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

Electronic supplementory information

Gas phase equilibrium structure of histamine

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Contents

List of Tables

List of Figures

General considerations

- The numeration of atoms is consistent for all of the tables.
- The dimensions of the values given are:
  - coordinates, r and l are in Å,
  - angles are in $^\circ$,
  - κ is in pm^3.
- The errors given are one standard deviation.
- **a-Value** denote r_a parameters.
- **g-Value** denote r_g parameters.
- **e-Value** denote r_e parameters.
- **stretch** denotes the bond distance between the atoms i and j.
- **bend** denotes valence angle between the atoms i, j and k.
- **torsion** denotes dihedral angle between the planes constructed by atoms $i-j-k$ and $j-k-l$.
- **o.o.p.** denotes out-of-plane coordinate value (angle between the bond $i-k$ and the plane $j-k-l$).

1 Results of quantum-chemical calculations

1.1 Geometries and thermochemical properties for histamine obtained by the MP2/def2-TZVP calculations

1.1.1 Histamine conformers

Table S1. Cartesian coordinates of ^{1}G−IVa conformer found using MP2/def2-TZVP calculations

At	X	Y	Z
N	−2.7239390212	1.2275499665	1.7956422089
C	−3.2907621995	0.1049539709	2.3112825350
N	−2.4251897655	−0.8952548033	2.3732372290
C	−1.2590573697	−0.3833754549	1.8631315019
C	−1.4176396863	0.9372077267	1.4918934249
C	−0.4910386474	1.9432478481	0.9026923214
C	−1.1239502209	2.7536824153	−0.2242745439
N	−2.1888602744	3.6133476092	0.3151966324
H	−3.1431762598	2.1212351743	1.5586724527
H	−4.3233699269	0.0642856861	2.6224176645
H	−0.3647880262	−0.9842788334	1.7876325718
H	0.3902022904	1.4184520507	0.5245116774
H	−0.1310088799	2.6400328956	1.6715889999
H	−0.3442016617	3.3213067287	−0.7475135583
H	−1.5777286832	2.0716057237	−0.9477082686
H	−1.7735827843	4.3519805800	0.8760700349
H	−2.6827779034	4.0738695830	−0.4424398242

Thermochemical data for 1G-IVa calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = -359.4829067171 Ha
ZPE = 0.146771 Ha = 385.348745 KJ/Mol

**** T = 10 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	9.156963	0.208	-0.761	20.786	96.921
ROT.	7.535684	0.125	-0.627	12.472	75.126
VIB.	0.000006	385.349	385.349	0.008	0.001
TOTAL	16.692653	385.681	383.961	33.265	172.048

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	-59.824	20.786	173.204
ROT.	13.040611	4.895	-42.557	12.472	120.897
VIB.	4.973809	407.504	369.117	127.574	97.801
TOTAL	36.346261	420.558	266.736	160.832	391.902

**** T = 403 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.398772	8.380	-61.672	20.786	173.761
ROT.	13.080769	5.028	-43.846	12.472	121.230
VIB.	5.158660	408.884	368.057	131.544	101.269
TOTAL	36.638201	422.292	262.539	164.802	396.261

Table S2. Cartesian coordinates of ^{3}G−Ib conformer found using MP2/def2-TZVP calculations

At	X	Y	Z
N	1.3548046555	−1.1868449832	0.0271554980
C	2.4542191502	−0.4566386195	−0.0391684945
N	2.1648345374	0.8714129322	−0.1018710613
C	0.7992307399	0.9978523077	−0.0739124963
C	0.3108143537	−0.2890728524	0.0122820705
C	−1.1070315674	−0.7462255564	0.0233036923
C	−1.4666112343	−1.4582256097	−1.2766835781
N	−1.3323934154	−0.5248346489	−2.3954084777
H	2.8322622376	1.6252102680	−0.1498304385
H	3.4664083107	−0.8312606036	−0.0403555242
H	0.3050631745	1.9550386946	−0.1148076827
H	−1.7683531715	0.1147812001	0.1530347643
H	−1.2611196083	−1.4282757421	0.8645246238
H	−0.8351403300	−2.3515635100	−1.3673285195
H	−2.5083162093	−1.7868961514	−1.2315999563
H	−0.3583422791	−0.2465854789	−2.4757019558
H	−1.5700524792	−0.9906539341	−3.2649142037

Thermochemical data for 3G-Ib calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −359.4796646003 Ha
ZPE = 0.145989 Ha = 383.294777 KJ/Mol

**** T = 10 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	9.156963	0.208	−0.761	20.786	96.921
ROT.	7.543347	0.125	−0.627	12.472	75.190
VIB.	0.005317	383.297	383.294	1.225	0.277
TOTAL	16.705627	383.630	381.906	34.482	172.387

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	−59.824	20.786	173.204
ROT.	13.048274	4.895	−42.582	12.472	120.960
VIB.	6.323261	406.825	362.659	130.324	112.523
TOTAL	37.703377	419.878	260.253	163.581	406.688

**** T = 403 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.398772	8.380	-61.672	20.786	173.761
ROT.	13.088433	5.028	-43.872	12.472	121.294
VIB.	6.519356	408.233	361.442	134.226	116.064
TOTAL	38.006561	421.641	255.899	167.484	411.119

Table S3. Cartesian coordinates of ^{3}G−Ic conformer found using MP2/def2-TZVP calculations

At	X	Y	Z
N	1.4370031580	−1.1519499858	0.4074819117
C	2.5124893789	−0.4078505101	0.2199494987
N	2.1851017302	0.8327741076	−0.2322053194
C	0.8184809676	0.8844298494	−0.3400464108
C	0.3680883528	−0.3543086574	0.0662812020
C	−1.0252576980	−0.8762360010	0.1083224006
C	−1.2337652302	−1.9969996334	−0.9182767986
N	−1.0072582271	−1.6188730370	−2.3080191522
H	2.8286541053	1.5797672101	−0.4414395097
H	3.5332998919	−0.7117387245	0.3944383224
H	0.2995319342	1.7688369280	−0.6731522135
H	−1.7279091142	−0.0594830434	−0.0902687862
H	−1.2418809421	−1.2600826879	1.1109737569
H	−0.5548092746	−2.8180094054	−0.6770367817
H	−2.2529890302	−2.3833632332	−0.8304009069
H	−1.6158903365	−0.8460481075	−2.5598145451
H	−0.0552687438	−1.2807173407	−2.4122030693

Thermochemical data for 3G-Ic calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −359.4791003894 Ha
ZPE = 0.145890 Ha = 383.034235 KJ/Mol

