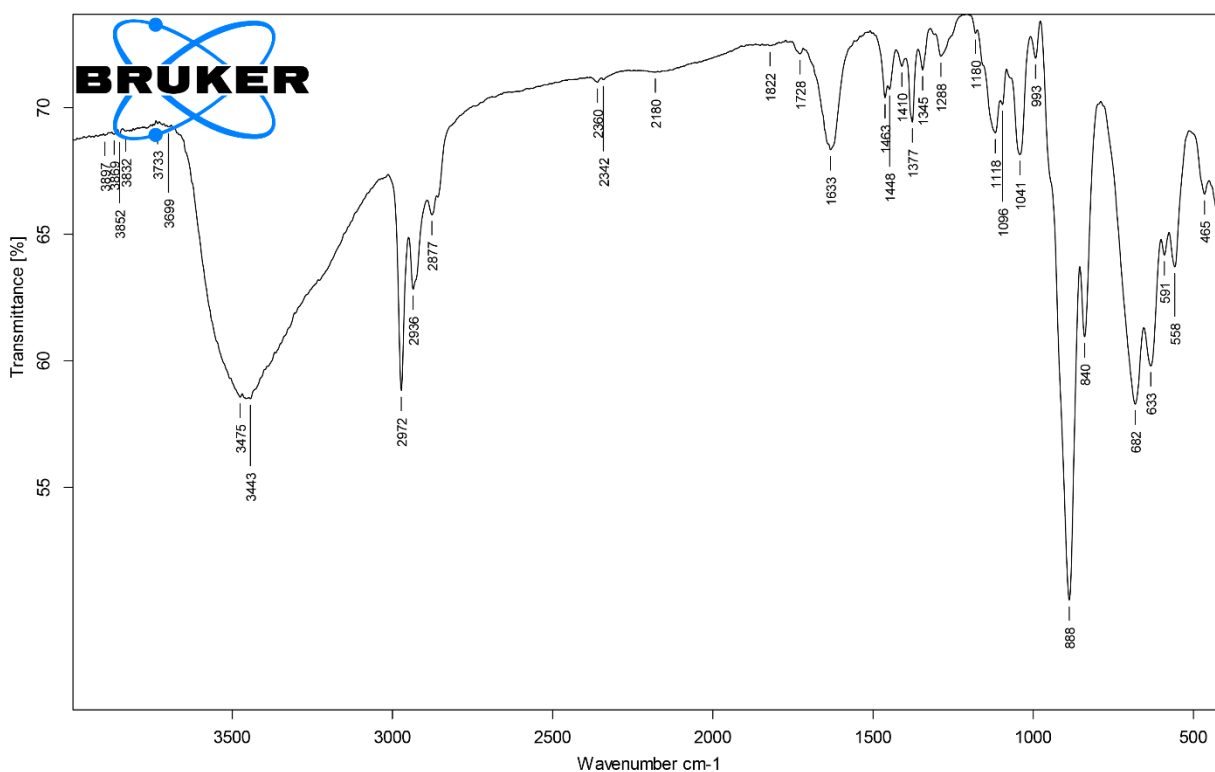


Figure S8. IR spectrum of (1S*,2S*)-1,2,3-Triethyldiaziridine (CDCl₃).

S3. Gas-phase electron diffraction experiment, quantum chemistry and the results of structural analysis

A modified apparatus EG-100M was used to obtain diffractograms in GED. The photo films (MACO EM-Film EMS) were recorded at the nominal long (LD) and short (SD) nozzle-to-film distances with the accelerating voltage of ca. 60kV. The conditions of the experiment are given in Table S3.

Table S3. The GED experiment conditions for the long (LD) and short (SD) camera distances

Parameter	LD = 362.3 mm	SD = 193.9 mm
Beam current, μA	1.6	2.2
Exposure time, sec.	25, 30	35
Nozzle temperature, K	291	285
Residual gas pressure, mm Hg	$3.0 \cdot 10^{-5}$	$3.0 \cdot 10^{-5}$
Number of the diffraction patterns for substance	2	2
Number of the diffraction patterns for standard (CCl_4)	2	2
Wavelength of electrons (λ), $\text{\AA}$	0.049687	0.049934
Range of scattering angles (s), $\text{\AA}^{-1}$	4.000 – 17.625 ($\Delta s = 0.125$)	7.00 – 28.00 ($\Delta s = 0.25$)

The incident electron wavelength was calibrated using the CCl_4 standard at the temperature of the experiment. The optical densities were measured using an Epson Perfection 4870 PHOTO commercial scanner. The wavelengths and the total intensities of electron scattering $I^{tot}(s)$ were determined with use of Plate program.^{S2}

The total electron scattering intensities $I(s)$ for both distances are shown in Fig. S9. The background lines were approximated by polynomial curves and checked qualitatively in the Plate program. The values of the total scattering intensity functions $I^{tot}(s)$ and the background lines $I^b(s)$ for the long and short camera distances are given in Tables S4 and S5.

In this work we used Gaussian-4 method as quantum-chemical approximation to calculate the enthalpy of TEDA formation and conformer composition. This is a composite technique aimed at getting accurate energies without requiring extensive computer resources.^{S3} Previously, we used MP2/cc-PVTZ and B3LYP/cc-PVTZ approximations to calculate starting equilibrium parameters for further structural analysis. Quadratic and cubic force fields were calculated at MP2/cc-PVTZ level to calculate harmonic and anharmonic corrections. More information one can get from our previous work on the quantum-chemical study of TEDA.^{S4} All quantum-chemical calculations were performed via Gaussian 09 Rev. C01.^{S5}

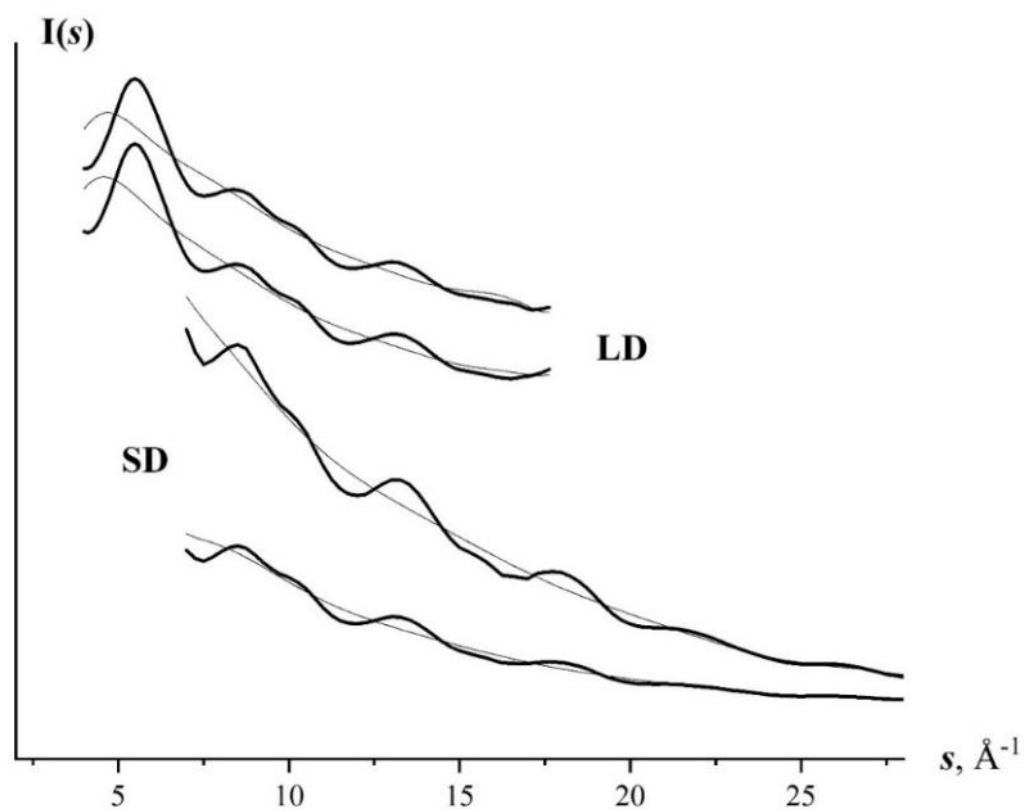


Figure S9. Experimental intensity curves $I(s)$ with the background lines for long (LD) and short (SD) camera distances

Table S4. The total scattering intensity functions $I^{tot}(s)$ and the background lines $I^b(s)$ for TEDA. Long camera distance (LD=362.3 mm).

Diffractogram №1

$s, \text{\AA}^{-1}$	$I^{tot}(s)$	$I^b(s)$	$s, \text{\AA}^{-1}$	$I^{tot}(s)$	$I^b(s)$	$s, \text{\AA}^{-1}$	$I^{tot}(s)$	$I^b(s)$
4.000	0.36172	0.39592	8.625	0.34193	0.33539	13.250	0.27978	0.26940
4.125	0.36203	0.40067	8.750	0.34056	0.33297	13.375	0.27866	0.26814
4.250	0.36489	0.40449	8.875	0.33867	0.33054	13.500	0.27710	0.26690
4.375	0.37007	0.40732	9.000	0.33523	0.32810	13.625	0.27528	0.26570
4.500	0.37701	0.40914	9.125	0.33189	0.32567	13.750	0.27318	0.26454
4.625	0.38557	0.41000	9.250	0.32848	0.32324	13.875	0.27076	0.26343
4.750	0.39505	0.40998	9.375	0.32502	0.32084	14.000	0.26819	0.26238
4.875	0.40561	0.40917	9.500	0.32185	0.31847	14.125	0.26563	0.26139
5.000	0.41648	0.40771	9.625	0.31911	0.31613	14.250	0.26313	0.26047
5.125	0.42659	0.40570	9.750	0.31713	0.31384	14.375	0.26071	0.25962
5.250	0.43392	0.40327	9.875	0.31532	0.31160	14.500	0.25852	0.25885
5.375	0.43823	0.40054	10.000	0.31373	0.30942	14.625	0.25649	0.25816
5.500	0.43952	0.39761	10.125	0.31185	0.30731	14.750	0.25492	0.25753
5.625	0.43738	0.39455	10.250	0.30949	0.30526	14.875	0.25358	0.25698
5.750	0.43272	0.39144	10.375	0.30664	0.30327	15.000	0.25264	0.25649
5.875	0.42599	0.38834	10.500	0.30332	0.30136	15.125	0.25189	0.25604
6.000	0.41747	0.38529	10.625	0.29950	0.29951	15.250	0.25129	0.25564
6.125	0.40843	0.38233	10.750	0.29545	0.29774	15.375	0.25080	0.25525
6.250	0.39898	0.37946	10.875	0.29136	0.29602	15.500	0.25017	0.25486
6.375	0.38935	0.37670	11.000	0.28747	0.29436	15.625	0.24951	0.25445
6.500	0.37961	0.37405	11.125	0.28399	0.29277	15.750	0.24884	0.25399
6.625	0.37063	0.37151	11.250	0.28123	0.29122	15.875	0.24793	0.25345
6.750	0.36228	0.36908	11.375	0.27899	0.28971	16.000	0.24718	0.25281
6.875	0.35485	0.36672	11.500	0.27721	0.28825	16.125	0.24630	0.25204
7.000	0.34858	0.36445	11.625	0.27604	0.28682	16.250	0.24571	0.25111
7.125	0.34354	0.36222	11.750	0.27542	0.28542	16.375	0.24525	0.25002
7.250	0.34040	0.36004	11.875	0.27527	0.28404	16.500	0.24493	0.24876
7.375	0.33836	0.35789	12.000	0.27542	0.28267	16.625	0.24423	0.24732
7.500	0.33787	0.35574	12.125	0.27591	0.28132	16.750	0.24299	0.24573
7.625	0.33808	0.35359	12.250	0.27649	0.27998	16.8750	0.24140	0.24403
7.750	0.33896	0.35142	12.375	0.27714	0.27864	17.0000	0.23996	0.24228
7.875	0.33998	0.34923	12.500	0.27795	0.27730	17.1250	0.23936	0.24057
8.000	0.34125	0.34702	12.625	0.27881	0.27597	17.2500	0.23942	0.23901
8.125	0.34224	0.34476	12.750	0.27964	0.27464	17.3750	0.24000	0.23777
8.250	0.34309	0.34247	12.875	0.28025	0.27331	17.5000	0.24066	0.23705
8.375	0.34339	0.34014	13.000	0.28048	0.27200	17.6250	0.24125	0.23712
8.500	0.34316	0.33778	13.125	0.28042	0.27069			

Diffractogram №2

$s, \text{\AA}^{-1}$	$I^{\text{tot}}(s)$	$I^b(s)$	$s, \text{\AA}^{-1}$	$I^{\text{tot}}(s)$	$I^b(s)$	$s, \text{\AA}^{-1}$	$I^{\text{tot}}(s)$	$I^b(s)$
4.000	0.40701	0.44428	8.625	0.37764	0.37050	13.250	0.31776	0.30632
4.125	0.40605	0.44828	8.750	0.37645	0.36811	13.375	0.31672	0.30512
4.250	0.40806	0.45124	8.875	0.37479	0.36573	13.500	0.31533	0.30393
4.375	0.41270	0.45318	9.000	0.37142	0.36335	13.625	0.31340	0.30275
4.500	0.41957	0.45413	9.125	0.36817	0.36098	13.750	0.31113	0.30159
4.625	0.42796	0.45420	9.250	0.36455	0.35862	13.875	0.30852	0.30045
4.750	0.43777	0.45346	9.375	0.36114	0.35629	14.000	0.30584	0.29933
4.875	0.44851	0.45204	9.500	0.35789	0.35399	14.125	0.30294	0.29825
5.000	0.45975	0.45004	9.625	0.35530	0.35172	14.250	0.30004	0.29720
5.125	0.47010	0.44759	9.750	0.35298	0.34949	14.375	0.29716	0.29619
5.250	0.47756	0.44478	9.875	0.35135	0.34730	14.500	0.29452	0.29522
5.375	0.48184	0.44171	10.000	0.34981	0.34517	14.625	0.29213	0.29430
5.500	0.48297	0.43847	10.125	0.34801	0.34309	14.750	0.29019	0.29343
5.625	0.48079	0.43513	10.250	0.34572	0.34107	14.875	0.28850	0.29261
5.750	0.47582	0.43175	10.375	0.34274	0.33911	15.000	0.28733	0.29185
5.875	0.46855	0.42838	10.500	0.33931	0.33721	15.125	0.28645	0.29114
6.000	0.45955	0.42504	10.625	0.33532	0.33537	15.250	0.28573	0.29047
6.125	0.44956	0.42178	10.750	0.33094	0.33359	15.375	0.28518	0.28986
6.250	0.43962	0.41860	10.875	0.32658	0.33187	15.500	0.28452	0.28928
6.375	0.42926	0.41553	11.000	0.32261	0.33022	15.625	0.28386	0.28875
6.500	0.41891	0.41255	11.125	0.31899	0.32862	15.750	0.28315	0.28824
6.625	0.40894	0.40968	11.250	0.31574	0.32707	15.875	0.28228	0.28775
6.750	0.40015	0.40690	11.375	0.31344	0.32557	16.000	0.28137	0.28727
6.875	0.39195	0.40422	11.500	0.31175	0.32413	16.125	0.28069	0.28679
7.000	0.38500	0.40161	11.625	0.31080	0.32272	16.250	0.28019	0.28630
7.125	0.37953	0.39907	11.750	0.31024	0.32135	16.375	0.27986	0.28580
7.250	0.37589	0.39660	11.875	0.31034	0.32001	16.500	0.27970	0.28528
7.375	0.37359	0.39416	12.000	0.31095	0.31870	16.625	0.28001	0.28473
7.500	0.37248	0.39177	12.125	0.31157	0.31741	16.750	0.28054	0.28418
7.625	0.37244	0.38939	12.250	0.31245	0.31614	16.8750	0.28121	0.28362
7.750	0.37314	0.38704	12.375	0.31356	0.31489	17.0000	0.28177	0.28309
7.875	0.37427	0.38469	12.500	0.31473	0.31364	17.1250	0.28245	0.28262
8.000	0.37557	0.38234	12.625	0.31585	0.31241	17.2500	0.28330	0.28227
8.125	0.37671	0.37998	12.750	0.31680	0.31118	17.3750	0.28430	0.28210
8.250	0.37777	0.37763	12.875	0.31785	0.30996	17.5000	0.28583	0.28223
8.375	0.37848	0.37526	13.000	0.31831	0.30874	17.6250	0.28760	0.28279
8.500	0.37859	0.37288	13.125	0.31824	0.30753			

Table S5. The total scattering intensity functions $I^{tot}(s)$ and the background lines $I^b(s)$ for TEDA. Short camera distance (SD=193.9 mm).

Diffractionogram №1

$s, \text{\AA}^{-1}$	$I^{tot}(s)$	$I^b(s)$	$s, \text{\AA}^{-1}$	$I^{tot}(s)$	$I^b(s)$	$s, \text{\AA}^{-1}$	$I^{tot}(s)$	$I^b(s)$
7.00	0.82226	0.85089	14.00	0.67166	0.65843	21.00	0.56329	0.56540
7.25	0.80245	0.84004	14.25	0.66043	0.65436	21.25	0.56309	0.56290
7.50	0.79188	0.83053	14.50	0.64965	0.65029	21.50	0.56192	0.56043
7.75	0.79540	0.82167	14.75	0.64037	0.64624	21.75	0.56052	0.55797
8.00	0.80126	0.81303	15.00	0.63340	0.64220	22.00	0.55862	0.55554
8.25	0.80697	0.80441	15.25	0.62961	0.63817	22.25	0.55636	0.55315
8.50	0.80917	0.79570	15.50	0.62576	0.63417	22.50	0.55372	0.55081
8.75	0.80549	0.78693	15.75	0.62118	0.63021	22.75	0.55075	0.54853
9.00	0.79287	0.77813	16.00	0.61523	0.62629	23.00	0.54769	0.54634
9.25	0.77875	0.76940	16.25	0.60902	0.62244	23.25	0.54496	0.54425
9.50	0.76688	0.76081	16.50	0.60819	0.61865	23.50	0.54220	0.54228
9.75	0.75675	0.75245	16.75	0.60728	0.61495	23.75	0.53993	0.54043
10.00	0.75048	0.74439	17.00	0.60634	0.61134	24.00	0.53776	0.53873
10.25	0.74262	0.73668	17.25	0.61036	0.60784	24.25	0.53569	0.53718
10.50	0.73240	0.72936	17.50	0.61176	0.60443	24.50	0.53392	0.53579
10.75	0.71823	0.72244	17.75	0.61231	0.60113	24.75	0.53273	0.53455
11.00	0.70423	0.71592	18.00	0.61137	0.59794	25.00	0.53235	0.53346
11.25	0.69223	0.70979	18.25	0.60835	0.59485	25.25	0.53206	0.53250
11.50	0.68396	0.70402	18.50	0.60377	0.59186	25.50	0.53221	0.53165
11.75	0.67944	0.69859	18.75	0.59735	0.58897	25.75	0.53208	0.53088
12.00	0.67864	0.69345	19.00	0.58978	0.58615	26.00	0.53202	0.53015
12.25	0.67926	0.68857	19.25	0.58198	0.58341	26.25	0.53144	0.52944
12.50	0.68365	0.68391	19.50	0.57546	0.58073	26.50	0.53039	0.52870
12.75	0.68827	0.67942	19.75	0.57025	0.57810	26.75	0.52898	0.52790
13.00	0.69168	0.67507	20.00	0.56682	0.57551	27.00	0.52728	0.52701
13.25	0.69191	0.67082	20.25	0.56472	0.57295	27.25	0.52538	0.52602
13.50	0.68849	0.66665	20.50	0.56424	0.57042	27.50	0.52355	0.52496
13.75	0.68132	0.66252	20.75	0.56378	0.56790	27.75	0.52227	0.52388
						28.00	0.52100	0.52291

Diffractogram №2

$s, \text{\AA}^{-1}$	$I^{\text{tot}}(s)$	$I^b(s)$	$s, \text{\AA}^{-1}$	$I^{\text{tot}}(s)$	$I^b(s)$	$s, \text{\AA}^{-1}$	$I^{\text{tot}}(s)$	$I^b(s)$
7.00	0.35088	0.36508	14.00	0.28233	0.27611	21.00	0.23489	0.23564
7.25	0.34365	0.36212	14.25	0.27696	0.27406	21.25	0.23462	0.23473
7.50	0.34135	0.35968	14.50	0.27148	0.27205	21.50	0.23417	0.23383
7.75	0.34475	0.35729	14.75	0.26706	0.27005	21.75	0.23370	0.23294
8.00	0.34941	0.35467	15.00	0.26380	0.26809	22.00	0.23300	0.23206
8.25	0.35319	0.35169	15.25	0.26178	0.26615	22.25	0.23215	0.23120
8.50	0.35470	0.34832	15.50	0.25973	0.26425	22.50	0.23137	0.23036
8.75	0.35252	0.34457	15.75	0.25777	0.26238	22.75	0.23050	0.22956
9.00	0.34679	0.34052	16.00	0.25521	0.26056	23.00	0.22945	0.22879
9.25	0.34033	0.33626	16.25	0.25317	0.25879	23.25	0.22854	0.22808
9.50	0.33482	0.33189	16.50	0.25275	0.25707	23.50	0.22758	0.22741
9.75	0.33023	0.32750	16.75	0.25252	0.25541	23.75	0.22688	0.22681
10.00	0.32712	0.32315	17.00	0.25259	0.25381	24.00	0.22603	0.22626
10.25	0.32321	0.31892	17.25	0.25366	0.25228	24.25	0.22532	0.22579
10.50	0.31740	0.31486	17.50	0.25401	0.25081	24.50	0.22467	0.22537
10.75	0.30941	0.31098	17.75	0.25404	0.24942	24.75	0.22443	0.22502
11.00	0.30106	0.30731	18.00	0.25352	0.24809	25.00	0.22429	0.22472
11.25	0.29427	0.30386	18.25	0.25236	0.24682	25.25	0.22434	0.22446
11.50	0.28972	0.30062	18.50	0.25054	0.24562	25.50	0.22435	0.22424
11.75	0.28750	0.29758	18.75	0.24796	0.24447	25.75	0.22448	0.22402
12.00	0.28720	0.29472	19.00	0.24493	0.24337	26.00	0.22434	0.22381
12.25	0.28791	0.29203	19.25	0.24180	0.24232	26.25	0.22422	0.22358
12.50	0.28973	0.28948	19.50	0.23926	0.24130	26.50	0.22389	0.22333
12.75	0.29194	0.28705	19.75	0.23730	0.24031	26.75	0.22355	0.22306
13.00	0.29319	0.28473	20.00	0.23589	0.23935	27.00	0.22296	0.22278
13.25	0.29294	0.28249	20.25	0.23516	0.23841	27.25	0.22246	0.22253
13.50	0.29080	0.28031	20.50	0.23500	0.23748	27.50	0.22208	0.22237
13.75	0.28711	0.27819	20.75	0.23481	0.23655	27.75	0.22176	0.22242
						28.00	0.22162	0.22284

Table S6. Relative electronic energies (ΔE_e), Gibbs free energies (ΔG°_{298}) and molar content (p) of TEDA conformations, calculated by quantum chemistry methods.

Conformer	B3LYP/cc-pVTZ	MP2/cc-pVTZ	Gaussian-4			
	ΔE_e , kJ·mol ⁻¹		ΔG°_{298} , kJ·mol ⁻¹	p , %	$p(\Delta E_e < 2.3)$, %	$p(\Delta E_e < 1.2)$, %
1a	0.00	0.00	0.00	25.9	27.6	34.6
1b	0.96	0.96	1.33	15.2	16.2	20.3
1c	1.17	0.84	0.61	20.3	21.6	27.1
1d	1.34	1.17	1.62	13.5	14.4	18.0
1e	1.84	2.09	2.19	10.7	11.4	-
1f	2.97	2.22	2.82	8.3	8.8	-
1g	4.06	5.31	4.73	3.9	-	-
1h	4.44	6.78	6.12	2.2	-	-

Table S7. Low harmonic frequencies (cm⁻¹), calculated in MP2/cc-pVTZ approximation for the lowest energy TEDA conformers.

1a	1b	1c	1d	1e	1f	1g	1h
59.3	58.1	60.7	69.1	64.5	70.4	69.1	64.5
70.1	69.0	64.5	80.9	88.4	85.5	81.2	80.9
83.9	94.9	99.7	92.6	94.2	93.7	91.2	90.5

Table S8. Correlation matrices for the GED refinement of the geometric parameters combined in independent groups.

1. For mixture of 8 conformers (**1a–h**)

	C_{cyc}NC	NC3H	CH	HC3C	NNC_{eth}	NC3C	CC	NN	CN
C_{cyc}NC	1.0000								
NC3H	0.1716	1.0000							
CH	0.1362	0.2811	1.0000						
HC3C	-0.1598	-0.3023	-0.5569	1.0000					
NNC_{eth}	-0.0320	0.6275	0.4133	-0.3164	1.0000				
NC3C	-0.3410	-0.2156	0.3800	-0.0048	-0.3506	1.0000			
CC	-0.0971	-0.0276	0.4646	-0.3861	0.4926	0.0875	1.0000		
NN	0.1457	0.0062	-0.2392	0.2997	-0.6241	0.2861	-0.6350	1.0000	
CN	-0.2879	-0.4225	-0.7069	0.3932	-0.2457	-0.4739	-0.3709	-0.1756	1.0000

1. For mixture of 6 conformers (**1a–f**)

	C_{cyc}NC	NC3H	CH	HC3C	NNC_{eth}	NC3C	CC	NN	CN
C_{cyc}NC	1.0000								
NC3H	0.1422	1.0000							
CH	0.1480	0.1827	1.0000						
HC3C	-0.1287	-0.1516	-0.6191	1.0000					
NNC_{eth}	-0.0758	0.3840	0.3948	-0.2814	1.0000				
NC3C	-0.3091	-0.1158	0.4248	-0.1023	-0.3074	1.0000			
CC	-0.0809	-0.0097	0.5352	-0.4820	0.6066	0.1142	1.0000		
NN	0.1507	0.0192	-0.3133	0.3757	-0.7447	0.2451	-0.6574	1.0000	
CN	-0.2942	-0.2771	-0.7039	0.3997	-0.1133	-0.5686	-0.4407	-0.1281	1.0000

1. For mixture of 4 conformers (**1a–d**)

	C_{cyc}NC	NC3H	CH	HC3C	NNC_{eth}	NC3C	CC	NN	CN
C_{cyc}NC	1.0000								
NC3H	0.1377	1.0000							
CH	0.2638	0.1900	1.0000						
HC3C	-0.2154	-0.1096	-0.7312	1.0000					
NNC_{eth}	0.0046	0.3451	0.3997	-0.3353	1.0000				
NC3C	-0.2283	-0.1319	0.3837	-0.1472	-0.4099	1.0000			
CC	0.0122	0.0591	0.5783	-0.5716	0.6590	0.0482	1.0000		
NN	0.0965	-0.0709	-0.3533	0.4318	-0.8228	0.3247	-0.6858	1.0000	
CN	-0.3787	-0.2133	-0.7370	0.5036	-0.0678	-0.5841	-0.4723	-0.0817	1.0000

Table S9. Equilibrium (r_e) and thermal average (r_g , r_a) distances, vibrational corrections (Δ), and mean amplitudes (u) for internuclear distances of TEDA conformation **1a** (in Å), obtained for 291 K by GED refinement (initial approximation MP2/cc-PVTZ). n – number of equivalent parameters.

Atomic pair	n	r_e	r_g	r_a	Δr	$\Delta r(\text{har})$	$\Delta r(\text{kin})$	$\Delta r(\text{dyn})$	$\Delta r(\text{rot})$	u
C6-H15	1	1.0891	1.1127	1.1101	0.0236	0.0494	-0.0442	0.0184	0.0000	0.0550
C7-H19	1	1.0909	1.1155	1.1136	0.0246	0.0621	-0.0563	0.0188	0.0000	0.0467
C8-H20	1	1.0910	1.1141	1.1111	0.0231	0.0534	-0.0484	0.0181	0.0000	0.0580
C9-H23	1	1.0911	1.1122	1.1086	0.0211	0.0429	-0.0383	0.0166	-0.0001	0.0639
C8-H22	1	1.0912	1.1147	1.1116	0.0235	0.0523	-0.0474	0.0186	0.0000	0.0588
C7-H18	1	1.0913	1.1158	1.1141	0.0246	0.0646	-0.0586	0.0186	0.0000	0.0445
C8-H21	1	1.0917	1.1133	1.1092	0.0216	0.0376	-0.0335	0.0175	0.0000	0.0676
C9-H24	1	1.0918	1.1175	1.1175	0.0256	0.0781	-0.0707	0.0182	0.0000	0.0093
C7-H17	1	1.0919	1.1135	1.1095	0.0216	0.0382	-0.0340	0.0174	0.0000	0.0672
C3-H10	1	1.0920	1.1134	1.1083	0.0215	0.0169	-0.0130	0.0176	0.0000	0.0753
C9-H25	1	1.0926	1.1176	1.1174	0.0250	0.0735	-0.0664	0.0178	0.0001	0.0163
C4-H12	1	1.0932	1.1174	1.1140	0.0242	0.0434	-0.0386	0.0194	0.0000	0.0625
C4-H11	1	1.0949	1.1185	1.1153	0.0236	0.0458	-0.0407	0.0185	0.0000	0.0605
C5-H13	1	1.0949	1.1174	1.1131	0.0225	0.0347	-0.0302	0.0180	0.0000	0.0689
C6-H16	1	1.0950	1.1186	1.1160	0.0235	0.0529	-0.0474	0.0180	0.0000	0.0538
C5-H14	1	1.0973	1.1199	1.1155	0.0226	0.0328	-0.0284	0.0182	0.0000	0.0705
N2-C3	1	1.4216	1.4312	1.4295	0.0096	0.0060	-0.0046	0.0082	0.0000	0.0487
N1-C3	1	1.4270	1.4369	1.4352	0.0100	0.0065	-0.0050	0.0085	0.0000	0.0491
N1-C4	1	1.4393	1.4506	1.4489	0.0113	0.0064	-0.0046	0.0094	0.0001	0.0491
N2-C5	1	1.4401	1.4503	1.4486	0.0102	0.0054	-0.0036	0.0083	0.0001	0.0491
N1-N2	1	1.4859	1.4981	1.4961	0.0122	0.0067	-0.0061	0.0115	0.0001	0.0542
C3-C6	1	1.4985	1.5094	1.5078	0.0109	0.0067	-0.0053	0.0096	-0.0001	0.0492
C5-C8	1	1.5117	1.5248	1.5237	0.0132	0.0259	-0.0244	0.0117	0.0000	0.0416
C4-C7	1	1.5131	1.5280	1.5273	0.0149	0.0342	-0.0324	0.0131	0.0000	0.0329
C6-C9	1	1.5224	1.5375	1.5374	0.0151	0.0434	-0.0412	0.0128	0.0001	0.0147
H23-H25	1	1.7655	1.7939	1.7901	0.0284	0.0871	-0.0846	0.0260	-0.0001	0.0825
H24-H25	1	1.7683	1.8007	1.8004	0.0324	0.1213	-0.1160	0.0271	0.0000	0.0264
H23-H24	1	1.7689	1.7969	1.7940	0.0280	0.0971	-0.0939	0.0247	0.0001	0.0721
H17-H18	1	1.7698	1.7982	1.7933	0.0283	0.0814	-0.0798	0.0267	0.0000	0.0929
H20-H21	1	1.7703	1.7993	1.7933	0.0290	0.0699	-0.0692	0.0283	0.0000	0.1036
H18-H19	1	1.7710	1.8017	1.7986	0.0307	0.1006	-0.0976	0.0277	0.0000	0.0752
H20-H22	1	1.7721	1.8021	1.7969	0.0300	0.0836	-0.0822	0.0285	0.0001	0.0964
H21-H22	1	1.7730	1.8012	1.7951	0.0282	0.0665	-0.0659	0.0275	0.0001	0.1043
H17-H19	1	1.7744	1.8023	1.7969	0.0279	0.0734	-0.0722	0.0267	0.0000	0.0982
H15-H16	1	1.7859	1.8138	1.8098	0.0279	0.0788	-0.0738	0.0229	0.0000	0.0856
H11-H12	1	1.7976	1.8279	1.8225	0.0303	0.0674	-0.0632	0.0260	0.0001	0.0989
H13-H14	1	1.7998	1.8275	1.8207	0.0277	0.0496	-0.0463	0.0244	0.0000	0.1109
H12-H15	1	1.9586	2.1083	2.0829	0.1497	0.0712	0.0487	0.0297	0.0001	0.2312

N2-H13	1	2.0136	2.0327	2.0276	0.0191	0.0248	-0.0266	0.0210	-0.0001	0.1022
N1-H11	1	2.0166	2.0404	2.0352	0.0239	0.0348	-0.0364	0.0255	0.0000	0.1027
N2-H14	1	2.0659	2.0915	2.0865	0.0256	0.0214	-0.0232	0.0274	0.0000	0.1017
N1-H12	1	2.0812	2.1007	2.0962	0.0195	0.0282	-0.0297	0.0210	0.0000	0.0969
N1-H10	1	2.0928	2.1118	2.1070	0.0191	0.0135	-0.0177	0.0233	0.0000	0.1004
C3-H16	1	2.0980	2.1196	2.1147	0.0216	0.0378	-0.0400	0.0238	0.0000	0.1018
C3-H15	1	2.1102	2.1265	2.1218	0.0163	0.0308	-0.0330	0.0186	-0.0001	0.1004
N2-H10	1	2.1360	2.1581	2.1535	0.0221	0.0139	-0.0178	0.0260	0.0000	0.1000
C5-H20	1	2.1446	2.1651	2.1618	0.0205	0.0570	-0.0584	0.0218	0.0001	0.0852
C7-H12	1	2.1467	2.1766	2.1740	0.0299	0.0658	-0.0661	0.0303	-0.0001	0.0754
C4-H18	1	2.1469	2.1786	2.1754	0.0317	0.0729	-0.0741	0.0329	0.0000	0.0830
C9-H15	1	2.1503	2.1792	2.1778	0.0289	0.0789	-0.0787	0.0288	-0.0001	0.0546
C5-H22	1	2.1509	2.1769	2.1730	0.0260	0.0580	-0.0596	0.0276	0.0000	0.0916
C4-H19	1	2.1523	2.1806	2.1788	0.0283	0.0770	-0.0772	0.0286	-0.0001	0.0644
C8-H14	1	2.1560	2.1797	2.1759	0.0237	0.0465	-0.0472	0.0244	0.0000	0.0914
C7-H11	1	2.1564	2.1804	2.1755	0.0241	0.0338	-0.0356	0.0258	0.0001	0.1037
C5-H21	1	2.1568	2.1881	2.1864	0.0313	0.0930	-0.0928	0.0310	0.0001	0.0610
C6-H24	1	2.1571	2.1785	2.1738	0.0214	0.0362	-0.0378	0.0229	0.0001	0.1014
C4-H17	1	2.1578	2.1793	2.1766	0.0215	0.0632	-0.0634	0.0216	0.0001	0.0768
C8-H13	1	2.1592	2.1833	2.1794	0.0241	0.0467	-0.0475	0.0249	0.0000	0.0917
C9-H16	1	2.1615	2.1831	2.1817	0.0216	0.0785	-0.0780	0.0211	0.0000	0.0550
H10-H14	1	2.1657	2.2057	2.1866	0.0400	0.0244	-0.0047	0.0204	-0.0001	0.2041
C6-H25	1	2.1693	2.1976	2.1979	0.0283	0.0941	-0.0926	0.0268	0.0000	0.0000
C6-H23	1	2.1720	2.1946	2.1903	0.0226	0.0435	-0.0447	0.0238	0.0000	0.0971
C6-H10	1	2.1791	2.2029	2.1982	0.0238	0.0130	-0.0142	0.0249	0.0001	0.1017
N1-C5	1	2.3886	2.4085	2.4064	0.0198	0.0061	-0.0075	0.0212	0.0000	0.0696
N2-C4	1	2.4082	2.4272	2.4252	0.0190	0.0073	-0.0090	0.0208	-0.0001	0.0706
C5-C3	1	2.4160	2.4396	2.4378	0.0236	0.0050	-0.0056	0.0243	-0.0001	0.0664
N1-H14	1	2.4219	2.4823	2.4713	0.0604	0.0156	-0.0117	0.0564	0.0001	0.1651
N1-C7	1	2.4387	2.4606	2.4588	0.0219	0.0183	-0.0187	0.0223	0.0000	0.0666
N2-H12	1	2.4405	2.4569	2.4460	0.0164	0.0244	-0.0127	0.0048	-0.0001	0.1639
N2-C8	1	2.4527	2.4662	2.4644	0.0135	0.0160	-0.0163	0.0137	0.0001	0.0664
C4-C3	1	2.4595	2.4752	2.4735	0.0157	0.0076	-0.0081	0.0162	0.0000	0.0650
H12-H18	1	2.4665	2.5013	2.4935	0.0349	0.0176	-0.0099	0.0271	0.0001	0.1400
C3-H14	1	2.4676	2.5164	2.5058	0.0488	0.0861	-0.0865	0.0491	0.0001	0.1624
H14-H20	1	2.4736	2.5070	2.4963	0.0334	0.0644	-0.0643	0.0333	0.0000	0.1630
H15-H24	1	2.4831	2.5463	2.5354	0.0631	0.1047	-0.1054	0.0638	0.0000	0.1655
H11-H19	1	2.4960	2.5489	2.5327	0.0529	0.0369	-0.0373	0.0533	0.0000	0.2025
H10-H16	1	2.4992	2.5285	2.5203	0.0293	0.0887	-0.0871	0.0277	0.0000	0.1428
H13-H22	1	2.5002	2.5322	2.5211	0.0320	0.0657	-0.0658	0.0321	0.0000	0.1667
H12-H17	1	2.5027	2.5300	2.5279	0.0274	0.0240	-0.0254	0.0287	0.0001	0.0744
C3-C9	1	2.5027	2.5335	2.5216	0.0308	0.0615	-0.0604	0.0296	0.0001	0.1727
H11-H17	1	2.5063	2.5179	2.5159	0.0116	0.0068	-0.0064	0.0112	0.0000	0.0703
H15-H23	1	2.5081	2.5346	2.5238	0.0264	0.0559	-0.0539	0.0245	-0.0001	0.1638
N2-C6	1	2.5085	2.5227	2.5123	0.0142	0.0731	-0.0704	0.0115	0.0000	0.1609

H13-H21	1	2.5102	2.5476	2.5355	0.0374	0.0474	-0.0460	0.0360	0.0000	0.1746
H16-H25	1	2.5114	2.5258	2.5205	0.0144	0.1096	-0.1051	0.0099	0.0000	0.1136
H14-H21	1	2.5161	2.5435	2.5320	0.0274	0.0490	-0.0475	0.0259	0.0000	0.1704
H16-H23	1	2.5180	2.5624	2.5518	0.0444	0.0669	-0.0649	0.0424	0.0000	0.1639
H18-H20	1	2.5256	2.6470	2.6034	0.1214	0.0747	0.0662	-0.0196	0.0001	0.3381
C5-H10	1	2.5306	2.5693	2.5614	0.0387	0.0107	-0.0140	0.0420	0.0000	0.1421
C3-H12	1	2.5868	2.6365	2.6281	0.0496	0.0271	-0.0144	0.0369	0.0000	0.1478
H10-H25	1	2.5984	2.6884	2.6663	0.0900	0.0689	-0.0292	0.0503	0.0000	0.2441
N1-C6	1	2.6020	2.6119	2.6102	0.0099	0.0072	-0.0054	0.0081	0.0000	0.0672
N2-H15	1	2.6295	2.6370	2.6253	0.0075	0.0254	-0.0118	-0.0061	0.0000	0.1750
C4-H15	1	2.6448	2.7044	2.6893	0.0597	0.0332	0.0104	0.0160	0.0001	0.2028
C6-H12	1	2.6521	2.7253	2.7111	0.0733	0.0285	0.0086	0.0362	0.0000	0.1974
N1-H19	1	2.6749	2.7139	2.7040	0.0390	0.0533	-0.0529	0.0386	0.0000	0.1631
N2-H22	1	2.6959	2.7232	2.7134	0.0273	0.0423	-0.0415	0.0266	-0.0001	0.1625
N1-H18	1	2.7284	2.7635	2.7545	0.0351	0.0463	-0.0466	0.0354	0.0000	0.1571
N2-H20	1	2.7410	2.7553	2.7462	0.0143	0.0389	-0.0389	0.0143	0.0000	0.1577
C3-H24	1	2.7605	2.7816	2.7725	0.0212	0.0615	-0.0606	0.0203	0.0000	0.1580
C3-H25	1	2.7620	2.8278	2.8173	0.0658	0.0641	-0.0642	0.0659	0.0000	0.1717
N1-H15	1	2.7621	2.7946	2.7864	0.0326	0.0285	-0.0124	0.0165	0.0000	0.1512
C9-H10	1	2.7860	2.8114	2.8008	0.0254	0.0235	-0.0172	0.0191	0.0000	0.1724
C3-H11	1	2.8482	2.8402	2.8314	-0.0080	0.0262	-0.0308	-0.0034	0.0000	0.1568
C3-H13	1	2.8494	2.9027	2.8936	0.0533	0.0158	-0.0225	0.0600	0.0000	0.1616
H10-H13	1	2.8547	2.9381	2.9177	0.0834	0.0166	-0.0241	0.0909	0.0000	0.2442
N1-H20	1	2.9213	2.9186	2.8564	-0.0027	0.0301	-0.0118	-0.0210	0.0000	0.4088
H11-H15	1	2.9247	2.9066	2.8848	-0.0181	0.0324	-0.0156	-0.0350	0.0001	0.2471
C4-C6	1	2.9853	2.9954	2.9919	0.0101	0.0082	-0.0029	0.0049	-0.0001	0.1027
N1-H16	1	3.0130	3.0068	2.9974	-0.0061	0.0271	-0.0277	-0.0055	0.0000	0.1671
N2-H24	1	3.0233	3.1094	3.0761	0.0861	0.0474	-0.0264	0.0651	0.0000	0.3232
N2-H18	1	3.0240	3.1418	3.1119	0.1178	0.0346	-0.0209	0.1041	0.0000	0.3088
H19-H20	1	3.0454	3.1917	3.1076	0.1462	0.0539	0.0310	0.0614	-0.0001	0.5163
H18-H22	1	3.0510	3.1621	3.0810	0.1111	0.0591	0.0407	0.0113	0.0000	0.5016
H12-H19	1	3.0535	3.0687	3.0643	0.0152	0.0276	-0.0505	0.0382	-0.0001	0.1170
H10-H15	1	3.0554	3.0908	3.0905	0.0355	0.1055	-0.1188	0.0488	0.0000	0.0307
H13-H20	1	3.0603	3.0857	3.0832	0.0254	0.0759	-0.0905	0.0399	0.0001	0.0873
H11-H18	1	3.0603	3.0921	3.0914	0.0318	0.1028	-0.1162	0.0452	0.0000	0.0506
H14-H22	1	3.0631	3.0923	3.0896	0.0293	0.0753	-0.0903	0.0442	0.0001	0.0931
H15-H25	1	3.0644	3.0982	3.1007	0.0338	0.1275	-0.1397	0.0460	0.0000	0.0000
H16-H24	1	3.0655	3.0963	3.0979	0.0308	0.1296	-0.1419	0.0431	0.0000	0.0000
H11-H16	1	3.0674	2.9905	2.9336	-0.0768	0.0306	0.0007	-0.1082	0.0001	0.4048
H10-H24	1	3.1273	3.1023	3.0772	-0.0250	0.0503	-0.0568	-0.0185	0.0000	0.2715
H12-H16	1	3.1359	3.1543	3.1059	0.0184	0.0279	-0.0189	0.0094	0.0000	0.3764
C7-H20	1	3.1434	3.2312	3.2028	0.0878	0.0388	0.0421	0.0069	0.0000	0.3039
C6-H11	1	3.1488	3.1042	3.0773	-0.0446	0.0167	-0.0151	-0.0462	0.0000	0.2816
N1-C8	1	3.1584	3.2622	3.2314	0.1038	0.0437	0.0450	0.0151	0.0000	0.3193
C8-H18	1	3.1603	3.1455	3.1384	-0.0148	0.0123	-0.0162	-0.0109	0.0000	0.1477

N2-C7	1	3.2307	3.2987	3.2886	0.0680	0.0131	-0.0198	0.0747	0.0000	0.1832
N2-H11	1	3.2521	3.2528	3.2495	0.0007	0.0240	-0.0444	0.0211	0.0000	0.1033
N2-C9	1	3.2569	3.2887	3.2851	0.0318	0.0186	-0.0341	0.0473	0.0000	0.1090
N1-H13	1	3.2579	3.3152	3.3033	0.0573	0.0164	-0.0216	0.0625	0.0000	0.1990
C4-H16	1	3.2844	3.2483	3.2229	-0.0361	0.0181	-0.0168	-0.0373	-0.0001	0.2809
H13-H24	1	3.3369	3.4690	3.4276	0.1321	0.0576	0.0265	0.0480	0.0000	0.3775
C4-H10	1	3.3518	3.3740	3.3709	0.0222	0.0125	-0.0208	0.0306	-0.0001	0.1023
N2-H16	1	3.3574	3.3554	3.3524	-0.0021	0.0249	-0.0459	0.0189	0.0000	0.0986
N1-H17	1	3.3836	3.4047	3.4020	0.0210	0.0246	-0.0390	0.0354	0.0000	0.0956
N2-H21	1	3.3940	3.4109	3.4082	0.0169	0.0242	-0.0387	0.0314	0.0000	0.0961
C3-H23	1	3.4544	3.4786	3.4759	0.0242	0.0302	-0.0466	0.0405	0.0001	0.0971
C4-C5	1	3.5513	3.5718	3.5702	0.0205	0.0065	-0.0119	0.0260	-0.0001	0.0759
C4-H20	1	3.5605	3.5579	3.5395	-0.0026	0.0258	-0.0015	-0.0269	0.0000	0.2542
H10-H11	1	3.5904	3.5971	3.5886	0.0067	0.0286	-0.0358	0.0139	0.0000	0.1743
C5-H18	1	3.6143	3.7173	3.6951	0.1030	0.0294	0.0016	0.0719	0.0001	0.2889
N1-H22	1	3.6272	3.6039	3.5888	-0.0233	0.0316	-0.0490	-0.0059	0.0000	0.2301
H10-H12	1	3.6433	3.6958	3.6888	0.0524	0.0278	-0.0306	0.0552	0.0000	0.1607
N2-H25	1	3.6762	3.7741	3.7464	0.0979	0.0399	-0.0681	0.1262	-0.0001	0.3212
C3-C8	1	3.6882	3.6927	3.6911	0.0045	0.0117	-0.0227	0.0155	0.0000	0.0770
N2-H19	1	3.6946	3.7702	3.7494	0.0756	0.0345	-0.0612	0.1023	0.0000	0.2787
C5-C6	1	3.7074	3.7325	3.7309	0.0251	0.0053	-0.0105	0.0304	-0.0001	0.0782
C3-C7	1	3.7324	3.7588	3.7570	0.0263	0.0116	-0.0282	0.0429	0.0000	0.0819
C5-H24	1	3.7811	3.8632	3.8376	0.0820	0.0381	-0.0036	0.0475	0.0000	0.3145
H10-H23	1	3.7884	3.7885	3.7801	0.0001	0.0165	-0.0205	0.0041	0.0000	0.1772
C5-H12	1	3.7905	3.8513	3.8439	0.0608	0.0121	-0.0193	0.0680	0.0000	0.1690
C4-H14	1	3.7913	3.8275	3.8194	0.0363	0.0296	-0.0455	0.0521	0.0001	0.1761
C3-H20	1	3.8408	3.8267	3.8175	-0.0141	0.0283	-0.0361	-0.0063	0.0000	0.1859
N1-C9	1	3.8436	3.8642	3.8623	0.0206	0.0137	-0.0330	0.0400	-0.0001	0.0868
C7-C8	1	3.8564	3.9134	3.8938	0.0569	0.0166	0.0089	0.0315	-0.0001	0.2781
C6-H13	1	3.8804	3.9347	3.9264	0.0544	0.0139	-0.0215	0.0619	0.0001	0.1806
C6-H14	1	3.9093	3.9377	3.9324	0.0285	0.0141	-0.0175	0.0319	0.0000	0.1449
C3-H18	1	3.9133	4.0479	4.0241	0.1346	0.0229	-0.0025	0.1142	0.0000	0.3119
C9-H13	1	3.9146	3.9785	3.9672	0.0639	0.0295	-0.0457	0.0801	0.0000	0.2119
C8-H10	1	3.9414	3.9537	3.9482	0.0123	0.0164	-0.0365	0.0324	0.0000	0.1473
C9-H12	1	3.9452	4.0219	4.0093	0.0766	0.0292	-0.0238	0.0713	-0.0001	0.2226
C7-H22	1	3.9486	3.9847	3.9316	0.0361	0.0276	-0.0137	0.0223	-0.0001	0.4529
C8-H19	1	3.9564	4.0511	3.9914	0.0946	0.0269	-0.0194	0.0871	0.0000	0.4896
H13-H25	1	3.9721	4.2075	4.1443	0.2354	0.0338	-0.0295	0.2311	0.0000	0.5184
C4-C8	1	3.9767	3.9652	3.9585	-0.0115	0.0103	-0.0129	-0.0088	-0.0001	0.1614
N1-H24	1	3.9960	4.0323	4.0200	0.0363	0.0372	-0.0576	0.0567	0.0000	0.2218
C5-C7	1	4.0130	4.0812	4.0725	0.0683	0.0103	-0.0111	0.0690	0.0001	0.1898
C5-H15	1	4.0155	4.0189	4.0107	0.0034	0.0171	-0.0201	0.0064	0.0000	0.1809
C7-H15	1	4.0199	4.0863	4.0773	0.0664	0.0318	-0.0150	0.0496	0.0000	0.1920
H12-H24	1	4.0370	4.1609	4.1203	0.1239	0.0462	-0.0426	0.1203	0.0000	0.4025
H12-H20	1	4.0689	4.0302	4.0053	-0.0387	0.0270	-0.0292	-0.0365	0.0000	0.3117

N1-H21	1	4.0904	4.0828	4.0764	-0.0076	0.0197	-0.0399	0.0126	0.0000	0.1606
C3-H19	1	4.0918	4.1104	4.1043	0.0186	0.0330	-0.0609	0.0466	-0.0001	0.1576
C3-H22	1	4.0925	4.1066	4.1006	0.0141	0.0293	-0.0496	0.0343	0.0001	0.1565
H14-H18	1	4.1246	4.2220	4.2004	0.0974	0.0280	-0.0221	0.0915	0.0000	0.3008
H17-H20	1	4.1377	4.2095	4.1865	0.0718	0.0374	0.0082	0.0262	0.0000	0.3120
H18-H21	1	4.1413	4.2122	4.1882	0.0709	0.0425	0.0151	0.0133	0.0000	0.3189
H10-H20	1	4.1491	4.1316	4.1178	-0.0175	0.0318	-0.0520	0.0027	0.0000	0.2352
N2-H17	1	4.1547	4.2092	4.2013	0.0544	0.0199	-0.0415	0.0761	-0.0001	0.1823
C5-C9	1	4.1573	4.1268	4.1043	-0.0306	0.0245	-0.0355	-0.0195	-0.0001	0.3005
C4-H22	1	4.1578	4.2359	4.2258	0.0781	0.0122	-0.0136	0.0795	0.0000	0.2071
N1-H25	1	4.1873	4.2270	4.2205	0.0397	0.0384	-0.0699	0.0713	-0.0001	0.1650
C5-H19	1	4.1995	4.2961	4.2677	0.0966	0.0256	-0.0409	0.1119	0.0000	0.3485
H12-H22	1	4.2092	4.1550	4.1206	-0.0543	0.0273	-0.0288	-0.0527	-0.0001	0.3727
N2-H23	1	4.2174	4.2448	4.2364	0.0273	0.0242	-0.0469	0.0500	0.0000	0.1877
H13-H15	1	4.2458	4.2495	4.2340	0.0037	0.0224	-0.0361	0.0173	0.0001	0.2546
H15-H18	1	4.2529	4.3636	4.3398	0.1107	0.0449	-0.0323	0.0981	0.0000	0.3186
H14-H19	1	4.2574	4.3883	4.3582	0.1309	0.0276	-0.0311	0.1344	0.0000	0.3624
H12-H14	1	4.2575	4.2943	4.2862	0.0368	0.0232	-0.0392	0.0528	0.0000	0.1862
H14-H24	1	4.2718	4.2308	4.2159	-0.0410	0.0146	-0.0241	-0.0315	0.0000	0.2479
C8-H12	1	4.2740	4.2801	4.2575	0.0061	0.0394	-0.0300	-0.0033	0.0000	0.3078
H19-H22	1	4.2839	4.3395	4.2470	0.0556	0.0337	-0.0609	0.0829	-0.0001	0.6192
C5-H25	1	4.2895	4.4390	4.4065	0.1495	0.0291	-0.0453	0.1657	0.0000	0.3799
C7-H14	1	4.3113	4.4034	4.3912	0.0921	0.0120	-0.0191	0.0992	0.0000	0.2311
H14-H25	1	4.3376	4.4497	4.4222	0.1121	0.0397	-0.0343	0.1067	0.0000	0.3489
C5-H11	1	4.3741	4.3925	4.3898	0.0183	0.0200	-0.0467	0.0451	-0.0001	0.1083
C4-H13	1	4.3833	4.4031	4.4004	0.0198	0.0168	-0.0379	0.0409	0.0000	0.1099
C4-C9	1	4.4017	4.4148	4.4111	0.0131	0.0111	-0.0406	0.0426	0.0000	0.1271
H11-H14	1	4.4056	4.4773	4.4676	0.0717	0.0254	-0.0431	0.0894	0.0000	0.2078
H12-H13	1	4.4154	4.4177	4.4072	0.0023	0.0260	-0.0349	0.0112	0.0000	0.2144
C9-H14	1	4.4290	4.4447	4.4374	0.0158	0.0246	-0.0392	0.0303	0.0001	0.1796
H14-H15	1	4.4301	4.4714	4.4616	0.0413	0.0189	-0.0218	0.0441	0.0001	0.2088
H11-H20	1	4.4402	4.4438	4.4218	0.0037	0.0330	-0.0355	0.0062	0.0000	0.3090
C6-C7	1	4.4416	4.5153	4.5022	0.0737	0.0375	-0.0107	0.0469	0.0000	0.2435
H15-H17	1	4.4437	4.4586	4.4562	0.0149	0.0104	-0.0327	0.0372	0.0000	0.1039
H12-H23	1	4.4560	4.5172	4.5033	0.0612	0.0360	-0.0218	0.0470	0.0000	0.2500
H14-H16	1	4.4864	4.5309	4.5222	0.0445	0.0286	-0.0427	0.0587	-0.0001	0.1972
H13-H18	1	4.4948	4.5925	4.5673	0.0977	0.0330	-0.0231	0.0878	0.0000	0.3418
C5-H16	1	4.4986	4.5208	4.5179	0.0222	0.0190	-0.0482	0.0514	0.0000	0.1146
C3-H21	1	4.5201	4.5348	4.5318	0.0147	0.0181	-0.0412	0.0378	0.0000	0.1161
C7-H10	1	4.5305	4.5517	4.5488	0.0211	0.0117	-0.0370	0.0464	0.0000	0.1142
H10-H22	1	4.5480	4.5711	4.5649	0.0231	0.0326	-0.0691	0.0596	0.0000	0.1683
H10-H21	1	4.5678	4.5957	4.5874	0.0279	0.0214	-0.0464	0.0529	0.0000	0.1947
C3-H17	1	4.5760	4.5981	4.5953	0.0221	0.0179	-0.0450	0.0493	-0.0001	0.1140
C4-H24	1	4.5841	4.6408	4.6206	0.0567	0.0291	-0.0660	0.0935	0.0001	0.3016
C9-H11	1	4.6655	4.5953	4.5775	-0.0702	0.0130	-0.0571	-0.0262	0.0001	0.2810

H10-H19	1	4.6819	4.6952	4.6859	0.0132	0.0283	-0.0587	0.0437	-0.0001	0.2084
C6-H18	1	4.7103	4.7767	4.7637	0.0664	0.0247	-0.0530	0.0947	0.0000	0.2478
N1-H23	1	4.7164	4.7261	4.7235	0.0097	0.0205	-0.0502	0.0394	0.0000	0.1106
H10-H18	1	4.7227	4.7737	4.7642	0.0510	0.0260	-0.0539	0.0788	0.0001	0.2122
H12-H25	1	4.7320	4.7891	4.7793	0.0571	0.0476	-0.0833	0.0928	0.0000	0.2159
H13-H16	1	4.7695	4.8293	4.8199	0.0598	0.0235	-0.0646	0.1009	0.0000	0.2124
H15-H19	1	4.7803	4.8131	4.8045	0.0327	0.0464	-0.0666	0.0530	-0.0001	0.2030
C7-H16	1	4.7963	4.7365	4.7194	-0.0598	0.0141	-0.0487	-0.0252	0.0000	0.2811
H17-H22	1	4.8001	4.8188	4.7732	0.0187	0.0301	-0.0342	0.0228	0.0000	0.4642
H19-H21	1	4.8012	4.8899	4.8388	0.0887	0.0300	-0.0356	0.0944	-0.0001	0.4996
C7-H21	1	4.8412	4.8827	4.8664	0.0415	0.0211	-0.0207	0.0411	0.0000	0.2821
C8-H17	1	4.8470	4.8860	4.8700	0.0390	0.0207	-0.0231	0.0414	0.0000	0.2810
C8-H11	1	4.9222	4.9111	4.9030	-0.0111	0.0205	-0.0531	0.0214	0.0001	0.1975
C6-C8	1	4.9472	5.0398	5.0205	0.0925	0.0278	-0.0410	0.1057	0.0000	0.3122
H13-H23	1	4.9497	4.9603	4.9589	0.0106	0.0076	-0.0243	0.0273	0.0000	0.0847
C7-H13	1	4.9609	5.0188	5.0090	0.0579	0.0179	-0.0425	0.0825	0.0000	0.2220
H22-H24	1	4.9867	5.1755	5.1260	0.1888	0.0366	-0.0085	0.1607	0.0000	0.5078
C4-H25	1	4.9955	5.0001	4.9964	0.0046	0.0310	-0.0855	0.0591	0.0000	0.1359
H15-H22	1	5.0057	5.0192	5.0011	0.0135	0.0311	-0.0195	0.0018	0.0001	0.3005
C6-H19	1	5.0126	4.9986	4.9928	-0.0140	0.0164	-0.0429	0.0125	0.0000	0.1693
C4-H21	1	5.0144	5.0028	4.9989	-0.0116	0.0272	-0.0708	0.0321	-0.0001	0.1399
C8-H15	1	5.0237	5.0250	5.0170	0.0013	0.0187	-0.0179	0.0005	0.0000	0.2008
C8-H24	1	5.0306	5.1494	5.1214	0.1188	0.0270	-0.0130	0.1049	-0.0001	0.3807
C6-H17	1	5.0353	5.0469	5.0418	0.0116	0.0158	-0.0399	0.0357	0.0000	0.1612
C4-H23	1	5.0469	5.0978	5.0907	0.0508	0.0161	-0.0408	0.0755	0.0000	0.1895
C5-H17	1	5.0476	5.0446	5.0390	-0.0030	0.0176	-0.0473	0.0267	0.0000	0.1676
H11-H24	1	5.0774	5.0412	5.0178	-0.0362	0.0301	-0.1007	0.0343	0.0001	0.3367
C6-H22	1	5.1296	5.1539	5.1461	0.0243	0.0202	-0.0402	0.0442	0.0001	0.2000
C6-H20	1	5.1547	5.1422	5.1355	-0.0125	0.0192	-0.0366	0.0048	0.0001	0.1851
H15-H20	1	5.1700	5.1696	5.1571	-0.0003	0.0313	-0.0253	-0.0063	0.0000	0.2539
H11-H25	1	5.1831	5.0976	5.0819	-0.0855	0.0331	-0.0932	-0.0255	0.0001	0.2793
H11-H23	1	5.2023	5.1222	5.0981	-0.0801	0.0164	-0.0540	-0.0425	0.0000	0.3453
H11-H22	1	5.2043	5.2162	5.2126	0.0120	0.0259	-0.0710	0.0570	0.0001	0.1363
C5-H23	1	5.2056	5.1644	5.1457	-0.0413	0.0306	-0.0796	0.0078	-0.0001	0.3064
H11-H13	1	5.2086	5.2545	5.2465	0.0459	0.0183	-0.0477	0.0753	0.0000	0.2045
H13-H19	1	5.2485	5.3289	5.3050	0.0805	0.0291	-0.0757	0.1270	0.0001	0.3554
H16-H19	1	5.2495	5.1650	5.1460	-0.0845	0.0308	-0.0757	-0.0396	0.0000	0.3087
H16-H18	1	5.2740	5.2556	5.2379	-0.0184	0.0274	-0.0860	0.0401	0.0001	0.3001
H16-H17	1	5.3063	5.2393	5.2159	-0.0671	0.0162	-0.0485	-0.0347	-0.0001	0.3447
H12-H21	1	5.3527	5.3059	5.2939	-0.0468	0.0193	-0.0560	-0.0101	0.0000	0.2494
H14-H17	1	5.3893	5.4677	5.4579	0.0785	0.0167	-0.0505	0.1123	0.0000	0.2312
H10-H17	1	5.4431	5.4595	5.4562	0.0164	0.0172	-0.0572	0.0564	0.0000	0.1333
C8-C9	1	5.5114	5.5902	5.5798	0.0788	0.0085	-0.0338	0.1041	0.0000	0.2413
H14-H23	1	5.5118	5.5369	5.5287	0.0251	0.0235	-0.0566	0.0582	0.0000	0.2118
C9-H22	1	5.6121	5.7275	5.7046	0.1154	0.0182	-0.0446	0.1418	0.0000	0.3609

H20-H24	1	5.6445	5.7207	5.6963	0.0762	0.0333	-0.0569	0.0999	-0.0001	0.3725
H18-H24	1	5.6882	5.9016	5.8551	0.2133	0.0352	-0.0595	0.2377	-0.0001	0.5151
H21-H24	1	5.7278	5.8468	5.8214	0.1191	0.0302	-0.0196	0.1084	0.0001	0.3855
C8-H16	1	5.7504	5.7332	5.7306	-0.0171	0.0162	-0.0609	0.0276	0.0000	0.1226
C8-H25	1	5.7554	5.8912	5.8652	0.1358	0.0200	-0.0719	0.1877	0.0000	0.3900
C7-C9	1	5.7837	5.8234	5.8188	0.0398	0.0093	-0.0655	0.0960	0.0000	0.1630
C7-H24	1	5.8051	5.9176	5.8941	0.1126	0.0234	-0.0759	0.1651	0.0000	0.3681
H16-H20	1	5.8234	5.7750	5.7645	-0.0484	0.0262	-0.0612	-0.0133	-0.0001	0.2445
C6-H21	1	5.8302	5.8485	5.8462	0.0183	0.0126	-0.0460	0.0518	-0.0001	0.1157
H17-H21	1	5.8338	5.8540	5.8391	0.0202	0.0229	-0.0547	0.0520	0.0000	0.2957
C9-H18	1	5.8713	5.9932	5.9737	0.1219	0.0214	-0.0710	0.1715	0.0000	0.3377
H11-H21	1	5.9099	5.9002	5.8921	-0.0097	0.0241	-0.0797	0.0459	0.0000	0.2162
H13-H17	1	5.9462	5.9827	5.9739	0.0365	0.0218	-0.0691	0.0839	-0.0001	0.2299
C9-H20	1	5.9760	6.0098	6.0004	0.0338	0.0171	-0.0622	0.0789	0.0000	0.2374
H16-H21	1	6.0051	6.0021	5.9946	-0.0030	0.0217	-0.0473	0.0226	0.0000	0.2116
H22-H25	1	6.0176	6.1813	6.1427	0.1637	0.0268	-0.0961	0.2330	0.0000	0.4833
H16-H22	1	6.0380	6.0187	6.0116	-0.0193	0.0248	-0.0835	0.0395	-0.0001	0.2056
C9-H21	1	6.2517	6.3441	6.3331	0.0924	0.0126	-0.0459	0.1257	0.0000	0.2633
H20-H25	1	6.2531	6.3240	6.3056	0.0709	0.0291	-0.1007	0.1424	0.0001	0.3402
H21-H25	1	6.3614	6.5290	6.5010	0.1676	0.0218	-0.0717	0.2175	0.0000	0.4268
C7-H25	1	6.3810	6.4082	6.4036	0.0271	0.0222	-0.1084	0.1133	0.0000	0.1705
C9-H19	1	6.3812	6.3857	6.3815	0.0045	0.0201	-0.1028	0.0872	0.0000	0.1634
C9-H17	1	6.4051	6.4309	6.4241	0.0258	0.0119	-0.0778	0.0917	0.0000	0.2082
C7-H23	1	6.4585	6.4677	6.4620	0.0092	0.0138	-0.0776	0.0730	0.0000	0.1908
H17-H24	1	6.4604	6.5659	6.5392	0.1055	0.0236	-0.0916	0.1734	0.0001	0.4120
H19-H24	1	6.4648	6.5343	6.5168	0.0695	0.0333	-0.1196	0.1558	0.0000	0.3344
H18-H25	1	6.4959	6.6109	6.5933	0.1150	0.0327	-0.1178	0.2000	0.0001	0.3368
C8-H23	1	6.5126	6.5520	6.5428	0.0395	0.0121	-0.0640	0.0914	0.0000	0.2443
H22-H23	1	6.5262	6.5944	6.5730	0.0682	0.0198	-0.0683	0.1168	-0.0001	0.3736
H18-H23	1	6.5977	6.6822	6.6628	0.0845	0.0244	-0.0888	0.1489	0.0000	0.3564
H16-H21	1	6.6148	6.6120	6.6087	-0.0027	0.0193	-0.0820	0.0600	0.0000	0.1475
H19-H25	1	6.8353	6.8334	6.8268	-0.0019	0.0304	-0.1325	0.1002	0.0000	0.2118
H17-H23	1	6.9470	6.9428	6.9335	-0.0041	0.0153	-0.0805	0.0610	0.0001	0.2527
H20-H23	1	6.9567	6.9558	6.9471	-0.0010	0.0187	-0.0871	0.0674	0.0000	0.2439
H17-H25	1	7.0971	7.0962	7.0912	-0.0009	0.0224	-0.1266	0.1033	0.0000	0.1879
H19-H23	1	7.1303	7.1016	7.0969	-0.0287	0.0224	-0.1190	0.0679	0.0000	0.1818
H21-H23	1	7.2850	7.3374	7.3273	0.0524	0.0147	-0.0811	0.1188	0.0000	0.2709

Table S10. Equilibrium (r_e) and thermal average (r_g , r_a) distances, vibrational corrections (Δ), and mean amplitudes (u) for internuclear distances of TEDA conformation **1b** (in Å), obtained for 291 K by GED refinement (initial approximation MP2/cc-PVTZ). n – number of equivalent parameters.

Atomic pair	n	r_e	r_g	r_a	Δr	$\Delta r(\text{har})$	$\Delta r(\text{kin})$	$\Delta r(\text{dyn})$	$\Delta r(\text{rot})$	u
C6-H15	1	1.0895	1.1122	1.1078	0.0226	0.0321	-0.0280	0.0185	0.0000	0.0698
C7-H19	1	1.0909	1.1132	1.1101	0.0223	0.0515	-0.0465	0.0174	-0.0001	0.0593
C8-H20	1	1.0911	1.1151	1.1134	0.0240	0.0637	-0.0577	0.0181	-0.0001	0.0443
C9-H23	1	1.0911	1.1130	1.1095	0.0220	0.0442	-0.0396	0.0174	0.0000	0.0633
C8-H22	1	1.0911	1.1156	1.1139	0.0246	0.0624	-0.0565	0.0187	0.0000	0.0452
C7-H18	1	1.0912	1.1145	1.1113	0.0233	0.0512	-0.0464	0.0185	0.0000	0.0601
C8-H21	1	1.0916	1.1145	1.1123	0.0229	0.0587	-0.0531	0.0173	0.0000	0.0505
C9-H24	1	1.0917	1.1133	1.1092	0.0216	0.0375	-0.0334	0.0174	0.0001	0.0678
C7-H17	1	1.0918	1.1133	1.1093	0.0215	0.0378	-0.0336	0.0173	0.0000	0.0673
C3-H10	1	1.0918	1.1134	1.1083	0.0216	0.0165	-0.0125	0.0176	0.0000	0.0753
C9-H25	1	1.0924	1.1162	1.1138	0.0237	0.0590	-0.0534	0.0182	-0.0001	0.0517
C4-H12	1	1.0935	1.1174	1.1144	0.0239	0.0467	-0.0416	0.0188	0.0000	0.0585
C4-H11	1	1.0946	1.1183	1.1152	0.0237	0.0471	-0.0419	0.0185	0.0000	0.0589
C5-H13	1	1.0949	1.1167	1.1124	0.0218	0.0335	-0.0291	0.0174	0.0000	0.0693
C6-H16	1	1.0949	1.1162	1.1117	0.0213	0.0320	-0.0277	0.0170	0.0000	0.0706
C5-H14	1	1.0973	1.1200	1.1156	0.0227	0.0323	-0.0279	0.0183	0.0000	0.0709
N2-C3	1	1.4196	1.4290	1.4274	0.0094	0.0055	-0.0041	0.0080	0.0000	0.0487
N1-C3	1	1.4305	1.4415	1.4399	0.0110	0.0058	-0.0042	0.0094	0.0000	0.0493
N1-C4	1	1.4391	1.4521	1.4504	0.0130	0.0067	-0.0049	0.0112	0.0000	0.0492
N2-C5	1	1.4401	1.4502	1.4486	0.0102	0.0059	-0.0040	0.0083	0.0000	0.0490
N1-N2	1	1.4855	1.4987	1.4967	0.0132	0.0063	-0.0057	0.0126	0.0000	0.0542
C3-C6	1	1.4988	1.5095	1.5079	0.0108	0.0053	-0.0040	0.0094	0.0001	0.0492
C5-C8	1	1.5117	1.5259	1.5247	0.0143	0.0254	-0.0239	0.0128	0.0000	0.0432
C4-C7	1	1.5132	1.5262	1.5255	0.0131	0.0322	-0.0304	0.0113	0.0000	0.0344
C6-C9	1	1.5222	1.5344	1.5333	0.0122	0.0266	-0.0251	0.0107	0.0000	0.0422
H23-H25	1	1.7636	1.7935	1.7894	0.0299	0.0931	-0.0907	0.0275	0.0000	0.0850
H24-H25	1	1.7653	1.7925	1.7879	0.0272	0.0823	-0.0804	0.0253	0.0000	0.0902
H23-H24	1	1.7667	1.7936	1.7889	0.0269	0.0797	-0.0780	0.0252	0.0000	0.0917
H17-H18	1	1.7702	1.7988	1.7925	0.0286	0.0678	-0.0672	0.0280	0.0000	0.1054
H20-H21	1	1.7705	1.7985	1.7936	0.0279	0.0793	-0.0777	0.0263	0.0000	0.0930
H18-H19	1	1.7716	1.8015	1.7985	0.0299	0.0993	-0.0962	0.0268	0.0000	0.0738
H20-H22	1	1.7717	1.7986	1.7915	0.0269	0.0465	-0.0438	0.0243	-0.0001	0.1130
H21-H22	1	1.7720	1.8017	1.7963	0.0297	0.0808	-0.0795	0.0285	-0.0001	0.0987
H17-H19	1	1.7728	1.8017	1.7954	0.0288	0.0656	-0.0651	0.0283	0.0000	0.1058
H15-H16	1	1.7740	1.8032	1.7981	0.0292	0.0764	-0.0751	0.0279	0.0000	0.0964
H11-H12	1	1.7976	1.8260	1.8211	0.0284	0.0707	-0.0661	0.0238	0.0000	0.0941
H13-H14	1	1.8001	1.8278	1.8209	0.0277	0.0478	-0.0446	0.0245	0.0000	0.1121
H12-H15	1	1.9534	2.0586	2.0321	0.1052	0.0704	0.0378	-0.0030	0.0000	0.2319

N2-H13	1	2.0135	2.0311	2.0260	0.0176	0.0244	-0.0262	0.0194	0.0000	0.1019
N1-H11	1	2.0139	2.0377	2.0324	0.0238	0.0351	-0.0369	0.0256	0.0000	0.1039
N2-H14	1	2.0655	2.0925	2.0875	0.0270	0.0217	-0.0236	0.0289	0.0000	0.1024
N1-H12	1	2.0746	2.0963	2.0908	0.0217	0.0197	-0.0227	0.0247	0.0000	0.1069
N1-H10	1	2.0856	2.1057	2.1016	0.0201	0.0339	-0.0350	0.0212	0.0000	0.0929
C3-H16	1	2.0911	2.1128	2.1080	0.0217	0.0128	-0.0172	0.0261	0.0000	0.1003
C3-H15	1	2.1109	2.1239	2.1187	0.0130	0.0210	-0.0234	0.0154	0.0000	0.1040
N2-H10	1	2.1369	2.1586	2.1540	0.0217	0.0126	-0.0164	0.0255	0.0000	0.0998
C5-H20	1	2.1453	2.1657	2.1623	0.0204	0.0549	-0.0562	0.0218	-0.0001	0.0856
C7-H12	1	2.1463	2.1718	2.1690	0.0255	0.0731	-0.0739	0.0262	0.0001	0.0772
C4-H18	1	2.1464	2.1729	2.1706	0.0266	0.0651	-0.0653	0.0268	0.0000	0.0717
C9-H15	1	2.1511	2.1768	2.1728	0.0257	0.0567	-0.0583	0.0274	-0.0001	0.0933
C5-H22	1	2.1522	2.1788	2.1766	0.0265	0.0739	-0.0743	0.0269	0.0000	0.0686
C4-H19	1	2.1551	2.1821	2.1791	0.0270	0.0644	-0.0649	0.0275	0.0000	0.0809
C8-H14	1	2.1558	2.1805	2.1755	0.0247	0.0343	-0.0361	0.0265	0.0000	0.1044
C7-H11	1	2.1559	2.1797	2.1758	0.0237	0.0457	-0.0465	0.0245	0.0000	0.0918
C5-H21	1	2.1567	2.1796	2.1747	0.0229	0.0320	-0.0337	0.0245	0.0001	0.1029
C6-H24	1	2.1571	2.1808	2.1768	0.0238	0.0460	-0.0475	0.0252	0.0001	0.0934
C4-H17	1	2.1585	2.1827	2.1787	0.0242	0.0450	-0.0460	0.0251	0.0001	0.0935
C8-H13	1	2.1670	2.1871	2.1841	0.0200	0.0623	-0.0629	0.0207	-0.0001	0.0807
C9-H16	1	2.1672	2.1991	2.1950	0.0319	0.0595	-0.0612	0.0336	0.0000	0.0945
H10-H14	1	2.1673	2.2034	2.1844	0.0361	0.0241	-0.0044	0.0164	0.0000	0.2034
C6-H25	1	2.1686	2.1858	2.1816	0.0172	0.0443	-0.0455	0.0185	-0.0001	0.0952
C6-H23	1	2.1699	2.1905	2.1859	0.0206	0.0380	-0.0393	0.0219	0.0000	0.1001
C6-H10	1	2.1795	2.2053	2.2005	0.0257	0.0114	-0.0126	0.0269	0.0000	0.1020
N1-C5	1	2.3887	2.4124	2.4104	0.0237	0.0070	-0.0084	0.0251	0.0000	0.0697
N2-C4	1	2.4039	2.4225	2.4204	0.0186	0.0075	-0.0093	0.0204	0.0000	0.0704
C5-C3	1	2.4125	2.4368	2.4350	0.0243	0.0050	-0.0057	0.0250	0.0000	0.0664
N1-H14	1	2.4178	2.4896	2.4785	0.0718	0.0174	-0.0136	0.0680	0.0000	0.1660
N1-C7	1	2.4352	2.4709	2.4579	0.0357	0.0240	-0.0237	0.0353	0.0001	0.1779
N2-H12	1	2.4397	2.4593	2.4575	0.0196	0.0140	-0.0144	0.0200	0.0000	0.0671
N2-C8	1	2.4539	2.4687	2.4669	0.0147	0.0163	-0.0165	0.0149	0.0000	0.0661
C4-C3	1	2.4652	2.4810	2.4793	0.0158	0.0074	-0.0076	0.0161	-0.0001	0.0644
H12-H18	1	2.4658	2.5001	2.4922	0.0343	0.0182	-0.0106	0.0267	0.0000	0.1398
C3-H14	1	2.4678	2.5070	2.4974	0.0392	0.0872	-0.0868	0.0388	0.0000	0.1543
H14-H20	1	2.4730	2.4827	2.4714	0.0097	0.0285	-0.0178	-0.0011	0.0001	0.1662
H15-H24	1	2.4749	2.4970	2.4866	0.0221	0.0631	-0.0625	0.0216	-0.0001	0.1604
H11-H19	1	2.4952	2.5326	2.5236	0.0375	0.0883	-0.0876	0.0368	0.0000	0.1503
H10-H16	1	2.4989	2.5400	2.5285	0.0411	0.0635	-0.0642	0.0418	0.0000	0.1699
H13-H22	1	2.5005	2.5318	2.5201	0.0313	0.0561	-0.0551	0.0302	0.0001	0.1711
H12-H17	1	2.5026	2.5495	2.5369	0.0469	0.0505	-0.0487	0.0451	0.0000	0.1787
C3-C9	1	2.5045	2.5416	2.5302	0.0370	0.0548	-0.0536	0.0358	0.0000	0.1692
H11-H17	1	2.5092	2.5362	2.5242	0.0270	0.0473	-0.0458	0.0255	0.0000	0.1735
H15-H23	1	2.5109	2.5399	2.5275	0.0290	0.0660	-0.0663	0.0292	0.0001	0.1763
N2-C6	1	2.5148	2.5521	2.5403	0.0373	0.0488	-0.0477	0.0361	0.0001	0.1724

H13-H21	1	2.5164	2.5533	2.5422	0.0369	0.0671	-0.0661	0.0359	0.0000	0.1670
H16-H25	1	2.5166	2.5278	2.4807	0.0112	0.0846	0.0390	-0.1123	-0.0001	0.3436
H14-H21	1	2.5191	2.5262	2.5242	0.0071	0.0050	-0.0042	0.0063	0.0000	0.0708
H16-H23	1	2.5281	2.5547	2.5524	0.0266	0.0189	-0.0198	0.0275	0.0000	0.0763
H18-H20	1	2.5295	2.5690	2.5611	0.0395	0.0097	-0.0128	0.0426	0.0000	0.1419
C5-H10	1	2.5303	2.5358	2.5240	0.0055	0.0481	-0.0456	0.0030	0.0000	0.1717
C3-H12	1	2.5467	2.6835	2.6391	0.1368	0.0684	0.0611	0.0074	-0.0001	0.3462
H10-H25	1	2.5705	2.6151	2.6066	0.0446	0.0333	-0.0191	0.0305	-0.0001	0.1482
N1-C6	1	2.5951	2.6047	2.6030	0.0096	0.0059	-0.0042	0.0078	0.0001	0.0658
N2-H15	1	2.5968	2.6592	2.6429	0.0623	0.0350	0.0056	0.0217	0.0000	0.2095
C4-H15	1	2.6134	2.6158	2.6054	0.0023	0.0197	-0.0100	-0.0073	-0.0001	0.1632
C6-H12	1	2.6614	2.7824	2.7562	0.1211	0.0440	-0.0174	0.0945	0.0000	0.2718
N1-H19	1	2.6744	2.7089	2.6990	0.0345	0.0455	-0.0452	0.0342	0.0000	0.1633
N2-H22	1	2.6965	2.7127	2.6980	0.0163	0.0190	0.0060	-0.0088	0.0001	0.1990
N1-H18	1	2.6987	2.7130	2.7035	0.0143	0.0417	-0.0407	0.0132	0.0001	0.1598
N2-H20	1	2.7307	2.7560	2.7472	0.0253	0.0441	-0.0442	0.0254	0.0000	0.1550
C3-H24	1	2.7426	2.7709	2.7619	0.0283	0.0378	-0.0379	0.0285	-0.0001	0.1579
C3-H25	1	2.7739	2.8495	2.8388	0.0756	0.0438	-0.0424	0.0742	0.0000	0.1745
N1-H15	1	2.7881	2.7989	2.7906	0.0107	0.0167	-0.0096	0.0036	0.0000	0.1514
C9-H10	1	2.8232	2.8361	2.8258	0.0129	0.0464	-0.0449	0.0115	-0.0001	0.1700
C3-H11	1	2.8388	2.8982	2.8890	0.0594	0.0153	-0.0221	0.0662	0.0000	0.1632
C3-H13	1	2.8466	2.9412	2.9208	0.0946	0.0152	-0.0225	0.1018	0.0001	0.2446
H10-H13	1	2.8536	2.9048	2.8936	0.0512	0.0175	-0.0180	0.0517	0.0000	0.1811
N1-H20	1	2.9018	2.8911	2.8838	-0.0106	0.0250	-0.0298	-0.0058	0.0000	0.1426
H11-H15	1	2.9148	3.0712	2.9970	0.1565	0.0591	0.0378	0.0596	0.0000	0.4816
C4-C6	1	2.9274	2.9463	2.9374	0.0190	0.0115	-0.0148	0.0222	0.0001	0.1612
N1-H16	1	2.9325	3.0351	3.0061	0.1025	0.0355	-0.0178	0.0848	0.0000	0.2987
N2-H24	1	2.9373	2.9214	2.8998	-0.0160	0.0334	-0.0167	-0.0327	0.0000	0.2449
N2-H18	1	2.9657	3.0150	2.9421	0.0493	0.0648	0.0461	-0.0616	0.0000	0.4578
H19-H20	1	2.9781	2.9840	2.9811	0.0059	0.0081	-0.0025	0.0003	0.0000	0.0927
H18-H22	1	3.0234	3.0802	2.9684	0.0568	0.0498	-0.0238	0.0308	0.0000	0.5572
H12-H19	1	3.0520	3.0712	3.0664	0.0191	0.0198	-0.0377	0.0370	0.0000	0.1211
H10-H15	1	3.0552	3.0878	3.0878	0.0327	0.1052	-0.1183	0.0457	0.0001	0.0078
H13-H20	1	3.0578	3.0899	3.0892	0.0321	0.1050	-0.1182	0.0453	0.0000	0.0464
H11-H18	1	3.0602	3.0848	3.0822	0.0246	0.0725	-0.0870	0.0391	0.0000	0.0895
H14-H22	1	3.0617	3.0737	3.0343	0.0120	0.0469	-0.0018	-0.0331	0.0000	0.3387
H15-H25	1	3.0632	3.0914	3.0885	0.0282	0.0736	-0.0885	0.0431	0.0000	0.0952
H16-H24	1	3.0695	3.0923	3.0899	0.0228	0.0775	-0.0941	0.0394	0.0000	0.0863
H11-H16	1	3.0761	3.1038	3.1007	0.0277	0.0746	-0.0917	0.0447	0.0001	0.0980
H10-H24	1	3.0832	3.0293	2.9668	-0.0539	0.0114	-0.0139	-0.0514	0.0000	0.4065
H12-H16	1	3.1018	3.2105	3.1855	0.1087	0.0401	0.0421	0.0264	0.0001	0.2850
C7-H20	1	3.1191	3.2038	3.1766	0.0847	0.0447	0.0461	-0.0062	0.0001	0.2947
C6-H11	1	3.1665	3.2307	3.2213	0.0643	0.0110	-0.0154	0.0687	0.0000	0.1765
N1-C8	1	3.1686	3.1501	3.1430	-0.0185	0.0135	-0.0173	-0.0148	0.0001	0.1472
C8-H18	1	3.1722	3.1872	3.1700	0.0150	0.0444	-0.0187	-0.0107	0.0000	0.2320

N2-C7	1	3.2183	3.1676	3.1450	-0.0507	0.0155	-0.0149	-0.0514	0.0001	0.2549
N2-H11	1	3.2545	3.2916	3.2879	0.0372	0.0183	-0.0337	0.0527	-0.0001	0.1102
N2-C9	1	3.2561	3.2710	3.2438	0.0149	0.0338	-0.0472	0.0283	0.0000	0.2943
N1-H13	1	3.2703	3.2716	3.2688	0.0014	0.0241	-0.0451	0.0224	0.0000	0.0951
C4-H16	1	3.2890	3.2413	3.2154	-0.0476	0.0331	0.0010	-0.0817	0.0000	0.2894
H13-H24	1	3.3427	3.3813	3.3312	0.0385	0.0300	-0.0171	0.0257	-0.0001	0.4044
C4-H10	1	3.3530	3.3782	3.3751	0.0253	0.0124	-0.0207	0.0335	0.0001	0.1020
N2-H16	1	3.3552	3.3726	3.3672	0.0173	0.0170	-0.0164	0.0167	0.0000	0.1344
N1-H17	1	3.3838	3.4058	3.4030	0.0220	0.0198	-0.0341	0.0363	0.0000	0.0966
N2-H21	1	3.3946	3.4118	3.4091	0.0172	0.0252	-0.0396	0.0316	0.0000	0.0959
C3-H23	1	3.4062	3.4213	3.4179	0.0150	0.0126	-0.0263	0.0287	0.0000	0.1075
C4-C5	1	3.4707	3.4939	3.4911	0.0232	0.0287	-0.0461	0.0407	-0.0001	0.0991
C4-H20	1	3.5228	3.5714	3.5606	0.0486	0.0294	-0.0107	0.0299	0.0000	0.1960
H10-H11	1	3.5472	3.5711	3.5695	0.0239	0.0080	-0.0135	0.0294	0.0000	0.0753
C5-H18	1	3.5485	3.5417	3.5272	-0.0068	0.0178	-0.0136	-0.0110	0.0000	0.2234
N1-H22	1	3.5534	3.6417	3.6213	0.0883	0.0302	0.0044	0.0538	-0.0001	0.2728
H10-H12	1	3.5638	3.5803	3.5625	0.0165	0.0286	-0.0045	-0.0076	0.0000	0.2512
N2-H25	1	3.6161	3.6888	3.6671	0.0727	0.0296	-0.0540	0.0971	0.0000	0.2826
C3-C8	1	3.6224	3.6712	3.6640	0.0488	0.0329	-0.0353	0.0512	0.0000	0.1630
N2-H19	1	3.6262	3.6338	3.6262	0.0076	0.0282	-0.0354	0.0148	0.0000	0.1656
C5-C6	1	3.6389	3.5882	3.5739	-0.0507	0.0316	-0.0482	-0.0341	0.0000	0.2229
C3-C7	1	3.6896	3.6933	3.6916	0.0037	0.0116	-0.0225	0.0146	0.0000	0.0771
C5-H24	1	3.6995	3.7651	3.7481	0.0655	0.0331	-0.0452	0.0777	-0.0001	0.2506
H10-H23	1	3.7165	3.7428	3.7407	0.0263	0.0080	-0.0236	0.0418	0.0001	0.0868
C5-H12	1	3.7202	3.7420	3.7404	0.0218	0.0036	-0.0083	0.0265	0.0000	0.0771
C4-H14	1	3.7634	3.8458	3.8277	0.0824	0.0178	-0.0080	0.0726	0.0000	0.2636
C3-H20	1	3.7833	3.8582	3.8508	0.0749	0.0144	-0.0217	0.0822	0.0000	0.1694
N1-C9	1	3.7944	3.8437	3.8271	0.0493	0.0180	0.0118	0.0195	0.0000	0.2535
C7-C8	1	3.8031	3.8126	3.8111	0.0095	0.0123	-0.0246	0.0219	-0.0001	0.0768
C6-H13	1	3.8239	3.9088	3.8530	0.0849	0.0282	-0.0115	0.0681	0.0001	0.4680
C6-H14	1	3.8302	3.8267	3.8181	-0.0035	0.0205	-0.0263	0.0023	0.0000	0.1795
C3-H18	1	3.8322	3.8884	3.8794	0.0562	0.0269	-0.0497	0.0790	0.0000	0.1872
C9-H13	1	3.8489	3.8370	3.8279	-0.0119	0.0274	-0.0353	-0.0040	0.0000	0.1846
C8-H10	1	3.8645	3.8487	3.7994	-0.0158	0.0296	-0.0089	-0.0365	0.0000	0.4255
C9-H12	1	3.8645	3.9192	3.9071	0.0548	0.0283	-0.0422	0.0687	0.0000	0.2170
C7-H22	1	3.8917	3.8735	3.8327	-0.0181	0.0420	-0.0419	-0.0182	0.0000	0.3908
C8-H19	1	3.8954	3.9491	3.9409	0.0537	0.0115	-0.0184	0.0606	0.0000	0.1799
H13-H25	1	3.8978	3.9347	3.9271	0.0370	0.0097	-0.0136	0.0409	0.0000	0.1733
C4-C8	1	3.9178	3.9434	3.9381	0.0256	0.0128	-0.0159	0.0286	0.0001	0.1440
N1-H24	1	3.9435	3.9556	3.9132	0.0122	0.0405	-0.0207	-0.0076	0.0000	0.4048
C5-C7	1	3.9438	3.9539	3.9483	0.0101	0.0152	-0.0351	0.0300	0.0000	0.1481
C5-H15	1	3.9565	4.0242	4.0166	0.0677	0.0096	-0.0073	0.0654	0.0000	0.1759
C7-H15	1	3.9678	3.9732	3.9690	0.0054	0.0105	-0.0269	0.0218	0.0000	0.1293
H12-H24	1	3.9784	3.9651	3.9586	-0.0133	0.0126	-0.0151	-0.0107	-0.0001	0.1593
H12-H20	1	3.9911	3.9886	3.9806	-0.0025	0.0334	-0.0425	0.0066	0.0000	0.1770