**** T = 10 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	9.156963	0.208	−0.761	20.786	96.921
ROT.	7.557537	0.125	−0.628	12.472	75.308
VIB.	0.001691	383.035	383.034	0.577	0.104
TOTAL	16.716191	383.368	381.644	33.834	172.333

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	−59.824	20.786	173.204
ROT.	13.062464	4.895	−42.628	12.472	121.078
VIB.	6.143720	406.511	362.985	130.644	110.896
TOTAL	37.538026	419.565	260.532	163.901	405.179

**** T = 403 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.398772	8.380	-61.672	20.786	173.761
ROT.	13.102622	5.028	-43.919	12.472	121.412
VIB.	6.339403	407.924	361.785	134.549	114.446
TOTAL	37.840797	421.331	256.194	167.807	409.619

Table S4. Cartesian coordinates of ^{3}G−Vb conformer found using MP2/def2-TZVP calculations

At	X	Y	Z
N	−0.3557969173	−0.4041423327	1.7505502294
C	−1.6682382823	−0.5411095260	1.8282077361
N	−2.2568691927	−0.3444323363	0.6192164819
C	−1.2640834781	−0.0627164344	−0.2835223554
C	−0.0858171063	−0.1041052383	0.4326460738
C	1.2982748435	0.1515995088	−0.0606141487
C	1.9837545123	1.3012220305	0.6732992047
N	2.3667513998	0.8734060988	2.0155306960
H	−3.2434075137	−0.4026867095	0.4212383421
H	−2.2299423886	−0.7806429128	2.7179056224
H	−1.4698389672	0.1361510399	−1.3228776548
H	1.2480589005	0.3763105489	−1.1302173118
H	1.9138742208	−0.7452167346	0.0631180667
H	2.8920288471	1.5779109931	0.1294574365
H	1.3125915078	2.1738190244	0.6537721346
H	1.5429725781	0.5198562619	2.4955743032
H	2.7180292357	1.6620193273	2.5475406450

Thermochemical data for 3G-Vb calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −359.4790211364 Ha
ZPE = 0.146435 Ha = 384.466030 KJ/Mol

**** T = 10 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	9.156963	0.208	−0.761	20.786	96.921
ROT.	7.548073	0.125	−0.628	12.472	75.229
VIB.	0.000309	384.466	384.466	0.168	0.023
TOTAL	16.705345	384.799	383.077	33.426	172.173

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	−59.824	20.786	173.204
ROT.	13.053000	4.895	−42.597	12.472	121.000
VIB.	5.508146	407.385	366.491	129.641	104.190
TOTAL	36.892988	420.439	264.069	162.899	398.394

**** T = 403 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.398772	8.380	-61.672	20.786	173.761
ROT.	13.093159	5.028	-43.888	12.472	121.333
VIB.	5.699269	408.787	365.362	133.557	107.713
TOTAL	37.191200	422.195	259.803	166.815	402.807

Table S5. Cartesian coordinates of ^{3}G−Vc conformer found using MP2/def2-TZVP calculations

At	X	Y	Z
N	1.3995275063	−1.1840913851	0.1600494811
C	2.4961533759	−0.4521162162	0.0572791056
N	2.1980214294	0.8631386870	−0.1096639592
C	0.8322854488	0.9810131887	−0.1158462594
C	0.3472876086	−0.2996494808	0.0541171147
C	−1.0729164019	−0.7484349744	0.0719146726
C	−1.4369671097	−1.5836895583	−1.1648046571
N	−0.7778881920	−2.8798114411	−1.2634234792
H	2.8613523926	1.6163928949	−0.2025409990
H	3.5101357219	−0.8187913482	0.1003694695
H	0.3364337718	1.9313661330	−0.2305304066
H	−1.7207289032	0.1336963892	0.1211158705
H	−1.2623643017	−1.3428687232	0.9723187837
H	−2.5185214758	−1.7474905370	−1.1814348637
H	−1.1913174946	−1.0036123729	−2.0602007744
H	0.2182206804	−2.7507745356	−1.1045182632
H	−1.0980294469	−3.4730166209	−0.5040967595

Thermochemical data for 3G-Vc calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −359.4792209647 Ha
ZPE = 0.146138 Ha = 383.685849 KJ/Mol

**** T = 10 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	9.156963	0.208	−0.761	20.786	96.921
ROT.	7.556718	0.125	−0.628	12.472	75.301
VIB.	0.000631	383.686	383.686	0.285	0.044
TOTAL	16.714312	384.019	382.296	33.543	172.266

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	−59.824	20.786	173.204
ROT.	13.061645	4.895	−42.625	12.472	121.071
VIB.	5.729404	406.849	364.988	130.002	106.652
TOTAL	37.122890	419.903	262.539	163.260	400.928

**** T = 403 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.398772	8.380	-61.672	20.786	173.761
ROT.	13.101803	5.028	-43.917	12.472	121.405
VIB.	5.922521	408.255	363.834	133.909	110.185
TOTAL	37.423096	421.663	258.245	167.167	405.351

Table S6. Cartesian coordinates of ^{3}T−a conformer found using MP2/def2-TZVP calculations

At	X	Y	Z
N	1.3741841553	−1.1872903166	0.0708520729
C	2.4762676811	−0.4596163269	0.0281142614
N	2.1911187492	0.8678914308	−0.0548704458
C	0.8257418912	0.9967694202	−0.0645089394
C	0.3329383552	−0.2887425751	0.0152659550
C	−1.0844574142	−0.7425284682	0.0054352520
C	−1.4332087424	−1.4777939331	−1.2831161568
N	−2.8248671508	−1.9283493464	−1.2337156012
H	2.8608243747	1.6201195633	−0.0923967407
H	3.4872117490	−0.8361908506	0.0579542983
H	0.3375041785	1.9560842625	−0.1240181243
H	−1.7580512876	0.1101031911	0.1248036553
H	−1.2517185962	−1.4141167485	0.8548710935
H	−1.3290973769	−0.7860964446	−2.1240457763
H	−0.7033084098	−2.2837781142	−1.4305895737
H	−3.0712968624	−2.3913371025	−2.1019845930
H	−2.9264523001	−2.6243426328	−0.5015890878

Thermochemical data for 3T-a calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −359.4774582506 Ha
ZPE = 0.145748 Ha = 382.660676 KJ/Mol

**** T = 10 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	9.156963	0.208	−0.761	20.786	96.921
ROT.	7.615359	0.125	−0.633	12.472	75.789
VIB.	0.000326	382.661	382.661	0.181	0.025
TOTAL	16.772648	382.993	381.266	33.439	172.734

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	−59.824	20.786	173.204
ROT.	13.120286	4.895	−42.817	12.472	121.559
VIB.	6.545535	406.804	361.300	130.868	115.934
TOTAL	37.997663	419.858	258.659	164.126	410.698

**** T = 403 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.398772	8.380	-61.672	20.786	173.761
ROT.	13.160445	5.028	-44.113	12.472	121.893
VIB.	6.746620	408.218	360.046	134.732	119.489
TOTAL	38.305836	421.626	254.261	167.989	415.143

Table S7. Harmonic frequencies of LAM in $N_{(3)}-H$ conformers computed at MP2/def2-TZVP level of theory. **ir** denotes internal rotation, **inv** denotes inversion.