N1-H21	1	3.9927	3.9959	3.9887	0.0032	0.0135	-0.0170	0.0067	0.0000	0.1689
C3-H19	1	4.0146	4.0375	4.0281	0.0229	0.0154	-0.0199	0.0274	0.0000	0.1949
C3-H22	1	4.0835	3.9849	3.9540	-0.0987	0.0340	-0.0222	-0.1104	-0.0001	0.3444
H14-H18	1	4.0921	4.1121	4.1056	0.0200	0.0258	-0.0534	0.0476	0.0000	0.1626
H17-H20	1	4.0936	4.0957	4.0899	0.0021	0.0283	-0.0482	0.0220	0.0000	0.1540
H18-H21	1	4.0961	4.0972	4.0906	0.0011	0.0215	-0.0415	0.0211	0.0000	0.1640
H10-H20	1	4.1000	4.1953	4.1742	0.0953	0.0386	0.0087	0.0481	-0.0001	0.2987
N2-H17	1	4.1050	4.1564	4.1490	0.0514	0.0171	-0.0370	0.0712	0.0001	0.1745
C5-C9	1	4.1067	4.2033	4.1828	0.0966	0.0280	-0.0211	0.0898	-0.0001	0.2918
C4-H22	1	4.1074	4.2053	4.1776	0.0979	0.0226	-0.0328	0.1081	0.0000	0.3420
N1-H25	1	4.1196	4.1805	4.1585	0.0609	0.0433	0.0158	0.0019	-0.0001	0.3031
C5-H19	1	4.1275	4.1292	4.0371	0.0017	0.0349	-0.0525	0.0193	0.0000	0.6009
H12-H22	1	4.1394	4.1269	4.1038	-0.0125	0.0306	-0.0348	-0.0083	0.0000	0.3039
N2-H23	1	4.1427	4.1613	4.1508	0.0185	0.0197	-0.0255	0.0244	-0.0001	0.2083
H13-H15	1	4.1578	4.1307	4.1169	-0.0271	0.0298	-0.0499	-0.0070	0.0000	0.2347
H15-H18	1	4.1642	4.0966	4.0750	-0.0675	0.0255	-0.0359	-0.0571	0.0000	0.2932
H14-H19	1	4.1672	4.2347	4.2059	0.0676	0.0330	-0.0378	0.0725	-0.0001	0.3454
H12-H14	1	4.1795	4.2347	4.2283	0.0552	0.0271	-0.0488	0.0769	0.0000	0.1649
H14-H24	1	4.1968	4.2421	4.1983	0.0453	0.0396	-0.0701	0.0758	0.0000	0.4206
C8-H12	1	4.2024	4.2156	4.2017	0.0132	0.0217	-0.0309	0.0224	0.0000	0.2399
H19-H22	1	4.2030	4.2239	4.1985	0.0209	0.0291	-0.0561	0.0479	0.0000	0.3194
C5-H25	1	4.2041	4.3516	4.3220	0.1475	0.0240	-0.0241	0.1476	0.0000	0.3578
C7-H14	1	4.2799	4.3218	4.3139	0.0419	0.0285	-0.0457	0.0591	0.0000	0.1842
H14-H25	1	4.2830	4.3887	4.3772	0.1057	0.0113	-0.0167	0.1111	0.0000	0.2243
C5-H11	1	4.2975	4.2392	4.2213	-0.0583	0.0149	-0.0440	-0.0292	0.0000	0.2669
C4-H13	1	4.2976	4.2080	4.1727	-0.0896	0.0276	-0.0325	-0.0846	-0.0001	0.3777
C4-C9	1	4.3410	4.3366	4.3320	-0.0044	0.0249	-0.0453	0.0160	0.0000	0.1412
H11-H14	1	4.3427	4.2989	4.2838	-0.0437	0.0177	-0.0297	-0.0317	0.0000	0.2501
H12-H13	1	4.3540	4.3116	4.2986	-0.0424	0.0260	-0.0355	-0.0329	0.0000	0.2348
C9-H14	1	4.3694	4.3938	4.3910	0.0245	0.0217	-0.0488	0.0516	0.0000	0.1120
H14-H15	1	4.3790	4.3986	4.3959	0.0196	0.0170	-0.0380	0.0406	0.0000	0.1095
H11-H20	1	4.3885	4.4772	4.4668	0.0888	0.0276	-0.0457	0.1069	0.0000	0.2157
C6-C7	1	4.3998	4.4197	4.3960	0.0198	0.0377	-0.0390	0.0211	0.0000	0.3185
H15-H17	1	4.4048	4.4788	4.4552	0.0739	0.0340	-0.0183	0.0583	-0.0001	0.3254
H12-H23	1	4.4108	4.4213	4.4182	0.0105	0.0078	-0.0296	0.0323	0.0000	0.1165
H14-H16	1	4.4187	4.4321	4.4251	0.0135	0.0198	-0.0338	0.0274	0.0001	0.1755
H13-H18	1	4.4528	4.4809	4.4679	0.0281	0.0204	-0.0176	0.0253	0.0000	0.2414
C5-H16	1	4.4544	4.4468	4.4358	-0.0075	0.0284	-0.0390	0.0031	0.0000	0.2198
C3-H21	1	4.5176	4.4772	4.4497	-0.0404	0.0290	-0.0273	-0.0422	0.0001	0.3462
C7-H10	1	4.5190	4.5370	4.5339	0.0180	0.0187	-0.0419	0.0412	0.0000	0.1183
H10-H22	1	4.5268	4.5518	4.5489	0.0250	0.0079	-0.0323	0.0494	0.0000	0.1137
H10-H21	1	4.5497	4.5662	4.5600	0.0166	0.0305	-0.0664	0.0524	0.0001	0.1677
C3-H17	1	4.5661	4.5904	4.5875	0.0244	0.0137	-0.0401	0.0508	0.0000	0.1164
C4-H24	1	4.5672	4.6000	4.5915	0.0328	0.0210	-0.0460	0.0578	0.0000	0.1973
C9-H11	1	4.6290	4.6815	4.6654	0.0525	0.0242	-0.0502	0.0784	0.0001	0.2728

H10-H19	1	4.6468	4.6456	4.6429	-0.0013	0.0207	-0.0453	0.0233	0.0000	0.1117
C6-H18	1	4.6759	4.7757	4.7284	0.0998	0.0323	-0.0278	0.0954	-0.0001	0.4781
N1-H23	1	4.6934	4.7383	4.7287	0.0449	0.0239	-0.0499	0.0709	0.0000	0.2124
H10-H18	1	4.6970	4.7167	4.7074	0.0196	0.0208	-0.0507	0.0495	0.0000	0.2084
H12-H25	1	4.7301	4.6937	4.6513	-0.0364	0.0315	-0.0295	-0.0384	0.0000	0.4387
H13-H16	1	4.7878	4.8353	4.8211	0.0475	0.0231	-0.0182	0.0426	0.0000	0.2624
H15-H19	1	4.7947	4.8255	4.8115	0.0307	0.0218	-0.0202	0.0292	-0.0001	0.2599
C7-H16	1	4.8028	4.9280	4.9110	0.1252	0.0272	-0.0210	0.1190	0.0000	0.2907
H17-H22	1	4.8052	4.7976	4.7894	-0.0077	0.0259	-0.0677	0.0341	0.0000	0.1975
H19-H21	1	4.8617	4.8345	4.7964	-0.0272	0.0325	-0.0201	-0.0396	0.0000	0.4214
C7-H21	1	4.8789	4.9358	4.9288	0.0569	0.0144	-0.0221	0.0645	0.0001	0.1850
C8-H17	1	4.8931	4.9435	4.9345	0.0504	0.0167	-0.0374	0.0711	0.0000	0.2114
C8-H11	1	4.8997	4.8893	4.8804	-0.0104	0.0239	-0.0561	0.0218	0.0000	0.2059
C6-C8	1	4.9305	4.8588	4.8342	-0.0717	0.0383	-0.0439	-0.0662	0.0001	0.3450
H13-H23	1	4.9361	4.9697	4.9680	0.0336	0.0064	-0.0259	0.0531	0.0000	0.0911
C7-H13	1	4.9635	4.9712	4.9698	0.0077	0.0062	-0.0221	0.0236	0.0000	0.0839
H22-H24	1	4.9834	4.9790	4.9620	-0.0044	0.0278	-0.0224	-0.0099	0.0001	0.2886
C4-H25	1	5.0007	5.0506	5.0444	0.0499	0.0149	-0.0369	0.0719	0.0000	0.1772
H15-H22	1	5.0082	5.0058	4.9985	-0.0024	0.0147	-0.0191	0.0021	-0.0001	0.1893
C6-H19	1	5.0084	5.0181	5.0126	0.0097	0.0126	-0.0365	0.0336	0.0000	0.1656
C4-H21	1	5.0097	4.9979	4.9942	-0.0118	0.0214	-0.0657	0.0325	0.0000	0.1364
C8-H15	1	5.0130	5.0082	5.0024	-0.0048	0.0192	-0.0453	0.0212	0.0001	0.1698
C8-H24	1	5.0608	5.0270	5.0164	-0.0338	0.0125	-0.0444	-0.0018	-0.0001	0.2287
C6-H17	1	5.0713	5.1667	5.1579	0.0954	0.0175	-0.0379	0.1157	0.0001	0.2133
C4-H23	1	5.0720	5.1118	5.0967	0.0398	0.0269	-0.0361	0.0490	0.0000	0.2766
C5-H17	1	5.1470	5.1557	5.1480	0.0086	0.0181	-0.0371	0.0276	0.0000	0.1987
H11-H24	1	5.1508	5.2278	5.2040	0.0771	0.0256	-0.0668	0.1182	0.0001	0.3534
C6-H22	1	5.1668	5.1613	5.1546	-0.0055	0.0176	-0.0342	0.0112	-0.0001	0.1849
C6-H20	1	5.1722	5.1789	5.1718	0.0067	0.0214	-0.0434	0.0287	0.0000	0.1903
H15-H20	1	5.1732	5.1784	5.1664	0.0052	0.0245	-0.0280	0.0087	0.0000	0.2481
H11-H25	1	5.1874	5.1585	5.1279	-0.0289	0.0399	-0.0779	0.0090	0.0001	0.3879
H11-H23	1	5.1968	5.1217	5.1030	-0.0751	0.0329	-0.0816	-0.0264	0.0000	0.3049
H11-H22	1	5.2140	5.2299	5.2266	0.0159	0.0260	-0.0718	0.0618	-0.0001	0.1327
C5-H23	1	5.2182	5.2881	5.2808	0.0699	0.0093	-0.0385	0.0990	0.0001	0.1960
H11-H13	1	5.2470	5.2806	5.2740	0.0336	0.0083	-0.0307	0.0559	0.0001	0.1858
H13-H19	1	5.3126	5.4511	5.4346	0.1385	0.0170	-0.0441	0.1656	0.0000	0.2999
H16-H19	1	5.3262	5.3512	5.3469	0.0249	0.0112	-0.0488	0.0626	-0.0001	0.1515
H16-H18	1	5.3639	5.4568	5.4475	0.0929	0.0156	-0.0478	0.1251	0.0000	0.2256
H16-H17	1	5.3856	5.4384	5.4231	0.0527	0.0171	-0.0396	0.0753	-0.0001	0.2870
H12-H21	1	5.3935	5.4729	5.4556	0.0794	0.0254	-0.0569	0.1108	0.0001	0.3056
H14-H17	1	5.4205	5.3742	5.3621	-0.0463	0.0225	-0.0617	-0.0072	0.0001	0.2524
H10-H17	1	5.4419	5.4646	5.4613	0.0227	0.0130	-0.0523	0.0619	0.0001	0.1330
C8-C9	1	5.5188	5.4829	5.4668	-0.0359	0.0165	-0.0462	-0.0062	0.0000	0.2939
H14-H23	1	5.5363	5.4784	5.4680	-0.0578	0.0232	-0.0691	-0.0119	0.0000	0.2387
C9-H22	1	5.5526	5.5485	5.5314	-0.0041	0.0257	-0.0793	0.0495	0.0000	0.3032

H20-H24	1	5.6517	5.6606	5.6525	0.0089	0.0188	-0.0547	0.0448	0.0000	0.2141
H18-H24	1	5.6546	5.6854	5.6766	0.0308	0.0230	-0.0684	0.0763	-0.0001	0.2226
H21-H24	1	5.6904	5.6873	5.6690	-0.0031	0.0227	-0.0805	0.0547	0.0000	0.3176
C8-H16	1	5.7865	5.8102	5.7969	0.0237	0.0247	-0.0519	0.0509	0.0000	0.2785
C8-H25	1	5.8364	5.8615	5.8592	0.0251	0.0133	-0.0503	0.0621	0.0000	0.1151
C7-C9	1	5.8426	5.7675	5.7554	-0.0752	0.0180	-0.0679	-0.0253	0.0000	0.2611
C7-H24	1	5.8431	5.8583	5.8561	0.0152	0.0117	-0.0443	0.0478	0.0000	0.1145
H16-H20	1	5.8689	5.9137	5.9076	0.0449	0.0204	-0.0541	0.0786	0.0000	0.1893
C6-H21	1	5.8811	5.8869	5.8779	0.0058	0.0280	-0.0829	0.0608	-0.0001	0.2283
H17-H21	1	5.8901	5.9172	5.9089	0.0272	0.0199	-0.0640	0.0713	0.0000	0.2209
C9-H18	1	5.9306	5.9354	5.9305	0.0048	0.0240	-0.0865	0.0673	0.0000	0.1701
H11-H21	1	5.9668	5.9825	5.9762	0.0157	0.0131	-0.0581	0.0607	0.0000	0.1945
H13-H17	1	5.9846	5.9780	5.9712	-0.0066	0.0190	-0.0476	0.0219	0.0001	0.2001
C9-H20	1	6.0043	5.9890	5.9675	-0.0153	0.0327	-0.0924	0.0444	0.0000	0.3560
H16-H21	1	6.0094	6.0782	6.0701	0.0688	0.0158	-0.0561	0.1091	0.0000	0.2214
H22-H25	1	6.0205	6.0610	6.0536	0.0406	0.0139	-0.0475	0.0742	0.0000	0.2117
H16-H22	1	6.1059	6.0592	6.0397	-0.0467	0.0298	-0.0334	-0.0432	0.0001	0.3396
C9-H21	1	6.1712	6.0859	6.0666	-0.0853	0.0206	-0.0616	-0.0442	-0.0001	0.3393
H20-H25	1	6.1834	6.1795	6.1777	-0.0039	0.0062	-0.0406	0.0305	0.0000	0.1047
H21-H25	1	6.1906	6.2152	6.1969	0.0246	0.0352	-0.1131	0.1025	0.0000	0.3335
C7-H25	1	6.2231	6.1974	6.1881	-0.0257	0.0165	-0.0430	0.0008	0.0000	0.2377
C9-H19	1	6.2560	6.2189	6.2103	-0.0371	0.0191	-0.0471	-0.0090	-0.0001	0.2308
C9-H17	1	6.2569	6.2390	6.2161	-0.0179	0.0242	-0.0909	0.0488	0.0000	0.3719
C7-H23	1	6.3134	6.2782	6.2587	-0.0352	0.0294	-0.0986	0.0341	-0.0001	0.3447
H17-H24	1	6.4185	6.3129	6.3014	-0.1056	0.0255	-0.1009	-0.0302	0.0000	0.2673
H19-H24	1	6.4189	6.4701	6.4630	0.0512	0.0144	-0.0598	0.0966	0.0000	0.2143
H18-H25	1	6.4845	6.5006	6.4843	0.0161	0.0246	-0.0660	0.0575	0.0000	0.3215
C8-H23	1	6.4858	6.4633	6.4574	-0.0225	0.0147	-0.0618	0.0246	0.0000	0.1943
H22-H23	1	6.5843	6.5176	6.5042	-0.0667	0.0274	-0.0717	-0.0223	-0.0001	0.2925
H18-H23	1	6.8667	6.8943	6.8866	0.0277	0.0216	-0.0905	0.0966	0.0000	0.2310
H16-H21	1	7.0446	7.0583	7.0557	0.0137	0.0088	-0.0614	0.0662	0.0001	0.1356
H19-H25	1	7.0827	7.0665	7.0643	-0.0163	0.0102	-0.0635	0.0370	0.0000	0.1221
H17-H23	1	7.1653	7.2459	7.2370	0.0806	0.0153	-0.0707	0.1360	0.0000	0.2544
H20-H23	1	7.1664	7.1422	7.1338	-0.0242	0.0193	-0.0711	0.0276	0.0000	0.2438
H17-H25	1	7.1721	7.1287	7.1208	-0.0434	0.0189	-0.0698	0.0075	0.0000	0.2357
H19-H23	1	7.2823	7.2497	7.2423	-0.0326	0.0169	-0.0748	0.0254	-0.0001	0.2306
H21-H23	1	7.9639	7.9644	7.9618	0.0005	0.0117	-0.0866	0.0754	0.0000	0.1426

Table S11. Equilibrium (r_e) and thermal average (r_g , r_a) distances, vibrational corrections (Δ), and mean amplitudes (u) for internuclear distances of TEDA conformation **1c** (in Å), obtained for 291 K by GED refinement (initial approximation MP2/cc-PVTZ). n – number of equivalent parameters.

Atomic pair	n	r_e	r_g	r_a	Δr	$\Delta r(\text{har})$	$\Delta r(\text{kin})$	$\Delta r(\text{dyn})$	$\Delta r(\text{rot})$	u
C6-H15	1	1.0892	1.1130	1.1105	0.0238	0.0512	-0.0459	0.0185	0.0000	0.0536
C7-H19	1	1.0907	1.1149	1.1131	0.0242	0.0626	-0.0567	0.0184	-0.0001	0.0459
C8-H20	1	1.0910	1.1143	1.1113	0.0233	0.0521	-0.0471	0.0183	0.0000	0.0586
C9-H23	1	1.0911	1.1120	1.1083	0.0209	0.0411	-0.0366	0.0164	0.0000	0.0649
C8-H22	1	1.0914	1.1132	1.1092	0.0218	0.0390	-0.0347	0.0176	-0.0001	0.0668
C7-H18	1	1.0916	1.1160	1.1146	0.0244	0.0676	-0.0614	0.0182	0.0000	0.0412
C8-H21	1	1.0918	1.1130	1.1091	0.0212	0.0405	-0.0362	0.0169	0.0000	0.0658
C9-H24	1	1.0918	1.1179	1.1177	0.0262	0.0754	-0.0683	0.0191	0.0000	0.0203
C7-H17	1	1.0924	1.1152	1.1122	0.0229	0.0529	-0.0479	0.0179	0.0000	0.0585
C3-H10	1	1.0926	1.1135	1.1084	0.0209	0.0167	-0.0128	0.0170	0.0000	0.0754
C9-H25	1	1.0927	1.1150	1.1107	0.0223	0.0328	-0.0285	0.0180	0.0000	0.0700
C4-H12	1	1.0928	1.1187	1.1185	0.0259	0.0731	-0.0661	0.0189	0.0000	0.0194
C4-H11	1	1.0933	1.1161	1.1126	0.0228	0.0423	-0.0375	0.0180	0.0000	0.0630
C5-H13	1	1.0947	1.1176	1.1143	0.0228	0.0461	-0.0410	0.0177	0.0000	0.0603
C6-H16	1	1.0951	1.1192	1.1166	0.0240	0.0531	-0.0476	0.0185	0.0000	0.0537
C5-H14	1	1.0971	1.1196	1.1150	0.0225	0.0305	-0.0262	0.0182	0.0000	0.0716
N2-C3	1	1.4225	1.4332	1.4315	0.0107	0.0067	-0.0052	0.0092	0.0000	0.0487
N1-C3	1	1.4264	1.4361	1.4344	0.0097	0.0064	-0.0049	0.0082	0.0000	0.0492
N1-C4	1	1.4384	1.4488	1.4471	0.0104	0.0070	-0.0051	0.0085	0.0000	0.0488
N2-C5	1	1.4398	1.4502	1.4485	0.0103	0.0056	-0.0037	0.0084	0.0000	0.0491
N1-N2	1	1.4836	1.4939	1.4919	0.0102	0.0061	-0.0055	0.0097	-0.0001	0.0541
C3-C6	1	1.4985	1.5113	1.5097	0.0129	0.0066	-0.0052	0.0115	0.0000	0.0493
C5-C8	1	1.5134	1.5280	1.5274	0.0146	0.0364	-0.0344	0.0127	-0.0001	0.0299
C4-C7	1	1.5142	1.5274	1.5262	0.0132	0.0247	-0.0233	0.0117	0.0001	0.0428
C6-C9	1	1.5222	1.5373	1.5371	0.0152	0.0414	-0.0392	0.0130	0.0000	0.0198
H23-H25	1	1.7653	1.7961	1.7921	0.0309	0.0861	-0.0840	0.0287	0.0001	0.0851
H24-H25	1	1.7682	1.7954	1.7896	0.0272	0.0715	-0.0706	0.0262	0.0001	0.1014
H23-H24	1	1.7683	1.7996	1.7990	0.0313	0.1186	-0.1135	0.0262	0.0000	0.0336
H17-H18	1	1.7687	1.7978	1.7927	0.0291	0.0828	-0.0814	0.0277	0.0000	0.0960
H20-H21	1	1.7688	1.7968	1.7937	0.0281	0.0932	-0.0903	0.0251	0.0001	0.0756
H18-H19	1	1.7705	1.8021	1.7990	0.0316	0.1037	-0.1006	0.0285	0.0000	0.0749
H20-H22	1	1.7708	1.7999	1.7953	0.0291	0.0858	-0.0840	0.0273	0.0000	0.0912
H21-H22	1	1.7717	1.7993	1.7933	0.0276	0.0679	-0.0672	0.0269	0.0000	0.1031
H17-H19	1	1.7751	1.8025	1.7974	0.0274	0.0751	-0.0736	0.0259	0.0000	0.0955
H15-H16	1	1.7858	1.8181	1.8137	0.0323	0.0795	-0.0749	0.0277	0.0000	0.0894
H11-H12	1	1.7895	1.8171	1.8101	0.0276	0.0461	-0.0430	0.0244	0.0001	0.1123
H13-H14	1	1.7979	1.8233	1.8183	0.0254	0.0674	-0.0628	0.0208	0.0000	0.0956
H12-H15	1	1.9556	2.0855	2.0617	0.1299	0.0741	0.0491	0.0067	0.0000	0.2230

N2-H13	1	2.0170	2.0327	2.0281	0.0157	0.0358	-0.0371	0.0169	0.0001	0.0962
N1-H11	1	2.0237	2.0414	2.0364	0.0177	0.0240	-0.0262	0.0198	0.0001	0.1009
N2-H14	1	2.0654	2.0901	2.0852	0.0248	0.0201	-0.0219	0.0266	0.0000	0.1010
N1-H12	1	2.0831	2.1109	2.1059	0.0278	0.0262	-0.0281	0.0297	0.0000	0.1029
N1-H10	1	2.0914	2.1116	2.1066	0.0201	0.0131	-0.0174	0.0244	0.0000	0.1017
C3-H16	1	2.0966	2.1252	2.1197	0.0286	0.0376	-0.0403	0.0313	0.0000	0.1082
C3-H15	1	2.1088	2.1228	2.1188	0.0140	0.0338	-0.0356	0.0158	0.0000	0.0919
N2-H10	1	2.1366	2.1628	2.1581	0.0261	0.0143	-0.0182	0.0300	0.0000	0.1006
C5-H20	1	2.1437	2.1688	2.1669	0.0251	0.0778	-0.0781	0.0254	0.0000	0.0645
C7-H12	1	2.1471	2.1729	2.1705	0.0258	0.0668	-0.0669	0.0260	-0.0001	0.0734
C4-H18	1	2.1501	2.1810	2.1798	0.0309	0.0785	-0.0784	0.0308	0.0000	0.0516
C9-H15	1	2.1522	2.1803	2.1783	0.0281	0.0784	-0.0787	0.0284	0.0000	0.0658
C5-H22	1	2.1536	2.1798	2.1763	0.0262	0.0564	-0.0579	0.0277	0.0000	0.0875
C4-H19	1	2.1567	2.1797	2.1749	0.0230	0.0340	-0.0356	0.0246	0.0000	0.1025
C8-H14	1	2.1581	2.1822	2.1780	0.0241	0.0548	-0.0565	0.0258	0.0000	0.0958
C7-H11	1	2.1581	2.1926	2.1903	0.0345	0.0893	-0.0895	0.0347	0.0000	0.0713
C5-H21	1	2.1589	2.1821	2.1778	0.0232	0.0438	-0.0450	0.0243	0.0001	0.0967
C6-H24	1	2.1597	2.1837	2.1788	0.0240	0.0404	-0.0419	0.0255	0.0000	0.1024
C4-H17	1	2.1604	2.1859	2.1834	0.0255	0.0647	-0.0648	0.0257	-0.0001	0.0748
C8-H13	1	2.1604	2.1840	2.1824	0.0236	0.0774	-0.0771	0.0233	0.0000	0.0595
C9-H16	1	2.1692	2.1930	2.1935	0.0238	0.0928	-0.0910	0.0220	0.0000	0.0000
H10-H14	1	2.1704	2.1936	2.1896	0.0232	0.0430	-0.0436	0.0239	-0.0001	0.0928
C6-H25	1	2.1710	2.1968	2.1922	0.0258	0.0394	-0.0409	0.0273	0.0000	0.1005
C6-H23	1	2.1806	2.2026	2.1979	0.0220	0.0127	-0.0137	0.0230	0.0000	0.1011
C6-H10	1	2.1913	2.2434	2.2233	0.0521	0.0223	-0.0082	0.0380	0.0000	0.2116
N1-C5	1	2.3962	2.4126	2.4106	0.0165	0.0050	-0.0065	0.0179	0.0001	0.0697
N2-C4	1	2.4002	2.4206	2.4186	0.0205	0.0068	-0.0086	0.0224	-0.0001	0.0710
C5-C3	1	2.4082	2.4582	2.4482	0.0500	0.0157	-0.0102	0.0446	-0.0001	0.1564
N1-H14	1	2.4115	2.4385	2.4366	0.0270	0.0062	-0.0069	0.0277	0.0000	0.0669
N1-C7	1	2.4302	2.4490	2.4474	0.0188	0.0223	-0.0229	0.0193	0.0001	0.0637
N2-H12	1	2.4394	2.4565	2.4546	0.0171	0.0157	-0.0157	0.0172	-0.0001	0.0692
N2-C8	1	2.4495	2.5326	2.5192	0.0831	0.0205	-0.0109	0.0735	0.0000	0.1847
C4-C3	1	2.4652	2.4866	2.4848	0.0214	0.0073	-0.0077	0.0218	0.0000	0.0667
H12-H18	1	2.4709	2.5098	2.5008	0.0389	0.0899	-0.0890	0.0380	0.0000	0.1492
C3-H14	1	2.4810	2.5185	2.5104	0.0376	0.0165	-0.0113	0.0324	0.0000	0.1430
H14-H20	1	2.4816	2.5154	2.5046	0.0338	0.1044	-0.1038	0.0332	0.0000	0.1637
H15-H24	1	2.4952	2.5306	2.5210	0.0354	0.0888	-0.0878	0.0345	-0.0001	0.1554
H11-H19	1	2.4988	2.5278	2.5171	0.0290	0.0662	-0.0640	0.0269	-0.0001	0.1632
H10-H16	1	2.5015	2.5339	2.5235	0.0324	0.0634	-0.0631	0.0320	0.0001	0.1611
H13-H22	1	2.5024	2.5930	2.5742	0.0906	0.0346	-0.0373	0.0934	-0.0001	0.2208
H12-H17	1	2.5048	2.5408	2.5289	0.0360	0.0607	-0.0607	0.0361	-0.0001	0.1729
C3-C9	1	2.5065	2.5412	2.5296	0.0347	0.0461	-0.0442	0.0328	0.0000	0.1708
H11-H17	1	2.5072	2.5260	2.5239	0.0188	0.0203	-0.0212	0.0197	0.0000	0.0725
H15-H23	1	2.5103	2.5189	2.5170	0.0086	0.0077	-0.0071	0.0080	0.0000	0.0695
N2-C6	1	2.5107	2.5681	2.5571	0.0574	0.0680	-0.0672	0.0567	-0.0001	0.1676

H13-H21	1	2.5120	2.5291	2.5186	0.0171	0.0653	-0.0627	0.0145	0.0000	0.1620
H16-H25	1	2.5134	2.5574	2.5518	0.0440	0.1073	-0.1046	0.0412	0.0001	0.1195
H14-H21	1	2.5218	2.5709	2.5628	0.0491	0.0124	-0.0157	0.0524	0.0000	0.1436
H16-H23	1	2.5221	2.5568	2.5450	0.0348	0.0580	-0.0567	0.0334	0.0001	0.1731
H18-H20	1	2.5301	2.5563	2.5440	0.0263	0.0464	-0.0447	0.0246	0.0000	0.1765
C5-H10	1	2.5860	2.6163	2.6090	0.0303	0.0261	-0.0115	0.0157	0.0000	0.1378
C3-H12	1	2.5958	2.5694	2.5485	-0.0263	0.0652	-0.0226	-0.0690	0.0001	0.2291
H10-H25	1	2.6002	2.6170	2.6153	0.0168	0.0075	-0.0057	0.0151	-0.0001	0.0665
N1-C6	1	2.6265	2.5955	2.5868	-0.0310	0.0299	-0.0147	-0.0463	0.0001	0.1480
N2-H15	1	2.6446	2.6563	2.6456	0.0117	0.0307	0.0110	-0.0300	0.0000	0.1683
C4-H15	1	2.6600	2.7891	2.7706	0.1292	0.0310	0.0085	0.0897	0.0000	0.2277
C6-H12	1	2.6713	2.7031	2.6949	0.0318	0.0588	-0.0573	0.0304	-0.0001	0.1483
N1-H19	1	2.6817	2.7130	2.7023	0.0314	0.0410	-0.0404	0.0308	0.0000	0.1699
N2-H22	1	2.7045	2.7323	2.7227	0.0278	0.0519	-0.0524	0.0283	0.0000	0.1611
N1-H18	1	2.7348	2.7609	2.7514	0.0261	0.0378	-0.0369	0.0252	0.0000	0.1609
N2-H20	1	2.7631	2.8231	2.8135	0.0600	0.0299	-0.0158	0.0459	0.0000	0.1640
C3-H24	1	2.7639	2.9044	2.8623	0.1405	0.0312	-0.0100	0.1193	0.0000	0.3519
C3-H25	1	2.7641	2.7714	2.7615	0.0073	0.0610	-0.0593	0.0056	0.0000	0.1635
N1-H15	1	2.7724	2.8241	2.8153	0.0517	0.0557	-0.0553	0.0513	0.0000	0.1570
C9-H10	1	2.7860	2.7560	2.7453	-0.0300	0.0189	-0.0120	-0.0369	0.0000	0.1705
C3-H11	1	2.8020	2.7952	2.7863	-0.0068	0.0165	-0.0217	-0.0016	0.0000	0.1563
C3-H13	1	2.8500	2.9706	2.9250	0.1206	0.0755	0.0629	-0.0179	0.0001	0.3664
H10-H13	1	2.8805	2.9402	2.9282	0.0597	0.0231	-0.0306	0.0672	0.0000	0.1873
N1-H20	1	2.9426	2.9111	2.8808	-0.0315	0.0440	-0.0243	-0.0511	-0.0001	0.2907
H11-H15	1	2.9809	3.2279	3.1718	0.2471	0.0253	-0.0140	0.2358	0.0000	0.4262
C4-C6	1	2.9952	3.0257	3.0222	0.0306	0.0080	-0.0027	0.0253	0.0000	0.1040
N1-H16	1	3.0004	2.9763	2.9695	-0.0241	0.0293	-0.0285	-0.0249	0.0000	0.1394
N2-H24	1	3.0249	3.0418	3.0016	0.0170	0.0589	0.0285	-0.0704	0.0000	0.3457
N2-H18	1	3.0300	3.1209	3.1006	0.0909	0.0284	-0.0159	0.0784	0.0000	0.2523
H19-H20	1	3.0536	3.0636	3.0596	0.0101	0.0304	-0.0526	0.0323	0.0000	0.1114
H18-H22	1	3.0555	3.0872	3.0870	0.0317	0.1057	-0.1191	0.0451	0.0000	0.0247
H12-H19	1	3.0589	3.2247	3.1930	0.1657	0.0412	-0.0226	0.1471	0.0000	0.3213
H10-H15	1	3.0596	3.0888	3.0887	0.0293	0.1068	-0.1200	0.0425	0.0000	0.0181
H13-H20	1	3.0644	3.0964	3.0991	0.0320	0.1281	-0.1398	0.0438	-0.0001	0.0000
H11-H18	1	3.0658	3.1010	3.1021	0.0352	0.1267	-0.1392	0.0478	-0.0001	0.0000
H14-H22	1	3.0680	3.0950	3.0918	0.0270	0.0718	-0.0871	0.0423	0.0000	0.1006
H15-H25	1	3.0737	3.1022	3.0994	0.0286	0.0709	-0.0860	0.0437	0.0000	0.0939
H16-H24	1	3.1066	2.9446	2.8951	-0.1620	0.0320	-0.0164	-0.1776	0.0000	0.3564
H11-H16	1	3.1082	3.1211	3.0678	0.0129	0.0288	0.0003	-0.0161	-0.0001	0.4023
H10-H24	1	3.1317	3.0918	3.0695	-0.0400	0.0459	-0.0504	-0.0355	0.0000	0.2545
H12-H16	1	3.1612	3.2561	3.2380	0.0949	0.0151	-0.0215	0.1012	0.0001	0.2436
C7-H20	1	3.1815	3.1490	3.1380	-0.0325	0.0161	-0.0225	-0.0260	-0.0001	0.1840
C6-H11	1	3.2000	3.3092	3.2811	0.1092	0.0132	-0.0154	0.1114	0.0000	0.3047
N1-C8	1	3.2062	3.5182	3.4312	0.3119	0.0508	0.0332	0.2279	0.0000	0.5675
C8-H18	1	3.2172	3.2754	3.2689	0.0582	0.0113	-0.0161	0.0630	0.0000	0.1468

N2-C7	1	3.2460	3.2604	3.2572	0.0144	0.0187	-0.0316	0.0273	0.0000	0.1021
N2-H11	1	3.2591	3.2900	3.2859	0.0309	0.0225	-0.0445	0.0529	0.0000	0.1151
N2-C9	1	3.2796	3.3682	3.3577	0.0886	0.0144	-0.0186	0.0928	0.0000	0.1895
N1-H13	1	3.2819	3.2023	3.1804	-0.0796	0.0205	-0.0169	-0.0832	0.0000	0.2536
C4-H16	1	3.2905	3.5980	3.5213	0.3075	0.0576	0.0461	0.2037	0.0001	0.5287
H13-H24	1	3.3555	3.3431	3.3408	-0.0125	0.0269	-0.0467	0.0073	0.0000	0.0870
C4-H10	1	3.3572	3.3827	3.3794	0.0254	0.0121	-0.0206	0.0339	0.0000	0.1040
N2-H16	1	3.3791	3.3986	3.3960	0.0195	0.0299	-0.0449	0.0345	0.0000	0.0939
N1-H17	1	3.3835	3.4018	3.3991	0.0183	0.0247	-0.0396	0.0332	0.0000	0.0963
N2-H21	1	3.3977	3.5745	3.5426	0.1768	0.0357	0.0403	0.1008	0.0000	0.3390
C3-H23	1	3.4346	3.6214	3.5880	0.1868	0.0462	0.0433	0.0972	0.0001	0.3480
C4-C5	1	3.4570	3.4775	3.4748	0.0205	0.0255	-0.0412	0.0361	0.0001	0.0976
C4-H20	1	3.5030	3.5344	3.5273	0.0315	0.0221	-0.0428	0.0522	0.0000	0.1588
H10-H11	1	3.5428	3.5360	3.5100	-0.0068	0.0356	-0.0006	-0.0419	0.0001	0.2999
C5-H18	1	3.5515	3.5665	3.5647	0.0149	0.0051	-0.0112	0.0210	0.0000	0.0799
N1-H22	1	3.6200	3.6698	3.6592	0.0497	0.0264	-0.0358	0.0591	0.0000	0.1967
H10-H12	1	3.6422	3.6698	3.6634	0.0276	0.0263	-0.0276	0.0289	0.0000	0.1523
N2-H25	1	3.6494	3.5955	3.5760	-0.0539	0.0403	-0.0647	-0.0295	0.0000	0.2574
C3-C8	1	3.6526	3.7127	3.6961	0.0601	0.0282	-0.0472	0.0790	0.0001	0.2471
N2-H19	1	3.6699	3.6123	3.5866	-0.0577	0.0239	-0.0022	-0.0793	-0.0001	0.3018
C5-C6	1	3.6833	3.6722	3.6635	-0.0112	0.0145	-0.0202	-0.0056	0.0001	0.1770
C3-C7	1	3.6956	3.7718	3.7455	0.0762	0.0378	-0.0640	0.1024	0.0000	0.3129
C5-H24	1	3.7026	3.7267	3.7251	0.0241	0.0070	-0.0120	0.0291	0.0000	0.0767
H10-H23	1	3.7029	3.7301	3.7282	0.0272	0.0111	-0.0237	0.0398	0.0000	0.0830
C5-H12	1	3.7189	3.7144	3.7127	-0.0045	0.0141	-0.0313	0.0126	0.0001	0.0798
C4-H14	1	3.7657	3.8119	3.8050	0.0463	0.0124	-0.0180	0.0519	0.0000	0.1622
C3-H20	1	3.7791	3.8681	3.8495	0.0890	0.0226	-0.0047	0.0711	0.0000	0.2684
N1-C9	1	3.7900	3.7639	3.7557	-0.0261	0.0247	-0.0392	-0.0117	0.0001	0.1743
C7-C8	1	3.7989	3.9415	3.9190	0.1426	0.0339	-0.0008	0.1095	0.0000	0.2977
C6-H13	1	3.8046	3.6677	3.5986	-0.1369	0.0352	-0.0295	-0.1427	0.0001	0.4867
C6-H14	1	3.8054	3.8848	3.8755	0.0794	0.0136	-0.0185	0.0843	0.0000	0.1901
C3-H18	1	3.8495	3.8787	3.8769	0.0292	0.0114	-0.0295	0.0473	0.0000	0.0840
C9-H13	1	3.8604	3.9486	3.9246	0.0882	0.0310	-0.0625	0.1197	0.0000	0.3066
C8-H10	1	3.8676	3.8415	3.8306	-0.0261	0.0347	-0.0500	-0.0109	0.0001	0.2022
C9-H12	1	3.8925	3.9468	3.9372	0.0543	0.0261	-0.0370	0.0653	-0.0001	0.1948
C7-H22	1	3.9296	3.9622	3.9567	0.0327	0.0131	-0.0188	0.0384	0.0000	0.1479
C8-H19	1	3.9382	4.0275	4.0097	0.0893	0.0225	-0.0403	0.1070	0.0001	0.2670
H13-H25	1	3.9523	4.0489	4.0384	0.0966	0.0289	-0.0202	0.0880	-0.0001	0.2062
C4-C8	1	3.9724	3.9398	3.9287	-0.0326	0.0118	-0.0135	-0.0310	0.0001	0.2072
N1-H24	1	3.9891	4.0654	4.0498	0.0764	0.0201	-0.0326	0.0888	0.0001	0.2522
C5-C7	1	4.0063	3.9640	3.9573	-0.0422	0.0211	-0.0236	-0.0398	0.0001	0.1606
C5-H15	1	4.0158	4.0590	4.0494	0.0433	0.0321	-0.0179	0.0290	0.0001	0.1971
C7-H15	1	4.0161	4.1127	4.1008	0.0965	0.0335	-0.0529	0.1159	0.0000	0.2202
H12-H24	1	4.0261	4.0839	4.0606	0.0578	0.0347	-0.0242	0.0473	0.0000	0.3065
H12-H20	1	4.0627	4.2907	4.2554	0.2279	0.0445	-0.0388	0.2222	0.0000	0.3876

N1-H21	1	4.0710	4.2377	4.2181	0.1667	0.0170	0.0081	0.1416	0.0000	0.2922
C3-H19	1	4.0839	4.3323	4.2718	0.2484	0.0286	-0.0185	0.2382	0.0001	0.5198
C3-H22	1	4.0884	4.0971	4.0916	0.0086	0.0361	-0.0650	0.0376	-0.0001	0.1500
H14-H18	1	4.1084	4.0898	4.0816	-0.0187	0.0244	-0.0468	0.0037	0.0000	0.1817
H17-H20	1	4.1240	4.1454	4.1393	0.0214	0.0283	-0.0502	0.0434	-0.0001	0.1584
H18-H21	1	4.1414	4.3724	4.3233	0.2310	0.0263	-0.0117	0.2164	0.0000	0.4661
H10-H20	1	4.1578	4.2095	4.2034	0.0517	0.0194	-0.0408	0.0731	0.0000	0.1599
N2-H17	1	4.1581	4.0838	4.0525	-0.0743	0.0288	-0.0440	-0.0591	0.0000	0.3499
C5-C9	1	4.1641	4.2573	4.2489	0.0932	0.0111	-0.0111	0.0932	0.0000	0.1901
C4-H22	1	4.1705	4.2261	4.2196	0.0556	0.0097	-0.0154	0.0613	0.0000	0.1659
N1-H25	1	4.1791	4.1979	4.1692	0.0189	0.0363	-0.0340	0.0166	0.0000	0.3443
C5-H19	1	4.1880	4.1690	4.1629	-0.0191	0.0360	-0.0650	0.0099	0.0000	0.1586
H12-H22	1	4.2148	4.1573	4.1306	-0.0575	0.0479	-0.0361	-0.0693	0.0000	0.3233
N2-H23	1	4.2384	4.3164	4.3087	0.0779	0.0208	-0.0420	0.0992	-0.0001	0.1820
H13-H15	1	4.2405	4.2748	4.2629	0.0343	0.0169	-0.0210	0.0384	0.0000	0.2252
H15-H18	1	4.2541	4.3355	4.3269	0.0814	0.0206	-0.0363	0.0970	0.0001	0.1922
H14-H19	1	4.2940	4.4036	4.3730	0.1097	0.0280	-0.0416	0.1233	0.0000	0.3662
H12-H14	1	4.3289	4.3763	4.3561	0.0475	0.0319	-0.0259	0.0414	0.0001	0.2956
H14-H24	1	4.3464	4.4082	4.3859	0.0618	0.0217	-0.0362	0.0763	0.0000	0.3116
C8-H12	1	4.3479	4.2904	4.2659	-0.0576	0.0265	-0.0354	-0.0487	0.0000	0.3184
H19-H22	1	4.3746	4.6789	4.5882	0.3043	0.0334	-0.0592	0.3301	0.0000	0.6538
C5-H25	1	4.3797	4.3849	4.3822	0.0052	0.0177	-0.0464	0.0340	-0.0001	0.1073
C7-H14	1	4.3864	4.4180	4.4090	0.0317	0.0258	-0.0428	0.0487	0.0000	0.1987
H14-H25	1	4.3874	4.4254	4.3977	0.0380	0.0321	-0.0309	0.0368	0.0000	0.3461
C5-H11	1	4.4066	4.5470	4.5206	0.1404	0.0355	0.0014	0.1035	0.0000	0.3462
C4-H13	1	4.4171	4.4778	4.4743	0.0607	0.0101	-0.0378	0.0884	0.0000	0.1257
C4-C9	1	4.4366	4.4304	4.4240	-0.0062	0.0270	-0.0419	0.0087	0.0000	0.1672
H11-H14	1	4.4382	4.4224	4.4199	-0.0158	0.0114	-0.0347	0.0076	-0.0001	0.1052
H12-H13	1	4.4419	4.5876	4.5605	0.1458	0.0449	0.0118	0.0891	0.0000	0.3522
C9-H14	1	4.4469	4.5323	4.5186	0.0853	0.0387	-0.0141	0.0607	0.0000	0.2489
H14-H15	1	4.4594	4.5606	4.5481	0.1012	0.0341	-0.0174	0.0846	-0.0001	0.2387
H11-H20	1	4.4741	4.5083	4.4987	0.0343	0.0131	-0.0190	0.0402	0.0000	0.2074
C6-C7	1	4.4931	4.5283	4.5251	0.0352	0.0218	-0.0500	0.0633	0.0001	0.1204
H15-H17	1	4.4969	4.4170	4.3833	-0.0799	0.0275	-0.0325	-0.0750	0.0001	0.3776
H12-H23	1	4.5044	4.5748	4.5655	0.0704	0.0278	-0.0447	0.0873	0.0000	0.2068
H14-H16	1	4.5118	4.5386	4.5354	0.0268	0.0181	-0.0423	0.0510	0.0000	0.1217
H13-H18	1	4.5129	4.5269	4.5241	0.0140	0.0167	-0.0352	0.0325	0.0000	0.1117
C5-H16	1	4.5200	4.5353	4.5324	0.0153	0.0145	-0.0407	0.0415	0.0000	0.1136
C3-H21	1	4.5428	4.4708	4.4568	-0.0720	0.0169	-0.0297	-0.0592	0.0000	0.2444
C7-H10	1	4.5708	4.5758	4.5730	0.0050	0.0216	-0.0497	0.0331	0.0000	0.1133
H10-H22	1	4.6104	4.7646	4.7461	0.1542	0.0275	-0.0621	0.1887	0.0001	0.2961
H10-H21	1	4.6125	4.7814	4.7585	0.1689	0.0313	-0.0439	0.1815	0.0000	0.3314
C3-H17	1	4.6126	4.5659	4.5565	-0.0466	0.0233	-0.0593	-0.0106	0.0000	0.2053
C4-H24	1	4.6176	4.5777	4.5691	-0.0399	0.0305	-0.0342	-0.0362	0.0000	0.1963
C9-H11	1	4.6534	4.8476	4.8221	0.1942	0.0351	-0.0231	0.1822	0.0000	0.3530

H10-H19	1	4.6690	4.5991	4.5852	-0.0699	0.0275	-0.0560	-0.0414	0.0000	0.2474
C6-H18	1	4.6764	4.6772	4.6673	0.0008	0.0305	-0.0585	0.0289	-0.0001	0.2139
N1-H23	1	4.6767	4.6182	4.5978	-0.0585	0.0293	-0.0373	-0.0505	0.0000	0.3044
H10-H18	1	4.6824	4.7149	4.7058	0.0325	0.0319	-0.0638	0.0644	0.0000	0.2066
H12-H25	1	4.7171	4.8068	4.7887	0.0897	0.0109	-0.0550	0.1339	-0.0001	0.2952
H13-H16	1	4.7192	4.7517	4.7490	0.0324	0.0171	-0.0458	0.0611	0.0000	0.1118
H15-H19	1	4.7340	4.7573	4.7491	0.0233	0.0476	-0.0785	0.0542	0.0000	0.1978
C7-H16	1	4.7821	4.6659	4.6119	-0.1161	0.0373	-0.0089	-0.1445	0.0000	0.4901
H17-H22	1	4.7868	4.8478	4.8394	0.0610	0.0462	-0.0705	0.0853	0.0000	0.2018
H19-H21	1	4.7917	4.8904	4.8703	0.0987	0.0272	-0.0214	0.0929	0.0000	0.3138
C7-H21	1	4.7936	4.6887	4.6735	-0.1049	0.0161	-0.0513	-0.0696	-0.0001	0.2599
C8-H17	1	4.8045	4.7285	4.6980	-0.0761	0.0256	-0.0106	-0.0911	0.0000	0.3741
C8-H11	1	4.8166	4.8328	4.8313	0.0162	0.0073	-0.0261	0.0351	-0.0001	0.0852
C6-C8	1	4.8280	4.9119	4.9023	0.0839	0.0149	-0.0193	0.0884	-0.0001	0.2176
H13-H23	1	4.9564	5.1865	5.1349	0.2301	0.0320	-0.0359	0.2340	0.0000	0.5246
C7-H13	1	4.9919	5.0021	4.9943	0.0102	0.0204	-0.0418	0.0316	0.0000	0.1976
H22-H24	1	5.0052	4.9736	4.9649	-0.0316	0.0188	-0.0459	-0.0045	0.0000	0.2063
C4-H25	1	5.0054	4.9939	4.9902	-0.0116	0.0302	-0.0817	0.0399	0.0000	0.1345
H15-H22	1	5.0209	5.0286	5.0246	0.0077	0.0278	-0.0738	0.0537	0.0000	0.1405
C6-H19	1	5.0409	5.0425	5.0371	0.0016	0.0181	-0.0430	0.0265	0.0000	0.1637
C4-H21	1	5.0415	5.1278	5.1140	0.0864	0.0270	-0.0289	0.0882	0.0001	0.2655
C8-H15	1	5.0422	5.2462	5.2035	0.2040	0.0289	-0.0389	0.2140	0.0000	0.4734
C8-H24	1	5.0617	5.1342	5.1286	0.0725	0.0151	-0.0439	0.1013	0.0000	0.1688
C6-H17	1	5.0724	5.2130	5.1961	0.1406	0.0216	-0.0233	0.1423	0.0000	0.2985
C4-H23	1	5.0740	5.1701	5.1614	0.0961	0.0207	-0.0602	0.1355	0.0001	0.2122
C5-H17	1	5.0782	5.1199	5.1135	0.0418	0.0185	-0.0399	0.0631	0.0001	0.1812
H11-H24	1	5.0874	5.2244	5.2077	0.1369	0.0208	-0.0288	0.1449	0.0000	0.2962
C6-H22	1	5.0908	5.1989	5.1892	0.1082	0.0171	-0.0408	0.1319	0.0000	0.2255
C6-H20	1	5.1349	5.2928	5.2700	0.1579	0.0273	-0.0969	0.2274	0.0001	0.3461
H15-H20	1	5.2065	5.2521	5.2463	0.0456	0.0162	-0.0465	0.0759	0.0000	0.1756
H11-H25	1	5.2159	5.2917	5.2849	0.0758	0.0166	-0.0433	0.1025	0.0000	0.1886
H11-H23	1	5.2270	5.2230	5.2064	-0.0040	0.0307	-0.0900	0.0553	0.0000	0.2933
H11-H22	1	5.2385	5.0841	5.0670	-0.1543	0.0308	-0.0902	-0.0950	0.0001	0.2864
C5-H23	1	5.2542	5.3726	5.3495	0.1183	0.0131	-0.0519	0.1571	0.0000	0.3519
H11-H13	1	5.2618	5.2172	5.2001	-0.0447	0.0317	-0.0794	0.0031	-0.0001	0.2948
H13-H19	1	5.3107	5.3025	5.2992	-0.0082	0.0274	-0.0713	0.0357	0.0000	0.1330
H16-H19	1	5.3184	5.2077	5.1857	-0.1107	0.0189	-0.0518	-0.0778	0.0000	0.3301
H16-H18	1	5.3216	5.3473	5.3375	0.0257	0.0225	-0.0551	0.0583	0.0000	0.2277
H16-H17	1	5.3282	5.4365	5.4111	0.1083	0.0295	-0.0759	0.1547	0.0000	0.3706
H12-H21	1	5.3409	5.2701	5.2582	-0.0708	0.0086	-0.0335	-0.0459	0.0000	0.2477
H14-H17	1	5.3657	5.4403	5.4217	0.0746	0.0292	-0.0869	0.1322	0.0001	0.3168
H10-H17	1	5.4425	5.4593	5.4561	0.0167	0.0210	-0.0624	0.0581	0.0000	0.1324
C8-C9	1	5.4480	5.3438	5.3192	-0.1041	0.0194	-0.0446	-0.0790	0.0001	0.3569
H14-H23	1	5.4499	5.3970	5.3696	-0.0529	0.0302	-0.0163	-0.0668	0.0000	0.3806
C9-H22	1	5.4798	5.4010	5.3752	-0.0788	0.0326	-0.0534	-0.0580	0.0000	0.3679

H20-H24	1	5.5538	5.5767	5.5687	0.0229	0.0175	-0.0520	0.0574	0.0000	0.2102
H18-H24	1	5.6190	5.5397	5.5285	-0.0793	0.0216	-0.0625	-0.0385	0.0001	0.2451
H21-H24	1	5.6338	5.5203	5.4935	-0.1136	0.0194	-0.0689	-0.0640	-0.0001	0.3768
C8-H16	1	5.6451	5.7486	5.7006	0.1036	0.0369	-0.0575	0.1241	0.0001	0.5132
C8-H25	1	5.6508	5.6773	5.6747	0.0265	0.0143	-0.0605	0.0727	0.0000	0.1214
C7-C9	1	5.6802	5.6914	5.6890	0.0113	0.0129	-0.0475	0.0458	0.0001	0.1172
C7-H24	1	5.7771	5.7969	5.7921	0.0198	0.0100	-0.0647	0.0745	0.0000	0.1644
H16-H20	1	5.7774	5.8524	5.8424	0.0750	0.0231	-0.0637	0.1156	0.0000	0.2408
C6-H21	1	5.7951	5.8730	5.8643	0.0779	0.0190	-0.0485	0.1074	0.0000	0.2261
H17-H21	1	5.8005	5.9155	5.8924	0.1150	0.0240	-0.0738	0.1648	0.0000	0.3658
C9-H18	1	5.8266	5.8200	5.7994	-0.0066	0.0231	-0.0704	0.0406	0.0001	0.3384
H11-H21	1	5.8633	5.8157	5.8059	-0.0475	0.0178	-0.0620	-0.0034	0.0001	0.2377
H13-H17	1	5.9114	5.7493	5.7106	-0.1620	0.0279	-0.0923	-0.0976	0.0000	0.4596
C9-H20	1	5.9224	5.9438	5.9363	0.0214	0.0232	-0.0814	0.0796	0.0000	0.2099
H16-H21	1	6.0452	5.9799	5.9670	-0.0653	0.0134	-0.0450	-0.0337	0.0000	0.2743
H22-H25	1	6.0573	6.1517	6.1428	0.0943	0.0244	-0.0872	0.1572	-0.0001	0.2333
H16-H22	1	6.0894	6.2009	6.1851	0.1115	0.0231	-0.0622	0.1506	0.0000	0.3132
C9-H21	1	6.1002	6.1929	6.1845	0.0927	0.0210	-0.0697	0.1414	0.0000	0.2282
H20-H25	1	6.1725	6.1042	6.0861	-0.0684	0.0287	-0.0968	-0.0003	0.0000	0.3280
H21-H25	1	6.2052	6.0918	6.0609	-0.1134	0.0214	-0.0692	-0.0656	0.0000	0.4261
C7-H25	1	6.3149	6.2433	6.2324	-0.0716	0.0126	-0.0624	-0.0218	0.0000	0.2579
C9-H19	1	6.3178	6.2159	6.1916	-0.1020	0.0208	-0.0659	-0.0568	-0.0001	0.3825
C9-H17	1	6.3713	6.3293	6.3245	-0.0420	0.0238	-0.1070	0.0413	-0.0001	0.1728
C7-H23	1	6.3848	6.3925	6.3884	0.0078	0.0205	-0.1027	0.0899	0.0001	0.1614
H17-H24	1	6.4076	6.4475	6.4407	0.0400	0.0144	-0.0787	0.1043	0.0000	0.2089
H19-H24	1	6.4469	6.4000	6.3814	-0.0469	0.0358	-0.1166	0.0339	0.0000	0.3385
H18-H25	1	6.4550	6.4802	6.4743	0.0252	0.0125	-0.0757	0.0884	0.0000	0.1943
C8-H23	1	6.4598	6.6031	6.5775	0.1433	0.0264	-0.0914	0.2083	0.0000	0.4079
H22-H23	1	6.4685	6.5441	6.5270	0.0756	0.0336	-0.1178	0.1598	0.0000	0.3315
H18-H23	1	6.5082	6.5167	6.5135	0.0085	0.0181	-0.0817	0.0720	0.0001	0.1431
H16-H21	1	6.5583	6.5420	6.5211	-0.0163	0.0239	-0.0869	0.0467	0.0000	0.3619
H19-H25	1	6.8259	6.7776	6.7683	-0.0483	0.0196	-0.0872	0.0193	0.0000	0.2499
H17-H23	1	6.8362	6.7832	6.7766	-0.0530	0.0318	-0.1318	0.0469	0.0001	0.2103
H20-H23	1	6.9541	7.0073	6.9980	0.0533	0.0158	-0.0804	0.1179	0.0000	0.2541
H17-H25	1	7.0523	6.9777	6.9655	-0.0746	0.0156	-0.0785	-0.0118	0.0001	0.2884
H19-H23	1	7.0980	7.0624	7.0573	-0.0356	0.0258	-0.1271	0.0657	0.0000	0.1896
H21-H23	1	7.1366	7.1512	7.1466	0.0146	0.0207	-0.1179	0.1118	0.0000	0.1818

Table S12. Equilibrium (r_e) and thermal average (r_g , r_a) distances, vibrational corrections (Δ), and mean amplitudes (u) for internuclear distances of TEDA conformation **1d** (in Å), obtained for 291 K by GED refinement (initial approximation MP2/cc-PVTZ). n – number of equivalent parameters.

Atomic pair	n	r_e	r_g	r_a	Δr	$\Delta r(\text{har})$	$\Delta r(\text{kin})$	$\Delta r(\text{dyn})$	$\Delta r(\text{rot})$	u
C6-H15	1	1.0897	1.1114	1.1079	0.0216	0.0420	-0.0373	0.0169	0.0000	0.0621
C7-H19	1	1.0909	1.1143	1.1112	0.0233	0.0523	-0.0473	0.0184	-0.0001	0.0587
C8-H20	1	1.0910	1.1138	1.1106	0.0229	0.0506	-0.0458	0.0180	0.0001	0.0599
C9-H23	1	1.0912	1.1125	1.1088	0.0214	0.0422	-0.0377	0.0169	0.0000	0.0645
C8-H22	1	1.0914	1.1146	1.1117	0.0232	0.0546	-0.0495	0.0182	-0.0001	0.0576
C7-H18	1	1.0915	1.1135	1.1098	0.0220	0.0417	-0.0373	0.0176	0.0000	0.0647
C8-H21	1	1.0916	1.1157	1.1143	0.0242	0.0660	-0.0598	0.0179	0.0001	0.0413
C9-H24	1	1.0916	1.1133	1.1094	0.0217	0.0396	-0.0354	0.0174	0.0001	0.0665
C7-H17	1	1.0917	1.1151	1.1118	0.0233	0.0504	-0.0456	0.0185	0.0000	0.0602
C3-H10	1	1.0918	1.1134	1.1083	0.0216	0.0160	-0.0121	0.0177	0.0000	0.0754
C9-H25	1	1.0927	1.1170	1.1155	0.0243	0.0644	-0.0583	0.0181	0.0001	0.0416
C4-H12	1	1.0929	1.1149	1.1102	0.0220	0.0269	-0.0228	0.0178	0.0001	0.0727
C4-H11	1	1.0936	1.1156	1.1108	0.0219	0.0264	-0.0223	0.0179	-0.0001	0.0729
C5-H13	1	1.0946	1.1173	1.1136	0.0226	0.0423	-0.0376	0.0179	0.0000	0.0639
C6-H16	1	1.0948	1.1169	1.1126	0.0221	0.0338	-0.0294	0.0177	0.0000	0.0696
C5-H14	1	1.0974	1.1196	1.1151	0.0222	0.0315	-0.0272	0.0178	0.0001	0.0710
N2-C3	1	1.4209	1.4314	1.4298	0.0106	0.0051	-0.0036	0.0091	0.0000	0.0488
N1-C3	1	1.4296	1.4376	1.4359	0.0080	0.0055	-0.0039	0.0064	0.0000	0.0494
N1-C4	1	1.4388	1.4492	1.4476	0.0105	0.0051	-0.0032	0.0086	0.0000	0.0490
N2-C5	1	1.4393	1.4504	1.4488	0.0111	0.0058	-0.0040	0.0093	0.0000	0.0491
N1-N2	1	1.4832	1.4952	1.4933	0.0121	0.0051	-0.0046	0.0115	0.0001	0.0543
C3-C6	1	1.4989	1.5105	1.5089	0.0115	0.0065	-0.0051	0.0102	-0.0001	0.0493
C5-C8	1	1.5120	1.5256	1.5244	0.0136	0.0260	-0.0245	0.0121	0.0000	0.0422
C4-C7	1	1.5148	1.5284	1.5270	0.0136	0.0200	-0.0187	0.0122	0.0001	0.0461
C6-C9	1	1.5227	1.5370	1.5361	0.0143	0.0325	-0.0308	0.0126	0.0000	0.0373
H23-H25	1	1.7655	1.7955	1.7911	0.0300	0.0829	-0.0810	0.0281	0.0000	0.0889
H24-H25	1	1.7676	1.7972	1.7918	0.0296	0.0802	-0.0790	0.0284	0.0000	0.0978
H23-H24	1	1.7685	1.7969	1.7913	0.0284	0.0714	-0.0705	0.0274	0.0001	0.1004
H17-H18	1	1.7686	1.7981	1.7956	0.0296	0.1032	-0.0997	0.0261	0.0000	0.0682
H20-H21	1	1.7701	1.7973	1.7930	0.0272	0.0852	-0.0830	0.0250	0.0000	0.0872
H18-H19	1	1.7710	1.7994	1.7936	0.0284	0.0726	-0.0717	0.0275	0.0000	0.1017
H20-H22	1	1.7718	1.7999	1.7942	0.0281	0.0713	-0.0704	0.0272	0.0000	0.1003
H21-H22	1	1.7718	1.8010	1.7960	0.0292	0.0847	-0.0832	0.0277	0.0000	0.0951
H17-H19	1	1.7737	1.8007	1.7948	0.0271	0.0683	-0.0674	0.0262	0.0000	0.1027
H15-H16	1	1.7801	1.8083	1.8008	0.0281	0.0385	-0.0358	0.0255	-0.0001	0.1158
H11-H12	1	1.7854	1.8132	1.8073	0.0278	0.0629	-0.0593	0.0241	0.0001	0.1032
H13-H14	1	1.8005	1.8281	1.8211	0.0276	0.0479	-0.0447	0.0243	0.0001	0.1122
H12-H15	1	1.9478	2.0338	2.0108	0.0860	0.0541	0.0350	-0.0031	0.0000	0.2156

N2-H13	1	2.0084	2.0274	2.0222	0.0189	0.0181	-0.0204	0.0212	0.0000	0.1022
N1-H11	1	2.0158	2.0371	2.0318	0.0212	0.0244	-0.0263	0.0231	0.0000	0.1033
N2-H14	1	2.0661	2.0880	2.0831	0.0219	0.0205	-0.0222	0.0236	0.0000	0.1007
N1-H12	1	2.0836	2.1083	2.1033	0.0247	0.0169	-0.0187	0.0265	0.0000	0.1027
N1-H10	1	2.0946	2.1123	2.1075	0.0178	0.0114	-0.0157	0.0220	0.0001	0.1014
C3-H16	1	2.0987	2.1165	2.1113	0.0178	0.0300	-0.0323	0.0202	-0.0001	0.1052
C3-H15	1	2.1129	2.1327	2.1279	0.0198	0.0288	-0.0310	0.0221	-0.0001	0.1010
N2-H10	1	2.1357	2.1594	2.1547	0.0236	0.0118	-0.0157	0.0275	0.0000	0.1000
C5-H20	1	2.1419	2.1666	2.1630	0.0247	0.0576	-0.0592	0.0264	-0.0001	0.0888
C7-H12	1	2.1509	2.1752	2.1724	0.0244	0.0597	-0.0605	0.0251	0.0001	0.0776
C4-H18	1	2.1509	2.1785	2.1746	0.0276	0.0571	-0.0587	0.0293	-0.0001	0.0926
C9-H15	1	2.1520	2.1741	2.1701	0.0221	0.0481	-0.0499	0.0239	0.0000	0.0934
C5-H22	1	2.1551	2.1789	2.1741	0.0237	0.0343	-0.0359	0.0253	0.0000	0.1016
C4-H19	1	2.1559	2.1839	2.1808	0.0280	0.0742	-0.0751	0.0289	0.0000	0.0824
C8-H14	1	2.1566	2.1792	2.1751	0.0225	0.0451	-0.0460	0.0234	0.0000	0.0940
C7-H11	1	2.1569	2.1807	2.1757	0.0238	0.0331	-0.0348	0.0255	0.0000	0.1042
C5-H21	1	2.1588	2.1810	2.1762	0.0222	0.0363	-0.0378	0.0238	-0.0001	0.1023
C6-H24	1	2.1603	2.1869	2.1835	0.0266	0.0604	-0.0615	0.0276	0.0001	0.0858
C4-H17	1	2.1603	2.1871	2.1826	0.0267	0.0476	-0.0495	0.0287	-0.0001	0.0987
C8-H13	1	2.1616	2.1852	2.1813	0.0236	0.0455	-0.0463	0.0244	0.0000	0.0921
C9-H16	1	2.1689	2.1928	2.1909	0.0239	0.0735	-0.0735	0.0239	0.0000	0.0653
H10-H14	1	2.1708	2.1941	2.1898	0.0233	0.0338	-0.0347	0.0242	0.0000	0.0975
C6-H25	1	2.1714	2.2115	2.1919	0.0401	0.0234	-0.0037	0.0205	-0.0001	0.2071
C6-H23	1	2.1722	2.1983	2.1935	0.0261	0.0367	-0.0382	0.0276	0.0000	0.1018
C6-H10	1	2.1808	2.1987	2.1940	0.0179	0.0125	-0.0135	0.0189	0.0000	0.1014
N1-C5	1	2.3812	2.3940	2.3920	0.0128	0.0052	-0.0068	0.0144	0.0000	0.0696
N2-C4	1	2.4123	2.4333	2.4312	0.0210	0.0045	-0.0063	0.0228	0.0000	0.0710
C5-C3	1	2.4213	2.4414	2.4396	0.0201	0.0050	-0.0056	0.0206	0.0001	0.0671
N1-H14	1	2.4240	2.4587	2.4480	0.0347	0.0149	-0.0109	0.0307	0.0000	0.1617
N1-C7	1	2.4398	2.4531	2.4512	0.0133	0.0152	-0.0152	0.0133	0.0000	0.0686
N2-H12	1	2.4446	2.4634	2.4616	0.0189	0.0180	-0.0185	0.0194	0.0000	0.0671
N2-C8	1	2.4477	2.5070	2.4967	0.0594	0.0145	-0.0107	0.0556	0.0000	0.1603
C4-C3	1	2.4614	2.4813	2.4796	0.0198	0.0056	-0.0060	0.0203	-0.0001	0.0649
H12-H18	1	2.4626	2.5212	2.5058	0.0586	0.0308	-0.0312	0.0590	0.0000	0.1962
C3-H14	1	2.4705	2.4992	2.4912	0.0287	0.0173	-0.0094	0.0209	-0.0001	0.1413
H14-H20	1	2.4774	2.5211	2.5099	0.0437	0.0634	-0.0639	0.0442	0.0000	0.1674
H15-H24	1	2.4812	2.5038	2.4929	0.0226	0.0844	-0.0838	0.0220	0.0000	0.1639
H11-H19	1	2.4961	2.5218	2.5107	0.0257	0.0641	-0.0638	0.0254	0.0000	0.1662
H10-H16	1	2.4961	2.5198	2.5076	0.0237	0.0417	-0.0392	0.0212	0.0000	0.1741
H13-H22	1	2.4988	2.5391	2.5273	0.0403	0.0513	-0.0518	0.0408	0.0000	0.1722
H12-H17	1	2.5000	2.5204	2.5185	0.0204	0.0064	-0.0061	0.0202	-0.0001	0.0700
C3-C9	1	2.5028	2.5218	2.5197	0.0190	0.0179	-0.0191	0.0202	0.0000	0.0728
H11-H17	1	2.5104	2.5374	2.5252	0.0270	0.0510	-0.0502	0.0262	0.0000	0.1750
H15-H23	1	2.5106	2.5601	2.5478	0.0495	0.0546	-0.0541	0.0490	0.0000	0.1765
N2-C6	1	2.5115	2.5608	2.5512	0.0493	0.0841	-0.0839	0.0491	0.0000	0.1556

H13-H21	1	2.5124	2.5296	2.5182	0.0171	0.0506	-0.0484	0.0149	0.0000	0.1679
H16-H25	1	2.5142	2.5383	2.5273	0.0241	0.0563	-0.0540	0.0218	0.0000	0.1654
H14-H21	1	2.5238	2.5646	2.5522	0.0409	0.0475	-0.0463	0.0396	0.0001	0.1774
H16-H23	1	2.5311	2.5727	2.5595	0.0417	0.0397	-0.0383	0.0403	0.0000	0.1833
H18-H20	1	2.5409	2.5743	2.5664	0.0334	0.0097	-0.0128	0.0365	0.0000	0.1431
C5-H10	1	2.5787	2.6708	2.6186	0.0922	0.0494	0.0377	0.0051	0.0000	0.3692
C3-H12	1	2.5975	2.6187	2.6112	0.0213	0.0142	-0.0098	0.0168	0.0001	0.1400
H10-H25	1	2.6089	2.6205	2.6188	0.0116	0.0066	-0.0045	0.0094	0.0001	0.0659
N1-C6	1	2.6114	2.7119	2.6974	0.1005	0.0299	0.0068	0.0637	0.0001	0.1988
N2-H15	1	2.6436	2.6196	2.5965	-0.0240	0.0522	-0.0183	-0.0578	-0.0001	0.2426
C4-H15	1	2.6572	2.6549	2.6444	-0.0023	0.0231	-0.0141	-0.0113	0.0000	0.1661
C6-H12	1	2.6633	2.6715	2.6608	0.0081	0.0374	-0.0352	0.0059	0.0000	0.1677
N1-H19	1	2.6689	2.6773	2.6661	0.0084	0.0152	0.0068	-0.0135	-0.0001	0.1725
N2-H22	1	2.6940	2.7410	2.7310	0.0470	0.0430	-0.0428	0.0467	0.0001	0.1649
N1-H18	1	2.7170	2.7317	2.7220	0.0146	0.0415	-0.0418	0.0150	-0.0001	0.1619
N2-H20	1	2.7465	2.7971	2.7889	0.0507	0.0265	-0.0137	0.0379	0.0000	0.1513
C3-H24	1	2.7552	2.7940	2.7839	0.0387	0.0356	-0.0349	0.0380	0.0000	0.1670
C3-H25	1	2.7583	2.7659	2.7561	0.0076	0.0495	-0.0480	0.0062	-0.0001	0.1631
N1-H15	1	2.7615	2.8122	2.8025	0.0506	0.0484	-0.0486	0.0508	0.0000	0.1647
C9-H10	1	2.7838	3.0551	2.9770	0.2713	0.0391	-0.0123	0.2445	0.0000	0.4813
C3-H11	1	2.8266	2.8153	2.8067	-0.0113	0.0112	-0.0165	-0.0060	0.0000	0.1546
C3-H13	1	2.8298	2.8090	2.7985	-0.0209	0.0173	-0.0144	-0.0237	-0.0001	0.1708
H10-H13	1	2.8643	2.8662	2.8431	0.0020	0.0346	-0.0178	-0.0148	0.0000	0.2558
N1-H20	1	2.8709	2.9106	2.9018	0.0397	0.0156	-0.0221	0.0462	0.0000	0.1601
H11-H15	1	2.8865	2.9435	2.9230	0.0570	0.0160	-0.0232	0.0641	0.0001	0.2437
C4-C6	1	2.9391	3.0961	3.0699	0.1570	0.0400	-0.0195	0.1365	0.0000	0.2854
N1-H16	1	2.9619	3.1255	3.0931	0.1637	0.0306	0.0028	0.1302	0.0001	0.3206
N2-H24	1	2.9723	2.9707	2.9332	-0.0016	0.0420	0.0207	-0.0644	0.0001	0.3303
N2-H18	1	2.9942	3.0194	3.0165	0.0253	0.0074	-0.0017	0.0195	0.0001	0.0939
H19-H20	1	3.0555	3.0746	3.0701	0.0191	0.0264	-0.0462	0.0389	0.0000	0.1179
H18-H22	1	3.0598	3.0871	3.0844	0.0272	0.0752	-0.0903	0.0423	0.0000	0.0918
H12-H19	1	3.0635	3.0926	3.0896	0.0292	0.0730	-0.0882	0.0444	0.0000	0.0965
H10-H15	1	3.0636	3.0955	3.0942	0.0318	0.1011	-0.1156	0.0463	0.0000	0.0631
H13-H20	1	3.0647	3.0910	3.0906	0.0264	0.0991	-0.1132	0.0405	0.0000	0.0364
H11-H18	1	3.0648	3.0317	3.0244	-0.0331	0.0216	-0.0219	-0.0327	-0.0001	0.1467
H14-H22	1	3.0664	3.0944	3.0904	0.0279	0.0584	-0.0752	0.0448	-0.0001	0.1104
H15-H25	1	3.0713	3.0950	3.0915	0.0237	0.0579	-0.0745	0.0403	0.0000	0.1044
H16-H24	1	3.0792	3.1882	3.1713	0.1090	0.0313	-0.0170	0.0947	0.0000	0.2324
H11-H16	1	3.1249	3.1236	3.1163	-0.0013	0.0132	-0.0176	0.0031	0.0000	0.1508
H10-H24	1	3.1885	3.3921	3.3548	0.2037	0.0266	-0.0106	0.1877	0.0000	0.3553
H12-H16	1	3.1945	3.2828	3.2736	0.0883	0.0133	-0.0165	0.0916	-0.0001	0.1743
C7-H20	1	3.1962	3.1822	3.1592	-0.0140	0.0384	-0.0481	-0.0043	0.0000	0.2660
C6-H11	1	3.2296	3.1199	3.0877	-0.1097	0.0148	-0.0122	-0.1123	0.0000	0.3070
N1-C8	1	3.2504	3.3077	3.3025	0.0572	0.0128	-0.0167	0.0611	0.0000	0.1307
C8-H18	1	3.2588	3.2802	3.2767	0.0214	0.0170	-0.0325	0.0369	0.0000	0.1072

N2-C7	1	3.2805	3.2884	3.2850	0.0079	0.0128	-0.0245	0.0196	0.0000	0.1055
N2-H11	1	3.3225	3.5085	3.4731	0.1860	0.0476	0.0209	0.1175	0.0000	0.3513
N2-C9	1	3.3511	3.3759	3.3727	0.0248	0.0096	-0.0179	0.0330	0.0001	0.1036
N1-H13	1	3.3676	3.3686	3.3658	0.0010	0.0202	-0.0373	0.0181	0.0000	0.0973
C4-H16	1	3.3703	3.3057	3.2897	-0.0646	0.0153	-0.0125	-0.0674	0.0000	0.2243
H13-H24	1	3.3821	3.3956	3.3929	0.0135	0.0256	-0.0417	0.0295	0.0001	0.0951
C4-H10	1	3.3889	3.3967	3.3689	0.0078	0.0228	0.0010	-0.0159	-0.0001	0.3029
N2-H16	1	3.3898	3.4093	3.4066	0.0195	0.0276	-0.0427	0.0345	0.0001	0.0951
N1-H17	1	3.4546	3.4749	3.4722	0.0203	0.0259	-0.0422	0.0366	0.0000	0.0972
N2-H21	1	3.4920	3.4879	3.4650	-0.0041	0.0262	-0.0022	-0.0282	0.0001	0.2809
C3-H23	1	3.4943	3.5879	3.5755	0.0936	0.0130	-0.0113	0.0919	0.0000	0.2120
C4-C5	1	3.5466	3.5610	3.5593	0.0144	0.0036	-0.0097	0.0204	0.0001	0.0794
C4-H20	1	3.5801	3.6389	3.6283	0.0588	0.0297	-0.0074	0.0365	0.0000	0.1963
H10-H11	1	3.5916	3.6602	3.6363	0.0686	0.0318	-0.0531	0.0899	0.0000	0.2926
C5-H18	1	3.5995	3.6162	3.6002	0.0167	0.0308	-0.0494	0.0352	0.0001	0.2384
N1-H22	1	3.6283	3.5981	3.5777	-0.0302	0.0167	-0.0030	-0.0438	-0.0001	0.2694
H10-H12	1	3.6322	3.6714	3.6558	0.0392	0.0267	-0.0426	0.0551	0.0000	0.2375
N2-H25	1	3.6525	3.6766	3.6701	0.0241	0.0155	-0.0237	0.0323	0.0000	0.1543
C3-C8	1	3.6753	3.6595	3.6514	-0.0158	0.0095	-0.0150	-0.0103	0.0000	0.1725
N2-H19	1	3.6787	3.6892	3.6876	0.0105	0.0125	-0.0238	0.0218	0.0000	0.0771
C5-C6	1	3.6867	3.7816	3.7625	0.0949	0.0290	-0.0149	0.0808	0.0000	0.2684
C3-C7	1	3.7075	3.7380	3.7363	0.0305	0.0054	-0.0107	0.0357	0.0001	0.0780
C5-H24	1	3.7091	3.7442	3.7424	0.0351	0.0102	-0.0219	0.0468	0.0000	0.0808
H10-H23	1	3.7389	3.8899	3.8684	0.1510	0.0306	-0.0028	0.1232	0.0000	0.2890
C5-H12	1	3.7453	3.9734	3.9357	0.2280	0.0346	-0.0153	0.2087	0.0000	0.3866
C4-H14	1	3.7576	3.7267	3.6770	-0.0309	0.0261	-0.0215	-0.0355	0.0000	0.4236
C3-H20	1	3.7874	3.8462	3.8391	0.0587	0.0104	-0.0175	0.0658	0.0000	0.1649
N1-C9	1	3.7942	3.8261	3.8189	0.0320	0.0095	-0.0169	0.0394	0.0000	0.1665
C7-C8	1	3.8065	3.8067	3.7970	0.0002	0.0295	-0.0378	0.0084	0.0001	0.1907
C6-H13	1	3.8221	3.7988	3.7909	-0.0233	0.0256	-0.0433	-0.0057	0.0001	0.1724
C6-H14	1	3.8286	3.8614	3.8593	0.0328	0.0101	-0.0247	0.0473	0.0001	0.0885
C3-H18	1	3.8797	4.0495	3.9952	0.1698	0.0307	-0.0207	0.1599	-0.0001	0.4671
C9-H13	1	3.8799	4.0214	4.0017	0.1414	0.0208	-0.0037	0.1243	0.0000	0.2817
C8-H10	1	3.8954	3.9498	3.9416	0.0543	0.0138	-0.0216	0.0621	0.0000	0.1790
C9-H12	1	3.9004	3.9806	3.9721	0.0802	0.0254	-0.0346	0.0894	0.0000	0.1838
C7-H22	1	3.9011	3.9829	3.9702	0.0817	0.0156	-0.0191	0.0853	-0.0001	0.2232
C8-H19	1	3.9100	3.9390	3.9335	0.0290	0.0138	-0.0170	0.0322	0.0000	0.1467
H13-H25	1	3.9285	4.1025	4.0652	0.1740	0.0331	-0.0353	0.1762	0.0000	0.3855
C4-C8	1	3.9372	3.9863	3.9794	0.0491	0.0144	-0.0221	0.0567	0.0001	0.1651
N1-H24	1	3.9388	3.9370	3.9287	-0.0018	0.0090	-0.0132	0.0024	0.0000	0.1795
C5-C7	1	3.9400	3.9567	3.9512	0.0167	0.0156	-0.0358	0.0370	-0.0001	0.1472
C5-H15	1	3.9476	4.0422	4.0308	0.0946	0.0304	-0.0444	0.1086	0.0000	0.2136
C7-H15	1	3.9707	3.9864	3.9481	0.0157	0.0345	-0.0350	0.0162	0.0000	0.3855
H12-H24	1	3.9862	4.0076	3.9949	0.0214	0.0142	-0.0268	0.0340	0.0000	0.2244
H12-H20	1	4.0006	4.0079	4.0043	0.0074	0.0123	-0.0222	0.0173	0.0000	0.1205

N1-H21	1	4.0055	4.0534	4.0301	0.0478	0.0275	-0.0255	0.0459	-0.0001	0.3046
C3-H19	1	4.0500	4.0434	4.0363	-0.0066	0.0162	-0.0218	-0.0010	0.0000	0.1690
C3-H22	1	4.0539	4.0435	4.0371	-0.0104	0.0225	-0.0436	0.0107	0.0000	0.1603
H14-H18	1	4.0741	4.2424	4.2083	0.1683	0.0367	-0.0589	0.1905	0.0000	0.3767
H17-H20	1	4.0787	4.1126	4.0914	0.0339	0.0255	-0.0384	0.0468	0.0000	0.2928
H18-H21	1	4.0899	4.1228	4.1167	0.0329	0.0291	-0.0498	0.0536	0.0000	0.1590
H10-H20	1	4.0963	4.1173	4.1128	0.0210	0.0150	-0.0365	0.0425	0.0000	0.1360
N2-H17	1	4.1117	4.1183	4.1120	0.0066	0.0240	-0.0437	0.0263	0.0000	0.1600
C5-C9	1	4.1154	4.2090	4.2013	0.0936	0.0100	-0.0119	0.0955	0.0000	0.1807
C4-H22	1	4.1252	4.1327	4.1188	0.0074	0.0309	-0.0517	0.0282	0.0000	0.2373
N1-H25	1	4.1267	4.1464	4.1219	0.0197	0.0217	-0.0350	0.0330	0.0000	0.3164
C5-H19	1	4.1684	4.2526	4.2452	0.0842	0.0213	-0.0431	0.1060	0.0000	0.1775
H12-H22	1	4.1693	4.2405	4.2195	0.0713	0.0242	-0.0494	0.0964	0.0001	0.2958
N2-H23	1	4.1778	4.1786	4.1482	0.0008	0.0260	-0.0227	-0.0025	0.0000	0.3505
H13-H15	1	4.1810	4.2861	4.2581	0.1051	0.0281	-0.0308	0.1077	0.0001	0.3445
H15-H18	1	4.1852	4.1782	4.1715	-0.0070	0.0286	-0.0533	0.0178	-0.0001	0.1673
H14-H19	1	4.2117	4.3027	4.2749	0.0909	0.0235	-0.0343	0.1017	0.0000	0.3423
H12-H14	1	4.2147	4.2706	4.2653	0.0560	0.0212	-0.0443	0.0791	0.0000	0.1509
H14-H24	1	4.2393	4.3039	4.2923	0.0646	0.0142	-0.0232	0.0736	0.0000	0.2226
C8-H12	1	4.2641	4.3210	4.3132	0.0569	0.0153	-0.0322	0.0737	0.0001	0.1836
H19-H22	1	4.2718	4.3436	4.3221	0.0718	0.0304	-0.0276	0.0690	0.0000	0.3038
C5-H25	1	4.2739	4.3761	4.3618	0.1021	0.0206	-0.0328	0.1144	-0.0001	0.2493
C7-H14	1	4.3008	4.3352	4.3096	0.0344	0.0316	-0.0253	0.0281	0.0000	0.3304
H14-H25	1	4.3105	4.2944	4.2809	-0.0160	0.0212	-0.0368	-0.0004	0.0000	0.2398
C5-H11	1	4.3726	4.4326	4.4284	0.0600	0.0090	-0.0298	0.0809	-0.0001	0.1368
C4-H13	1	4.3853	4.4046	4.4018	0.0193	0.0128	-0.0349	0.0414	0.0000	0.1112
C4-C9	1	4.4168	4.4578	4.4484	0.0410	0.0152	-0.0201	0.0459	0.0000	0.2037
H11-H14	1	4.4215	4.4860	4.4767	0.0644	0.0193	-0.0345	0.0796	0.0000	0.2031
H12-H13	1	4.4241	4.5193	4.5048	0.0952	0.0223	-0.0210	0.0939	0.0000	0.2550
C9-H14	1	4.4481	4.3811	4.3686	-0.0671	0.0185	-0.0366	-0.0490	0.0000	0.2296
H14-H15	1	4.4491	4.4591	4.4523	0.0101	0.0235	-0.0383	0.0249	0.0000	0.1743
H11-H20	1	4.4580	4.5882	4.5651	0.1303	0.0222	-0.0257	0.1337	0.0001	0.3275
C6-C7	1	4.4791	4.5225	4.5136	0.0434	0.0251	-0.0360	0.0543	0.0000	0.2003
H15-H17	1	4.4973	4.5261	4.5229	0.0288	0.0162	-0.0407	0.0534	-0.0001	0.1204
H12-H23	1	4.4986	4.6320	4.6133	0.1334	0.0253	-0.0498	0.1579	0.0000	0.2916
H14-H16	1	4.5166	4.5265	4.5237	0.0099	0.0206	-0.0442	0.0335	0.0000	0.1130
H13-H18	1	4.5284	4.5674	4.5641	0.0390	0.0182	-0.0426	0.0634	0.0000	0.1230
C5-H16	1	4.5523	4.5844	4.5781	0.0321	0.0307	-0.0676	0.0690	0.0000	0.1698
C3-H21	1	4.5731	4.5904	4.5822	0.0173	0.0226	-0.0476	0.0423	0.0000	0.1928
C7-H10	1	4.6076	4.5800	4.5714	-0.0276	0.0159	-0.0427	-0.0008	0.0000	0.1977
H10-H22	1	4.6324	4.5863	4.5692	-0.0461	0.0237	-0.0375	-0.0324	0.0001	0.2785
H10-H21	1	4.6779	4.5864	4.5443	-0.0915	0.0278	-0.0014	-0.1179	0.0000	0.4329
C3-H17	1	4.7065	4.7351	4.7251	0.0286	0.0296	-0.0678	0.0669	-0.0001	0.2165
C4-H24	1	4.7077	4.7430	4.7401	0.0352	0.0176	-0.0439	0.0615	0.0000	0.1161
C9-H11	1	4.7280	4.6687	4.6446	-0.0593	0.0185	-0.0082	-0.0695	-0.0001	0.3332