Conformer	3G-Ib	3G-Ic	3G-Vb	3G-Vc	3T-a
ir(-(CH2)2NH2)	36.42	44.37	56.17	51.21	55.99
ir(-CH2NH2)	97.17	91.21	148.85	156.25	80.84
ir(-NH2)	254.04	306.94	326.79	301.61	212.44
inv(-NH2)	889.68	855.84	862.80	891.76	871.61

1.1.2 Single-molecule tautomerization reaction

Table S8. Cartesian coordinates of ^{2}G−Vc conformer found using MP2/def2-TZVP calculations

At	X	Y	Z
N	3.4085907266	−1.4363853885	−0.5797081089
C	3.3660100825	−2.2853260599	0.5962145579
N	2.0638988245	−2.1989762755	1.2341458004
C	1.4097812009	−1.3678259233	0.4903710983
C	2.2289628177	−0.8940503308	−0.6384992211
C	1.8172801310	0.1156175770	−1.6480587522
C	2.1122357308	1.5381129066	−1.1300743611
N	3.5182683084	1.8443450330	−0.9289354142
H	4.1418754782	−1.9795630847	1.3067008246
H	3.5682209313	−3.3237654180	0.3122267375
H	0.3828314904	−1.0875919398	0.7040592788
H	0.7467630769	0.0163585265	−1.8554296136
H	2.3657570500	−0.0527027419	−2.5779886059
H	1.7000254410	2.2614424655	−1.8377615138
H	1.5861691464	1.6918287674	−0.1826434664
H	4.0080262263	1.8002580912	−1.8168059073
H	3.9466036680	1.1345330123	−0.3418546179

Thermochemical data for 2G-Vc calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −359.4501520520 Ha
ZPE = 0.144976 Ha = 380.633605 KJ/Mol

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	−59.824	20.786	173.204
ROT.	13.081146	4.895	−42.689	12.472	121.234
VIB.	6.334497	404.096	359.962	128.602	112.443
TOTAL	37.747484	417.149	257.448	161.860	406.881

Table S9. Cartesian coordinates of ^{1}TS between ^{1}G−VIa and ^{2}G−Vc conformers in the single-molecule tautomerization found using MP2/def2-TZVP calculations

At	X	Y	Z
N	1.8254197214	−2.3838604525	2.3276743464
C	0.8590596468	−2.1042582551	3.3690180397
N	−0.1843502876	−1.3619397850	2.9417014932
C	0.1023859040	−1.1168342750	1.6497320085
C	1.3279543254	−1.6838730093	1.2783577137
C	2.1321357952	−1.4579942294	0.0471020531
C	2.8149142296	−0.0902377160	0.0950631936
N	3.5440792307	0.0518181462	1.3540252749
H	2.0093392421	−1.5503742634	3.3017253417
H	0.8541944624	−2.6991320028	4.2724831221
H	−0.5591379937	−0.5169173666	1.0373562420
H	1.5012039882	−1.5166988934	−0.8443410211
H	2.8862006771	−2.2466243232	−0.0312373749
H	3.4391441180	0.0280531459	−0.8014013930
H	2.0496468409	0.6905037556	0.0659061701
H	4.2800564911	−0.6460684301	1.4091156791
H	3.9944791329	0.9594945226	1.3989741828

Thermochemical data for 1TS between 1G-VIa and 2G-Vc conformers
in the single-molecule tautomerization calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −359.4019210596 Ha
ZPE = 0.141086 Ha = 370.422552 KJ/Mol
Imaginary frequency absolute value = 1403.77 cm-1

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	−59.824	20.786	173.204
ROT.	13.019355	4.895	−42.487	12.472	120.720
VIB.	5.477401	392.502	352.548	124.288	101.794
TOTAL	36.828598	405.555	250.236	157.546	395.718

Table S10. Cartesian coordinates of ^{3}TS between ^{2}G−Vc and ^{3}G−Vc conformers in the single-molecule tautomerization found using MP2/def2-TZVP calculations

At	X	Y	Z
N	2.2059367479	−2.8998596764	−0.7142040653
C	1.6583507166	−3.7294324238	0.1949488703
N	0.3606936112	−3.2844701791	0.6647505906
C	0.2297882714	−2.1037397996	0.0192337361
C	1.3132382968	−1.8897008012	−0.8423317647
C	1.5651114753	−0.7093960051	−1.7141182048
C	2.6483262782	0.2122346680	−1.1255111260
N	3.9913091958	−0.3457840259	−1.0770772724
H	1.9590713550	−4.7576184195	0.3468481318
H	1.4465339193	−3.2643669081	1.3645251707
H	−0.6101705990	−1.4543897380	0.2227156828
H	0.6317799063	−0.1498754593	−1.8332243775
H	1.8813239445	−1.0462257523	−2.7060354814
H	2.6822253555	1.1355532033	−1.7099003321
H	2.3532147560	0.4944758996	−0.1096998327
H	3.9564434220	−1.2727038265	−0.6617812516
H	4.3330952474	−0.4826846317	−2.0229931312

Thermochemical data for 3TS between 2G-Vc and 3G-Vc conformers
in the single-molecule tautomerization calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −359.4022622386 Ha
ZPE = 0.141277 Ha = 370.923991 KJ/Mol
Imaginary frequency absolute value = 1406.82 cm-1

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	−59.824	20.786	173.204
ROT.	13.065489	4.895	−42.638	12.472	121.103
VIB.	5.760837	393.097	352.124	124.479	104.389
TOTAL	37.158167	406.150	249.662	157.736	398.697

1.1.3 Transition states for N3H confomational interconversion

Table S11. Cartesian coordinates of TS between ^{3}G−Ib and ^{3}G−Vb conformers through the rotation of $-(CH_2)_2NH_2$ group found using MP2/def2-TZVP calculations