H10-H19	1	4.7386	4.7366	4.7183	-0.0020	0.0220	-0.0192	-0.0048	0.0000	0.2936
C6-H18	1	4.7667	4.8386	4.8289	0.0719	0.0210	-0.0560	0.1069	0.0000	0.2158
N1-H23	1	4.7979	4.8192	4.8112	0.0213	0.0110	-0.0200	0.0303	0.0000	0.1964
H10-H18	1	4.8025	4.8105	4.8090	0.0080	0.0059	-0.0230	0.0252	-0.0001	0.0862
H12-H25	1	4.8296	4.9856	4.9557	0.1560	0.0273	-0.0185	0.1473	-0.0001	0.3876
H13-H16	1	4.8771	5.1504	5.1103	0.2733	0.0358	-0.0075	0.2450	0.0000	0.4562
H15-H19	1	4.9217	5.0459	5.0291	0.1242	0.0258	-0.0414	0.1399	-0.0001	0.2917
C7-H16	1	4.9371	4.9601	4.9587	0.0231	0.0087	-0.0258	0.0401	0.0001	0.0850
H17-H22	1	4.9525	5.1501	5.1275	0.1976	0.0241	-0.0129	0.1864	0.0000	0.3420
H19-H21	1	4.9536	4.9271	4.9189	-0.0264	0.0165	-0.0336	-0.0093	0.0000	0.1997
C7-H21	1	4.9629	5.0259	5.0045	0.0630	0.0339	-0.0475	0.0767	-0.0001	0.3282
C8-H17	1	4.9708	4.9532	4.9461	-0.0176	0.0165	-0.0455	0.0114	0.0000	0.1864
C8-H11	1	4.9831	5.0258	5.0197	0.0427	0.0212	-0.0548	0.0763	0.0000	0.1746
C6-C8	1	4.9900	4.9953	4.9909	0.0053	0.0238	-0.0669	0.0485	-0.0001	0.1475
H13-H23	1	5.0105	5.0950	5.0856	0.0845	0.0105	-0.0430	0.1171	-0.0001	0.2189
C7-H13	1	5.0189	5.0755	5.0617	0.0566	0.0220	-0.0300	0.0646	0.0000	0.2644
H22-H24	1	5.0283	5.1017	5.0954	0.0733	0.0159	-0.0390	0.0965	-0.0001	0.1774
C4-H25	1	5.0389	5.0621	5.0451	0.0232	0.0306	-0.0260	0.0186	0.0000	0.2928
H15-H22	1	5.0400	5.0384	5.0310	-0.0016	0.0190	-0.0233	0.0027	0.0000	0.1917
C6-H19	1	5.0498	5.2128	5.1860	0.1630	0.0367	-0.0753	0.2016	0.0000	0.3712
C4-H21	1	5.0786	5.1319	5.1255	0.0533	0.0172	-0.0370	0.0731	0.0000	0.1819
C8-H15	1	5.1155	5.1160	5.1088	0.0005	0.0208	-0.0387	0.0183	0.0001	0.1914
C8-H24	1	5.1224	5.1752	5.1675	0.0528	0.0208	-0.0411	0.0730	0.0001	0.1994
C6-H17	1	5.1400	5.1393	5.1261	-0.0007	0.0322	-0.0311	-0.0018	0.0000	0.2594
C4-H23	1	5.1744	5.2567	5.2500	0.0824	0.0164	-0.0461	0.1120	0.0001	0.1876
C5-H17	1	5.2637	5.3852	5.3645	0.1215	0.0245	-0.0536	0.1507	-0.0001	0.3320
H11-H24	1	5.2895	5.3358	5.3302	0.0463	0.0117	-0.0459	0.0804	0.0001	0.1722
C6-H22	1	5.2907	5.2502	5.2415	-0.0405	0.0061	-0.0286	-0.0180	0.0000	0.2122
C6-H20	1	5.3210	5.3722	5.3627	0.0512	0.0203	-0.0571	0.0880	0.0000	0.2251
H15-H20	1	5.3691	5.2838	5.2644	-0.0853	0.0144	-0.0334	-0.0663	0.0000	0.3162
H11-H25	1	5.3727	5.3089	5.2853	-0.0638	0.0241	-0.0188	-0.0690	-0.0001	0.3513
H11-H23	1	5.4158	5.5516	5.5348	0.1358	0.0244	-0.0771	0.1886	-0.0001	0.3027
H11-H22	1	5.4174	5.3777	5.3565	-0.0397	0.0266	-0.0469	-0.0194	0.0000	0.3345
C5-H23	1	5.4492	5.5579	5.5498	0.1088	0.0083	-0.0322	0.1326	0.0001	0.2128
H11-H13	1	5.4999	5.5284	5.5206	0.0285	0.0207	-0.0549	0.0628	-0.0001	0.2080
H13-H19	1	5.5038	5.6133	5.5994	0.1095	0.0163	-0.0449	0.1381	0.0000	0.2788
H16-H19	1	5.5319	5.6978	5.6785	0.1659	0.0187	-0.0416	0.1888	0.0000	0.3305
H16-H18	1	5.5412	5.6960	5.6752	0.1549	0.0314	-0.0548	0.1782	0.0001	0.3440
H16-H17	1	5.5564	5.5708	5.5620	0.0145	0.0223	-0.0711	0.0632	0.0001	0.2214
H12-H21	1	5.5932	5.5767	5.5566	-0.0164	0.0146	-0.0549	0.0239	0.0000	0.3325
H14-H17	1	5.6551	5.6820	5.6795	0.0269	0.0114	-0.0483	0.0638	0.0000	0.1176
H10-H17	1	5.6663	5.7557	5.7334	0.0895	0.0166	-0.0611	0.1339	0.0001	0.3552
C8-C9	1	5.6696	5.6740	5.6716	0.0044	0.0124	-0.0465	0.0385	0.0000	0.1170
H14-H23	1	5.6762	5.7172	5.7018	0.0409	0.0180	-0.0766	0.0996	-0.0001	0.2947
C9-H22	1	5.6865	5.8826	5.8609	0.1961	0.0274	-0.0240	0.1927	0.0000	0.3565

H20-H24	1	5.7500	5.7414	5.7388	-0.0086	0.0150	-0.0551	0.0314	0.0001	0.1207
H18-H24	1	5.7532	5.8618	5.8488	0.1086	0.0153	-0.0645	0.1578	0.0000	0.2752
H21-H24	1	5.7683	5.7796	5.7723	0.0114	0.0164	-0.0508	0.0457	0.0001	0.2048
C8-H16	1	5.8016	5.8879	5.8793	0.0863	0.0209	-0.0537	0.1191	0.0000	0.2248
C8-H25	1	5.8096	5.7643	5.7541	-0.0453	0.0253	-0.0574	-0.0132	0.0000	0.2415
C7-C9	1	5.8271	5.8506	5.8483	0.0235	0.0150	-0.0491	0.0576	0.0000	0.1142
C7-H24	1	5.8305	5.8268	5.8185	-0.0037	0.0157	-0.0554	0.0360	0.0000	0.2186
H16-H20	1	5.8435	5.7715	5.7431	-0.0720	0.0212	-0.0714	-0.0218	0.0000	0.3991
C6-H21	1	5.8971	5.9620	5.9536	0.0649	0.0173	-0.0601	0.1078	-0.0001	0.2231
H17-H21	1	5.8985	5.8933	5.8870	-0.0052	0.0241	-0.0840	0.0548	-0.0001	0.1921
C9-H18	1	5.9005	5.8869	5.8794	-0.0137	0.0190	-0.0636	0.0309	0.0000	0.2086
H11-H21	1	5.9040	6.0439	6.0101	0.1399	0.0245	-0.0832	0.1985	0.0001	0.4471
H13-H17	1	5.9888	6.0470	6.0400	0.0582	0.0168	-0.0575	0.0989	0.0000	0.2051
C9-H20	1	5.9958	5.9525	5.9422	-0.0434	0.0118	-0.0437	-0.0115	0.0000	0.2454
H16-H21	1	6.0324	6.0224	6.0158	-0.0100	0.0233	-0.0538	0.0206	-0.0001	0.1985
H22-H25	1	6.0486	6.0568	6.0500	0.0082	0.0233	-0.0766	0.0615	0.0000	0.2027
H16-H22	1	6.0628	6.0335	6.0142	-0.0293	0.0273	-0.0924	0.0358	0.0000	0.3382
C9-H21	1	6.1096	6.1941	6.1779	0.0845	0.0304	-0.1098	0.1639	0.0000	0.3153
H20-H25	1	6.1166	6.2834	6.2605	0.1669	0.0265	-0.0933	0.2337	0.0000	0.3746
H21-H25	1	6.1208	6.2663	6.2469	0.1455	0.0193	-0.0582	0.1844	0.0000	0.3464
C7-H25	1	6.1515	6.1777	6.1625	0.0262	0.0241	-0.0817	0.0838	0.0000	0.3050
C9-H19	1	6.1661	6.1980	6.1814	0.0319	0.0257	-0.0905	0.0968	-0.0001	0.3185
C9-H17	1	6.1661	6.1529	6.1287	-0.0132	0.0181	-0.0593	0.0280	0.0000	0.3830
C7-H23	1	6.2119	6.3245	6.3156	0.1126	0.0133	-0.0471	0.1465	-0.0001	0.2381
H17-H24	1	6.2296	6.1109	6.0898	-0.1187	0.0165	-0.0547	-0.0805	0.0000	0.3542
H19-H24	1	6.2596	6.1921	6.1831	-0.0675	0.0104	-0.0577	-0.0202	0.0000	0.2345
H18-H25	1	6.2632	6.3242	6.3054	0.0610	0.0223	-0.0859	0.1246	0.0000	0.3429
C8-H23	1	6.2894	6.3942	6.3701	0.1048	0.0201	-0.0640	0.1488	-0.0001	0.3899
H22-H23	1	6.4104	6.4388	6.4287	0.0283	0.0245	-0.1010	0.1049	-0.0001	0.2543
H18-H23	1	6.4581	6.6257	6.6068	0.1676	0.0201	-0.0657	0.2131	0.0001	0.3526
H16-H21	1	6.4594	6.5620	6.5542	0.1027	0.0121	-0.0626	0.1532	0.0000	0.2255
H19-H25	1	6.5171	6.5391	6.5360	0.0220	0.0160	-0.0712	0.0772	0.0000	0.1429
H17-H23	1	6.6127	6.6116	6.6082	-0.0011	0.0198	-0.0775	0.0567	-0.0001	0.1487
H20-H23	1	6.7905	6.7626	6.7537	-0.0280	0.0176	-0.0816	0.0361	-0.0001	0.2434
H17-H25	1	6.8841	6.9428	6.9345	0.0587	0.0191	-0.0856	0.1252	0.0000	0.2382
H19-H23	1	6.9956	6.9182	6.9076	-0.0773	0.0141	-0.0767	-0.0148	0.0001	0.2687
H21-H23	1	7.2526	7.3554	7.3468	0.1028	0.0155	-0.0820	0.1693	0.0000	0.2514

Table S13. Equilibrium (r_e) and thermal average (r_g , r_a) distances, vibrational corrections (Δ), and mean amplitudes (u) for internuclear distances of TEDA conformation **1e** (in Å), obtained for 291 K by GED refinement (initial approximation MP2/cc-PVTZ). n – number of equivalent parameters.

Atomic pair	n	r_e	r_g	r_a	Δr	$\Delta r(\text{har})$	$\Delta r(\text{kin})$	$\Delta r(\text{dyn})$	$\Delta r(\text{rot})$	u
C6-H15	1	1.0897	1.1105	1.1062	0.0208	0.0326	-0.0284	0.0165	0.0001	0.0686
C7-H19	1	1.0908	1.1140	1.1109	0.0231	0.0523	-0.0473	0.0182	-0.0001	0.0585
C8-H20	1	1.0908	1.1145	1.1128	0.0237	0.0620	-0.0561	0.0178	0.0000	0.0448
C9-H23	1	1.0911	1.1127	1.1091	0.0216	0.0432	-0.0387	0.0170	0.0001	0.0635
C8-H22	1	1.0913	1.1132	1.1094	0.0219	0.0410	-0.0366	0.0175	0.0000	0.0656
C7-H18	1	1.0914	1.1160	1.1142	0.0246	0.0645	-0.0586	0.0186	0.0001	0.0454
C8-H21	1	1.0917	1.1152	1.1129	0.0235	0.0591	-0.0535	0.0180	-0.0001	0.0514
C9-H24	1	1.0917	1.1135	1.1097	0.0218	0.0407	-0.0364	0.0175	0.0000	0.0656
C7-H17	1	1.0925	1.1156	1.1133	0.0231	0.0592	-0.0535	0.0175	-0.0001	0.0509
C3-H10	1	1.0925	1.1145	1.1094	0.0220	0.0160	-0.0121	0.0181	0.0000	0.0755
C9-H25	1	1.0925	1.1154	1.1125	0.0229	0.0543	-0.0491	0.0178	-0.0001	0.0578
C4-H12	1	1.0927	1.1144	1.1100	0.0217	0.0321	-0.0278	0.0174	0.0000	0.0704
C4-H11	1	1.0937	1.1169	1.1134	0.0232	0.0425	-0.0377	0.0184	0.0000	0.0624
C5-H13	1	1.0945	1.1176	1.1141	0.0231	0.0437	-0.0388	0.0182	0.0000	0.0630
C6-H16	1	1.0950	1.1170	1.1126	0.0220	0.0327	-0.0285	0.0178	0.0000	0.0705
C5-H14	1	1.0971	1.1193	1.1147	0.0222	0.0293	-0.0250	0.0179	0.0000	0.0722
N2-C3	1	1.4202	1.4295	1.4278	0.0093	0.0053	-0.0039	0.0079	0.0000	0.0488
N1-C3	1	1.4300	1.4390	1.4373	0.0090	0.0053	-0.0037	0.0074	0.0000	0.0492
N1-C4	1	1.4384	1.4495	1.4479	0.0112	0.0070	-0.0051	0.0093	0.0000	0.0492
N2-C5	1	1.4395	1.4501	1.4484	0.0106	0.0060	-0.0041	0.0088	-0.0001	0.0491
N1-N2	1	1.4834	1.4957	1.4937	0.0123	0.0053	-0.0047	0.0117	0.0000	0.0540
C3-C6	1	1.4985	1.5087	1.5071	0.0102	0.0047	-0.0034	0.0089	0.0000	0.0493
C5-C8	1	1.5135	1.5277	1.5268	0.0142	0.0317	-0.0300	0.0124	0.0001	0.0364
C4-C7	1	1.5144	1.5280	1.5268	0.0137	0.0250	-0.0236	0.0122	0.0001	0.0430
C6-C9	1	1.5221	1.5368	1.5356	0.0147	0.0266	-0.0251	0.0132	0.0000	0.0425
H23-H25	1	1.7637	1.7920	1.7880	0.0283	0.0943	-0.0918	0.0258	0.0000	0.0839
H24-H25	1	1.7653	1.7939	1.7891	0.0286	0.0807	-0.0791	0.0269	0.0001	0.0925
H23-H24	1	1.7669	1.7950	1.7902	0.0281	0.0791	-0.0775	0.0265	0.0000	0.0929
H17-H18	1	1.7681	1.7960	1.7903	0.0279	0.0742	-0.0732	0.0269	0.0000	0.1003
H20-H21	1	1.7682	1.7968	1.7918	0.0286	0.0847	-0.0831	0.0271	-0.0001	0.0943
H18-H19	1	1.7713	1.8001	1.7972	0.0287	0.1002	-0.0969	0.0255	-0.0001	0.0713
H20-H22	1	1.7714	1.7979	1.7935	0.0266	0.0827	-0.0807	0.0246	0.0000	0.0889
H21-H22	1	1.7716	1.7998	1.7927	0.0281	0.0480	-0.0453	0.0254	0.0000	0.1126
H17-H19	1	1.7720	1.7998	1.7940	0.0277	0.0694	-0.0686	0.0269	0.0000	0.1018
H15-H16	1	1.7749	1.8033	1.7985	0.0284	0.0788	-0.0771	0.0268	-0.0001	0.0933
H11-H12	1	1.7897	1.8178	1.8106	0.0281	0.0450	-0.0419	0.0250	0.0000	0.1138
H13-H14	1	1.7978	1.8291	1.8232	0.0313	0.0645	-0.0606	0.0274	0.0000	0.1038
H12-H15	1	1.9576	2.0574	2.0343	0.0998	0.0634	0.0392	-0.0028	0.0000	0.2176

N2-H13	1	2.0148	2.0460	2.0399	0.0312	0.0319	-0.0343	0.0336	0.0000	0.1115
N1-H11	1	2.0242	2.0436	2.0384	0.0194	0.0234	-0.0256	0.0216	0.0000	0.1025
N2-H14	1	2.0654	2.0894	2.0846	0.0241	0.0190	-0.0209	0.0259	0.0001	0.1004
N1-H12	1	2.0751	2.0959	2.0904	0.0208	0.0196	-0.0226	0.0238	0.0000	0.1069
N1-H10	1	2.0873	2.0992	2.0955	0.0118	0.0306	-0.0313	0.0126	-0.0001	0.0873
C3-H16	1	2.0900	2.1087	2.1040	0.0187	0.0121	-0.0164	0.0230	0.0000	0.0995
C3-H15	1	2.1090	2.1345	2.1291	0.0254	0.0201	-0.0229	0.0282	0.0000	0.1068
N2-H10	1	2.1375	2.1549	2.1501	0.0174	0.0120	-0.0158	0.0212	0.0000	0.1015
C5-H20	1	2.1431	2.1735	2.1696	0.0304	0.0721	-0.0738	0.0320	0.0001	0.0918
C7-H12	1	2.1476	2.1701	2.1677	0.0225	0.0606	-0.0607	0.0226	0.0000	0.0711
C4-H18	1	2.1518	2.1802	2.1783	0.0285	0.0718	-0.0722	0.0289	0.0000	0.0646
C9-H15	1	2.1536	2.1793	2.1753	0.0257	0.0556	-0.0573	0.0274	0.0000	0.0930
C5-H22	1	2.1575	2.1814	2.1766	0.0239	0.0367	-0.0383	0.0254	0.0001	0.1025
C4-H19	1	2.1575	2.1823	2.1785	0.0247	0.0557	-0.0572	0.0262	0.0000	0.0902
C8-H14	1	2.1579	2.1852	2.1813	0.0273	0.0601	-0.0611	0.0282	0.0001	0.0911
C7-H11	1	2.1580	2.1799	2.1753	0.0219	0.0462	-0.0479	0.0236	0.0000	0.1000
C5-H21	1	2.1596	2.1823	2.1774	0.0227	0.0349	-0.0364	0.0242	0.0000	0.1034
C6-H24	1	2.1597	2.1834	2.1793	0.0237	0.0429	-0.0439	0.0247	0.0000	0.0938
C4-H17	1	2.1665	2.1972	2.1932	0.0307	0.0616	-0.0631	0.0322	0.0000	0.0936
C8-H13	1	2.1672	2.1880	2.1853	0.0207	0.0609	-0.0615	0.0213	0.0000	0.0757
C9-H16	1	2.1688	2.1922	2.1888	0.0234	0.0449	-0.0459	0.0244	0.0000	0.0863
H10-H14	1	2.1700	2.1956	2.1908	0.0256	0.0371	-0.0386	0.0272	-0.0001	0.1027
C6-H25	1	2.1709	2.1931	2.1889	0.0222	0.0416	-0.0424	0.0231	-0.0001	0.0968
C6-H23	1	2.1814	2.1933	2.1885	0.0119	0.0105	-0.0116	0.0130	0.0000	0.1023
C6-H10	1	2.1928	2.2212	2.2011	0.0285	0.0210	-0.0062	0.0137	0.0000	0.2109
N1-C5	1	2.3958	2.4096	2.4076	0.0138	0.0069	-0.0088	0.0157	0.0000	0.0691
N2-C4	1	2.3974	2.4236	2.4215	0.0262	0.0057	-0.0071	0.0276	0.0000	0.0707
C5-C3	1	2.4082	2.4247	2.4229	0.0165	0.0056	-0.0064	0.0173	0.0000	0.0663
N1-H14	1	2.4093	2.4619	2.4520	0.0526	0.0161	-0.0104	0.0469	0.0000	0.1564
N1-C7	1	2.4310	2.4481	2.4463	0.0171	0.0175	-0.0181	0.0177	0.0000	0.0659
N2-H12	1	2.4329	2.5292	2.5156	0.0963	0.0216	-0.0225	0.0971	0.0001	0.1849
N2-C8	1	2.4364	2.4523	2.4503	0.0158	0.0182	-0.0184	0.0161	-0.0001	0.0691
C4-C3	1	2.4706	2.5162	2.5033	0.0456	0.0819	-0.0835	0.0471	0.0001	0.1789
H12-H18	1	2.4707	2.4811	2.4794	0.0105	0.0068	-0.0069	0.0105	0.0001	0.0646
C3-H14	1	2.4809	2.5112	2.5030	0.0303	0.0155	-0.0101	0.0250	-0.0001	0.1433
H14-H20	1	2.4818	2.4026	2.3945	-0.0793	0.0273	-0.0157	-0.0908	-0.0001	0.1353
H15-H24	1	2.4923	2.5233	2.5159	0.0310	0.0848	-0.0826	0.0289	-0.0001	0.1351
H11-H19	1	2.4993	2.5158	2.5033	0.0165	0.0552	-0.0538	0.0151	0.0000	0.1760
H10-H16	1	2.5005	2.5248	2.5135	0.0243	0.0614	-0.0612	0.0241	0.0000	0.1676
H13-H22	1	2.5035	2.5372	2.5254	0.0336	0.0510	-0.0485	0.0311	0.0000	0.1718
H12-H17	1	2.5064	2.5492	2.5377	0.0428	0.0599	-0.0597	0.0426	0.0000	0.1703
C3-C9	1	2.5108	2.5539	2.5414	0.0431	0.0466	-0.0451	0.0416	0.0000	0.1774
H11-H17	1	2.5126	2.5372	2.5274	0.0247	0.0676	-0.0664	0.0235	0.0000	0.1565
H15-H23	1	2.5154	2.5571	2.5435	0.0417	0.0655	-0.0660	0.0422	0.0000	0.1856
N2-C6	1	2.5178	2.5641	2.5530	0.0463	0.0541	-0.0527	0.0450	-0.0001	0.1684

H13-H21	1	2.5200	2.5440	2.5420	0.0240	0.0045	-0.0038	0.0233	0.0000	0.0709
H16-H25	1	2.5220	2.5416	2.5334	0.0197	0.0105	-0.0135	0.0227	0.0000	0.1445
H14-H21	1	2.5280	2.5379	2.5360	0.0099	0.0185	-0.0190	0.0104	0.0000	0.0690
H16-H23	1	2.5296	2.5490	2.5372	0.0194	0.0485	-0.0462	0.0171	0.0000	0.1721
H18-H20	1	2.5312	2.5635	2.5505	0.0323	0.0471	-0.0458	0.0310	0.0000	0.1818
C5-H10	1	2.5510	2.7406	2.6898	0.1896	0.0643	0.0397	0.0856	0.0000	0.3864
C3-H12	1	2.5721	2.6434	2.6347	0.0713	0.0281	-0.0157	0.0588	0.0001	0.1509
H10-H25	1	2.5931	2.7754	2.7573	0.1823	0.0275	0.0081	0.1467	0.0000	0.2236
N1-C6	1	2.5936	2.6120	2.6103	0.0184	0.0051	-0.0034	0.0168	-0.0001	0.0660
N2-H15	1	2.6075	2.7119	2.7005	0.1044	0.0170	-0.0094	0.0968	0.0000	0.1752
C4-H15	1	2.6684	2.7192	2.7074	0.0508	0.0471	-0.0479	0.0517	-0.0001	0.1785
C6-H12	1	2.6728	2.5813	2.5605	-0.0914	0.0506	-0.0170	-0.1251	0.0001	0.2284
N1-H19	1	2.6800	2.7192	2.7088	0.0392	0.0430	-0.0422	0.0384	0.0000	0.1675
N2-H22	1	2.7080	2.7196	2.7124	0.0115	0.0492	-0.0482	0.0105	0.0000	0.1388
N1-H18	1	2.7116	2.6318	2.6199	-0.0798	0.0190	0.0076	-0.1065	0.0001	0.1740
N2-H20	1	2.7277	2.7409	2.7311	0.0131	0.0410	-0.0401	0.0122	0.0000	0.1625
C3-H24	1	2.7542	2.8280	2.7861	0.0738	0.0341	-0.0097	0.0495	-0.0001	0.3447
C3-H25	1	2.7744	2.7872	2.7768	0.0128	0.0449	-0.0423	0.0101	0.0001	0.1693
N1-H15	1	2.7893	2.7647	2.7574	-0.0246	0.0161	-0.0087	-0.0320	0.0000	0.1412
C9-H10	1	2.8070	2.8280	2.8181	0.0210	0.0162	-0.0219	0.0267	0.0000	0.1661
C3-H11	1	2.8220	2.8471	2.8393	0.0250	0.0470	-0.0445	0.0226	-0.0001	0.1483
C3-H13	1	2.8556	3.1089	3.0763	0.2533	0.0345	-0.0210	0.2397	0.0001	0.3210
H10-H13	1	2.8630	2.7727	2.7633	-0.0903	0.0187	-0.0169	-0.0920	-0.0001	0.1595
N1-H20	1	2.9313	2.8379	2.8321	-0.0934	0.0238	-0.0273	-0.0899	0.0000	0.1228
H11-H15	1	2.9368	2.8729	2.8646	-0.0639	0.0127	-0.0151	-0.0615	0.0000	0.1520
C4-C6	1	2.9791	3.6689	3.5939	0.6898	0.0368	-0.0193	0.6723	0.0000	0.5526
N1-H16	1	2.9825	3.1393	3.0978	0.1568	0.0504	0.0267	0.0798	-0.0001	0.3591
N2-H24	1	2.9881	3.0101	3.0071	0.0220	0.0071	-0.0014	0.0163	0.0000	0.0940
N2-H18	1	3.0115	3.0533	3.0338	0.0417	0.0325	-0.0185	0.0278	-0.0001	0.2442
H19-H20	1	3.0517	3.0814	3.0765	0.0297	0.0193	-0.0368	0.0472	0.0000	0.1228
H18-H22	1	3.0531	3.4300	3.3903	0.3769	0.0340	0.0002	0.3427	0.0000	0.3807
H12-H19	1	3.0556	3.0853	3.0850	0.0297	0.0987	-0.1122	0.0432	0.0000	0.0291
H10-H15	1	3.0573	3.0920	3.0900	0.0347	0.1003	-0.1148	0.0492	0.0000	0.0775
H13-H20	1	3.0681	3.0949	3.0919	0.0268	0.0715	-0.0869	0.0422	0.0000	0.0963
H11-H18	1	3.0699	3.0982	3.0950	0.0284	0.0780	-0.0950	0.0454	0.0000	0.0996
H14-H22	1	3.0740	3.1011	3.0979	0.0272	0.0687	-0.0843	0.0428	0.0000	0.1006
H15-H25	1	3.0764	3.0979	3.0960	0.0215	0.0761	-0.0923	0.0378	-0.0001	0.0772
H16-H24	1	3.1186	3.2972	3.2876	0.1786	0.0127	-0.0182	0.1841	0.0000	0.1820
H11-H16	1	3.1382	2.7437	2.6856	-0.3946	0.0139	-0.0117	-0.3968	0.0000	0.3723
H10-H24	1	3.1560	3.1948	3.1771	0.0388	0.0154	-0.0209	0.0444	-0.0001	0.2379
H12-H16	1	3.1582	3.3328	3.3124	0.1746	0.0384	-0.0179	0.1541	0.0000	0.2608
C7-H20	1	3.2056	3.2329	3.2270	0.0273	0.0131	-0.0180	0.0322	0.0000	0.1390
C6-H11	1	3.2456	3.2599	3.2563	0.0143	0.0168	-0.0302	0.0276	0.0001	0.1082
N1-C8	1	3.2666	3.0658	3.0460	-0.2009	0.0156	-0.0131	-0.2033	-0.0001	0.2311
C8-H18	1	3.2674	3.1349	3.1146	-0.1325	0.0396	-0.0469	-0.1252	0.0000	0.2429

N2-C7	1	3.2742	3.2460	3.2437	-0.0282	0.0222	-0.0417	-0.0087	0.0000	0.0855
N2-H11	1	3.3140	3.8034	3.7644	0.4894	0.0239	-0.0138	0.4792	0.0001	0.3954
N2-C9	1	3.3302	3.3616	3.3368	0.0313	0.0284	0.0016	0.0013	0.0000	0.2901
N1-H13	1	3.3354	3.3399	3.3057	0.0045	0.0394	0.0196	-0.0544	-0.0001	0.3368
C4-H16	1	3.3454	3.4609	3.4541	0.1155	0.0145	-0.0155	0.1165	0.0000	0.1535
H13-H24	1	3.3584	3.3797	3.3767	0.0213	0.0116	-0.0198	0.0295	0.0000	0.1008
C4-H10	1	3.3794	3.3985	3.3958	0.0191	0.0250	-0.0400	0.0341	0.0000	0.0954
N2-H16	1	3.3818	3.3996	3.3969	0.0178	0.0287	-0.0440	0.0332	-0.0001	0.0962
N1-H17	1	3.4075	3.4027	3.3994	-0.0048	0.0129	-0.0261	0.0084	0.0000	0.1049
N2-H21	1	3.4706	3.4826	3.4800	0.0120	0.0274	-0.0446	0.0291	0.0001	0.0959
C3-H23	1	3.4873	3.6561	3.6311	0.1688	0.0311	0.0003	0.1374	0.0000	0.3030
C4-C5	1	3.5045	3.5166	3.5088	0.0120	0.0191	-0.0399	0.0329	-0.0001	0.1646
C4-H20	1	3.5291	3.5651	3.5540	0.0360	0.0275	-0.0100	0.0185	0.0000	0.1983
H10-H11	1	3.5476	3.7780	3.7638	0.2304	0.0144	-0.0122	0.2282	0.0000	0.2372
C5-H18	1	3.5480	3.5750	3.5732	0.0270	0.0063	-0.0125	0.0332	0.0000	0.0797
N1-H22	1	3.5691	3.8169	3.7905	0.2477	0.0276	-0.0561	0.2763	-0.0001	0.3187
H10-H12	1	3.6086	3.8141	3.7916	0.2055	0.0214	-0.0008	0.1848	0.0001	0.2962
N2-H25	1	3.6234	3.7097	3.7021	0.0863	0.0278	-0.0312	0.0897	0.0000	0.1670
C3-C8	1	3.6424	3.6866	3.6719	0.0442	0.0299	-0.0483	0.0626	0.0000	0.2314
N2-H19	1	3.6544	3.6054	3.5986	-0.0490	0.0259	-0.0331	-0.0419	0.0001	0.1550
C5-C6	1	3.6793	4.0999	4.0444	0.4206	0.0274	-0.0218	0.4150	0.0000	0.4955
C3-C7	1	3.6817	3.7101	3.7013	0.0284	0.0154	-0.0213	0.0343	0.0000	0.1800
C5-H24	1	3.6875	3.8304	3.8094	0.1429	0.0297	-0.0449	0.1580	0.0001	0.2805
H10-H23	1	3.7006	3.7264	3.7249	0.0258	0.0126	-0.0256	0.0387	0.0001	0.0755
C5-H12	1	3.7013	3.7730	3.7708	0.0717	0.0106	-0.0254	0.0865	0.0000	0.0927
C4-H14	1	3.7125	3.7338	3.7322	0.0213	0.0037	-0.0088	0.0263	0.0001	0.0778
C3-H20	1	3.7638	3.8169	3.8100	0.0531	0.0131	-0.0186	0.0585	0.0001	0.1624
N1-C9	1	3.7818	3.8085	3.7877	0.0267	0.0230	-0.0046	0.0083	0.0000	0.2813
C7-C8	1	3.7999	3.8577	3.8557	0.0578	0.0115	-0.0240	0.0703	0.0000	0.0874
C6-H13	1	3.8180	3.9751	3.9614	0.1571	0.0299	-0.0443	0.1716	-0.0001	0.2335
C6-H14	1	3.8400	3.7718	3.7643	-0.0681	0.0269	-0.0475	-0.0475	0.0000	0.1672
C3-H18	1	3.8455	3.7451	3.7387	-0.1004	0.0185	-0.0237	-0.0953	0.0001	0.1517
C9-H13	1	3.8574	3.9066	3.8850	0.0492	0.0311	-0.0612	0.0793	0.0000	0.2887
C8-H10	1	3.8844	3.9172	3.9087	0.0328	0.0284	-0.0392	0.0436	0.0000	0.1821
C9-H12	1	3.8910	3.8484	3.8409	-0.0426	0.0109	-0.0148	-0.0387	0.0000	0.1688
C7-H22	1	3.9166	4.3871	4.3491	0.4704	0.0318	-0.0181	0.4568	-0.0001	0.4120
C8-H19	1	3.9183	4.0889	4.0799	0.1706	0.0105	-0.0110	0.1711	0.0000	0.1942
H13-H25	1	3.9213	4.0871	4.0485	0.1657	0.0373	-0.0415	0.1700	-0.0001	0.4042
C4-C8	1	3.9305	3.9516	3.9348	0.0211	0.0252	-0.0423	0.0382	0.0000	0.2569
N1-H24	1	3.9363	3.9608	3.9551	0.0245	0.0096	-0.0151	0.0300	0.0000	0.1493
C5-C7	1	3.9480	3.9079	3.8902	-0.0401	0.0177	-0.0041	-0.0537	0.0000	0.2621
C5-H15	1	3.9793	4.0956	4.0880	0.1163	0.0123	-0.0172	0.1212	0.0000	0.1769
C7-H15	1	3.9801	3.9403	3.9363	-0.0398	0.0115	-0.0267	-0.0246	0.0000	0.1258
H12-H24	1	3.9805	4.1201	4.1100	0.1396	0.0308	-0.0417	0.1505	0.0000	0.2033
H12-H20	1	4.0072	4.0986	4.0892	0.0914	0.0154	-0.0168	0.0928	0.0000	0.1969

N1-H21	1	4.0188	4.0601	4.0378	0.0413	0.0316	-0.0235	0.0332	0.0000	0.2990
C3-H19	1	4.0496	3.8971	3.8830	-0.1525	0.0239	-0.0368	-0.1397	0.0001	0.2297
C3-H22	1	4.0606	4.1838	4.1764	0.1232	0.0209	-0.0426	0.1449	0.0000	0.1763
H14-H18	1	4.0660	4.3796	4.3486	0.3136	0.0209	-0.0359	0.3286	0.0000	0.3746
H17-H20	1	4.0755	4.0223	3.9793	-0.0533	0.0263	-0.0205	-0.0590	-0.0001	0.4106
H18-H21	1	4.0834	4.1393	4.1315	0.0559	0.0279	-0.0553	0.0832	0.0001	0.1787
H10-H20	1	4.1228	4.1539	4.1480	0.0311	0.0288	-0.0512	0.0534	0.0001	0.1566
N2-H17	1	4.1256	4.4681	4.4388	0.3425	0.0300	-0.0344	0.3470	-0.0001	0.3641
C5-C9	1	4.1292	4.0778	4.0477	-0.0515	0.0301	-0.0216	-0.0600	0.0000	0.3423
C4-H22	1	4.1305	4.3588	4.3284	0.2282	0.0275	-0.0261	0.2269	-0.0001	0.3638
N1-H25	1	4.1464	4.1630	4.1577	0.0165	0.0230	-0.0449	0.0385	-0.0001	0.1483
C5-H19	1	4.1689	4.6247	4.5880	0.4558	0.0348	-0.0671	0.4881	0.0000	0.4151
H12-H22	1	4.1714	4.1796	4.1691	0.0082	0.0161	-0.0257	0.0178	0.0000	0.2089
N2-H23	1	4.1799	4.2060	4.1989	0.0261	0.0083	-0.0146	0.0324	0.0000	0.1728
H13-H15	1	4.1802	4.1882	4.1817	0.0080	0.0279	-0.0488	0.0289	0.0000	0.1639
H15-H18	1	4.1983	4.4583	4.4325	0.2600	0.0258	-0.0554	0.2896	0.0000	0.3404
H14-H19	1	4.2197	4.3245	4.3133	0.1047	0.0143	-0.0185	0.1090	-0.0001	0.2197
H12-H14	1	4.2785	4.4351	4.4117	0.1566	0.0260	-0.0290	0.1595	0.0001	0.3204
H14-H24	1	4.2795	4.2462	4.2394	-0.0333	0.0246	-0.0400	-0.0180	0.0001	0.1689
C8-H12	1	4.3328	4.4219	4.4159	0.0891	0.0220	-0.0438	0.1109	0.0000	0.1621
H19-H22	1	4.3450	4.1334	4.1173	-0.2116	0.0166	-0.0429	-0.1854	0.0001	0.2475
C5-H25	1	4.3557	4.5450	4.5305	0.1893	0.0215	-0.0336	0.2014	0.0000	0.2576
C7-H14	1	4.3606	4.4164	4.3948	0.0559	0.0202	-0.0349	0.0705	0.0001	0.3070
H14-H25	1	4.3736	4.4800	4.4694	0.1063	0.0246	-0.0406	0.1223	0.0000	0.2165
C5-H11	1	4.3744	4.4202	4.4168	0.0458	0.0176	-0.0449	0.0730	0.0001	0.1236
C4-H13	1	4.4033	4.5092	4.5058	0.1059	0.0088	-0.0285	0.1256	0.0000	0.1232
C4-C9	1	4.4248	4.5060	4.4987	0.0812	0.0162	-0.0318	0.0969	-0.0001	0.1812
H11-H14	1	4.4291	4.6635	4.6359	0.2345	0.0281	-0.0309	0.2372	0.0001	0.3584
H12-H13	1	4.4555	4.4959	4.4832	0.0404	0.0224	-0.0151	0.0331	0.0000	0.2386
C9-H14	1	4.4847	4.6551	4.6427	0.1704	0.0151	-0.0255	0.1807	0.0001	0.2403
H14-H15	1	4.5114	4.5389	4.5360	0.0275	0.0214	-0.0461	0.0521	0.0001	0.1151
H11-H20	1	4.5143	4.5492	4.5463	0.0349	0.0111	-0.0350	0.0588	0.0000	0.1155
C6-C7	1	4.5224	4.8370	4.8112	0.3147	0.0249	-0.0246	0.3144	0.0000	0.3642
H15-H17	1	4.5231	4.5477	4.5449	0.0246	0.0121	-0.0312	0.0437	0.0000	0.1125
H12-H23	1	4.5596	4.6116	4.6085	0.0520	0.0178	-0.0436	0.0778	0.0000	0.1183
H14-H16	1	4.5866	4.8541	4.8366	0.2675	0.0235	-0.0491	0.2931	0.0000	0.2916
H13-H18	1	4.5914	4.6801	4.6697	0.0888	0.0235	-0.0575	0.1228	0.0000	0.2203
C5-H16	1	4.5969	4.7135	4.7039	0.1166	0.0207	-0.0304	0.1264	-0.0001	0.2117
C3-H21	1	4.6266	4.7763	4.7585	0.1497	0.0275	-0.0364	0.1586	0.0000	0.2924
C7-H10	1	4.6448	4.6997	4.6965	0.0549	0.0190	-0.0441	0.0799	0.0001	0.1222
H10-H22	1	4.6475	4.7377	4.7275	0.0902	0.0273	-0.0528	0.1157	0.0000	0.2193
H10-H21	1	4.6529	5.0191	4.9727	0.3662	0.0352	-0.0061	0.3371	0.0000	0.4868
C3-H17	1	4.6914	4.7063	4.6968	0.0149	0.0249	-0.0540	0.0441	-0.0001	0.2118
C4-H24	1	4.7117	4.9689	4.9418	0.2571	0.0245	-0.0098	0.2425	-0.0001	0.3693
C9-H11	1	4.8056	4.8114	4.8028	0.0057	0.0262	-0.0647	0.0443	-0.0001	0.2027

H10-H19	1	4.8076	4.7441	4.7363	-0.0635	0.0160	-0.0406	-0.0389	0.0000	0.1909
C6-H18	1	4.8100	4.8252	4.8237	0.0152	0.0094	-0.0288	0.0346	0.0000	0.0867
N1-H23	1	4.8326	4.7749	4.7576	-0.0576	0.0265	-0.0221	-0.0621	0.0001	0.2865
H10-H18	1	4.8358	4.7147	4.6965	-0.1211	0.0326	-0.0285	-0.1252	0.0000	0.2891
H12-H25	1	4.8619	4.7550	4.7479	-0.1068	0.0205	-0.0268	-0.1006	0.0001	0.1822
H13-H16	1	4.8832	5.2812	5.2484	0.3980	0.0293	-0.0170	0.3857	0.0000	0.4316
H15-H19	1	4.9000	4.8830	4.8757	-0.0170	0.0120	-0.0215	-0.0075	0.0000	0.1878
C7-H16	1	4.9316	4.9311	4.9295	-0.0005	0.0063	-0.0260	0.0192	0.0000	0.0885
H17-H22	1	4.9522	5.0561	5.0330	0.1039	0.0365	-0.0418	0.1092	0.0000	0.3460
H19-H21	1	4.9615	5.0830	5.0758	0.1215	0.0172	-0.0438	0.1481	0.0000	0.1919
C7-H21	1	4.9637	4.9146	4.8996	-0.0491	0.0248	-0.0396	-0.0343	0.0000	0.2710
C8-H17	1	4.9782	4.7697	4.7278	-0.2085	0.0260	-0.0107	-0.2238	0.0000	0.4384
C8-H11	1	4.9853	5.0050	4.9967	0.0197	0.0218	-0.0438	0.0418	-0.0001	0.2032
C6-C8	1	5.0112	5.0406	5.0366	0.0294	0.0226	-0.0649	0.0717	0.0000	0.1422
H13-H23	1	5.0125	5.0969	5.0912	0.0844	0.0152	-0.0362	0.1055	-0.0001	0.1700
C7-H13	1	5.0271	4.9281	4.9053	-0.0989	0.0152	-0.0169	-0.0972	0.0000	0.3338
H22-H24	1	5.0510	4.9863	4.9739	-0.0647	0.0333	-0.0365	-0.0614	-0.0001	0.2468
C4-H25	1	5.0608	5.2760	5.2656	0.2151	0.0119	-0.0425	0.2457	0.0000	0.2369
H15-H22	1	5.0665	5.0766	5.0701	0.0100	0.0209	-0.0431	0.0322	0.0000	0.1802
C6-H19	1	5.0712	5.0032	4.9951	-0.0680	0.0192	-0.0386	-0.0485	-0.0001	0.2004
C4-H21	1	5.0827	5.0916	5.0777	0.0089	0.0262	-0.0348	0.0175	0.0000	0.2648
C8-H15	1	5.1648	5.5732	5.5445	0.4084	0.0358	-0.0762	0.4488	0.0000	0.4039
C8-H24	1	5.1664	5.2290	5.2221	0.0625	0.0209	-0.0432	0.0848	0.0000	0.1894
C6-H17	1	5.2138	5.2217	5.2156	0.0079	0.0160	-0.0478	0.0396	0.0001	0.1789
C4-H23	1	5.2698	5.4643	5.4547	0.1945	0.0094	-0.0318	0.2169	0.0000	0.2306
C5-H17	1	5.3036	5.3880	5.3789	0.0844	0.0199	-0.0527	0.1172	0.0000	0.2213
H11-H24	1	5.3148	5.3701	5.3656	0.0552	0.0133	-0.0489	0.0908	0.0000	0.1536
C6-H22	1	5.3444	5.5519	5.5335	0.2075	0.0261	-0.0566	0.2381	-0.0001	0.3208
C6-H20	1	5.3552	5.6048	5.5836	0.2495	0.0199	-0.0417	0.2713	0.0000	0.3453
H15-H20	1	5.3808	5.6008	5.5748	0.2199	0.0296	-0.0184	0.2087	0.0000	0.3812
H11-H25	1	5.3825	5.6207	5.5982	0.2382	0.0326	-0.0528	0.2584	0.0000	0.3572
H11-H23	1	5.4396	5.4666	5.4633	0.0270	0.0174	-0.0566	0.0662	0.0000	0.1327
H11-H22	1	5.5187	5.4605	5.4528	-0.0581	0.0048	-0.0351	-0.0278	0.0000	0.2044
C5-H23	1	5.5207	5.8512	5.8339	0.3305	0.0240	-0.0778	0.3843	0.0000	0.3181
H11-H13	1	5.5310	5.8527	5.8287	0.3217	0.0163	-0.0618	0.3672	0.0000	0.3810
H13-H19	1	5.5345	5.7920	5.7772	0.2575	0.0171	-0.0441	0.2845	0.0000	0.2970
H16-H19	1	5.5504	5.6095	5.6000	0.0591	0.0234	-0.0677	0.1034	0.0000	0.2335
H16-H18	1	5.5635	5.7153	5.7052	0.1518	0.0212	-0.0602	0.1908	0.0000	0.2399
H16-H17	1	5.5944	5.4249	5.4062	-0.1695	0.0144	-0.0411	-0.1428	0.0000	0.3132
H12-H21	1	5.6588	5.6455	5.6433	-0.0134	0.0158	-0.0606	0.0315	-0.0001	0.1101
H14-H17	1	5.6692	5.6013	5.5819	-0.0679	0.0262	-0.0602	-0.0339	0.0000	0.3277
H10-H17	1	5.6764	5.6969	5.6943	0.0205	0.0164	-0.0519	0.0560	0.0000	0.1202
C8-C9	1	5.6886	5.8933	5.8735	0.2047	0.0218	-0.0803	0.2631	0.0001	0.3415
H14-H23	1	5.7164	5.6316	5.6094	-0.0848	0.0205	-0.0287	-0.0766	0.0000	0.3523
C9-H22	1	5.7449	5.7826	5.7797	0.0377	0.0113	-0.0482	0.0746	0.0000	0.1286

H20-H24	1	5.7834	6.1561	6.1224	0.3727	0.0250	-0.0845	0.4321	0.0001	0.4611
H18-H24	1	5.7943	5.7443	5.7357	-0.0499	0.0249	-0.0646	-0.0102	0.0000	0.2220
H21-H24	1	5.7967	5.9532	5.9447	0.1565	0.0182	-0.0610	0.1993	0.0000	0.2259
C8-H16	1	5.8229	5.8117	5.7942	-0.0111	0.0128	-0.0611	0.0372	0.0000	0.3173
C8-H25	1	5.8306	5.8314	5.8292	0.0008	0.0124	-0.0498	0.0382	0.0000	0.1129
C7-C9	1	5.8354	5.7174	5.7106	-0.1180	0.0253	-0.0576	-0.0858	0.0001	0.1955
C7-H24	1	5.8405	5.9667	5.9564	0.1262	0.0238	-0.0555	0.1579	0.0000	0.2474
H16-H20	1	5.8445	6.0506	6.0381	0.2061	0.0161	-0.0645	0.2544	0.0001	0.2749
C6-H21	1	5.8914	5.8719	5.8657	-0.0194	0.0170	-0.0527	0.0163	0.0000	0.1918
H17-H21	1	5.9262	5.9480	5.9425	0.0218	0.0259	-0.0868	0.0827	0.0000	0.1799
C9-H18	1	5.9370	5.9015	5.8946	-0.0355	0.0244	-0.0811	0.0213	-0.0001	0.2016
H11-H21	1	5.9662	5.9799	5.9733	0.0137	0.0170	-0.0590	0.0557	0.0000	0.1968
H13-H17	1	5.9788	5.9486	5.9405	-0.0302	0.0204	-0.0663	0.0158	-0.0001	0.2180
C9-H20	1	5.9839	6.1786	6.1676	0.1946	0.0151	-0.0453	0.2248	0.0000	0.2615
H16-H21	1	6.0056	6.0054	5.9979	-0.0002	0.0169	-0.0656	0.0485	0.0000	0.2125
H22-H25	1	6.0168	6.0896	6.0668	0.0728	0.0327	-0.0929	0.1330	0.0000	0.3711
H16-H22	1	6.0668	5.9249	5.8986	-0.1419	0.0200	-0.0794	-0.0825	0.0000	0.3884
C9-H21	1	6.0912	6.3326	6.3147	0.2414	0.0247	-0.0911	0.3078	0.0000	0.3386
H20-H25	1	6.1040	6.4578	6.4313	0.3538	0.0205	-0.0634	0.3966	0.0001	0.4198
H21-H25	1	6.1573	6.4173	6.3964	0.2600	0.0333	-0.1133	0.3400	0.0000	0.3650
C7-H25	1	6.1900	6.4367	6.4179	0.2467	0.0198	-0.0577	0.2846	0.0000	0.3478
C9-H19	1	6.2387	6.4149	6.3934	0.1762	0.0213	-0.0635	0.2184	0.0000	0.3694
C9-H17	1	6.2549	6.3882	6.3791	0.1333	0.0131	-0.0612	0.1813	0.0001	0.2410
C7-H23	1	6.2709	6.5298	6.5076	0.2589	0.0250	-0.0907	0.3246	0.0000	0.3831
H17-H24	1	6.2720	6.2251	6.2162	-0.0469	0.0103	-0.0511	-0.0061	0.0000	0.2343
H19-H24	1	6.2822	6.6444	6.6247	0.3622	0.0265	-0.0955	0.4312	0.0000	0.3601
H18-H25	1	6.3272	6.3985	6.3847	0.0713	0.0247	-0.0917	0.1384	-0.0001	0.2962
C8-H23	1	6.4345	6.4671	6.4560	0.0326	0.0246	-0.0980	0.1060	0.0000	0.2672
H22-H23	1	6.4576	6.4629	6.4421	0.0053	0.0163	-0.0668	0.0558	0.0000	0.3643
H18-H23	1	6.4660	6.2523	6.2313	-0.2137	0.0160	-0.0625	-0.1672	0.0000	0.3566
H16-H21	1	6.4902	6.3957	6.3873	-0.0945	0.0090	-0.0644	-0.0390	-0.0001	0.2295
H19-H25	1	6.5080	6.5265	6.5234	0.0186	0.0210	-0.0831	0.0807	0.0000	0.1439
H17-H23	1	6.6437	6.6779	6.6747	0.0342	0.0157	-0.0714	0.0900	-0.0001	0.1446
H20-H23	1	6.7688	6.8677	6.8591	0.0990	0.0197	-0.0864	0.1657	0.0000	0.2421
H17-H25	1	6.9594	6.9184	6.9098	-0.0409	0.0181	-0.0911	0.0321	0.0000	0.2431
H19-H23	1	7.0001	7.1381	7.1276	0.1380	0.0173	-0.0792	0.2000	-0.0001	0.2739
H21-H23	1	7.2768	7.1888	7.1795	-0.0880	0.0126	-0.0848	-0.0158	0.0000	0.2568

Table S14. Equilibrium (r_e) and thermal average (r_g , r_a) distances, vibrational corrections (Δ), and mean amplitudes (u) for internuclear distances of TEDA conformation **1f** (in Å), obtained for 291 K by GED refinement (initial approximation MP2/cc-PVTZ). n – number of equivalent parameters.

Atomic pair	n	r_e	r_g	r_a	Δr	$\Delta r(\text{har})$	$\Delta r(\text{kin})$	$\Delta r(\text{dyn})$	$\Delta r(\text{rot})$	u
C6-H15	1	1.0898	1.1123	1.1090	0.0225	0.0435	-0.0387	0.0177	0.0000	0.0611
C7-H19	1	1.0909	1.1138	1.1106	0.0229	0.0506	-0.0457	0.0181	-0.0001	0.0599
C8-H20	1	1.0910	1.1142	1.1112	0.0232	0.0522	-0.0473	0.0183	0.0000	0.0589
C9-H23	1	1.0912	1.1126	1.1087	0.0214	0.0395	-0.0352	0.0171	0.0000	0.0662
C8-H22	1	1.0914	1.1131	1.1091	0.0217	0.0391	-0.0349	0.0175	0.0000	0.0668
C7-H18	1	1.0915	1.1154	1.1136	0.0239	0.0631	-0.0571	0.0179	0.0000	0.0450
C8-H21	1	1.0915	1.1139	1.1102	0.0224	0.0426	-0.0382	0.0180	0.0000	0.0647
C9-H24	1	1.0917	1.1147	1.1114	0.0230	0.0501	-0.0453	0.0181	0.0001	0.0603
C7-H17	1	1.0923	1.1155	1.1124	0.0232	0.0520	-0.0471	0.0182	0.0001	0.0593
C3-H10	1	1.0925	1.1141	1.1090	0.0216	0.0162	-0.0123	0.0177	0.0000	0.0755
C9-H25	1	1.0926	1.1146	1.1102	0.0219	0.0322	-0.0279	0.0176	0.0000	0.0701
C4-H12	1	1.0927	1.1144	1.1097	0.0217	0.0267	-0.0225	0.0176	-0.0001	0.0728
C4-H11	1	1.0929	1.1168	1.1151	0.0239	0.0629	-0.0568	0.0178	0.0000	0.0444
C5-H13	1	1.0937	1.1157	1.1109	0.0220	0.0263	-0.0222	0.0179	0.0000	0.0729
C6-H16	1	1.0947	1.1168	1.1133	0.0221	0.0430	-0.0381	0.0172	0.0000	0.0627
C5-H14	1	1.0972	1.1195	1.1149	0.0223	0.0307	-0.0264	0.0180	0.0000	0.0716
N2-C3	1	1.4217	1.4315	1.4299	0.0098	0.0059	-0.0044	0.0083	0.0000	0.0488
N1-C3	1	1.4290	1.4396	1.4379	0.0106	0.0057	-0.0042	0.0090	0.0001	0.0494
N1-C4	1	1.4386	1.4490	1.4473	0.0103	0.0059	-0.0040	0.0085	-0.0001	0.0490
N2-C5	1	1.4397	1.4499	1.4483	0.0103	0.0059	-0.0040	0.0084	0.0000	0.0490
N1-N2	1	1.4818	1.4924	1.4904	0.0106	0.0051	-0.0045	0.0101	-0.0001	0.0541
C3-C6	1	1.4990	1.5100	1.5084	0.0110	0.0062	-0.0049	0.0097	0.0000	0.0493
C5-C8	1	1.5143	1.5282	1.5270	0.0140	0.0249	-0.0235	0.0125	0.0001	0.0436
C4-C7	1	1.5149	1.5274	1.5260	0.0125	0.0206	-0.0192	0.0111	0.0000	0.0459
C6-C9	1	1.5224	1.5361	1.5352	0.0137	0.0311	-0.0293	0.0120	-0.0001	0.0376
H23-H25	1	1.7653	1.7932	1.7884	0.0279	0.0797	-0.0780	0.0262	0.0000	0.0924
H24-H25	1	1.7675	1.7958	1.7905	0.0283	0.0795	-0.0782	0.0270	0.0000	0.0972
H23-H24	1	1.7683	1.7961	1.7902	0.0279	0.0704	-0.0695	0.0270	0.0000	0.1023
H17-H18	1	1.7684	1.7965	1.7909	0.0282	0.0719	-0.0709	0.0272	0.0000	0.1007
H20-H21	1	1.7684	1.7977	1.7947	0.0293	0.0991	-0.0959	0.0261	0.0000	0.0737
H18-H19	1	1.7686	1.7977	1.7925	0.0292	0.0820	-0.0807	0.0278	0.0001	0.0970
H20-H22	1	1.7700	1.7977	1.7930	0.0277	0.0801	-0.0783	0.0259	0.0000	0.0919
H21-H22	1	1.7716	1.7998	1.7938	0.0282	0.0684	-0.0678	0.0276	0.0000	0.1036
H17-H19	1	1.7718	1.7994	1.7938	0.0276	0.0724	-0.0714	0.0267	-0.0001	0.1003
H15-H16	1	1.7805	1.8069	1.7994	0.0264	0.0377	-0.0350	0.0238	-0.0001	0.1159
H11-H12	1	1.7853	1.8134	1.8078	0.0281	0.0642	-0.0604	0.0243	0.0000	0.1004
H13-H14	1	1.7898	1.8185	1.8114	0.0287	0.0455	-0.0425	0.0257	0.0000	0.1134
H12-H15	1	1.9479	2.0040	1.9833	0.0561	0.0583	0.0332	-0.0354	0.0000	0.2039

N2-H13	1	2.0081	2.0274	2.0223	0.0193	0.0186	-0.0209	0.0217	-0.0001	0.1021
N1-H11	1	2.0234	2.0426	2.0376	0.0191	0.0235	-0.0256	0.0213	-0.0001	0.1008
N2-H14	1	2.0653	2.0894	2.0845	0.0241	0.0209	-0.0227	0.0260	-0.0001	0.1009
N1-H12	1	2.0843	2.1093	2.1044	0.0250	0.0179	-0.0196	0.0268	-0.0001	0.1021
N1-H10	1	2.0939	2.1132	2.1083	0.0193	0.0118	-0.0160	0.0235	0.0000	0.1009
C3-H16	1	2.0973	2.1214	2.1161	0.0240	0.0303	-0.0328	0.0265	0.0000	0.1055
C3-H15	1	2.1119	2.1266	2.1220	0.0147	0.0310	-0.0331	0.0168	0.0000	0.0990
N2-H10	1	2.1357	2.1597	2.1550	0.0240	0.0129	-0.0167	0.0278	0.0000	0.1001
C5-H20	1	2.1506	2.1732	2.1702	0.0226	0.0599	-0.0607	0.0234	0.0000	0.0802
C7-H12	1	2.1520	2.1811	2.1768	0.0291	0.0481	-0.0502	0.0312	0.0000	0.0967
C4-H18	1	2.1538	2.1777	2.1740	0.0240	0.0565	-0.0580	0.0255	0.0000	0.0902
C9-H15	1	2.1544	2.1781	2.1733	0.0237	0.0347	-0.0363	0.0254	-0.0001	0.1026
C5-H22	1	2.1564	2.1812	2.1764	0.0248	0.0346	-0.0363	0.0265	0.0000	0.1029
C4-H19	1	2.1569	2.1779	2.1731	0.0210	0.0346	-0.0361	0.0226	-0.0001	0.1019
C8-H14	1	2.1573	2.1837	2.1810	0.0264	0.0715	-0.0721	0.0270	0.0000	0.0767
C7-H11	1	2.1583	2.1809	2.1767	0.0226	0.0437	-0.0448	0.0237	0.0000	0.0954
C5-H21	1	2.1583	2.1840	2.1799	0.0257	0.0545	-0.0561	0.0274	-0.0001	0.0941
C6-H24	1	2.1588	2.1815	2.1784	0.0227	0.0605	-0.0613	0.0235	0.0000	0.0818
C4-H17	1	2.1606	2.1828	2.1785	0.0223	0.0481	-0.0499	0.0240	0.0001	0.0976
C8-H13	1	2.1689	2.1969	2.1945	0.0280	0.0713	-0.0718	0.0285	0.0000	0.0732
C9-H16	1	2.1702	2.1945	2.1904	0.0242	0.0432	-0.0439	0.0250	-0.0001	0.0947
H10-H14	1	2.1706	2.1879	2.1836	0.0173	0.0342	-0.0350	0.0180	0.0001	0.0966
C6-H25	1	2.1710	2.1933	2.1885	0.0223	0.0334	-0.0349	0.0238	0.0000	0.1027
C6-H23	1	2.1815	2.2052	2.2005	0.0237	0.0123	-0.0133	0.0247	0.0000	0.1018
C6-H10	1	2.1891	2.2494	2.2290	0.0603	0.0225	-0.0085	0.0462	0.0001	0.2135
N1-C5	1	2.3931	2.4138	2.4118	0.0207	0.0044	-0.0059	0.0222	0.0000	0.0695
N2-C4	1	2.4080	2.4533	2.4435	0.0453	0.0163	-0.0106	0.0396	0.0000	0.1545
C5-C3	1	2.4098	2.4260	2.4240	0.0162	0.0047	-0.0065	0.0180	0.0000	0.0708
N1-H14	1	2.4116	2.4359	2.4341	0.0243	0.0062	-0.0069	0.0250	0.0000	0.0668
N1-C7	1	2.4394	2.4577	2.4557	0.0183	0.0164	-0.0164	0.0184	-0.0001	0.0694
N2-H12	1	2.4398	2.4547	2.4527	0.0148	0.0163	-0.0163	0.0148	0.0000	0.0689
N2-C8	1	2.4484	2.5064	2.4960	0.0580	0.0153	-0.0113	0.0541	-0.0001	0.1608
C4-C3	1	2.4615	2.4849	2.4833	0.0235	0.0062	-0.0066	0.0239	0.0000	0.0649
H12-H18	1	2.4677	2.5174	2.5028	0.0496	0.0318	-0.0318	0.0496	0.0000	0.1902
C3-H14	1	2.4799	2.5237	2.5153	0.0438	0.0174	-0.0123	0.0386	0.0001	0.1451
H14-H20	1	2.4810	2.5151	2.5046	0.0341	0.0829	-0.0826	0.0338	0.0000	0.1610
H15-H24	1	2.4952	2.5496	2.5372	0.0544	0.0421	-0.0403	0.0527	-0.0001	0.1775
H11-H19	1	2.4980	2.5164	2.5052	0.0184	0.0529	-0.0525	0.0180	0.0000	0.1665
H10-H16	1	2.5001	2.5317	2.5210	0.0317	0.0632	-0.0631	0.0315	0.0001	0.1636
H13-H22	1	2.5054	2.5115	2.5095	0.0061	0.0071	-0.0065	0.0056	-0.0001	0.0695
H12-H17	1	2.5056	2.5403	2.5287	0.0347	0.0609	-0.0608	0.0345	0.0001	0.1705
C3-C9	1	2.5061	2.5377	2.5260	0.0316	0.0468	-0.0450	0.0298	0.0000	0.1716
H11-H17	1	2.5076	2.5296	2.5276	0.0221	0.0142	-0.0152	0.0230	0.0001	0.0720
H15-H23	1	2.5085	2.5382	2.5265	0.0297	0.0540	-0.0526	0.0283	0.0000	0.1713
N2-C6	1	2.5102	2.5582	2.5456	0.0480	0.0511	-0.0508	0.0477	0.0000	0.1783

H13-H21	1	2.5113	2.5388	2.5273	0.0275	0.0535	-0.0524	0.0264	0.0000	0.1701
H16-H25	1	2.5120	2.5475	2.5376	0.0354	0.0839	-0.0837	0.0352	0.0000	0.1575
H14-H21	1	2.5222	2.5643	2.5562	0.0420	0.0117	-0.0149	0.0453	-0.0001	0.1432
H16-H23	1	2.5288	2.5624	2.5501	0.0336	0.0467	-0.0452	0.0321	0.0000	0.1766
H18-H20	1	2.5307	2.5275	2.5148	-0.0032	0.0415	-0.0390	-0.0058	0.0001	0.1775
C5-H10	1	2.5621	2.7635	2.7150	0.2014	0.0491	0.0361	0.1162	0.0000	0.3707
C3-H12	1	2.5971	2.6182	2.6108	0.0211	0.0154	-0.0107	0.0164	0.0000	0.1395
H10-H25	1	2.6068	2.6228	2.6211	0.0160	0.0067	-0.0047	0.0140	0.0000	0.0656
N1-C6	1	2.6144	2.6830	2.6693	0.0686	0.0320	0.0048	0.0317	0.0001	0.1918
N2-H15	1	2.6405	2.6985	2.6738	0.0580	0.0422	-0.0124	0.0281	0.0001	0.2591
C4-H15	1	2.6560	2.6539	2.6432	-0.0022	0.0253	-0.0161	-0.0114	0.0000	0.1678
C6-H12	1	2.6623	2.7263	2.7147	0.0640	0.0367	-0.0359	0.0632	0.0000	0.1781
N1-H19	1	2.6667	2.6695	2.6585	0.0028	0.0164	0.0059	-0.0195	0.0000	0.1708
N2-H22	1	2.6833	2.7040	2.6934	0.0206	0.0413	-0.0404	0.0197	0.0000	0.1679
N1-H18	1	2.7349	2.7622	2.7528	0.0273	0.0382	-0.0374	0.0264	0.0001	0.1613
N2-H20	1	2.7469	2.7760	2.7681	0.0291	0.0290	-0.0163	0.0163	0.0001	0.1473
C3-H24	1	2.7555	2.7549	2.7454	-0.0006	0.0376	-0.0359	-0.0023	0.0000	0.1606
C3-H25	1	2.7620	2.8036	2.7941	0.0416	0.0440	-0.0431	0.0408	-0.0001	0.1627
N1-H15	1	2.7728	2.8032	2.7942	0.0304	0.0441	-0.0436	0.0299	0.0000	0.1587
C9-H10	1	2.7745	2.8603	2.8171	0.0858	0.0334	-0.0111	0.0635	0.0000	0.3476
C3-H11	1	2.7943	2.8123	2.8028	0.0180	0.0146	-0.0204	0.0238	0.0000	0.1618
C3-H13	1	2.7988	3.0608	2.9848	0.2620	0.0405	-0.0152	0.2367	0.0000	0.4886
H10-H13	1	2.8206	2.7971	2.7886	-0.0235	0.0109	-0.0160	-0.0184	0.0000	0.1527
N1-H20	1	2.8285	2.8520	2.8411	0.0235	0.0125	-0.0097	0.0207	0.0000	0.1765
H11-H15	1	2.8838	2.9724	2.9197	0.0885	0.0597	0.0480	-0.0191	-0.0001	0.3919
C4-C6	1	2.9641	3.1622	3.1297	0.1981	0.0314	0.0010	0.1657	0.0000	0.3276
N1-H16	1	2.9762	3.0371	3.0131	0.0609	0.0377	-0.0158	0.0390	0.0000	0.2677
N2-H24	1	2.9921	3.0256	3.0228	0.0335	0.0077	-0.0022	0.0280	0.0000	0.0932
N2-H18	1	3.0366	3.0949	3.0752	0.0583	0.0306	-0.0172	0.0449	0.0000	0.2456
H19-H20	1	3.0515	3.0655	3.0577	0.0140	0.0215	-0.0227	0.0151	0.0001	0.1542
H18-H22	1	3.0558	3.0736	3.0692	0.0177	0.0286	-0.0482	0.0374	-0.0001	0.1165
H12-H19	1	3.0637	3.0920	3.0911	0.0283	0.0995	-0.1134	0.0421	0.0001	0.0525
H10-H15	1	3.0647	3.0939	3.0931	0.0292	0.0988	-0.1129	0.0433	0.0000	0.0487
H13-H20	1	3.0660	3.0913	3.0873	0.0253	0.0585	-0.0753	0.0422	-0.0001	0.1108
H11-H18	1	3.0676	3.0950	3.0918	0.0274	0.0709	-0.0861	0.0425	0.0001	0.0990
H14-H22	1	3.0711	3.0974	3.0938	0.0263	0.0579	-0.0746	0.0430	0.0000	0.1060
H15-H25	1	3.0737	3.1009	3.0979	0.0271	0.0712	-0.0864	0.0423	0.0000	0.0966
H16-H24	1	3.0823	3.2669	3.1967	0.1846	0.0570	0.0369	0.0907	0.0000	0.4738
H11-H16	1	3.0852	3.1709	3.1535	0.0857	0.0328	-0.0183	0.0711	0.0001	0.2346
H10-H24	1	3.1680	3.2237	3.2054	0.0557	0.0157	-0.0215	0.0615	0.0000	0.2408
H12-H16	1	3.1981	3.2071	3.1842	0.0089	0.0328	-0.0422	0.0184	-0.0001	0.2673
C7-H20	1	3.1994	3.3691	3.3324	0.1697	0.0284	-0.0130	0.1543	0.0000	0.3542
C6-H11	1	3.2126	3.1530	3.1195	-0.0596	0.0152	-0.0132	-0.0617	0.0001	0.3128
N1-C8	1	3.2152	3.3288	3.2637	0.1137	0.0598	0.0399	0.0140	0.0000	0.4614
C8-H18	1	3.2186	3.2503	3.2421	0.0318	0.0113	-0.0133	0.0339	-0.0001	0.1631

N2-C7	1	3.2218	3.2542	3.2479	0.0324	0.0122	-0.0166	0.0368	0.0000	0.1430
N2-H11	1	3.2444	3.2657	3.2623	0.0213	0.0175	-0.0306	0.0344	0.0000	0.1057
N2-C9	1	3.2540	3.3269	3.3217	0.0729	0.0139	-0.0179	0.0769	0.0000	0.1323
N1-H13	1	3.2790	3.2869	3.2836	0.0079	0.0130	-0.0248	0.0197	0.0000	0.1050
C4-H16	1	3.3518	3.3797	3.3766	0.0280	0.0106	-0.0188	0.0362	0.0000	0.1030
H13-H24	1	3.3526	3.3623	3.3463	0.0097	0.0152	-0.0132	0.0077	0.0000	0.2291
C4-H10	1	3.3626	3.4702	3.4430	0.1076	0.0363	0.0335	0.0379	-0.0001	0.3073
N2-H16	1	3.3676	3.3730	3.3701	0.0054	0.0215	-0.0383	0.0222	0.0000	0.0993
N1-H17	1	3.3708	3.4961	3.4698	0.1253	0.0227	-0.0001	0.1027	0.0000	0.3051
N2-H21	1	3.3817	3.4012	3.3984	0.0195	0.0276	-0.0438	0.0356	0.0001	0.0963
C3-H23	1	3.3836	3.4009	3.3982	0.0173	0.0257	-0.0405	0.0320	0.0001	0.0962
C4-C5	1	3.4078	3.4882	3.4593	0.0804	0.0404	0.0352	0.0048	0.0000	0.3164
C4-H20	1	3.4574	3.4788	3.4760	0.0214	0.0212	-0.0368	0.0369	0.0001	0.0987
H10-H11	1	3.4946	3.6223	3.6101	0.1277	0.0138	-0.0124	0.1263	0.0000	0.2130
C5-H18	1	3.5015	3.5370	3.5296	0.0355	0.0202	-0.0412	0.0565	0.0000	0.1617
N1-H22	1	3.5038	3.4734	3.4545	-0.0304	0.0168	-0.0066	-0.0407	0.0001	0.2548
H10-H12	1	3.5617	3.5770	3.5752	0.0153	0.0032	-0.0089	0.0211	-0.0001	0.0787
N2-H25	1	3.5808	3.6053	3.5954	0.0245	0.0306	-0.0087	0.0026	0.0000	0.1887
C3-C8	1	3.6153	3.6621	3.6419	0.0468	0.0301	-0.0485	0.0652	0.0000	0.2670
N2-H19	1	3.6355	3.7629	3.7464	0.1273	0.0260	-0.0433	0.1446	0.0000	0.2481
C5-C6	1	3.6528	3.6764	3.6699	0.0236	0.0168	-0.0248	0.0316	0.0000	0.1540
C3-C7	1	3.6591	3.6803	3.6649	0.0212	0.0290	-0.0468	0.0391	-0.0001	0.2362
C5-H24	1	3.6937	3.7489	3.7295	0.0552	0.0309	-0.0163	0.0407	-0.0001	0.2685
H10-H23	1	3.6951	3.7020	3.6934	0.0069	0.0113	-0.0168	0.0124	0.0000	0.1784
C5-H12	1	3.6961	3.6734	3.6655	-0.0227	0.0081	-0.0133	-0.0175	0.0000	0.1697
C4-H14	1	3.6980	3.7161	3.7146	0.0181	0.0071	-0.0120	0.0231	-0.0001	0.0755
C3-H20	1	3.7028	3.7236	3.7219	0.0208	0.0108	-0.0234	0.0335	-0.0001	0.0803
N1-C9	1	3.7086	3.7450	3.7432	0.0364	0.0110	-0.0228	0.0482	0.0000	0.0811
C7-C8	1	3.7494	3.8035	3.7848	0.0541	0.0287	-0.0002	0.0256	0.0000	0.2666
C6-H13	1	3.7566	3.8812	3.8441	0.1245	0.0378	-0.0177	0.1044	0.0000	0.3780
C6-H14	1	3.7737	3.8108	3.8041	0.0371	0.0117	-0.0167	0.0421	0.0000	0.1598
C3-H18	1	3.7760	3.8320	3.8138	0.0560	0.0250	-0.0067	0.0377	0.0000	0.2642
C9-H13	1	3.8002	3.8591	3.8520	0.0589	0.0106	-0.0173	0.0656	0.0000	0.1655
C8-H10	1	3.8198	3.8450	3.8365	0.0252	0.0199	-0.0369	0.0421	0.0001	0.1815
C9-H12	1	3.8359	3.8560	3.8541	0.0201	0.0077	-0.0216	0.0340	0.0000	0.0839
C7-H22	1	3.8688	3.9076	3.8850	0.0388	0.0316	-0.0617	0.0689	0.0000	0.2944
C8-H19	1	3.8964	3.9328	3.9237	0.0365	0.0264	-0.0370	0.0471	0.0000	0.1885
H13-H25	1	3.9035	3.9618	3.9531	0.0583	0.0267	-0.0359	0.0675	0.0000	0.1846
C4-C8	1	3.9115	3.9355	3.9234	0.0240	0.0160	-0.0188	0.0268	0.0000	0.2168
N1-H24	1	3.9261	3.9649	3.9592	0.0388	0.0140	-0.0198	0.0445	0.0001	0.1501
C5-C7	1	3.9416	4.0087	4.0018	0.0671	0.0159	-0.0235	0.0747	0.0000	0.1654
C5-H15	1	3.9431	4.0047	3.9869	0.0616	0.0234	-0.0408	0.0789	0.0001	0.2658
C7-H15	1	3.9536	4.0330	3.9963	0.0793	0.0338	-0.0344	0.0799	0.0000	0.3740
H12-H24	1	3.9539	4.1636	4.1258	0.2097	0.0319	-0.0357	0.2135	0.0000	0.3968
H12-H20	1	3.9546	4.0729	4.0224	0.1183	0.0282	-0.0109	0.1010	0.0000	0.4473

N1-H21	1	3.9549	3.9728	3.9605	0.0179	0.0166	-0.0251	0.0264	0.0000	0.2201
C3-H19	1	3.9694	4.0055	3.9950	0.0360	0.0277	-0.0404	0.0487	0.0000	0.2028
C3-H22	1	3.9757	4.0409	4.0279	0.0652	0.0190	-0.0290	0.0752	0.0000	0.2278
H14-H18	1	3.9981	4.0055	4.0018	0.0074	0.0120	-0.0223	0.0177	0.0000	0.1204
H17-H20	1	4.0136	4.0821	4.0662	0.0685	0.0167	0.0058	0.0460	0.0000	0.2543
H18-H21	1	4.0407	4.0361	4.0288	-0.0046	0.0189	-0.0246	0.0011	0.0000	0.1710
H10-H20	1	4.0558	4.1206	4.0753	0.0648	0.0272	-0.0118	0.0494	0.0000	0.4287
N2-H17	1	4.0832	4.2223	4.2010	0.1392	0.0255	-0.0395	0.1531	0.0001	0.2989
C5-C9	1	4.0843	4.2662	4.2325	0.1819	0.0374	-0.0611	0.2055	0.0001	0.3785
C4-H22	1	4.0953	4.1177	4.1132	0.0224	0.0157	-0.0373	0.0439	0.0001	0.1355
N1-H25	1	4.1095	4.1645	4.1577	0.0549	0.0238	-0.0442	0.0754	-0.0001	0.1671
C5-H19	1	4.1146	4.1568	4.1503	0.0422	0.0090	-0.0095	0.0427	0.0000	0.1644
H12-H22	1	4.1234	4.1358	4.1298	0.0124	0.0274	-0.0492	0.0342	0.0000	0.1569
N2-H23	1	4.1599	4.2169	4.1875	0.0570	0.0270	-0.0243	0.0543	0.0000	0.3499
H13-H15	1	4.1610	4.1956	4.1896	0.0346	0.0206	-0.0417	0.0557	0.0000	0.1587
H15-H18	1	4.1670	4.1909	4.1845	0.0239	0.0107	-0.0162	0.0294	0.0000	0.1635
H14-H19	1	4.1692	4.3447	4.3235	0.1755	0.0234	-0.0500	0.2021	0.0000	0.3035
H12-H14	1	4.1890	4.2156	4.2092	0.0266	0.0249	-0.0486	0.0504	-0.0001	0.1644
H14-H24	1	4.1911	4.2109	4.2043	0.0197	0.0182	-0.0378	0.0394	-0.0001	0.1657
C8-H12	1	4.2083	4.2822	4.2582	0.0738	0.0226	-0.0307	0.0819	0.0000	0.3164
H19-H22	1	4.2111	4.3082	4.2209	0.0971	0.0330	-0.0488	0.1129	0.0000	0.5978
C5-H25	1	4.2177	4.2605	4.2556	0.0428	0.0234	-0.0462	0.0656	0.0000	0.1445
C7-H14	1	4.2533	4.3162	4.3087	0.0629	0.0174	-0.0328	0.0783	0.0000	0.1799
H14-H25	1	4.2746	4.3488	4.3352	0.0742	0.0226	-0.0346	0.0862	0.0000	0.2425
C5-H11	1	4.3233	4.3538	4.3343	0.0305	0.0260	-0.0255	0.0300	0.0000	0.2899
C4-H13	1	4.3443	4.3527	4.3311	0.0084	0.0223	-0.0361	0.0222	0.0000	0.3042
C4-C9	1	4.3492	4.4258	4.4020	0.0766	0.0248	-0.0237	0.0754	0.0001	0.3229
H11-H14	1	4.3734	4.4571	4.4334	0.0837	0.0361	-0.0025	0.0501	0.0000	0.3252
H12-H13	1	4.3801	4.4131	4.4091	0.0330	0.0080	-0.0282	0.0533	-0.0001	0.1319
C9-H14	1	4.4078	4.4131	4.3916	0.0052	0.0270	-0.0353	0.0135	0.0000	0.3053
H14-H15	1	4.4297	4.4858	4.4605	0.0560	0.0393	0.0016	0.0151	0.0000	0.3360
H11-H20	1	4.4306	4.4339	4.4212	0.0033	0.0180	-0.0370	0.0224	-0.0001	0.2358
C6-C7	1	4.4320	4.4451	4.4310	0.0131	0.0212	-0.0201	0.0120	0.0000	0.2487
H15-H17	1	4.4542	4.4745	4.4676	0.0203	0.0264	-0.0421	0.0359	0.0001	0.1753
H12-H23	1	4.4563	4.6339	4.6112	0.1776	0.0230	-0.0263	0.1809	0.0000	0.3296
H14-H16	1	4.4577	4.4996	4.4905	0.0419	0.0112	-0.0191	0.0498	0.0000	0.2010
H13-H18	1	4.4863	4.5152	4.5122	0.0289	0.0189	-0.0428	0.0528	0.0000	0.1176
C5-H16	1	4.4919	4.5546	4.5456	0.0628	0.0259	-0.0397	0.0765	0.0001	0.2017
C3-H21	1	4.5078	4.5201	4.5174	0.0123	0.0157	-0.0342	0.0308	0.0000	0.1108
C7-H10	1	4.5101	4.5373	4.5341	0.0272	0.0182	-0.0424	0.0514	0.0000	0.1209
H10-H22	1	4.5217	4.5790	4.5610	0.0572	0.0244	-0.0474	0.0802	0.0000	0.2816
H10-H21	1	4.5273	4.5506	4.5476	0.0233	0.0200	-0.0441	0.0474	0.0000	0.1181
C3-H17	1	4.5634	4.6435	4.6203	0.0801	0.0324	-0.0374	0.0851	0.0000	0.3252
C4-H24	1	4.5706	4.6322	4.6105	0.0617	0.0318	-0.0210	0.0508	0.0001	0.3152
C9-H11	1	4.5717	4.5407	4.5107	-0.0310	0.0258	-0.0342	-0.0226	0.0000	0.3652

H10-H19	1	4.6023	4.5848	4.5724	-0.0175	0.0162	-0.0307	-0.0030	0.0000	0.2369
C6-H18	1	4.6488	4.6421	4.6327	-0.0067	0.0270	-0.0357	0.0020	0.0000	0.2085
N1-H23	1	4.7114	4.7286	4.7259	0.0172	0.0140	-0.0397	0.0429	0.0000	0.1134
H10-H18	1	4.7125	4.7893	4.7717	0.0768	0.0239	-0.0192	0.0721	0.0000	0.2906
H12-H25	1	4.7134	4.7213	4.7123	0.0079	0.0300	-0.0659	0.0438	0.0000	0.2049
H13-H16	1	4.7781	4.8169	4.8094	0.0387	0.0136	-0.0209	0.0460	0.0000	0.1897
H15-H19	1	4.7878	4.8478	4.8302	0.0600	0.0248	-0.0268	0.0619	0.0001	0.2909
C7-H16	1	4.8154	4.8340	4.8325	0.0186	0.0061	-0.0231	0.0356	0.0000	0.0857
H17-H22	1	4.8203	5.0411	5.0119	0.2208	0.0266	-0.0196	0.2139	-0.0001	0.3898
H19-H21	1	4.8258	4.8816	4.8740	0.0558	0.0119	-0.0227	0.0665	0.0001	0.1921
C7-H21	1	4.8271	4.8397	4.8382	0.0126	0.0057	-0.0243	0.0312	0.0000	0.0855
C8-H17	1	4.8373	4.9527	4.9099	0.1154	0.0319	-0.0316	0.1151	0.0000	0.4572
C8-H11	1	4.9553	5.0872	5.0652	0.1319	0.0337	-0.0469	0.1452	-0.0001	0.3361
C6-C8	1	4.9670	5.0034	4.9953	0.0364	0.0158	-0.0333	0.0539	0.0000	0.2016
H13-H23	1	4.9689	5.0080	4.9682	0.0391	0.0296	-0.0375	0.0471	-0.0001	0.4441
C7-H13	1	4.9872	5.0280	5.0222	0.0408	0.0236	-0.0570	0.0742	0.0000	0.1708
H22-H24	1	4.9932	5.0168	5.0127	0.0237	0.0223	-0.0637	0.0651	0.0000	0.1433
C4-H25	1	5.0044	5.0086	5.0006	0.0043	0.0180	-0.0394	0.0257	0.0000	0.2003
H15-H22	1	5.0101	5.0309	5.0174	0.0208	0.0244	-0.0322	0.0286	0.0000	0.2583
C6-H19	1	5.0123	5.1213	5.1122	0.1090	0.0106	-0.0427	0.1411	0.0000	0.2184
C4-H21	1	5.0240	5.0806	5.0665	0.0566	0.0216	-0.0270	0.0620	0.0000	0.2674
C8-H15	1	5.0269	5.0643	5.0561	0.0374	0.0149	-0.0373	0.0598	0.0000	0.2035
C8-H24	1	5.0319	5.0648	5.0588	0.0328	0.0134	-0.0369	0.0563	0.0000	0.1735
C6-H17	1	5.0378	5.0827	5.0685	0.0449	0.0207	-0.0294	0.0536	0.0000	0.2682
C4-H23	1	5.0440	5.0820	5.0732	0.0379	0.0199	-0.0529	0.0709	0.0000	0.2103
C5-H17	1	5.0449	5.0299	5.0222	-0.0150	0.0097	-0.0322	0.0075	0.0000	0.1956
H11-H24	1	5.0456	5.1042	5.0916	0.0586	0.0225	-0.0339	0.0700	0.0000	0.2522
C6-H22	1	5.0575	5.0141	5.0070	-0.0434	0.0073	-0.0310	-0.0196	-0.0001	0.1876
C6-H20	1	5.0605	5.2354	5.2100	0.1749	0.0377	-0.0741	0.2113	0.0000	0.3667
H15-H20	1	5.0868	5.1169	5.1106	0.0302	0.0176	-0.0387	0.0513	0.0000	0.1802
H11-H25	1	5.0872	5.1132	5.1068	0.0261	0.0181	-0.0375	0.0455	0.0000	0.1811
H11-H23	1	5.1560	5.1359	5.1198	-0.0201	0.0171	-0.0366	-0.0006	0.0000	0.2854
H11-H22	1	5.1748	5.2003	5.1947	0.0255	0.0148	-0.0412	0.0519	0.0000	0.1710
C5-H23	1	5.1915	5.1288	5.1126	-0.0627	0.0173	-0.0404	-0.0396	0.0000	0.2860
H11-H13	1	5.2026	5.2230	5.2171	0.0204	0.0175	-0.0475	0.0503	0.0001	0.1745
H13-H19	1	5.2340	5.2953	5.2738	0.0614	0.0241	-0.0635	0.1008	0.0000	0.3336
H16-H19	1	5.2910	5.3037	5.2832	0.0127	0.0228	-0.0508	0.0407	0.0000	0.3239
H16-H18	1	5.2994	5.2977	5.2923	-0.0017	0.0101	-0.0436	0.0317	0.0001	0.1679
H16-H17	1	5.3186	5.3316	5.3280	0.0130	0.0234	-0.0635	0.0531	0.0000	0.1378
H12-H21	1	5.3445	5.3527	5.3337	0.0082	0.0278	-0.0784	0.0587	0.0001	0.3171
H14-H17	1	5.4323	5.5428	5.5267	0.1105	0.0245	-0.0754	0.1614	0.0000	0.2975
H10-H17	1	5.4993	5.6287	5.6151	0.1294	0.0149	-0.0447	0.1592	0.0000	0.2780
C8-C9	1	5.5218	5.5130	5.5042	-0.0088	0.0209	-0.0583	0.0285	0.0001	0.2191
H14-H23	1	5.5232	5.4962	5.4882	-0.0270	0.0188	-0.0566	0.0108	0.0000	0.2096
C9-H22	1	5.5388	5.5701	5.5625	0.0313	0.0161	-0.0514	0.0666	0.0000	0.2053

H20-H24	1	5.5523	5.6392	5.6300	0.0868	0.0217	-0.0693	0.1345	-0.0001	0.2274
H18-H24	1	5.6755	5.6510	5.6409	-0.0245	0.0215	-0.0634	0.0174	0.0000	0.2371
H21-H24	1	5.6763	5.8280	5.8127	0.1517	0.0167	-0.0753	0.2102	0.0001	0.2983
C8-H16	1	5.6843	5.6968	5.6944	0.0125	0.0132	-0.0472	0.0465	0.0000	0.1167
C8-H25	1	5.6905	5.7025	5.7001	0.0120	0.0117	-0.0460	0.0463	0.0000	0.1167
C7-C9	1	5.7460	5.7821	5.7753	0.0361	0.0199	-0.0521	0.0683	0.0000	0.1991
C7-H24	1	5.7563	5.8128	5.8002	0.0565	0.0168	-0.0653	0.1051	-0.0001	0.2699
H16-H20	1	5.7907	5.8435	5.8365	0.0527	0.0172	-0.0507	0.0863	-0.0001	0.2012
C6-H21	1	5.7931	5.7840	5.7753	-0.0090	0.0163	-0.0494	0.0240	0.0001	0.2238
H17-H21	1	5.8027	5.7641	5.7559	-0.0387	0.0129	-0.0469	-0.0047	0.0000	0.2157
C9-H18	1	5.9043	5.9020	5.8961	-0.0023	0.0223	-0.0800	0.0554	0.0000	0.1846
H11-H21	1	5.9956	5.9890	5.9821	-0.0066	0.0138	-0.0546	0.0342	0.0000	0.2019
H13-H17	1	6.0233	6.0627	6.0536	0.0394	0.0243	-0.0807	0.0958	0.0000	0.2333
C9-H20	1	6.0451	6.0761	6.0622	0.0310	0.0235	-0.0638	0.0713	0.0000	0.2899
H16-H21	1	6.0466	6.0640	6.0564	0.0174	0.0189	-0.0660	0.0645	0.0000	0.2146
H22-H25	1	6.0562	6.2056	6.1864	0.1494	0.0251	-0.0895	0.2139	-0.0001	0.3436
H16-H22	1	6.0921	6.1240	6.1225	0.0318	0.0056	-0.0396	0.0658	0.0000	0.0942
C9-H21	1	6.1178	6.1894	6.1702	0.0717	0.0193	-0.0596	0.1119	0.0001	0.3427
H20-H25	1	6.1211	6.2285	6.2114	0.1074	0.0253	-0.0358	0.1179	0.0000	0.3256
H21-H25	1	6.1249	6.2547	6.2384	0.1298	0.0291	-0.1070	0.2078	-0.0001	0.3185
C7-H25	1	6.1345	6.2037	6.1815	0.0692	0.0283	-0.0930	0.1338	0.0001	0.3653
C9-H19	1	6.1964	6.2670	6.2590	0.0706	0.0156	-0.0454	0.1004	0.0000	0.2222
C9-H17	1	6.2078	6.2687	6.2612	0.0610	0.0156	-0.0448	0.0902	0.0000	0.2175
C7-H23	1	6.2564	6.4263	6.4079	0.1699	0.0198	-0.0846	0.2348	-0.0001	0.3441
H17-H24	1	6.3438	6.3938	6.3874	0.0500	0.0125	-0.0557	0.0933	-0.0001	0.2025
H19-H24	1	6.3763	6.3964	6.3905	0.0201	0.0143	-0.0598	0.0656	0.0000	0.1931
H18-H25	1	6.4076	6.4381	6.4280	0.0305	0.0257	-0.1005	0.1052	0.0001	0.2546
C8-H23	1	6.4717	6.5755	6.5616	0.1038	0.0220	-0.0649	0.1467	0.0000	0.3008
H22-H23	1	6.5148	6.5801	6.5680	0.0653	0.0239	-0.0681	0.1095	0.0000	0.2814
H18-H23	1	6.7755	6.7976	6.7901	0.0220	0.0204	-0.0850	0.0866	0.0000	0.2260
H16-H21	1	6.9429	6.9640	6.9616	0.0211	0.0088	-0.0598	0.0721	0.0000	0.1279
H19-H25	1	6.9555	6.9662	6.9641	0.0107	0.0097	-0.0622	0.0632	0.0000	0.1234
H17-H23	1	7.0788	7.1198	7.1114	0.0410	0.0141	-0.0664	0.0933	0.0000	0.2433
H20-H23	1	7.1161	7.1557	7.1484	0.0397	0.0174	-0.0690	0.0913	0.0000	0.2280
H17-H25	1	7.1181	7.1566	7.1495	0.0385	0.0183	-0.0723	0.0925	0.0000	0.2245
H19-H23	1	7.1284	7.1252	7.1173	-0.0032	0.0165	-0.0726	0.0529	0.0000	0.2367
H21-H23	1	7.8231	7.8260	7.8232	0.0029	0.0117	-0.0843	0.0754	0.0001	0.1453

Table S15. Equilibrium (r_e) and thermal average (r_g , r_a) distances, vibrational corrections (Δ), and mean amplitudes (u) for internuclear distances of TEDA conformation **1g** (in Å), obtained for 291 K by GED refinement (initial approximation MP2/cc-PVTZ). n – number of equivalent parameters.