At	X	Y	Z
N	-0.4991848898	0.2594474768	1.7122051340
C	-1.7157487195	-0.2476270227	1.8289255367
N	-2.1607957474	-0.7313708478	0.6404404158
C	-1.1746750048	-0.5234103385	-0.2883899460
C	-0.1448324806	0.0941834649	0.3926841005
C	1.1748517589	0.5565105775	-0.1481451027
C	2.0226728415	1.2731067000	0.8919930719
N	2.4600712710	0.3324871337	1.9218671256
H	-3.0550292523	-1.1649020793	0.4716469918
H	-2.3029655714	-0.2884276942	2.7331036449
H	-1.2854163312	-0.8198087938	-1.3189240026
H	1.0014195128	1.2262352679	-0.9972730009
H	1.7447821830	-0.3007383815	-0.5198520922
H	2.9115484706	1.6719358453	0.3957391408
H	1.4549042780	2.1255820308	1.2891428915
H	1.6523400196	0.0999400666	2.4925900634
H	3.1335658108	0.7830566022	2.5321162650

Thermochemical data for TS between 3G-Ib and 3G-Vb conformers
through the rotation of -(CH2)2NH2 group calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = -359.4778582052 Ha
ZPE = 0.146239 Ha = 383.951719 KJ/Mol
Imaginary frequency absolute value = 66.72 cm-1

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	-59.824	20.786	173.204
ROT.	13.039585	4.895	-42.553	12.472	120.888
VIB.	3.759870	403.969	371.682	121.705	82.261
TOTAL	35.131297	417.023	269.304	154.963	376.354

Table S12. Cartesian coordinates of TS between ^{3}G−Ic and ^{3}G−Vc conformers through the rotation of $-(CH_2)_2NH_2$ group found using MP2/def2-TZVP calculations

At	X	Y	Z
N	1.3560652488	-1.0453485162	-0.4432387266
C	2.4871018066	-0.4024585833	-0.2036468948
N	2.2493831322	0.8508708719	0.2630977933
C	0.8907787981	1.0199376803	0.3259539352
C	0.3460169951	-0.1690849776	-0.1168944522
C	-1.1029735103	-0.5371600007	-0.2308023212
C	-1.3240775914	-1.9829266985	-0.6776250673
N	-0.8736043057	-2.3074494637	-2.0245384298
H	2.9461895882	1.5317712334	0.5220396473
H	3.4822628200	-0.7926527797	-0.3499707935
H	0.4422645168	1.9361803307	0.6746982655
H	-1.6016399278	0.1329949604	-0.9414068542
H	-1.5929246216	-0.3803139793	0.7373621715
H	-0.8117280124	-2.6541750550	0.0155569541
H	-2.3924598410	-2.2074923110	-0.6074974362
H	-1.3079254939	-1.6814060150	-2.6949286127
H	0.1280270183	-2.1490056921	-2.0679623498

Thermochemical data for TS between 3G-Ic and 3G-Vc conformers
through the rotation of -(CH2)2NH2 group calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = -359.4772127975 Ha
ZPE = 0.146077 Ha = 383.525918 KJ/Mol
Imaginary frequency absolute value = 49.04 cm-1

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	-59.824	20.786	173.204
ROT.	13.050562	4.895	-42.589	12.472	120.979
VIB.	3.780372	403.555	371.189	121.798	82.461
TOTAL	35.162775	416.609	268.776	155.056	376.645

Table S13. Cartesian coordinates of TS between ^{3}G−Ib and ^{3}G−Ic conformers through the $-NH_2$ group inversion found using MP2/def2-TZVP calculations

At	X	Y	Z
N	1.3735273279	-1.1852926592	0.1011762410
C	2.4666326204	-0.4481632075	0.0126819273
N	2.1651370819	0.8717574655	-0.1239847440
C	0.7977034946	0.9845736435	-0.1214930355
C	0.3203744109	-0.3009721184	0.0244997261
C	-1.0891509672	-0.7756688025	0.0275927271
C	-1.4476050414	-1.4399358114	-1.3100028241
N	-1.3580553512	-0.5497890271	-2.4308370498
H	2.8258264257	1.6292560563	-0.1972611475
H	3.4824372258	-0.8113587139	0.0459171786
H	0.2954143941	1.9333617299	-0.2178144482
H	-1.7638530301	0.0681433674	0.1977313303
H	-1.2244848631	-1.4962328981	0.8409389706
H	-0.7908755925	-2.3073402065	-1.4410786164
H	-2.4700494323	-1.8233938479	-1.2572522106
H	-0.4660100283	-0.2535085901	-2.7739380797
H	-2.1764377046	-0.2270867401	-2.9038362369

Thermochemical data for TS between 3G-Ib and 3G-Ic conformers
through the -NH2 group inversion calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = -359.4709839165 Ha
ZPE = 0.144256 Ha = 378.744256 KJ/Mol
Imaginary frequency absolute value = 691.25 cm-1

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	-59.824	20.786	173.204
ROT.	13.064723	4.895	-42.635	12.472	121.097
VIB.	6.537213	402.448	357.411	127.929	114.746
TOTAL	37.933777	415.502	254.951	161.187	409.047

Table S14. Cartesian coordinates of TS between ^{3}G−Vb and ^{3}G−Vc conformers through the $-NH_2$ group inversion found using MP2/def2-TZVP calculations

At	X	Y	Z
N	1.3933243199	−1.1910626698	0.1888196352
C	2.4901867702	−0.4633735616	0.0677588409
N	2.1932065483	0.8468987980	−0.1376917094
C	0.8272489895	0.9647925651	−0.1493414834
C	0.3414325113	−0.3101848022	0.0539933872
C	−1.0794287547	−0.7594534121	0.0877791197
C	−1.4595142556	−1.5763541592	−1.1499567187
N	−0.7146982139	−2.7979371530	−1.2177690999
H	2.8569428509	1.5976216892	−0.2454913934
H	3.5039034666	−0.8290135649	0.1229789411
H	0.3318943098	1.9114445950	−0.2926111851
H	−1.7256914207	0.1217750351	0.1515110218
H	−1.2492749489	−1.3733935934	0.9769497476
H	−2.5286967324	−1.8062799294	−1.0993037416
H	−1.3158813921	−0.9314608513	−2.0327167173
H	0.2221635140	−2.8239054110	−0.8586789373
H	−1.1383395791	−3.6405012773	−1.5469811000

Thermochemical data for TS between 3G-Vb and 3G-Vc conformers
through the -NH2 group inversion calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −359.4709149157 Ha
ZPE = 0.144537 Ha = 379.482611 KJ/Mol
Imaginary frequency absolute value = 664.16 cm-1

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	−59.824	20.786	173.204
ROT.	13.045800	4.895	−42.574	12.472	120.940
VIB.	3.848043	399.160	366.925	118.226	82.127
TOTAL	35.225684	412.214	264.527	151.484	376.272

Table S15. Cartesian coordinates of TS between ^{3}G−Ib and ^{3}G−Ic conformers through the $-NH_2$ group internal rotation found using MP2/def2-TZVP calculations

At	X	Y	Z
N	1.4274173821	−1.1635460185	0.3253037677
C	2.5046465734	−0.4139027073	0.1744008381
N	2.1797106289	0.8550723317	−0.1924987137
C	0.8123587003	0.9202166315	−0.2809272838
C	0.3603412902	−0.3407525662	0.0474902716
C	−1.0386214993	−0.8509411035	0.0833577142
C	−1.2401757166	−2.0157929379	−0.8834637669
N	−1.0021018198	−1.6346243251	−2.2810997125
H	2.8252586442	1.6102878932	−0.3624360983
H	3.5257459348	−0.7334966777	0.3165887519
H	0.2942308291	1.8273186465	−0.5484015117
H	−1.7284917231	−0.0391610104	−0.1735527884
H	−1.2906903348	−1.1800516749	1.0964585222
H	−0.5687370836	−2.8253202990	−0.5871138356
H	−2.2653122198	−2.3842738859	−0.7756334329
H	−0.7328878662	−0.6575015346	−2.3290393214
H	−0.2159569281	−2.1513539980	−2.6547911624

Thermochemical data for TS between 3G-Ib and 3G-Ic conformers
through the -NH2 group internal rotation calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −359.4754382219 Ha
ZPE = 0.145427 Ha = 381.819312 KJ/Mol
Imaginary frequency absolute value = 275.02 cm-1

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	−59.824	20.786	173.204
ROT.	13.055949	4.895	−42.607	12.472	121.024
VIB.	5.542367	403.389	363.732	122.784	101.036
TOTAL	36.930157	416.443	261.301	156.042	395.265

Table S16. Cartesian coordinates of TS between ^{3}G−Vb and ^{3}G−Vc conformers through the $-NH_2$ group internal rotation found using MP2/def2-TZVP calculations

At	X	Y	Z
N	1.3873032872	-1.1704402029	0.3830346561
C	2.4839429923	-0.4579771584	0.1879068729
N	2.1856010521	0.8030824078	-0.2239696633
C	0.8201951428	0.9050477951	-0.2933075084
C	0.3368034636	-0.3306187129	0.0857885318
C	-1.0740363826	-0.8018512173	0.1445431253
C	-1.5049733200	-1.5529993411	-1.1181763590
N	-0.6949609096	-2.7452876766	-1.3821139288
H	2.8478481388	1.5381138541	-0.4169712303
H	3.4975203487	-0.7989127915	0.3320090093
H	0.3254926561	1.8164184583	-0.5882249226
H	-1.7470750230	0.0458109610	0.3058664805
H	-1.1823693612	-1.4698620226	1.0051462009
H	-2.5558801254	-1.8401295947	-1.0011931099
H	-1.4581776199	-0.8673594305	-1.9705132312
H	-0.1446982463	-2.6167157584	-2.2214368198
H	-0.0200288497	-2.8731812662	-0.6345419412

Thermochemical data for TS between 3G-Vb and 3G-Vc conformers
through the -NH2 group internal rotation calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = -359.4755314499 Ha
ZPE = 0.145681 Ha = 382.485391 KJ/Mol
Imaginary frequency absolute value = 244.21 cm-1

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	-59.824	20.786	173.204
ROT.	13.053874	4.895	-42.600	12.472	121.007
VIB.	5.219502	403.836	365.452	122.442	97.793
TOTAL	36.605217	416.889	263.028	155.700	392.004

Table S17. Cartesian coordinates of TS between ^{3}T−a and ^{3}G−Vb conformers through the rotation of $-CH_2NH_2$ group found using MP2/def2-TZVP calculations

At	X	Y	Z
N	1.3785314297	−1.1692326619	−0.0245134288
C	2.4843290267	−0.4467428471	−0.0008896562
N	2.2062705720	0.8844831020	0.0217356917
C	0.8407987582	1.0205746799	0.0104985355
C	0.3415035041	−0.2637225892	−0.0154924781
C	−1.0730022093	−0.7266693560	−0.0498000151
C	−1.3979099050	−1.5571245724	−1.3062764044
N	−1.9521793802	−2.8564050633	−0.9173062569
H	2.8800788421	1.6335729482	0.0435193272
H	3.4934950170	−0.8293812245	0.0037187975
H	0.3575297890	1.9841077797	0.0244277061
H	−1.7414844376	0.1336684063	0.0349321785
H	−1.2652530851	−1.3552315008	0.8248872036
H	−2.1491388173	−1.0433450779	−1.9111471849
H	−0.4892181141	−1.6403060986	−1.9143422220
H	−2.1844628943	−3.3937785749	−1.7467095029
H	−1.2299155822	−3.3813583389	−0.4320600300

Thermochemical data for TS between 3T-a and 3G-Vb conformers
through the rotation of -CH2NH2 group calculated with MP2/def2-TZVP
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = -359.4726121038 Ha
ZPE = 0.145798 Ha = 382.793396 KJ/Mol
Imaginary frequency absolute value = 110.24 cm-1

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	-59.824	20.786	173.204
ROT.	13.114539	4.895	-42.798	12.472	121.511
VIB.	4.831216	403.621	367.027	122.075	93.234
TOTAL	36.277596	416.675	264.405	155.333	387.950

1.2 Results of calculation at BP86/def2-SV(P) level: two-molecule tautomerization reaction of histamine

Table S18. Cartesian coordinates of ^{1}G−IVa found using BP86/def2-SV(P) calculations

At	X	Y	Z
N	−2.7155199669	1.2327545682	1.7659401498
C	−3.3026681568	0.1185031345	2.3100756405
N	−2.4473021840	−0.8924229148	2.4126269843
C	−1.2592119865	−0.4118455942	1.9011658690
C	−1.3956749565	0.9117669241	1.4856674370
C	−0.4614068746	1.9219940919	0.8781707886
C	−1.1153957247	2.7882053038	−0.2202084839
N	−2.2222178639	3.5993479626	0.3353616396
H	−3.0944943112	2.1509880013	1.4654944021
H	−4.3597127959	0.0976915514	2.6137957408
H	−0.3577020705	−1.0402839420	1.8552468129
H	0.4168954746	1.3940639261	0.4479279239
H	−0.0467468388	2.6058746891	1.6614806839
H	−0.3254005173	3.4056308963	−0.7186794041
H	−1.5469583592	2.1230925550	−1.0003361286
H	−1.8461556652	4.3500906737	0.9357185873
H	−2.7434810824	4.0646804640	−0.4218350294

Thermochemical data for 1G-IVa calculated with BP86/def2-SV(P)
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −359.9351398862 Ha
ZPE = 0.141650 Ha = 371.903278 KJ/Mol