Atomic pair	n	r_e	r_g	r_a	Δr	$\Delta r(\text{har})$	$\Delta r(\text{kin})$	$\Delta r(\text{dyn})$	$\Delta r(\text{rot})$	u
C6-H15	1	1.0905	1.1132	1.1093	0.0227	0.0382	-0.0337	0.0182	0.0000	0.0658
C7-H19	1	1.0909	1.1141	1.1111	0.0232	0.0519	-0.0470	0.0183	0.0000	0.0590
C8-H20	1	1.0910	1.1143	1.1122	0.0234	0.0595	-0.0539	0.0178	0.0000	0.0500
C9-H23	1	1.0911	1.1152	1.1131	0.0241	0.0608	-0.0551	0.0185	-0.0001	0.0492
C8-H22	1	1.0911	1.1139	1.1109	0.0228	0.0497	-0.0448	0.0179	0.0000	0.0582
C7-H18	1	1.0914	1.1145	1.1115	0.0231	0.0543	-0.0492	0.0181	-0.0001	0.0580
C8-H21	1	1.0914	1.1154	1.1142	0.0240	0.0667	-0.0603	0.0175	0.0001	0.0375
C9-H24	1	1.0916	1.1139	1.1103	0.0224	0.0432	-0.0387	0.0179	0.0000	0.0635
C7-H17	1	1.0916	1.1134	1.1095	0.0218	0.0402	-0.0360	0.0176	0.0000	0.0664
C3-H10	1	1.0921	1.1136	1.1085	0.0215	0.0154	-0.0115	0.0176	0.0000	0.0755
C9-H25	1	1.0924	1.1171	1.1154	0.0247	0.0642	-0.0581	0.0186	0.0000	0.0436
C4-H12	1	1.0930	1.1144	1.1100	0.0215	0.0317	-0.0273	0.0171	0.0000	0.0700
C4-H11	1	1.0942	1.1161	1.1116	0.0219	0.0305	-0.0262	0.0177	-0.0001	0.0710
C5-H13	1	1.0947	1.1172	1.1132	0.0226	0.0384	-0.0340	0.0181	0.0001	0.0672
C6-H16	1	1.0947	1.1173	1.1130	0.0226	0.0337	-0.0293	0.0183	-0.0001	0.0701
C5-H14	1	1.0975	1.1197	1.1152	0.0222	0.0311	-0.0268	0.0179	0.0000	0.0712
N2-C3	1	1.4184	1.4275	1.4259	0.0091	0.0045	-0.0031	0.0077	0.0000	0.0487
N1-C3	1	1.4348	1.4442	1.4425	0.0094	0.0052	-0.0036	0.0078	0.0000	0.0498
N1-C4	1	1.4383	1.4484	1.4467	0.0101	0.0042	-0.0023	0.0082	0.0000	0.0491
N2-C5	1	1.4391	1.4501	1.4485	0.0110	0.0065	-0.0047	0.0092	0.0000	0.0490
N1-N2	1	1.4812	1.4937	1.4917	0.0124	0.0048	-0.0042	0.0119	-0.0001	0.0541
C3-C6	1	1.5007	1.5120	1.5104	0.0113	0.0066	-0.0052	0.0099	0.0000	0.0493
C5-C8	1	1.5120	1.5251	1.5240	0.0131	0.0263	-0.0248	0.0116	0.0000	0.0423
C4-C7	1	1.5145	1.5286	1.5274	0.0141	0.0254	-0.0239	0.0126	0.0000	0.0421
C6-C9	1	1.5222	1.5340	1.5328	0.0118	0.0251	-0.0236	0.0103	0.0000	0.0429
H23-H25	1	1.7620	1.7936	1.7911	0.0317	0.1047	-0.1012	0.0282	0.0000	0.0676
H24-H25	1	1.7645	1.7947	1.7918	0.0302	0.0953	-0.0924	0.0273	0.0000	0.0729
H23-H24	1	1.7659	1.7924	1.7893	0.0265	0.0914	-0.0884	0.0235	0.0000	0.0746
H17-H18	1	1.7667	1.7982	1.7935	0.0315	0.0823	-0.0807	0.0300	-0.0001	0.0921
H20-H21	1	1.7674	1.7979	1.7941	0.0305	0.0962	-0.0937	0.0280	0.0000	0.0821
H18-H19	1	1.7695	1.7940	1.7875	0.0245	0.0559	-0.0526	0.0213	-0.0001	0.1076
H20-H22	1	1.7708	1.7979	1.7922	0.0271	0.0731	-0.0721	0.0261	0.0000	0.1013
H21-H22	1	1.7717	1.8000	1.7952	0.0282	0.0795	-0.0780	0.0267	0.0000	0.0923
H17-H19	1	1.7719	1.8008	1.7957	0.0289	0.0837	-0.0822	0.0274	0.0000	0.0954
H15-H16	1	1.7737	1.8012	1.7952	0.0275	0.0685	-0.0677	0.0266	0.0001	0.1031
H11-H12	1	1.7787	1.8068	1.7997	0.0281	0.0460	-0.0432	0.0252	0.0001	0.1132
H13-H14	1	1.8007	1.8288	1.8218	0.0281	0.0470	-0.0438	0.0249	0.0000	0.1131
H12-H15	1	1.9291	2.0251	2.0009	0.0960	0.0519	0.0361	0.0079	0.0001	0.2210

N2-H13	1	2.0039	2.0269	2.0216	0.0230	0.0200	-0.0224	0.0254	0.0000	0.1027
N1-H11	1	2.0161	2.0356	2.0304	0.0195	0.0252	-0.0271	0.0214	0.0000	0.1030
N2-H14	1	2.0658	2.0867	2.0818	0.0209	0.0210	-0.0228	0.0226	0.0001	0.1004
N1-H12	1	2.0763	2.0902	2.0849	0.0139	0.0263	-0.0288	0.0164	0.0000	0.1047
N1-H10	1	2.0836	2.1051	2.1003	0.0215	0.0188	-0.0206	0.0233	0.0000	0.1008
C3-H16	1	2.0931	2.1115	2.1067	0.0184	0.0111	-0.0153	0.0226	0.0000	0.1010
C3-H15	1	2.1175	2.1389	2.1340	0.0213	0.0285	-0.0307	0.0236	-0.0001	0.1019
N2-H10	1	2.1322	2.1549	2.1503	0.0227	0.0103	-0.0141	0.0265	0.0000	0.1000
C5-H20	1	2.1420	2.1698	2.1656	0.0278	0.0572	-0.0593	0.0299	0.0000	0.0960
C7-H12	1	2.1510	2.1757	2.1721	0.0247	0.0572	-0.0587	0.0261	0.0001	0.0884
C4-H18	1	2.1515	2.1799	2.1763	0.0284	0.0611	-0.0626	0.0300	-0.0001	0.0889
C9-H15	1	2.1529	2.1782	2.1741	0.0253	0.0444	-0.0456	0.0264	0.0001	0.0942
C5-H22	1	2.1542	2.1746	2.1709	0.0204	0.0517	-0.0528	0.0215	0.0000	0.0894
C4-H19	1	2.1551	2.1810	2.1760	0.0259	0.0337	-0.0354	0.0276	0.0000	0.1038
C8-H14	1	2.1566	2.1821	2.1781	0.0255	0.0450	-0.0459	0.0264	0.0000	0.0936
C7-H11	1	2.1587	2.1806	2.1758	0.0219	0.0372	-0.0387	0.0234	0.0000	0.1018
C5-H21	1	2.1608	2.2258	2.2065	0.0650	0.0235	-0.0038	0.0453	0.0000	0.2067
C6-H24	1	2.1614	2.1820	2.1779	0.0205	0.0457	-0.0465	0.0214	-0.0001	0.0947
C4-H17	1	2.1624	2.1816	2.1787	0.0192	0.0619	-0.0626	0.0200	-0.0001	0.0799
C8-H13	1	2.1647	2.1921	2.1884	0.0273	0.0588	-0.0601	0.0286	0.0000	0.0899
C9-H16	1	2.1671	2.1904	2.1863	0.0233	0.0471	-0.0486	0.0249	-0.0001	0.0938
H10-H14	1	2.1692	2.1884	2.1838	0.0192	0.0370	-0.0382	0.0205	-0.0001	0.0994
C6-H25	1	2.1715	2.1937	2.1897	0.0222	0.0427	-0.0433	0.0228	0.0000	0.0936
C6-H23	1	2.1730	2.2001	2.1971	0.0271	0.0678	-0.0686	0.0279	0.0000	0.0821
C6-H10	1	2.1791	2.1982	2.1934	0.0190	0.0125	-0.0135	0.0201	-0.0001	0.1017
N1-C5	1	2.2972	2.4279	2.3877	0.1307	0.0964	0.0943	-0.0600	0.0000	0.3138
N2-C4	1	2.3816	2.4044	2.4024	0.0228	0.0062	-0.0077	0.0244	-0.0001	0.0698
C5-C3	1	2.3979	2.4213	2.4192	0.0234	0.0041	-0.0059	0.0252	0.0000	0.0703
N1-H14	1	2.4174	2.4357	2.4338	0.0182	0.0054	-0.0060	0.0188	0.0000	0.0669
N1-C7	1	2.4258	2.4514	2.4409	0.0256	0.0167	-0.0125	0.0214	0.0000	0.1597
N2-H12	1	2.4420	2.4834	2.4728	0.0414	0.0170	-0.0121	0.0365	0.0000	0.1613
N2-C8	1	2.4444	2.4651	2.4632	0.0207	0.0188	-0.0193	0.0212	0.0000	0.0677
C4-C3	1	2.4472	2.4584	2.4564	0.0112	0.0160	-0.0161	0.0113	0.0000	0.0705
H12-H18	1	2.4677	2.5094	2.5014	0.0418	0.0182	-0.0105	0.0341	0.0000	0.1419
C3-H14	1	2.4704	2.4871	2.4853	0.0166	0.0042	-0.0049	0.0173	0.0000	0.0660
H14-H20	1	2.4774	2.5202	2.5082	0.0428	0.0632	-0.0641	0.0436	0.0001	0.1726
H15-H24	1	2.4819	2.5450	2.5324	0.0631	0.0456	-0.0433	0.0608	0.0000	0.1784
H11-H19	1	2.4843	2.5243	2.5122	0.0400	0.0695	-0.0689	0.0394	0.0000	0.1738
H10-H16	1	2.4958	2.5231	2.5126	0.0273	0.0648	-0.0642	0.0267	0.0000	0.1618
H13-H22	1	2.5054	2.5367	2.5245	0.0313	0.0473	-0.0449	0.0290	-0.0001	0.1746
H12-H17	1	2.5056	2.5203	2.5086	0.0147	0.0665	-0.0659	0.0141	0.0000	0.1709
C3-C9	1	2.5059	2.5548	2.5437	0.0489	0.0652	-0.0636	0.0474	-0.0001	0.1682
H11-H17	1	2.5120	2.5412	2.5288	0.0292	0.0502	-0.0488	0.0278	0.0000	0.1763
H15-H23	1	2.5171	2.5367	2.5242	0.0196	0.0540	-0.0517	0.0173	0.0000	0.1767
N2-C6	1	2.5185	2.5270	2.5250	0.0085	0.0057	-0.0048	0.0076	0.0000	0.0706

H13-H21	1	2.5237	2.5527	2.5412	0.0290	0.0490	-0.0469	0.0269	0.0000	0.1699
H16-H25	1	2.5327	2.5639	2.5559	0.0312	0.0089	-0.0118	0.0341	0.0000	0.1428
H14-H21	1	2.5340	2.5617	2.5595	0.0277	0.0145	-0.0155	0.0287	0.0000	0.0746
H16-H23	1	2.5382	2.5448	2.5318	0.0066	0.0445	-0.0420	0.0041	0.0000	0.1803
H18-H20	1	2.5448	2.5789	2.5685	0.0341	0.0743	-0.0734	0.0333	-0.0001	0.1624
C5-H10	1	2.5539	2.6218	2.5983	0.0680	0.0406	-0.0080	0.0354	0.0000	0.2480
C3-H12	1	2.5726	2.6351	2.6206	0.0625	0.0237	0.0054	0.0333	0.0001	0.1960
H10-H25	1	2.5726	2.5871	2.5738	0.0144	0.0252	-0.0288	0.0179	0.0001	0.1838
N1-C6	1	2.5916	2.6260	2.6184	0.0344	0.0159	-0.0087	0.0272	0.0000	0.1409
N2-H15	1	2.6129	2.6321	2.6304	0.0192	0.0063	-0.0047	0.0175	0.0001	0.0659
C4-H15	1	2.6610	2.7163	2.7054	0.0553	0.0448	-0.0426	0.0531	0.0000	0.1715
C6-H12	1	2.6679	2.7149	2.7036	0.0470	0.0166	0.0104	0.0200	0.0000	0.1745
N1-H19	1	2.6945	2.7291	2.7188	0.0346	0.0435	-0.0432	0.0343	0.0000	0.1670
N2-H22	1	2.7025	2.8005	2.6550	0.0981	0.0348	-0.0151	0.0783	0.0001	0.5756
N1-H18	1	2.7166	2.7505	2.7407	0.0339	0.0414	-0.0422	0.0346	0.0001	0.1634
N2-H20	1	2.7177	2.7601	2.7503	0.0424	0.0175	-0.0139	0.0387	0.0001	0.1639
C3-H24	1	2.7267	2.7645	2.7562	0.0378	0.0240	-0.0150	0.0288	0.0000	0.1507
C3-H25	1	2.7353	2.7475	2.7381	0.0122	0.0228	-0.0155	0.0049	0.0000	0.1598
N1-H15	1	2.7629	2.7714	2.7619	0.0085	0.0201	-0.0197	0.0081	0.0000	0.1610
C9-H10	1	2.7792	2.8123	2.8024	0.0331	0.0124	-0.0167	0.0374	0.0000	0.1676
C3-H11	1	2.7816	2.7610	2.7513	-0.0206	0.0441	-0.0421	-0.0226	0.0000	0.1618
C3-H13	1	2.8019	2.8419	2.8321	0.0399	0.0367	-0.0343	0.0375	0.0000	0.1663
H10-H13	1	2.8125	2.8686	2.8562	0.0561	0.0445	-0.0447	0.0563	0.0000	0.1879
N1-H20	1	2.8647	2.8694	2.8608	0.0047	0.0162	-0.0223	0.0108	0.0000	0.1559
H11-H15	1	2.8649	2.9552	2.9308	0.0903	0.0339	-0.0193	0.0757	0.0000	0.2684
C4-C6	1	2.8800	2.8869	2.8664	0.0070	0.0152	-0.0216	0.0134	0.0000	0.2412
N1-H16	1	2.9277	3.0505	3.0121	0.1228	0.0447	0.0210	0.0570	0.0001	0.3426
N2-H24	1	2.9904	3.0583	3.0262	0.0679	0.0391	-0.0464	0.0751	0.0001	0.3106
N2-H18	1	3.0086	3.0381	3.0350	0.0295	0.0060	-0.0013	0.0248	0.0000	0.0966
H19-H20	1	3.0488	3.0713	3.0665	0.0225	0.0267	-0.0448	0.0405	0.0001	0.1213
H18-H22	1	3.0563	3.0969	3.0470	0.0407	0.0312	-0.0007	0.0102	0.0000	0.3724
H12-H19	1	3.0582	3.1206	3.0939	0.0624	0.0398	0.0435	-0.0210	0.0001	0.2911
H10-H15	1	3.0597	3.0878	3.0846	0.0281	0.0749	-0.0902	0.0434	0.0000	0.0988
H13-H20	1	3.0635	3.0926	3.0897	0.0291	0.0725	-0.0877	0.0443	0.0000	0.0950
H11-H18	1	3.0660	3.0897	3.0873	0.0237	0.0773	-0.0937	0.0400	0.0001	0.0857
H14-H22	1	3.0711	3.0971	3.0953	0.0260	0.0908	-0.1075	0.0427	0.0000	0.0748
H15-H25	1	3.0715	3.0999	3.0972	0.0284	0.0746	-0.0913	0.0450	0.0001	0.0911
H16-H24	1	3.0733	3.1021	3.0996	0.0288	0.0805	-0.0974	0.0457	0.0000	0.0885
H11-H16	1	3.1208	3.1840	3.1243	0.0632	0.0164	-0.0138	0.0606	0.0000	0.4148
H10-H24	1	3.1252	3.1782	3.1702	0.0530	0.0139	-0.0189	0.0580	0.0000	0.1596
H12-H16	1	3.1674	3.1554	3.1375	-0.0120	0.0352	-0.0204	-0.0269	0.0001	0.2339
C7-H20	1	3.2540	3.3407	3.3153	0.0867	0.0410	0.0410	0.0048	-0.0001	0.2949
C6-H11	1	3.2589	3.2747	3.2714	0.0157	0.0177	-0.0332	0.0312	0.0000	0.1040
N1-C8	1	3.2723	3.2936	3.2900	0.0213	0.0132	-0.0261	0.0342	0.0000	0.1092
C8-H18	1	3.3027	3.3119	3.3060	0.0092	0.0106	-0.0171	0.0157	0.0000	0.1383

N2-C7	1	3.3509	3.3643	3.3603	0.0135	0.0187	-0.0317	0.0264	0.0001	0.1160
N2-H11	1	3.3578	3.3788	3.3757	0.0210	0.0081	-0.0167	0.0296	0.0000	0.1030
N2-C9	1	3.3648	3.4191	3.4022	0.0543	0.0230	-0.0132	0.0445	0.0000	0.2389
N1-H13	1	3.3849	3.4023	3.3994	0.0174	0.0237	-0.0406	0.0342	0.0001	0.0983
C4-H16	1	3.3896	3.4100	3.4074	0.0204	0.0292	-0.0443	0.0355	0.0000	0.0947
H13-H24	1	3.4411	3.5166	3.5003	0.0755	0.0320	-0.0132	0.0567	0.0000	0.2396
C4-H10	1	3.4752	3.5641	3.5413	0.0889	0.0276	-0.0041	0.0654	0.0000	0.2855
N2-H16	1	3.4756	3.4972	3.4945	0.0215	0.0275	-0.0455	0.0396	-0.0001	0.0966
N1-H17	1	3.5334	3.5615	3.5597	0.0281	0.0044	-0.0104	0.0341	0.0000	0.0795
N2-H21	1	3.5528	3.5981	3.5882	0.0453	0.0204	-0.0131	0.0380	0.0000	0.1897
C3-H23	1	3.5536	3.5868	3.5824	0.0332	0.0087	-0.0097	0.0342	0.0000	0.1253
C4-C5	1	3.5564	3.5832	3.5644	0.0268	0.0094	-0.0139	0.0313	0.0000	0.2511
C4-H20	1	3.5710	3.6602	3.6380	0.0892	0.0198	-0.0019	0.0713	0.0000	0.2860
H10-H11	1	3.5994	3.6569	3.6391	0.0576	0.0299	-0.0498	0.0774	0.0001	0.2528
C5-H18	1	3.6087	3.7167	3.6645	0.1080	0.0428	0.0243	0.0409	0.0000	0.4303
N1-H22	1	3.6285	3.6699	3.6606	0.0414	0.0121	-0.0151	0.0444	0.0000	0.1849
H10-H12	1	3.6458	3.6827	3.6762	0.0369	0.0164	-0.0227	0.0432	0.0000	0.1546
N2-H25	1	3.6524	3.7074	3.6847	0.0549	0.0268	0.0036	0.0245	0.0000	0.2872
C3-C8	1	3.6545	3.8122	3.7579	0.1578	0.0483	0.0078	0.1017	0.0000	0.4483
N2-H19	1	3.6683	3.6650	3.6477	-0.0033	0.0268	-0.0114	-0.0187	0.0000	0.2508
C5-C6	1	3.6751	3.7268	3.7105	0.0518	0.0293	-0.0500	0.0725	0.0000	0.2439
C3-C7	1	3.6768	3.7050	3.7031	0.0282	0.0129	-0.0244	0.0397	0.0000	0.0830
C5-H24	1	3.6843	3.7996	3.7469	0.1153	0.0275	-0.0186	0.1064	0.0000	0.4435
H10-H23	1	3.6973	3.7201	3.6712	0.0228	0.0230	-0.0165	0.0164	-0.0001	0.4172
C5-H12	1	3.7165	3.7309	3.7293	0.0144	0.0096	-0.0247	0.0296	-0.0001	0.0775
C4-H14	1	3.7196	3.7358	3.6879	0.0162	0.0230	-0.0100	0.0032	0.0000	0.4144
C3-H20	1	3.7208	3.7337	3.7320	0.0129	0.0055	-0.0101	0.0175	0.0000	0.0784
N1-C9	1	3.7499	3.7764	3.7691	0.0265	0.0294	-0.0516	0.0487	0.0000	0.1659
C7-C8	1	3.7702	3.7870	3.7665	0.0168	0.0086	-0.0024	0.0106	0.0000	0.2760
C6-H13	1	3.7809	3.7491	3.7293	-0.0318	0.0298	-0.0155	-0.0461	0.0000	0.2696
C6-H14	1	3.7859	3.8246	3.8172	0.0387	0.0133	-0.0205	0.0459	0.0000	0.1673
C3-H18	1	3.7890	3.8097	3.8026	0.0207	0.0106	-0.0179	0.0281	-0.0001	0.1642
C9-H13	1	3.7915	3.7962	3.7886	0.0047	0.0170	-0.0180	0.0057	0.0000	0.1699
C8-H10	1	3.8070	3.8634	3.8527	0.0564	0.0290	-0.0384	0.0658	0.0000	0.2020
C9-H12	1	3.8476	3.8635	3.8622	0.0159	0.0085	-0.0206	0.0279	0.0001	0.0702
C7-H22	1	3.8534	3.8812	3.8733	0.0279	0.0153	-0.0313	0.0439	0.0000	0.1742
C8-H19	1	3.8974	3.8822	3.8562	-0.0152	0.0358	-0.0038	-0.0471	-0.0001	0.3153
H13-H25	1	3.9083	3.9440	3.9308	0.0357	0.0130	0.0024	0.0203	0.0000	0.2302
C4-C8	1	3.9109	3.9067	3.8985	-0.0043	0.0136	-0.0203	0.0024	0.0000	0.1783
N1-H24	1	3.9142	3.9540	3.9485	0.0398	0.0145	-0.0174	0.0427	0.0000	0.1478
C5-C7	1	3.9198	3.9792	3.9707	0.0594	0.0106	-0.0147	0.0635	0.0000	0.1842
C5-H15	1	3.9217	3.9478	3.9409	0.0262	0.0071	-0.0054	0.0245	0.0000	0.1640
C7-H15	1	3.9315	3.9703	3.9645	0.0388	0.0149	-0.0353	0.0592	0.0000	0.1516
H12-H24	1	3.9452	3.9352	3.9271	-0.0099	0.0296	-0.0432	0.0037	0.0000	0.1775
H12-H20	1	3.9608	3.9830	3.9701	0.0222	0.0173	-0.0284	0.0333	0.0000	0.2257

N1-H21	1	3.9745	4.0014	3.9897	0.0268	0.0222	-0.0347	0.0393	0.0000	0.2146
C3-H19	1	3.9908	3.9978	3.9908	0.0070	0.0112	-0.0211	0.0169	0.0000	0.1664
C3-H22	1	3.9962	4.0685	4.0149	0.0723	0.0309	-0.0717	0.1131	0.0000	0.4435
H14-H18	1	4.0016	4.0272	4.0235	0.0255	0.0116	-0.0249	0.0389	-0.0001	0.1209
H17-H20	1	4.0167	4.0743	4.0507	0.0576	0.0300	-0.0314	0.0590	0.0000	0.3078
H18-H21	1	4.0477	4.0488	4.0195	0.0011	0.0369	0.0129	-0.0487	0.0000	0.3407
H10-H20	1	4.0544	4.0994	4.0920	0.0450	0.0238	-0.0457	0.0669	0.0000	0.1737
N2-H17	1	4.0881	4.1134	4.1070	0.0254	0.0288	-0.0497	0.0462	0.0001	0.1616
C5-C9	1	4.0889	4.1152	4.1106	0.0263	0.0153	-0.0379	0.0489	0.0000	0.1367
C4-H22	1	4.1027	4.1794	4.1535	0.0767	0.0222	-0.0359	0.0904	0.0000	0.3262
N1-H25	1	4.1059	4.1468	4.1405	0.0409	0.0276	-0.0520	0.0652	0.0001	0.1604
C5-H19	1	4.1169	4.1868	4.1715	0.0699	0.0295	-0.0515	0.0918	0.0001	0.2507
H12-H22	1	4.1219	4.1507	4.1400	0.0288	0.0241	-0.0315	0.0362	0.0000	0.2097
N2-H23	1	4.1249	4.1839	4.1626	0.0590	0.0262	-0.0433	0.0761	0.0000	0.2963
H13-H15	1	4.1273	4.1368	4.1307	0.0095	0.0175	-0.0237	0.0158	-0.0001	0.1577
H15-H18	1	4.1366	4.1667	4.1226	0.0301	0.0302	-0.0363	0.0363	-0.0001	0.4083
H14-H19	1	4.1402	4.1811	4.1739	0.0409	0.0290	-0.0429	0.0548	0.0000	0.1734
H12-H14	1	4.1628	4.1915	4.1849	0.0286	0.0228	-0.0390	0.0448	0.0000	0.1650
H14-H24	1	4.1863	4.2598	4.2303	0.0736	0.0301	-0.0349	0.0784	0.0000	0.3522
C8-H12	1	4.2179	4.2752	4.2463	0.0573	0.0244	-0.0608	0.0937	0.0000	0.3384
H19-H22	1	4.2449	4.2951	4.2830	0.0502	0.0171	-0.0281	0.0613	-0.0001	0.2275
C5-H25	1	4.2638	4.2965	4.2887	0.0327	0.0185	-0.0353	0.0496	-0.0001	0.1829
C7-H14	1	4.2641	4.2555	4.2505	-0.0086	0.0173	-0.0431	0.0171	0.0001	0.1453
H14-H25	1	4.2915	4.3249	4.3029	0.0334	0.0202	-0.0087	0.0218	0.0001	0.3056
C5-H11	1	4.3476	4.3326	4.3162	-0.0150	0.0158	-0.0338	0.0030	0.0000	0.2623
C4-H13	1	4.3710	4.3982	4.3953	0.0272	0.0132	-0.0355	0.0495	0.0000	0.1125
C4-C9	1	4.4153	4.4618	4.4522	0.0465	0.0221	-0.0364	0.0608	0.0000	0.2058
H11-H14	1	4.4161	4.4066	4.3950	-0.0095	0.0236	-0.0384	0.0052	0.0001	0.2250
H12-H13	1	4.4279	4.5144	4.4785	0.0865	0.0236	-0.0396	0.1025	0.0000	0.3942
C9-H14	1	4.4841	4.5140	4.5090	0.0299	0.0198	-0.0406	0.0507	0.0000	0.1493
H14-H15	1	4.4875	4.5189	4.5125	0.0314	0.0248	-0.0393	0.0459	0.0000	0.1696
H11-H20	1	4.5138	4.5401	4.5370	0.0264	0.0216	-0.0455	0.0503	0.0000	0.1190
C6-C7	1	4.5262	4.5437	4.5407	0.0175	0.0159	-0.0425	0.0441	0.0000	0.1169
H15-H17	1	4.5448	4.5993	4.5722	0.0544	0.0203	-0.0216	0.0557	0.0000	0.3477
H12-H23	1	4.5457	4.5738	4.5674	0.0281	0.0295	-0.0663	0.0649	0.0000	0.1709
H14-H16	1	4.5539	4.5975	4.5876	0.0436	0.0180	-0.0426	0.0682	0.0000	0.2125
H13-H18	1	4.5632	4.6030	4.5944	0.0397	0.0226	-0.0478	0.0649	0.0000	0.1983
C5-H16	1	4.5804	4.6531	4.6343	0.0728	0.0275	-0.0372	0.0825	0.0000	0.2965
C3-H21	1	4.5910	4.6106	4.5912	0.0196	0.0162	-0.0494	0.0529	-0.0001	0.2897
C7-H10	1	4.6151	4.6195	4.6037	0.0044	0.0212	-0.0492	0.0324	0.0000	0.2671
H10-H22	1	4.6153	4.7465	4.7013	0.1312	0.0311	-0.0051	0.1052	0.0000	0.4639
H10-H21	1	4.6373	4.6732	4.6630	0.0359	0.0174	-0.0269	0.0455	-0.0001	0.2162
C3-H17	1	4.6475	4.6549	4.6443	0.0073	0.0193	-0.0450	0.0331	-0.0001	0.2176
C4-H24	1	4.6737	4.6809	4.6783	0.0072	0.0190	-0.0441	0.0323	0.0000	0.1097
C9-H11	1	4.6865	4.7847	4.7594	0.0982	0.0202	-0.0114	0.0895	-0.0001	0.3483

H10-H19	1	4.6948	4.6880	4.6720	-0.0068	0.0197	-0.0403	0.0137	0.0001	0.2713
C6-H18	1	4.7051	4.8012	4.7836	0.0961	0.0246	-0.0113	0.0829	-0.0001	0.2904
N1-H23	1	4.7054	4.6747	4.6606	-0.0307	0.0169	-0.0243	-0.0234	0.0001	0.2562
H10-H18	1	4.7211	4.7735	4.7560	0.0525	0.0276	-0.0219	0.0468	0.0000	0.2877
H12-H25	1	4.7337	4.7916	4.7728	0.0579	0.0238	-0.0232	0.0573	0.0000	0.2989
H13-H16	1	4.7430	4.7687	4.7616	0.0258	0.0202	-0.0488	0.0544	0.0000	0.1837
H15-H19	1	4.8025	4.8198	4.8181	0.0172	0.0052	-0.0258	0.0378	0.0000	0.0892
C7-H16	1	4.8066	4.8211	4.8131	0.0145	0.0101	-0.0215	0.0259	0.0000	0.1969
H17-H22	1	4.8155	4.8850	4.8774	0.0695	0.0140	-0.0187	0.0742	0.0000	0.1927
H19-H21	1	4.9018	4.9296	4.9275	0.0279	0.0053	-0.0238	0.0464	0.0000	0.1026
C7-H21	1	4.9381	4.9869	4.9780	0.0488	0.0186	-0.0396	0.0697	0.0001	0.2098
C8-H17	1	4.9535	4.9994	4.9918	0.0459	0.0186	-0.0478	0.0751	0.0000	0.1947
C8-H11	1	4.9536	5.0021	4.9922	0.0484	0.0155	-0.0279	0.0609	-0.0001	0.2226
C6-C8	1	4.9542	4.9681	4.9667	0.0139	0.0088	-0.0255	0.0306	0.0000	0.0847
H13-H23	1	4.9954	5.0993	5.0806	0.1039	0.0278	-0.0339	0.1100	0.0000	0.3077
C7-H13	1	4.9963	5.0200	5.0137	0.0237	0.0133	-0.0331	0.0435	0.0000	0.1770
H22-H24	1	5.0349	5.0234	5.0177	-0.0115	0.0166	-0.0534	0.0254	-0.0001	0.1690
C4-H25	1	5.0378	5.0939	5.0588	0.0561	0.0307	-0.0656	0.0911	-0.0001	0.4200
H15-H22	1	5.0569	5.0798	5.0575	0.0229	0.0180	-0.0314	0.0363	0.0000	0.3343
C6-H19	1	5.0654	5.0340	5.0198	-0.0314	0.0237	-0.0363	-0.0188	0.0000	0.2655
C4-H21	1	5.0862	5.0775	5.0706	-0.0088	0.0167	-0.0355	0.0100	0.0000	0.1863
C8-H15	1	5.1158	5.1128	5.1032	-0.0029	0.0099	-0.0365	0.0236	0.0001	0.2205
C8-H24	1	5.1201	5.0949	5.0887	-0.0252	0.0193	-0.0455	0.0010	0.0000	0.1776
C6-H17	1	5.1234	5.1391	5.1323	0.0157	0.0192	-0.0266	0.0232	-0.0001	0.1871
C4-H23	1	5.1300	5.1716	5.1642	0.0416	0.0207	-0.0388	0.0596	0.0001	0.1954
C5-H17	1	5.1458	5.1530	5.1455	0.0072	0.0203	-0.0401	0.0270	0.0000	0.1967
H11-H24	1	5.1500	5.1647	5.1480	0.0147	0.0298	-0.0303	0.0152	0.0000	0.2928
C6-H22	1	5.1695	5.1553	5.1394	-0.0142	0.0273	-0.0416	0.0001	0.0000	0.2843
C6-H20	1	5.1724	5.1573	5.1283	-0.0151	0.0220	-0.0344	-0.0026	-0.0001	0.3834
H15-H20	1	5.1872	5.2753	5.2279	0.0882	0.0275	-0.0744	0.1350	0.0001	0.4840
H11-H25	1	5.1936	5.2397	5.2267	0.0461	0.0309	-0.0335	0.0486	0.0001	0.2603
H11-H23	1	5.1993	5.2574	5.2485	0.0581	0.0203	-0.0456	0.0834	0.0000	0.2157
H11-H22	1	5.2628	5.3164	5.3069	0.0536	0.0072	-0.0325	0.0789	0.0000	0.2242
C5-H23	1	5.2641	5.3084	5.2864	0.0443	0.0307	-0.0943	0.1079	0.0000	0.3327
H11-H13	1	5.3080	5.4439	5.4187	0.1359	0.0248	-0.0193	0.1304	0.0000	0.3702
H13-H19	1	5.3220	5.4006	5.3787	0.0786	0.0173	-0.0388	0.1000	0.0001	0.3425
H16-H19	1	5.3264	5.3647	5.3548	0.0383	0.0237	-0.0625	0.0771	0.0000	0.2301
H16-H18	1	5.3395	5.3215	5.3006	-0.0180	0.0195	-0.0656	0.0280	0.0001	0.3269
H16-H17	1	5.4083	5.4501	5.4283	0.0419	0.0313	-0.0579	0.0685	0.0000	0.3438
H12-H21	1	5.4777	5.4861	5.4770	0.0083	0.0274	-0.0627	0.0436	0.0000	0.2223
H14-H17	1	5.5597	5.6232	5.6017	0.0635	0.0153	-0.0596	0.1078	0.0000	0.3446
H10-H17	1	5.5900	5.5203	5.5048	-0.0696	0.0229	-0.0751	-0.0174	0.0000	0.2889
C8-C9	1	5.6143	5.6303	5.6174	0.0160	0.0237	-0.0720	0.0643	0.0000	0.2673
H14-H23	1	5.6548	5.6843	5.6815	0.0294	0.0106	-0.0470	0.0659	-0.0001	0.1239
C9-H22	1	5.6641	5.6690	5.6667	0.0049	0.0097	-0.0514	0.0466	0.0000	0.1154

H20-H24	1	5.6742	5.6863	5.6769	0.0120	0.0269	-0.0694	0.0546	-0.0001	0.2287
H18-H24	1	5.7220	5.7483	5.7391	0.0262	0.0193	-0.0535	0.0604	0.0000	0.2279
H21-H24	1	5.7647	5.7858	5.7784	0.0211	0.0145	-0.0512	0.0578	0.0000	0.2068
C8-H16	1	5.7916	5.8635	5.8320	0.0720	0.0237	-0.0781	0.1264	0.0000	0.4253
C8-H25	1	5.8063	5.8150	5.8125	0.0087	0.0140	-0.0523	0.0469	0.0001	0.1213
C7-C9	1	5.8202	5.8673	5.8608	0.0471	0.0219	-0.0557	0.0809	0.0000	0.1942
C7-H24	1	5.8419	5.8435	5.8351	0.0015	0.0191	-0.0667	0.0491	0.0000	0.2208
H16-H20	1	5.8420	5.8514	5.8493	0.0094	0.0157	-0.0494	0.0431	0.0000	0.1132
C6-H21	1	5.8581	5.8210	5.8122	-0.0371	0.0210	-0.0618	0.0037	0.0000	0.2242
H17-H21	1	5.8947	5.9256	5.9182	0.0309	0.0197	-0.0703	0.0814	0.0001	0.2093
C9-H18	1	5.8996	5.8877	5.8802	-0.0119	0.0228	-0.0541	0.0193	0.0001	0.2087
H11-H21	1	5.9280	5.9049	5.8951	-0.0231	0.0178	-0.0590	0.0181	0.0000	0.2402
H13-H17	1	5.9455	6.0311	6.0198	0.0856	0.0120	-0.0447	0.1183	0.0000	0.2605
C9-H20	1	6.1074	6.2097	6.1843	0.1024	0.0182	-0.0602	0.1444	0.0000	0.3943
H16-H21	1	6.1161	6.1217	6.1157	0.0055	0.0245	-0.0576	0.0386	0.0000	0.1912
H22-H25	1	6.1588	6.1757	6.1599	0.0169	0.0273	-0.0942	0.0837	0.0001	0.3102
H16-H22	1	6.1821	6.2488	6.2253	0.0667	0.0188	-0.0593	0.1072	0.0000	0.3820
C9-H21	1	6.2070	6.2359	6.2344	0.0289	0.0045	-0.0405	0.0649	0.0000	0.0969
H20-H25	1	6.2325	6.2703	6.2603	0.0378	0.0114	-0.0619	0.0882	0.0001	0.2494
H21-H25	1	6.2853	6.4108	6.3919	0.1254	0.0248	-0.0388	0.1394	0.0000	0.3466
C7-H25	1	6.2888	6.3570	6.3484	0.0682	0.0138	-0.0450	0.0994	0.0000	0.2332
C9-H19	1	6.3712	6.4110	6.4042	0.0397	0.0115	-0.0520	0.0802	0.0000	0.2078
C9-H17	1	6.3890	6.4609	6.4526	0.0719	0.0162	-0.0520	0.1077	0.0000	0.2301
C7-H23	1	6.5116	6.5239	6.5208	0.0123	0.0133	-0.0720	0.0710	0.0000	0.1424
H17-H24	1	6.5366	6.5433	6.5383	0.0067	0.0124	-0.0622	0.0566	-0.0001	0.1821
H19-H24	1	6.5386	6.6098	6.5968	0.0712	0.0202	-0.0640	0.1150	0.0000	0.2916
H18-H25	1	6.7974	6.8406	6.8304	0.0432	0.0230	-0.0799	0.1001	0.0000	0.2629
C8-H23	1	6.8044	6.7844	6.7751	-0.0200	0.0203	-0.0930	0.0527	0.0000	0.2493
H22-H23	1	6.8112	6.8229	6.8148	0.0117	0.0189	-0.0819	0.0747	0.0000	0.2351
H18-H23	1	6.9442	7.0140	7.0023	0.0698	0.0146	-0.0783	0.1334	0.0001	0.2850
H16-H21	1	7.0310	7.0572	7.0544	0.0263	0.0092	-0.0617	0.0788	0.0000	0.1405
H19-H25	1	7.0678	7.1119	7.1025	0.0441	0.0145	-0.0618	0.0914	0.0000	0.2581
H17-H23	1	7.0937	7.0994	7.0974	0.0057	0.0103	-0.0666	0.0619	0.0001	0.1182
H20-H23	1	7.2094	7.2547	7.2472	0.0453	0.0185	-0.0738	0.1007	-0.0001	0.2339
H17-H25	1	7.2324	7.3010	7.2917	0.0686	0.0188	-0.0754	0.1253	-0.0001	0.2603
H19-H23	1	7.3146	7.3002	7.2934	-0.0144	0.0162	-0.0777	0.0471	0.0000	0.2221
H21-H23	1	7.9496	7.9474	7.9446	-0.0022	0.0136	-0.0912	0.0753	0.0001	0.1479

Table S16. Equilibrium (r_e) and thermal average (r_g , r_a) distances, vibrational corrections (Δ), and mean amplitudes (u) for internuclear distances of TEDA conformation **1h** (in Å), obtained for 291 K by GED refinement (initial approximation MP2/cc-PVTZ). n – number of equivalent parameters.