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	−59.824	20.786	173.204
ROT.	13.062298	4.895	−42.628	12.472	121.077
VIB.	4.883745	394.391	355.966	130.976	97.900
TOTAL	36.277884	407.445	253.514	164.233	392.181

Table S19. Cartesian coordinates of ^{3}G−Vc found using BP86/def2-SV(P) calculations

At	X	Y	Z
N	1.3846251141	−1.1788722009	0.0268198875
C	2.5006376020	−0.4650849460	0.0021923571
N	2.2357552355	0.8812894161	−0.0193790959
C	0.8569386694	1.0301973897	−0.0110474514
C	0.3399914013	−0.2617882883	0.0200004806
C	−1.1003898953	−0.6993478713	0.0055305993
C	−1.4452738847	−1.6471016242	−1.1828542418
N	−0.7874371178	−2.9537566346	−1.1789009496
H	2.9223817421	1.6383604927	−0.0298590239
H	3.5247489840	−0.8653355188	−0.0015585075
H	0.3776025941	2.0162230884	−0.0240525887
H	−1.7524050459	0.2031106593	−0.0277127756
H	−1.3418066355	−1.2312864077	0.9569890326
H	−2.5482349625	−1.8048870621	−1.2024737685
H	−1.1876246007	−1.1263328740	−2.1344368664
H	0.2251692692	−2.8039079270	−1.0292503220
H	−1.1032322579	−3.4897859788	−0.3552144125

Thermochemical data for 3G-Vc calculated with BP86/def2-SV(P)
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −359.9310647819 Ha
ZPE = 0.141152 Ha = 370.595886 KJ/Mol

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	18.331841	8.159	−59.824	20.786	173.204
ROT.	13.088407	4.895	−42.713	12.472	121.294
VIB.	5.539715	394.123	352.518	133.838	106.000
TOTAL	36.959963	407.176	249.981	167.096	400.499

Table S20. Cartesian coordinates of $(^1G{-}IVa)_2$ found using BP86/def2-SV(P) calculations

At	X	Y	Z
N	0.6832095997	−1.5095892573	−1.1315604757
N	−0.6832095997	1.5095892573	1.1315604757
C	−0.6725404997	−1.4652258167	−0.9766234637
C	0.6725404997	1.4652258167	0.9766234637
N	−1.0531087042	−1.9785936232	0.1929310959
N	1.0531087042	1.9785936232	−0.1929310959
C	0.1221827026	−2.3528608388	0.8237923462
C	−0.1221827026	2.3528608388	−0.8237923462
C	1.2225315242	−2.0601397634	0.0209055586
C	−1.2225315242	2.0601397634	−0.0209055586
C	2.7136449680	−2.1824353341	0.1501923016
C	−2.7136449680	2.1824353341	−0.1501923016
C	3.4571388396	−0.8260525917	−0.0383628587
C	−3.4571388396	0.8260525917	0.0383628587
N	3.0475396190	−0.1106613732	−1.2680356780
N	−3.0475396190	0.1106613732	1.2680356780
H	−2.5442514627	−0.7683014895	1.0214879521
H	2.5442514627	0.7683014895	−1.0214879521
H	−1.3404932151	−1.0509276558	−1.7438411212
H	1.3404932151	1.0509276558	1.7438411212
H	0.1161532427	−2.8190454142	1.8192187081
H	−0.1161532427	2.8190454142	−1.8192187081
H	2.9698819456	−2.6067851584	1.1453326189
H	−2.9698819456	2.6067851584	−1.1453326189
H	3.0975417388	−2.9012123568	−0.6118779465
H	−3.0975417388	2.9012123568	0.6118779465
H	4.5509042337	−1.0339139515	−0.0534758446
H	−4.5509042337	1.0339139515	0.0534758446
H	3.2701053533	−0.1935055629	0.8591777827
H	−3.2701053533	0.1935055629	−0.8591777827
H	1.3231633254	−1.0006633923	−1.7776391331
H	−1.3231633254	1.0006633923	1.7776391331
H	3.8602127618	0.1401343848	−1.8446561328
H	−3.8602127618	−0.1401343848	1.8446561328

Thermochemical data for (1G-IVa)2 calculated with BP86/def2-SV(P)
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = -719.8823215392 Ha
ZPE = 0.284704 Ha = 747.491780 KJ/Mol

**** T = 393 K ****

Ln Q	H	G	Cp	S

		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	19.371562	8.159	-63.217	20.786	181.849
ROT.	15.242884	4.895	-49.744	12.472	139.207
VIB.	18.303851	809.005	687.759	310.623	308.906
TOTAL	52.918297	822.058	574.798	343.881	629.963

Table S21. Cartesian coordinates of $(^3G-Vc)_2$ found using BP86/def2-SV(P) calculations

At	X	Y	Z
N	-0.0116950545	1.0090116188	-2.2676782142
N	0.0116950545	-1.0090116188	2.2676782142
C	-1.0553139676	0.3127475402	-1.8196819247
C	1.0553139676	-0.3127475402	1.8196819247
N	-0.7099679138	-0.9471323417	-1.4136625068
N	0.7099679138	0.9471323417	1.4136625068
C	0.6549795750	-1.0574907616	-1.6006243971
C	-0.6549795750	1.0574907616	1.6006243971
C	1.0757508630	0.1568959131	-2.1365185146
C	-1.0757508630	-0.1568959131	2.1365185146
C	2.4669890985	0.6689573998	-2.3989895532
C	-2.4669890985	-0.6689573998	2.3989895532
C	3.0513305653	1.4137332843	-1.1706022977
C	-3.0513305653	-1.4137332843	1.1706022977
N	2.0843235980	2.3795763887	-0.5855075101
N	-2.0843235980	-2.3795763887	0.5855075101
H	-1.3018069410	-1.6065090028	-0.8087611365
H	1.3018069410	1.6065090028	0.8087611365
H	-2.0903759848	0.6809522477	-1.7760111051
H	2.0903759848	-0.6809522477	1.7760111051
H	1.2016795729	-1.9691363444	-1.3301825469
H	-1.2016795729	1.9691363444	1.3301825469
H	3.1567601381	-0.1596079479	-2.6716344739
H	-3.1567601381	0.1596079479	2.6716344739
H	2.4275888445	1.3674551727	-3.2648475514
H	-2.4275888445	-1.3674551727	3.2648475514
H	3.9989702769	1.9227520333	-1.4626682672
H	-3.9989702769	-1.9227520333	1.4626682672
H	3.3231691668	0.6604750775	-0.3933006570
H	-3.3231691668	-0.6604750775	0.3933006570
H	1.2639433328	2.4725815325	-1.2155059806
H	-1.2639433328	-2.4725815325	1.2155059806
H	2.5044260748	3.3104131589	-0.4637366908
H	-2.5044260748	-3.3104131589	0.4637366908