Atomic pair	n	r_e	r_g	r_a	Δr	$\Delta r(\text{har})$	$\Delta r(\text{kin})$	$\Delta r(\text{dyn})$	$\Delta r(\text{rot})$	u
C6-H15	1	1.0906	1.1131	1.1093	0.0225	0.0386	-0.0341	0.0180	0.0000	0.0656
C7-H19	1	1.0908	1.1139	1.1108	0.0231	0.0520	-0.0471	0.0181	0.0001	0.0588
C8-H20	1	1.0909	1.1146	1.1125	0.0237	0.0606	-0.0550	0.0180	0.0001	0.0497
C9-H23	1	1.0911	1.1159	1.1139	0.0249	0.0612	-0.0555	0.0192	0.0000	0.0485
C8-H22	1	1.0911	1.1135	1.1105	0.0224	0.0486	-0.0437	0.0175	0.0000	0.0582
C7-H18	1	1.0913	1.1131	1.1093	0.0218	0.0414	-0.0371	0.0175	0.0000	0.0656
C8-H21	1	1.0914	1.1175	1.1160	0.0261	0.0666	-0.0605	0.0200	0.0000	0.0422
C9-H24	1	1.0915	1.1139	1.1104	0.0224	0.0443	-0.0397	0.0179	-0.0001	0.0633
C7-H17	1	1.0924	1.1174	1.1159	0.0250	0.0648	-0.0587	0.0188	0.0001	0.0418
C3-H10	1	1.0925	1.1157	1.1127	0.0232	0.0539	-0.0488	0.0181	0.0000	0.0583
C9-H25	1	1.0926	1.1144	1.1100	0.0218	0.0320	-0.0277	0.0175	0.0000	0.0706
C4-H12	1	1.0927	1.1140	1.1089	0.0212	0.0154	-0.0115	0.0173	0.0000	0.0756
C4-H11	1	1.0928	1.1142	1.1098	0.0214	0.0320	-0.0276	0.0170	0.0000	0.0699
C5-H13	1	1.0942	1.1167	1.1123	0.0225	0.0313	-0.0271	0.0182	0.0001	0.0709
C6-H16	1	1.0948	1.1168	1.1129	0.0221	0.0388	-0.0342	0.0175	0.0000	0.0662
C5-H14	1	1.0973	1.1192	1.1145	0.0219	0.0292	-0.0249	0.0176	0.0000	0.0722
N2-C3	1	1.4189	1.4290	1.4273	0.0100	0.0048	-0.0034	0.0086	0.0000	0.0488
N1-C3	1	1.4344	1.4447	1.4430	0.0103	0.0052	-0.0036	0.0087	0.0000	0.0498
N1-C4	1	1.4382	1.4488	1.4472	0.0107	0.0051	-0.0032	0.0088	0.0000	0.0491
N2-C5	1	1.4392	1.4510	1.4494	0.0118	0.0065	-0.0047	0.0100	0.0000	0.0490
N1-N2	1	1.4801	1.4918	1.4898	0.0117	0.0046	-0.0040	0.0112	-0.0001	0.0540
C3-C6	1	1.5006	1.5143	1.5127	0.0137	0.0056	-0.0043	0.0123	0.0001	0.0496
C5-C8	1	1.5144	1.5278	1.5265	0.0134	0.0257	-0.0242	0.0119	0.0000	0.0433
C4-C7	1	1.5145	1.5278	1.5267	0.0133	0.0274	-0.0258	0.0117	0.0000	0.0408
C6-C9	1	1.5222	1.5341	1.5329	0.0119	0.0245	-0.0230	0.0104	0.0000	0.0426
H23-H25	1	1.7619	1.7931	1.7908	0.0312	0.1062	-0.1026	0.0275	0.0001	0.0649
H24-H25	1	1.7645	1.7959	1.7928	0.0314	0.0944	-0.0916	0.0286	0.0000	0.0747
H23-H24	1	1.7659	1.7952	1.7917	0.0293	0.0903	-0.0876	0.0266	0.0000	0.0794
H17-H18	1	1.7666	1.8004	1.7956	0.0338	0.0829	-0.0815	0.0323	0.0001	0.0924
H20-H21	1	1.7674	1.7970	1.7934	0.0296	0.0971	-0.0944	0.0270	-0.0001	0.0807
H18-H19	1	1.7678	1.7963	1.7906	0.0284	0.0742	-0.0732	0.0274	0.0000	0.1008
H20-H22	1	1.7684	1.7979	1.7928	0.0295	0.0835	-0.0821	0.0281	0.0000	0.0958
H21-H22	1	1.7695	1.7966	1.7901	0.0271	0.0570	-0.0538	0.0239	0.0000	0.1079
H17-H19	1	1.7718	1.7996	1.7950	0.0278	0.0818	-0.0800	0.0261	-0.0001	0.0907
H15-H16	1	1.7721	1.7993	1.7935	0.0273	0.0699	-0.0690	0.0264	0.0000	0.1018
H11-H12	1	1.7792	1.8075	1.8004	0.0283	0.0466	-0.0437	0.0254	0.0000	0.1129
H13-H14	1	1.7903	1.8182	1.8110	0.0279	0.0443	-0.0413	0.0249	0.0000	0.1141
H12-H15	1	1.9305	2.0185	1.9911	0.0880	0.0513	0.0369	-0.0003	0.0001	0.2339

N2-H13	1	2.0037	2.0284	2.0232	0.0248	0.0206	-0.0230	0.0271	0.0001	0.1025
N1-H11	1	2.0243	2.0456	2.0404	0.0213	0.0238	-0.0261	0.0235	0.0001	0.1030
N2-H14	1	2.0649	2.0867	2.0818	0.0218	0.0198	-0.0217	0.0237	0.0000	0.1011
N1-H12	1	2.0765	2.1067	2.1003	0.0302	0.0249	-0.0281	0.0334	0.0000	0.1151
N1-H10	1	2.0840	2.0993	2.0946	0.0154	0.0208	-0.0224	0.0170	0.0000	0.0993
C3-H16	1	2.0923	2.1138	2.1089	0.0215	0.0112	-0.0155	0.0258	0.0000	0.1017
C3-H15	1	2.1172	2.1382	2.1333	0.0210	0.0275	-0.0298	0.0232	0.0001	0.1014
N2-H10	1	2.1318	2.1508	2.1461	0.0190	0.0107	-0.0144	0.0228	-0.0001	0.1004
C5-H20	1	2.1515	2.1788	2.1751	0.0273	0.0637	-0.0652	0.0288	0.0000	0.0899
C7-H12	1	2.1524	2.1791	2.1753	0.0267	0.0467	-0.0477	0.0277	0.0000	0.0900
C4-H18	1	2.1535	2.1791	2.1752	0.0256	0.0560	-0.0577	0.0272	0.0001	0.0922
C9-H15	1	2.1544	2.1814	2.1767	0.0270	0.0503	-0.0521	0.0288	0.0000	0.1014
C5-H22	1	2.1551	2.1817	2.1768	0.0266	0.0362	-0.0379	0.0283	0.0000	0.1034
C4-H19	1	2.1576	2.1816	2.1766	0.0240	0.0376	-0.0393	0.0256	0.0001	0.1041
C8-H14	1	2.1577	2.1809	2.1772	0.0232	0.0565	-0.0579	0.0246	0.0000	0.0890
C7-H11	1	2.1592	2.1839	2.1798	0.0247	0.0438	-0.0449	0.0258	0.0000	0.0947
C5-H21	1	2.1624	2.1815	2.1788	0.0191	0.0644	-0.0650	0.0197	0.0000	0.0762
C6-H24	1	2.1647	2.1878	2.1850	0.0231	0.0596	-0.0603	0.0237	0.0001	0.0772
C4-H17	1	2.1672	2.1851	2.1824	0.0179	0.0479	-0.0486	0.0186	0.0000	0.0767
C8-H13	1	2.1692	2.1945	2.1896	0.0252	0.0350	-0.0365	0.0267	0.0000	0.1026
C9-H16	1	2.1707	2.1925	2.1883	0.0219	0.0422	-0.0430	0.0227	0.0000	0.0962
H10-H14	1	2.1712	2.1951	2.1909	0.0239	0.0451	-0.0458	0.0246	0.0000	0.0966
C6-H25	1	2.1730	2.2003	2.1969	0.0273	0.0669	-0.0678	0.0283	-0.0001	0.0870
C6-H23	1	2.1795	2.2030	2.1983	0.0234	0.0114	-0.0124	0.0244	0.0000	0.1013
C6-H10	1	2.1802	2.2211	2.2009	0.0409	0.0218	-0.0072	0.0263	0.0000	0.2110
N1-C5	1	2.2967	2.6212	2.5665	0.3244	0.0793	0.0952	0.1499	0.0000	0.3786
N2-C4	1	2.3951	2.4124	2.4103	0.0173	0.0046	-0.0065	0.0191	0.0001	0.0701
C5-C3	1	2.3963	2.4161	2.4141	0.0198	0.0053	-0.0067	0.0212	0.0000	0.0706
N1-H14	1	2.4059	2.4202	2.4184	0.0143	0.0062	-0.0070	0.0151	0.0000	0.0665
N1-C7	1	2.4111	2.4398	2.4298	0.0288	0.0170	-0.0111	0.0229	0.0000	0.1563
N2-H12	1	2.4364	2.4540	2.4521	0.0176	0.0191	-0.0193	0.0178	0.0000	0.0679
N2-C8	1	2.4407	2.4316	2.4214	-0.0091	0.0194	-0.0137	-0.0149	0.0001	0.1558
C4-C3	1	2.4468	2.4599	2.4578	0.0132	0.0184	-0.0185	0.0132	0.0001	0.0715
H12-H18	1	2.4699	2.4718	2.4701	0.0020	0.0051	-0.0058	0.0026	0.0001	0.0659
C3-H14	1	2.4785	2.5098	2.5016	0.0313	0.0170	-0.0116	0.0260	-0.0001	0.1434
H14-H20	1	2.4814	2.5342	2.5210	0.0528	0.0483	-0.0461	0.0506	0.0000	0.1818
H15-H24	1	2.4849	2.5132	2.5034	0.0284	0.0705	-0.0684	0.0263	0.0000	0.1558
H11-H19	1	2.5005	2.5297	2.5182	0.0292	0.0623	-0.0624	0.0293	0.0000	0.1693
H10-H16	1	2.5049	2.5337	2.5208	0.0287	0.0686	-0.0688	0.0290	-0.0001	0.1790
H13-H22	1	2.5052	2.5418	2.5303	0.0365	0.0612	-0.0609	0.0362	0.0000	0.1697
H12-H17	1	2.5054	2.5448	2.5345	0.0394	0.0691	-0.0668	0.0370	0.0001	0.1609
C3-C9	1	2.5060	2.5230	2.5101	0.0170	0.0464	-0.0441	0.0147	0.0000	0.1794
H11-H17	1	2.5096	2.5507	2.5384	0.0412	0.0480	-0.0464	0.0396	0.0000	0.1768
H15-H23	1	2.5114	2.5289	2.5206	0.0175	0.0103	-0.0135	0.0206	0.0001	0.1437
N2-C6	1	2.5170	2.5700	2.5574	0.0529	0.0515	-0.0501	0.0515	0.0000	0.1790

H13-H21	1	2.5212	2.5415	2.5395	0.0203	0.0052	-0.0044	0.0195	0.0000	0.0717
H16-H25	1	2.5300	2.5537	2.5415	0.0236	0.0488	-0.0468	0.0216	0.0000	0.1749
H14-H21	1	2.5338	2.5463	2.5442	0.0125	0.0131	-0.0140	0.0134	0.0000	0.0721
H16-H23	1	2.5379	2.5635	2.5512	0.0256	0.0471	-0.0447	0.0232	0.0000	0.1762
H18-H20	1	2.5446	2.5868	2.5736	0.0423	0.0717	-0.0726	0.0432	0.0000	0.1843
C5-H10	1	2.5541	2.5766	2.5531	0.0225	0.0411	-0.0071	-0.0115	0.0000	0.2443
C3-H12	1	2.5718	2.6880	2.6725	0.1162	0.0212	-0.0271	0.1221	0.0000	0.2038
H10-H25	1	2.5747	2.5164	2.5056	-0.0583	0.0265	0.0063	-0.0912	0.0001	0.1617
N1-C6	1	2.5906	2.6198	2.6122	0.0292	0.0179	-0.0105	0.0218	0.0000	0.1415
N2-H15	1	2.6130	2.6255	2.6239	0.0125	0.0055	-0.0038	0.0108	0.0000	0.0649
C4-H15	1	2.6604	2.7050	2.6949	0.0446	0.0479	-0.0451	0.0418	0.0000	0.1643
C6-H12	1	2.6686	2.7201	2.7083	0.0515	0.0175	0.0096	0.0244	0.0000	0.1793
N1-H19	1	2.6795	2.7175	2.7075	0.0381	0.0436	-0.0427	0.0371	0.0001	0.1645
N2-H22	1	2.7063	2.3369	2.1501	-0.3694	0.0429	-0.0189	-0.3933	-0.0001	0.5830
N1-H18	1	2.7189	2.6764	2.6668	-0.0425	0.0168	-0.0123	-0.0470	0.0000	0.1593
N2-H20	1	2.7278	2.7134	2.7071	-0.0144	0.0243	-0.0137	-0.0251	0.0001	0.1300
C3-H24	1	2.7286	2.7453	2.7360	0.0167	0.0420	-0.0410	0.0157	0.0000	0.1590
C3-H25	1	2.7369	2.8363	2.8239	0.0994	0.0193	-0.0142	0.0943	0.0000	0.1869
N1-H15	1	2.7467	2.7610	2.7162	0.0144	0.0366	-0.0124	-0.0099	0.0001	0.3456
C9-H10	1	2.7678	2.7260	2.7179	-0.0418	0.0216	-0.0200	-0.0434	0.0000	0.1471
C3-H11	1	2.7748	2.8573	2.8471	0.0825	0.0117	-0.0163	0.0871	0.0000	0.1706
C3-H13	1	2.7813	2.7750	2.7642	-0.0063	0.0464	-0.0452	-0.0075	0.0000	0.1717
H10-H13	1	2.8015	2.8417	2.8308	0.0402	0.0356	-0.0338	0.0384	0.0000	0.1752
N1-H20	1	2.8049	2.8367	2.8265	0.0318	0.0147	-0.0206	0.0377	0.0000	0.1693
H11-H15	1	2.8125	2.8180	2.8102	0.0055	0.0463	-0.0432	0.0024	0.0000	0.1460
C4-C6	1	2.9931	2.8619	2.8361	-0.1312	0.0459	-0.0456	-0.1316	0.0001	0.2568
N1-H16	1	3.0084	3.0219	3.0022	0.0134	0.0350	-0.0208	-0.0008	0.0000	0.2423
N2-H24	1	3.0096	2.9983	2.9953	-0.0113	0.0062	-0.0014	-0.0161	0.0000	0.0944
N2-H18	1	3.0495	3.0559	3.0516	0.0065	0.0261	-0.0439	0.0243	0.0000	0.1144
H19-H20	1	3.0593	2.8802	2.8258	-0.1791	0.0369	-0.0046	-0.2113	-0.0001	0.3745
H18-H22	1	3.0593	3.1337	3.1085	0.0743	0.0422	0.0420	-0.0099	0.0000	0.2875
H12-H19	1	3.0656	3.0903	3.0883	0.0247	0.0799	-0.0961	0.0410	-0.0001	0.0791
H10-H15	1	3.0678	3.0946	3.0916	0.0268	0.0722	-0.0876	0.0422	0.0000	0.0965
H13-H20	1	3.0713	3.1021	3.0996	0.0308	0.0898	-0.1070	0.0480	0.0000	0.0886
H11-H18	1	3.0713	3.1000	3.0972	0.0287	0.0779	-0.0946	0.0454	0.0000	0.0934
H14-H22	1	3.0734	3.0948	3.0938	0.0213	0.0824	-0.0983	0.0372	0.0000	0.0557
H15-H25	1	3.0737	3.1005	3.0973	0.0268	0.0690	-0.0845	0.0423	0.0000	0.0999
H16-H24	1	3.1243	2.8364	2.7644	-0.2879	0.0195	-0.0157	-0.2917	0.0000	0.4157
H11-H16	1	3.1464	3.1470	3.1284	0.0006	0.0162	-0.0221	0.0066	-0.0001	0.2396
H10-H24	1	3.1695	3.0737	3.0552	-0.0958	0.0401	-0.0244	-0.1115	0.0000	0.2337
H12-H16	1	3.2022	3.2091	3.2030	0.0069	0.0144	-0.0194	0.0118	0.0001	0.1395
C7-H20	1	3.2445	3.2645	3.2608	0.0200	0.0168	-0.0302	0.0334	0.0000	0.1086
C6-H11	1	3.2529	3.5036	3.4755	0.2507	0.0362	0.0426	0.1719	0.0000	0.3187
N1-C8	1	3.2706	3.3724	3.3371	0.1018	0.0436	0.0125	0.0457	0.0000	0.3429
C8-H18	1	3.2711	3.3049	3.3012	0.0338	0.0134	-0.0266	0.0469	0.0001	0.1099

N2-C7	1	3.3038	3.2440	3.2380	-0.0598	0.0134	-0.0199	-0.0534	0.0001	0.1376
N2-H11	1	3.3521	3.3286	3.3253	-0.0235	0.0190	-0.0315	-0.0111	0.0001	0.1042
N2-C9	1	3.3580	3.3720	3.3688	0.0140	0.0092	-0.0178	0.0226	0.0000	0.1032
N1-H13	1	3.3669	3.2608	3.2452	-0.1061	0.0275	-0.0151	-0.1186	0.0001	0.2203
C4-H16	1	3.3817	3.4013	3.3986	0.0196	0.0301	-0.0453	0.0349	-0.0001	0.0958
H13-H24	1	3.3845	3.4027	3.3998	0.0182	0.0269	-0.0438	0.0351	0.0000	0.0988
C4-H10	1	3.4379	3.5762	3.5586	0.1383	0.0284	-0.0106	0.1205	0.0000	0.2505
N2-H16	1	3.4636	3.5978	3.5759	0.1341	0.0180	-0.0043	0.1205	-0.0001	0.2814
N1-H17	1	3.4755	3.4912	3.4885	0.0156	0.0247	-0.0428	0.0337	0.0000	0.0967
N2-H21	1	3.4944	3.5156	3.5079	0.0211	0.0184	-0.0393	0.0421	-0.0001	0.1634
C3-H23	1	3.5515	3.6413	3.6366	0.0898	0.0066	-0.0077	0.0909	0.0000	0.1302
C4-C5	1	3.5516	3.5830	3.5812	0.0314	0.0040	-0.0097	0.0371	0.0000	0.0798
C4-H20	1	3.5546	3.5506	3.5411	-0.0041	0.0196	-0.0120	-0.0117	0.0000	0.1828
H10-H11	1	3.5587	3.4244	3.4041	-0.1343	0.0114	-0.0163	-0.1294	0.0000	0.2550
C5-H18	1	3.6106	3.5804	3.5297	-0.0303	0.0465	0.0241	-0.1009	0.0000	0.4186
N1-H22	1	3.6382	3.6552	3.6407	0.0170	0.0308	-0.0489	0.0351	0.0000	0.2282
H10-H12	1	3.6456	3.6831	3.6765	0.0375	0.0184	-0.0245	0.0436	0.0000	0.1555
N2-H25	1	3.6501	3.9190	3.8938	0.2689	0.0207	0.0062	0.2420	0.0000	0.3173
C3-C8	1	3.6534	3.7884	3.7365	0.1350	0.0489	0.0088	0.0773	0.0000	0.4408
N2-H19	1	3.6557	3.7532	3.7438	0.0975	0.0100	-0.0129	0.1004	0.0000	0.1884
C5-C6	1	3.6764	3.6336	3.6176	-0.0428	0.0328	-0.0528	-0.0228	0.0000	0.2364
C3-C7	1	3.6886	3.7414	3.7321	0.0528	0.0119	-0.0173	0.0582	0.0000	0.1854
C5-H24	1	3.6997	3.7131	3.7115	0.0134	0.0130	-0.0259	0.0263	0.0000	0.0758
H10-H23	1	3.7009	3.4164	3.3599	-0.2845	0.0278	-0.0194	-0.2929	0.0000	0.4142
C5-H12	1	3.7052	3.7295	3.7278	0.0243	0.0056	-0.0108	0.0295	0.0000	0.0801
C4-H14	1	3.7148	3.7020	3.7005	-0.0128	0.0118	-0.0272	0.0025	0.0001	0.0754
C3-H20	1	3.7170	4.0751	4.0307	0.3581	0.0168	-0.0080	0.3493	0.0000	0.4364
N1-C9	1	3.7507	3.7296	3.7224	-0.0210	0.0270	-0.0487	0.0008	-0.0001	0.1642
C7-C8	1	3.7549	3.7834	3.7624	0.0284	0.0270	-0.0082	0.0097	-0.0001	0.2808
C6-H13	1	3.7681	3.7754	3.7676	0.0073	0.0182	-0.0194	0.0085	0.0000	0.1710
C6-H14	1	3.7694	3.9722	3.9529	0.2028	0.0076	-0.0018	0.1970	0.0000	0.2782
C3-H18	1	3.7696	3.8025	3.7956	0.0329	0.0118	-0.0167	0.0379	-0.0001	0.1610
C9-H13	1	3.7850	3.7088	3.6884	-0.0762	0.0336	-0.0192	-0.0906	0.0000	0.2719
C8-H10	1	3.7979	3.7850	3.7781	-0.0128	0.0147	-0.0210	-0.0065	0.0000	0.1615
C9-H12	1	3.8094	3.8436	3.8268	0.0342	0.0258	-0.0072	0.0156	0.0000	0.2531
C7-H22	1	3.8477	3.8473	3.8076	-0.0005	0.0384	-0.0192	-0.0196	-0.0001	0.3854
C8-H19	1	3.8486	3.8517	3.8296	0.0032	0.0315	-0.0616	0.0332	0.0001	0.2877
H13-H25	1	3.8492	3.8659	3.8646	0.0167	0.0071	-0.0194	0.0289	0.0001	0.0709
C4-C8	1	3.8553	3.7528	3.7462	-0.1025	0.0175	-0.0324	-0.0876	0.0000	0.1535
N1-H24	1	3.8853	3.8941	3.8855	0.0087	0.0296	-0.0404	0.0195	0.0000	0.1814
C5-C7	1	3.8975	4.0547	4.0285	0.1572	0.0359	-0.0060	0.1273	0.0000	0.3234
C5-H15	1	3.9087	3.9742	3.9614	0.0656	0.0134	0.0021	0.0501	0.0000	0.2295
C7-H15	1	3.9206	3.9137	3.8961	-0.0069	0.0266	-0.0441	0.0106	0.0000	0.2603
H12-H24	1	3.9208	4.0560	4.0491	0.1352	0.0056	-0.0041	0.1337	0.0000	0.1677
H12-H20	1	3.9296	3.9663	3.9607	0.0367	0.0123	-0.0178	0.0423	-0.0001	0.1491

N1-H21	1	3.9313	3.9987	3.9859	0.0675	0.0183	-0.0252	0.0744	0.0000	0.2258
C3-H19	1	3.9452	3.8779	3.8698	-0.0674	0.0334	-0.0469	-0.0539	0.0000	0.1750
C3-H22	1	3.9713	4.0987	4.0847	0.1274	0.0195	-0.0339	0.1418	0.0000	0.2386
H14-H18	1	3.9841	3.9675	3.9542	-0.0165	0.0226	-0.0336	-0.0055	0.0000	0.2279
H17-H20	1	3.9934	3.9536	3.9465	-0.0398	0.0138	-0.0238	-0.0298	0.0000	0.1663
H18-H21	1	3.9994	3.7056	3.6427	-0.2938	0.0342	-0.0740	-0.2541	0.0001	0.4494
H10-H20	1	4.0022	4.0233	4.0196	0.0211	0.0111	-0.0247	0.0348	-0.0001	0.1214
N2-H17	1	4.0471	4.3022	4.2718	0.2551	0.0332	0.0134	0.2085	0.0000	0.3613
C5-C9	1	4.0878	4.1215	4.1169	0.0337	0.0159	-0.0387	0.0565	0.0000	0.1372
C4-H22	1	4.1038	4.1296	4.1237	0.0258	0.0299	-0.0544	0.0503	0.0000	0.1555
N1-H25	1	4.1197	4.2184	4.2107	0.0987	0.0153	-0.0233	0.1067	0.0000	0.1799
C5-H19	1	4.1198	4.1458	4.1400	0.0260	0.0286	-0.0508	0.0482	0.0000	0.1540
H12-H22	1	4.1276	4.1029	4.0814	-0.0247	0.0291	-0.0459	-0.0080	0.0001	0.2929
N2-H23	1	4.1398	3.9131	3.8657	-0.2266	0.0357	-0.0407	-0.2216	0.0000	0.4084
H13-H15	1	4.1401	4.1963	4.1892	0.0563	0.0271	-0.0412	0.0703	0.0001	0.1725
H15-H18	1	4.1435	4.1455	4.1400	0.0020	0.0248	-0.0468	0.0240	0.0000	0.1508
H14-H19	1	4.1458	4.2093	4.1984	0.0635	0.0212	-0.0327	0.0750	0.0000	0.2128
H12-H14	1	4.1594	4.1806	4.1731	0.0211	0.0112	-0.0176	0.0275	0.0000	0.1755
H14-H24	1	4.1645	4.1523	4.1462	-0.0122	0.0230	-0.0390	0.0038	0.0000	0.1585
C8-H12	1	4.2199	4.0844	4.0544	-0.1354	0.0272	-0.0632	-0.0995	0.0001	0.3370
H19-H22	1	4.2523	4.2540	4.2465	0.0017	0.0204	-0.0357	0.0169	0.0001	0.1784
C5-H25	1	4.2649	4.2060	4.2010	-0.0589	0.0209	-0.0466	-0.0332	0.0000	0.1434
C7-H14	1	4.2920	4.4657	4.4440	0.1736	0.0178	-0.0068	0.1626	0.0000	0.3091
H14-H25	1	4.3391	4.3719	4.3500	0.0329	0.0225	-0.0371	0.0474	0.0001	0.3070
C5-H11	1	4.3500	4.2054	4.1880	-0.1447	0.0191	-0.0371	-0.1266	-0.0001	0.2640
C4-H13	1	4.4278	4.4444	4.4086	0.0166	0.0243	-0.0400	0.0324	-0.0001	0.3935
C4-C9	1	4.4721	4.2612	4.2084	-0.2108	0.0367	0.0016	-0.2491	0.0000	0.4620
H11-H14	1	4.4828	4.5395	4.5345	0.0566	0.0168	-0.0376	0.0774	0.0000	0.1494
H12-H13	1	4.4910	4.6175	4.5957	0.1265	0.0281	-0.0366	0.1349	0.0001	0.3166
C9-H14	1	4.4950	4.5558	4.5487	0.0608	0.0221	-0.0382	0.0769	0.0000	0.1794
H14-H15	1	4.5112	4.5274	4.5243	0.0162	0.0221	-0.0468	0.0409	0.0000	0.1182
H11-H20	1	4.5219	4.5466	4.5438	0.0247	0.0133	-0.0327	0.0440	0.0001	0.1134
C6-C7	1	4.5240	4.5245	4.5216	0.0006	0.0190	-0.0456	0.0272	0.0000	0.1152
H15-H17	1	4.5464	4.5149	4.4877	-0.0315	0.0200	-0.0208	-0.0307	0.0000	0.3464
H12-H23	1	4.5937	4.4022	4.3825	-0.1915	0.0197	-0.0525	-0.1588	0.0001	0.2815
H14-H16	1	4.6139	4.7793	4.7620	0.1653	0.0198	-0.0500	0.1955	0.0000	0.2869
H13-H18	1	4.6377	4.7198	4.7098	0.0821	0.0150	-0.0246	0.0917	0.0000	0.2158
C5-H16	1	4.6404	4.6101	4.6020	-0.0303	0.0244	-0.0445	-0.0102	0.0000	0.1922
C3-H21	1	4.6458	4.7996	4.7872	0.1539	0.0173	-0.0450	0.1816	0.0000	0.2425
C7-H10	1	4.6761	4.6987	4.6960	0.0226	0.0165	-0.0418	0.0479	0.0000	0.1121
H10-H22	1	4.6939	4.8392	4.8226	0.1453	0.0196	-0.0415	0.1672	0.0000	0.2818
H10-H21	1	4.7021	4.8966	4.8701	0.1945	0.0259	-0.0380	0.2067	-0.0001	0.3606
C3-H17	1	4.7045	4.8429	4.8307	0.1384	0.0162	-0.0329	0.1551	0.0000	0.2429
C4-H24	1	4.7064	4.7570	4.7434	0.0507	0.0182	-0.0257	0.0582	0.0000	0.2541
C9-H11	1	4.7108	4.8104	4.7928	0.0996	0.0265	-0.0231	0.0962	0.0000	0.2906

H10-H19	1	4.7185	4.9596	4.9406	0.2411	0.0230	-0.0197	0.2378	0.0000	0.3083
C6-H18	1	4.7274	4.7333	4.7150	0.0059	0.0225	-0.0139	-0.0027	0.0000	0.2934
N1-H23	1	4.7369	4.8424	4.8326	0.1055	0.0222	-0.0349	0.1182	0.0000	0.2172
H10-H18	1	4.7447	4.6811	4.6747	-0.0636	0.0213	-0.0495	-0.0354	0.0000	0.1715
H12-H25	1	4.7479	4.6200	4.5916	-0.1279	0.0223	-0.0169	-0.1332	-0.0001	0.3582
H13-H16	1	4.7722	4.7756	4.7579	0.0034	0.0304	-0.0305	0.0035	0.0000	0.2893
H15-H19	1	4.7885	4.8294	4.8219	0.0410	0.0127	-0.0222	0.0505	0.0000	0.1908
C7-H16	1	4.8108	4.8324	4.8308	0.0216	0.0077	-0.0270	0.0409	0.0000	0.0859
H17-H22	1	4.8124	4.7987	4.7912	-0.0137	0.0176	-0.0273	-0.0040	0.0000	0.1886
H19-H21	1	4.8192	4.8426	4.8409	0.0233	0.0061	-0.0269	0.0441	0.0000	0.0890
C7-H21	1	4.8320	4.8233	4.8151	-0.0088	0.0112	-0.0193	-0.0006	-0.0001	0.1976
C8-H17	1	4.8528	4.8846	4.8701	0.0318	0.0322	-0.0438	0.0435	-0.0001	0.2655
C8-H11	1	4.8845	4.8593	4.8571	-0.0251	0.0050	-0.0241	-0.0060	0.0000	0.1026
C6-C8	1	4.9303	4.8740	4.8644	-0.0563	0.0171	-0.0294	-0.0441	0.0001	0.2151
H13-H23	1	4.9580	5.0365	5.0278	0.0784	0.0189	-0.0404	0.0999	0.0000	0.2084
C7-H13	1	4.9837	5.0231	5.0149	0.0394	0.0195	-0.0415	0.0614	0.0000	0.2020
H22-H24	1	4.9951	5.1257	5.1191	0.1306	0.0114	-0.0319	0.1511	0.0000	0.1830
C4-H25	1	5.0043	4.9573	4.9397	-0.0469	0.0270	-0.0336	-0.0404	0.0001	0.2913
H15-H22	1	5.0085	5.1082	5.0998	0.0998	0.0096	-0.0319	0.1220	0.0001	0.2081
C6-H19	1	5.0213	5.0076	4.9948	-0.0137	0.0289	-0.0381	-0.0045	0.0000	0.2512
C4-H21	1	5.0361	5.1823	5.1470	0.1462	0.0308	-0.0667	0.1821	0.0000	0.4244
C8-H15	1	5.0372	4.9904	4.9847	-0.0468	0.0200	-0.0569	-0.0099	0.0000	0.1685
C8-H24	1	5.0381	5.1063	5.0979	0.0682	0.0099	-0.0358	0.0941	0.0000	0.2072
C6-H17	1	5.0568	5.0427	5.0284	-0.0141	0.0263	-0.0393	-0.0012	0.0001	0.2663
C4-H23	1	5.0661	5.0689	5.0626	0.0028	0.0200	-0.0423	0.0251	0.0000	0.1788
C5-H17	1	5.1295	5.0842	5.0776	-0.0453	0.0216	-0.0480	-0.0189	0.0000	0.1819
H11-H24	1	5.1325	5.2640	5.2461	0.1316	0.0187	-0.0398	0.1527	0.0000	0.3061
C6-H22	1	5.1354	5.2694	5.2506	0.1340	0.0194	-0.0423	0.1570	-0.0001	0.3134
C6-H20	1	5.1748	5.1225	5.0937	-0.0523	0.0227	-0.0349	-0.0400	-0.0001	0.3812
H15-H20	1	5.1880	5.0959	5.0465	-0.0921	0.0271	-0.0739	-0.0453	0.0000	0.4880
H11-H25	1	5.1889	5.1655	5.1579	-0.0234	0.0203	-0.0455	0.0018	0.0000	0.1954
H11-H23	1	5.1936	5.2020	5.1956	0.0084	0.0196	-0.0514	0.0403	-0.0001	0.1818
H11-H22	1	5.2173	5.0329	5.0064	-0.1845	0.0188	-0.0319	-0.1713	-0.0001	0.3577
C5-H23	1	5.2664	5.1121	5.0917	-0.1543	0.0351	-0.0972	-0.0922	0.0000	0.3108
H11-H13	1	5.3365	5.2355	5.2242	-0.1010	0.0078	-0.0362	-0.0726	0.0000	0.2400
H13-H19	1	5.3425	5.1105	5.0884	-0.2320	0.0240	-0.0697	-0.1863	0.0000	0.3235
H16-H19	1	5.4194	5.2415	5.2125	-0.1780	0.0355	-0.0659	-0.1476	0.0000	0.3814
H16-H18	1	5.4743	5.5411	5.5323	0.0668	0.0213	-0.0599	0.1054	0.0000	0.2199
H16-H17	1	5.4843	5.4125	5.3861	-0.0718	0.0275	-0.0343	-0.0649	-0.0001	0.3752
H12-H21	1	5.5507	5.5428	5.5339	-0.0079	0.0245	-0.0699	0.0374	0.0001	0.2203
H14-H17	1	5.5898	5.7041	5.6883	0.1144	0.0237	-0.0774	0.1681	0.0000	0.2978
H10-H17	1	5.6677	5.5778	5.5548	-0.0899	0.0147	-0.0637	-0.0410	0.0001	0.3535
C8-C9	1	5.6719	5.8206	5.8089	0.1487	0.0245	-0.0693	0.1935	0.0000	0.2605
H14-H23	1	5.6737	5.7126	5.7100	0.0389	0.0121	-0.0487	0.0755	0.0000	0.1229
C9-H22	1	5.6789	5.7059	5.7034	0.0269	0.0149	-0.0502	0.0622	0.0000	0.1200

H20-H24	1	5.6873	5.4781	5.4383	-0.2092	0.0237	-0.0716	-0.1613	0.0000	0.4560
H18-H24	1	5.7223	5.8058	5.7966	0.0835	0.0166	-0.0513	0.1181	0.0001	0.2287
H21-H24	1	5.7438	5.7908	5.7837	0.0469	0.0180	-0.0522	0.0811	0.0000	0.2016
C8-H16	1	5.7607	5.8697	5.8599	0.1090	0.0165	-0.0487	0.1412	0.0000	0.2396
C8-H25	1	5.7666	5.8621	5.8523	0.0955	0.0156	-0.0501	0.1300	0.0000	0.2395
C7-C9	1	5.7715	5.7735	5.7710	0.0019	0.0082	-0.0460	0.0397	0.0000	0.1186
C7-H24	1	5.7728	5.8920	5.8823	0.1191	0.0229	-0.0675	0.1638	-0.0001	0.2388
H16-H20	1	5.7829	5.7646	5.7578	-0.0183	0.0239	-0.0576	0.0154	0.0000	0.1981
C6-H21	1	5.7880	5.7783	5.7756	-0.0097	0.0126	-0.0515	0.0291	0.0001	0.1243
H17-H21	1	5.8381	5.8370	5.8303	-0.0011	0.0180	-0.0552	0.0361	0.0000	0.1973
C9-H18	1	5.8956	5.7770	5.7649	-0.1186	0.0211	-0.0733	-0.0664	0.0000	0.2596
H11-H21	1	5.9211	5.8860	5.8782	-0.0351	0.0172	-0.0575	0.0052	0.0000	0.2144
H13-H17	1	5.9857	6.0197	6.0110	0.0340	0.0193	-0.0577	0.0724	0.0000	0.2281
C9-H20	1	6.0658	5.8577	5.8298	-0.2081	0.0218	-0.0539	-0.1759	-0.0001	0.3974
H16-H21	1	6.0984	6.0800	6.0785	-0.0184	0.0055	-0.0459	0.0220	0.0000	0.0942
H22-H25	1	6.1155	6.0565	6.0445	-0.0590	0.0140	-0.0565	-0.0164	-0.0001	0.2665
H16-H22	1	6.1767	6.0466	6.0270	-0.1300	0.0275	-0.0470	-0.1106	0.0001	0.3405
C9-H21	1	6.2080	6.1517	6.1431	-0.0564	0.0153	-0.0525	-0.0192	0.0000	0.2275
H20-H25	1	6.2567	6.1564	6.1480	-0.1002	0.0181	-0.0572	-0.0611	0.0000	0.2258
H21-H25	1	6.2887	6.1620	6.1503	-0.1266	0.0133	-0.0665	-0.0734	0.0000	0.2667
C7-H25	1	6.3035	6.2282	6.2111	-0.0753	0.0272	-0.1036	0.0011	0.0000	0.3231
C9-H19	1	6.3154	6.2713	6.2456	-0.0441	0.0187	-0.0721	0.0093	0.0000	0.3969
C9-H17	1	6.3387	6.3678	6.3616	0.0292	0.0147	-0.0656	0.0801	0.0000	0.1987
C7-H23	1	6.3765	6.3629	6.3568	-0.0136	0.0143	-0.0669	0.0389	0.0001	0.1960
H17-H24	1	6.4735	6.4550	6.4410	-0.0185	0.0240	-0.0764	0.0339	0.0000	0.2986
H19-H24	1	6.5573	6.4552	6.4414	-0.1021	0.0263	-0.0817	-0.0467	0.0000	0.2948
H18-H25	1	6.6579	6.6635	6.6606	0.0057	0.0142	-0.0720	0.0634	0.0001	0.1391
C8-H23	1	6.7646	6.7915	6.7840	0.0269	0.0224	-0.0962	0.1007	0.0000	0.2259
H22-H23	1	6.8115	6.6533	6.6387	-0.1582	0.0229	-0.0987	-0.0824	0.0000	0.3060
H18-H23	1	6.9486	6.9438	6.9416	-0.0048	0.0087	-0.0663	0.0528	0.0000	0.1235
H16-H21	1	6.9497	6.9467	6.9445	-0.0029	0.0097	-0.0670	0.0544	0.0000	0.1256
H19-H25	1	7.0741	7.1286	7.1203	0.0546	0.0164	-0.0759	0.1140	0.0001	0.2433
H17-H23	1	7.1030	7.0140	7.0017	-0.0890	0.0174	-0.0916	-0.0149	0.0001	0.2905
H20-H23	1	7.1143	7.1204	7.1125	0.0062	0.0156	-0.0767	0.0673	0.0000	0.2376
H17-H25	1	7.1213	7.0659	7.0584	-0.0555	0.0169	-0.0778	0.0055	-0.0001	0.2284
H19-H23	1	7.1652	7.0722	7.0646	-0.0930	0.0202	-0.0826	-0.0305	-0.0001	0.2307
H21-H23	1	7.8147	7.8283	7.8255	0.0136	0.0117	-0.0893	0.0912	0.0000	0.1471

Table S17. Cartesian coordinates for the **1a** conformer of TEDA molecule obtained by GED (MP2/cc-PVTZ initial approximation) refinement (in Å).

Atom	X	Y	Z
N1	-0.032553	0.002921	-0.000358
N2	0.007119	0.031472	1.484734
C3	-0.455742	1.148682	0.737443
C4	1.298704	-0.000235	-0.547517
C5	-1.024810	-0.825764	2.008202
C6	0.297239	2.439168	0.851923
C7	1.791457	-1.410102	-0.790202
C8	-0.569287	-2.261310	2.138024
C9	-0.118682	3.231375	2.083641
H10	-1.539422	1.276697	0.697128
H11	1.210621	0.545872	-1.492415
H12	1.979254	0.519147	0.132386
H13	-1.258759	-0.400809	2.989801
H14	-1.896656	-0.758593	1.345279
H15	1.360660	2.209748	0.904029
H16	0.087486	3.012962	-0.056854
H17	2.775994	-1.400242	-1.262159
H18	1.870436	-1.945917	0.157189
H19	1.098000	-1.950146	-1.436429
H20	-0.335530	-2.667697	1.152903
H21	-1.350368	-2.876954	2.588280
H22	0.324766	-2.322054	2.760666
H23	0.425121	4.174865	2.151372
H24	0.084758	2.653721	2.987528
H25	-1.186756	3.460360	2.060469

Table S18. Cartesian coordinates for the **1b** conformer of TEDA molecule obtained by GED (MP2/cc-PVTZ initial approximation) refinement (in Å).

Atom	X	Y	Z
N1	-0.061570	0.031579	0.026448
N2	0.018905	0.018151	1.509665
C3	-0.464325	1.156651	0.812863
C4	1.256549	0.036202	-0.551029
C5	-1.000301	-0.851553	2.037586
C6	0.290416	2.448291	0.904095
C7	1.792690	-1.369099	-0.716484
C8	-0.541666	-2.289002	2.129869
C9	0.068721	3.369599	-0.287155
H10	-1.548656	1.283543	0.797062
H11	1.125418	0.512720	-1.527722
H12	1.938240	0.621924	0.071846
H13	-1.213655	-0.446927	3.032332
H14	-1.885886	-0.772315	1.394474
H15	1.347521	2.217336	1.031778
H16	-0.071546	2.927661	1.819501
H17	2.763394	-1.356121	-1.216119
H18	1.914506	-1.838464	0.260893
H19	1.102479	-1.972629	-1.307952
H20	-0.326660	-2.676411	1.132975
H21	-1.314054	-2.913503	2.582945
H22	0.363951	-2.361826	2.734229
H23	0.587476	4.320021	-0.152816
H24	-0.994092	3.583488	-0.421779
H25	0.434332	2.911337	-1.208003

Table S19. Cartesian coordinates for the **1c** conformer of TEDA molecule obtained by GED (MP2/cc-PVTZ initial approximation) refinement (in Å).

Atom	X	Y	Z
N1	-0.026562	-0.002738	-0.023887
N2	0.023597	0.003821	1.458898
C3	-0.993716	-0.864583	1.991920
C4	-0.468094	1.123362	0.732097
C5	1.303409	0.010080	-0.571568
C6	0.258037	2.428575	0.852870
C7	1.821083	-1.399529	-0.759573
C8	-1.408258	-0.436737	3.384042
C9	-0.177911	3.217924	2.079184
H10	-1.555301	1.227188	0.700179
H11	1.202768	0.519636	-1.535249
H12	1.973938	0.567215	0.088191
H13	-1.845757	-0.860036	1.300814
H14	-0.541877	-1.859354	2.010514
H15	0.043265	2.996626	-0.058448
H16	1.325203	2.218388	0.911127
H17	2.814200	-1.393574	-1.213013
H18	1.887464	-1.899216	0.208672
H19	1.145807	-1.971121	-1.397426
H20	-0.542693	-0.407522	4.047598
H21	-2.140284	-1.131833	3.798935
H22	-1.857401	0.558820	3.364939
H23	0.342581	4.175019	2.139709
H24	0.038508	2.653055	2.988048
H25	-1.251337	3.421202	2.053653

Table S20. Cartesian coordinates for the **1d** conformer of TEDA molecule obtained by GED (MP2/cc-PVTZ initial approximation) refinement (in Å).

Atom	X	Y	Z
N1	-0.018648	-0.044675	0.017036
N2	-0.009180	0.026163	1.498466
C3	-0.487132	1.111303	0.715615
C4	1.317741	-0.022457	-0.515523
C5	-1.017547	-0.858962	2.019302
C6	0.230406	2.422542	0.827849
C7	1.345471	0.563020	-1.912374
C8	-0.508730	-2.276939	2.148155
C9	-0.132580	3.159108	2.110114
H10	-1.572645	1.208648	0.650692
H11	1.981293	0.521228	0.162822
H12	1.614583	-1.074057	-0.536833
H13	-1.270864	-0.441917	2.999356
H14	-1.887210	-0.822460	1.351022
H15	1.302835	2.230376	0.805042
H16	-0.055104	3.019281	-0.044283
H17	2.346201	0.487455	-2.341566
H18	0.648772	0.029138	-2.560257
H19	1.058718	1.616318	-1.899151
H20	-0.236814	-2.660502	1.163263
H21	-1.273215	-2.929575	2.573894
H22	0.373900	-2.307606	2.788606
H23	0.378337	4.121174	2.173653
H24	0.151242	2.560760	2.977821
H25	-1.207871	3.346021	2.162971

Table S21. Cartesian coordinates for the **1e** conformer of TEDA molecule obtained by GED (MP2/cc-PVTZ initial approximation) refinement (in Å).

Atom	X	Y	Z
N1	-0.049732	0.025405	-0.010685
N2	0.023051	-0.010969	1.470489
C3	-0.472683	1.132509	0.789567
C4	1.274631	0.038084	-0.571779
C5	-0.991955	-0.885530	1.996779
C6	0.264152	2.432381	0.902921
C7	1.826314	-1.366959	-0.682519
C8	-1.381726	-0.484333	3.404042
C9	0.055872	3.357612	-0.287610
H10	-1.559358	1.242775	0.768486
H11	1.149170	0.482589	-1.564064
H12	1.940746	0.651731	0.041245
H13	-1.853914	-0.859334	1.318557
H14	-0.546931	-1.883472	1.986370
H15	1.320990	2.210987	1.049687
H16	-0.119947	2.902073	1.814425
H17	2.811235	-1.363557	-1.153404
H18	1.920742	-1.803744	0.313210
H19	1.155926	-1.992655	-1.273284
H20	-0.506781	-0.479981	4.055434
H21	-2.117376	-1.178398	3.814076
H22	-1.817878	0.517261	3.412769
H23	0.561253	4.312993	-0.138254
H24	-1.006357	3.560370	-0.442552
H25	0.444961	2.907718	-1.203000

Table S22. Cartesian coordinates for the **1f** conformer of TEDA molecule obtained by GED (MP2/cc-PVTZ initial approximation) refinement (in Å).

Atom	X	Y	Z
N1	-0.001663	-0.068251	0.004193
N2	0.028648	-0.008999	1.484476
C3	-0.478861	1.074738	0.716957
C4	1.326969	-0.022375	-0.545661
C5	-0.973912	-0.884784	2.032692
C6	0.216866	2.398682	0.817778
C7	1.325542	0.564344	-1.942345
C8	-1.410263	-0.429639	3.409433
C9	-0.152654	3.146636	2.091257
H10	-1.567519	1.152479	0.669283
H11	1.990673	0.532341	0.123571
H12	1.641130	-1.068590	-0.572878
H13	-1.819935	-0.917698	1.334865
H14	-0.500463	-1.868228	2.082484
H15	1.292067	2.222787	0.793467
H16	-0.080180	2.981597	-0.059970
H17	2.321398	0.505739	-2.385305
H18	0.628959	0.019200	-2.580861
H19	1.021569	1.612701	-1.924569
H20	-0.551933	-0.365528	4.079885
H21	-2.131766	-1.129003	3.835455
H22	-1.879444	0.555554	3.360746
H23	0.339611	4.119515	2.135767
H24	0.147474	2.568815	2.967268
H25	-1.231159	3.314092	2.147949

Table S23. Cartesian coordinates for the **1g** conformer of TEDA molecule obtained by GED (MP2/cc-PVTZ initial approximation) refinement (in Å).

Atom	X	Y	Z
N1	-0.001093	-0.065235	0.018963
N2	0.021734	0.005511	1.498343
C3	-0.450431	1.098641	0.727598
C4	1.338837	-0.078391	-0.503699
C5	-0.994393	-0.863229	2.031096
C6	0.270336	2.412891	0.801427
C7	1.394777	0.430760	-1.928909
C8	-0.506159	-2.288787	2.156174
C9	-0.282903	3.473666	-0.139726
H10	-1.536018	1.201328	0.667799
H11	1.623489	-1.132984	-0.466904
H12	2.002679	0.489734	0.154948
H13	-1.231008	-0.441718	3.013340
H14	-1.870256	-0.814146	1.371611
H15	1.330410	2.238686	0.614048
H16	0.157418	2.743970	1.838701
H17	2.394572	0.294343	-2.345189
H18	0.682437	-0.111538	-2.552361
H19	1.149911	1.492894	-1.977182
H20	-0.250115	-2.677342	1.168976
H21	-1.276470	-2.929221	2.589846
H22	0.382137	-2.332702	2.787916
H23	0.268617	4.410266	-0.044568
H24	-1.332150	3.679231	0.084154
H25	-0.224965	3.152084	-1.181052

Table S24. Cartesian coordinates for the **1h** conformer of TEDA molecule obtained by GED (MP2/cc-PVTZ initial approximation) refinement (in Å).

Atom	X	Y	Z
N1	0.009388	-0.107375	-0.003253
N2	0.047257	-0.053950	1.475360
C3	-0.438206	1.046245	0.722159
C4	1.344845	-0.109364	-0.537031
C5	-0.976295	-0.898354	2.032722
C6	0.274067	2.364737	0.800859
C7	1.385676	0.411646	-1.958514
C8	-1.394246	-0.415733	3.405977
C9	-0.293919	3.428962	-0.127516
H10	-1.525753	1.141913	0.675352
H11	1.634862	-1.162642	-0.512090
H12	2.011652	0.457207	0.120043
H13	-1.825124	-0.913549	1.337578
H14	-0.530214	-1.894040	2.090636
H15	1.333747	2.198916	0.603544
H16	0.167487	2.686835	1.841717
H17	2.382466	0.283733	-2.384572
H18	0.670577	-0.129115	-2.580088
H19	1.135188	1.472908	-1.995953
H20	-0.531949	-0.369274	4.072416
H21	-2.135740	-1.087027	3.842483
H22	-1.833578	0.582785	3.346832
H23	0.251410	4.368843	-0.028920
H24	-1.342954	3.625006	0.105924
H25	-0.241623	3.116125	-1.171790

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