Thermochemical data for (3G-Vc)2 calculated with BP86/def2-SV(P)
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = -719.8889174132 Ha
ZPE = 0.284636 Ha = 747.313239 KJ/Mol

**** T = 393 K ****

Ln Q	H	G	Cp	S

		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	19.371562	8.159	-63.217	20.786	181.849
ROT.	15.206229	4.895	-49.624	12.472	138.902
VIB.	17.092147	807.461	691.535	306.437	295.353
TOTAL	51.669938	820.514	578.693	339.695	616.104

Table S22. Cartesian coordinates of DTS between $(^1G{-}IVa)_2$ and $(^3G{-}Vc)_2$ dimers in the two-molecule tautomerization reaction estimated using BP86/def2-SV(P) calculations

At	X	Y	Z
N	0.0118580345	0.9825646644	−2.0682985833
N	−0.0272997842	−0.9786528380	2.0760342847
C	−1.0663556684	0.2329448286	−1.7638580968
C	1.0579435259	−0.2548752420	1.7457948835
N	−0.8195636007	−1.0988525473	−1.6451612144
N	0.8186231982	1.0764899028	1.6087846267
C	0.5376068694	−1.2095973180	−1.8886053806
C	−0.5345527144	1.2147331777	1.8628485244
C	1.0481330058	0.0626572307	−2.1539753410
C	−1.0536872100	−0.0445240515	2.1566996286
C	2.4500928761	0.5880788099	−2.3055639056
C	−2.4580411877	−0.5607779121	2.3095829430
C	2.8995468325	1.3408935655	−1.0213985006
C	−2.8924321481	−1.3414838664	1.0364486168
N	1.8089730435	2.2280540294	−0.4893881489
N	−1.7870264736	−2.2341613162	0.5327848303
H	−1.4620023270	−1.9025421591	−0.4701251639
H	1.4369384322	1.8237850331	0.5832883329
H	−2.0703671871	0.6663156142	−1.6278281859
H	2.0527908945	−0.7002484147	1.5937497331
H	1.0554011409	−2.1801795664	−1.8576465120
H	−1.0374633648	2.1908886004	1.8088811787
H	3.1747173425	−0.2315395799	−2.5001466281
H	−3.1823462897	0.2650198499	2.4740908466
H	2.5036508659	1.2864669288	−3.1723863125
H	−2.5243683790	−1.2362513848	3.1931787086
H	3.8147356820	1.9444761021	−1.2038727271
H	−3.8025974056	−1.9504008621	1.2215242990
H	3.1381046378	0.6021384973	−0.2267549937
H	−3.1201399474	−0.6259831683	0.2197372463
H	0.9362647270	2.0810563657	−1.1206469351
H	−0.9069122409	−2.0509027964	1.1706398598
H	2.0763805966	3.2231979800	−0.4728497465
H	−2.0405026819	−3.2335986078	0.5383268595

Thermochemical data for DTS between (1G-VIa)2 and (3G-Vc)2 dimers
in the two-molecule tautomerization calculated with BP86/def2-SV(P)
using ideal gas, rigid rotor, harmonic normal mode approximations.

Ee = −719.8644953278 Ha
ZPE = 0.281505 Ha = 739.093170 KJ/Mol
Imaginary frequency absolute value = 145.57 cm-1

**** T = 393 K ****

	Ln Q	H	G	Cp	S
		KJ/Mol	KJ/Mol	J/Mol-K	J/Mol-K
ELEC.	0.000000	0.000	0.000	0.000	0.000
TRANS.	19.371562	8.159	-63.217	20.786	181.849
ROT.	15.155692	4.895	-49.459	12.472	138.482
VIB.	14.070116	793.110	693.177	290.559	254.606
TOTAL	48.597370	806.163	580.500	323.817	574.938

2 Information used for the GED model

2.1 Histamine GED experimental intensity curves

Table S23. Experimental LD curve. Scale factor = 0.48(1), Nozzle-to-Plate distance = 362.3 mm, electrons' wavelength $\lambda = 0.049722$ Å, s in Å^{-1}

s	Total Int.	Background
3.4	0.66388886	0.70768236
3.6	0.67129387	0.72572792
3.8	0.68705060	0.74354537
4.0	0.69950463	0.75998163
4.2	0.71627151	0.77363117
4.4	0.73137858	0.78334425
4.6	0.74537254	0.78883059
4.8	0.75646311	0.79073539
5.0	0.77633137	0.79013375
5.2	0.80041060	0.78758807
5.4	0.82340644	0.78316262
5.6	0.84005488	0.77683323
5.8	0.84506403	0.76871511
6.0	0.83694658	0.75910413
6.2	0.81733661	0.74838856
6.4	0.78984916	0.73696063
6.6	0.75862894	0.72518428
6.8	0.72667662	0.71337902
7.0	0.69662120	0.70178400
7.2	0.66972509	0.69049962
7.4	0.64681036	0.67949085
7.6	0.62822564	0.66865854
7.8	0.61479521	0.65793108
8.0	0.60706188	0.64729500
8.2	0.60440396	0.63678421
8.4	0.60566417	0.62646895
8.6	0.60849646	0.61643689
8.8	0.60998215	0.60680496
9.0	0.60897034	0.59773370
9.2	0.60566702	0.58936025
9.4	0.60015916	0.58171983
9.6	0.59335472	0.57474937
9.8	0.58613106	0.56831821
10.0	0.57834335	0.56226804
10.2	0.56943809	0.55647829
10.4	0.55975643	0.55090362
10.6	0.54955568	0.54553879
10.8	0.53891095	0.54038754
11.0	0.52906406	0.53546087
11.2	0.52070945	0.53075247
11.4	0.51469544	0.52622917
11.6	0.51095874	0.52183029
11.8	0.50888846	0.51749846

12.0	0.50735359	0.51321856
12.2	0.50564914	0.50902970
12.4	0.50295006	0.50498707
12.6	0.49944490	0.50111875
12.8	0.49489058	0.49739854
13.0	0.49042154	0.49377643
13.2	0.48627242	0.49020428
13.4	0.48336184	0.48667587
13.6	0.48163696	0.48322377
13.8	0.48097143	0.47990935
14.0	0.48074008	0.47680470
14.2	0.48074324	0.47397980
14.4	0.48042413	0.47148450
14.6	0.47962490	0.46934750
14.8	0.47872332	0.46756513
15.0	0.47648449	0.46610019
15.2	0.47362519	0.46493709
15.4	0.46963331	0.46407433
15.6	0.46568071	0.46351311
15.8	0.46120679	0.46321692
16.0	0.45738587	0.46313170
16.2	0.45421519	0.46318232
16.4	0.45224721	0.46330267
16.6	0.45179646	0.46345066
16.8	0.45295420	0.46360628

Table S24. Experimental SD curve. Scale factor = 0.51(1), Nozzle-to-Plate distance = 193.9 mm, electrons' wavelength $\lambda = 0.049907$ Å, s in Å^{-1}

s	Total Int.	Background
6.4	0.65457589	0.60768234
6.6	0.63186933	0.60390888
6.8	0.61262617	0.60009203
7.0	0.59406240	0.59603718
7.2	0.57319596	0.59154878
7.4	0.55664408	0.58659795
7.6	0.54312051	0.58124066
7.8	0.53412561	0.57557416
8.0	0.53111345	0.56967561
8.2	0.53305732	0.56354871
8.4	0.53834552	0.55715463
8.6	0.54369572	0.55048973
8.8	0.54683990	0.54366022
9.0	0.54703742	0.53687175
9.2	0.54516655	0.53033224
9.4	0.54162213	0.52414618
9.6	0.53644857	0.51829527
9.8	0.53022232	0.51269495
10.0	0.52299486	0.50725839
10.2	0.51455629	0.50194030
10.4	0.50510230	0.49674585
10.6	0.49544840	0.49170176
10.8	0.48515192	0.48682266
11.0	0.47616979	0.48210835
11.2	0.46803377	0.47753564
11.4	0.46201769	0.47308666
11.6	0.45819877	0.46875149
11.8	0.45599718	0.46452793
12.0	0.45465418	0.46042288
12.2	0.45294652	0.45644514
12.4	0.45103226	0.45259252
12.6	0.44719946	0.44883852
12.8	0.44295121	0.44515747
13.0	0.43813746	0.44152230
13.2	0.43435946	0.43791776
13.4	0.43108501	0.43434172
13.6	0.42920457	0.43081910
13.8	0.42829963	0.42738301
14.0	0.42770348	0.42406079
14.2	0.42720226	0.42086814
14.4	0.42630167	0.41780057
14.6	0.42480596	0.41483503
14.8	0.42245771	0.41193708
15.0	0.41912928	0.40907363
15.2	0.41445767	0.40622743

15.4	0.40885201	0.40340754
15.6	0.40262555	0.40063963
15.8	0.39623888	0.39795345
16.0	0.38983004	0.39537696
16.2	0.38453712	0.39293397
16.4	0.38050341	0.39062940
16.6	0.37777525	0.38845304
16.8	0.37685562	0.38638635
17.0	0.37712088	0.38439910
17.2	0.37827724	0.38246119
17.4	0.37901289	0.38055601
17.6	0.37974209	0.37869113
17.8	0.37962638	0.37687663
18.0	0.37858032	0.37512074
18.2	0.37688725	0.37342740
18.4	0.37491886	0.37179189
18.6	0.37254206	0.37020592
18.8	0.37039096	0.36867047
19.0	0.36854370	0.36719072
19.2	0.36717081	0.36577000
19.4	0.36576846	0.36440828
19.6	0.36491910	0.36310677
19.8	0.36401000	0.36186023
20.0	0.36309400	0.36066620
20.2	0.36187873	0.35952838
20.4	0.36068629	0.35845401
20.6	0.35900805	0.35744404
20.8	0.35712843	0.35649627
21.0	0.35493850	0.35560291
21.2	0.35306838	0.35475082
21.4	0.35078881	0.35392290
21.6	0.34931938	0.35311366
21.8	0.34815474	0.35231812
22.0	0.34746792	0.35153908
22.2	0.34744323	0.35078592
22.4	0.34777245	0.35006566
22.6	0.34841420	0.34938196
22.8	0.34895891	0.34873591
23.0	0.34918740	0.34813247
23.2	0.34947806	0.34757897
23.4	0.34935849	0.34707606
23.6	0.34881107	0.34662592
23.8	0.34839145	0.34623341
24.0	0.34763497	0.34589723
24.2	0.34709335	0.34561486
24.4	0.34638375	0.34537998
24.6	0.34575034	0.34518933
24.8	0.34542117	0.34504010
25.0	0.34503483	0.34492784
25.2	0.34479273	0.34485538
25.4	0.34466383	0.34483229
25.6	0.34458961	0.34487115

25.8	0.34470498	0.34498216
26.0	0.34476624	0.34516624
26.2	0.34492538	0.34541539
26.4	0.34510810	0.34571245
26.6	0.34514239	0.34603860
26.8	0.34516879	0.34638370
27.0	0.34536703	0.34674547
27.2	0.34582341	0.34712240
27.4	0.34649957	0.34751094
27.6	0.34708629	0.34791119
27.8	0.34799109	0.34833285
28.0	0.34883328	0.34878756
28.2	0.34989389	0.34928793
28.4	0.35082540	0.34984330
28.6	0.35169842	0.35046376
28.8	0.35275470	0.35115818
29.0	0.35341216	0.35193237
29.2	0.35412895	0.35279723
29.4	0.35502943	0.35375899
29.6	0.35563345	0.35481534
29.8	0.35629032	0.35596496
30.0	0.35705248	0.35720211
30.2	0.35809457	0.35851033
30.4	0.35911786	0.35986370
30.6	0.36018657	0.36124001
30.8	0.36155754	0.36262554
31.0	0.36288490	0.36401364
31.2	0.36432572	0.36540996
31.4	0.36577426	0.36682777
31.6	0.36766738	0.36827862
31.8	0.36942736	0.36976335
32.0	0.37094768	0.37128547
32.2	0.37275287	0.37285381
32.4	0.37459963	0.37446737
32.6	0.37650172	0.37611421
32.8	0.37841585	0.37777701

2.2 Defenition of the internal coordinates used in GED+MW refinement

Table S25. UNEX Z-Matrix used for the GED+MW refinement of $N_{(1)}$−H species. The given coordinates' values correspond to ^{1}G−IVa conformer.

```
 ------------------------------------------------------------
  1 N
  2 C   1       rC2N1
  3 N   2       rN3C2  1     aN3C2N1
  4 C   3       rC4N3  2     aC4N3C2  1   dC4N3C2N1
  5 C   4       rC5C4  1       rC5N1  2   dC5C4N1C2  4
  6 C   5       rC6C5  1     aC6C5N1  2   dC6C5N1C2
  7 C   6       rC7C6  5     aC7C6C5  1   tC7C6C5N1
  8 N   7       rN8C7  6     aN8C7C6  5   tN8C7C6C5
  9 H   1       rH9N1  5     aH9N1C5  4   dH9N1C5C4
 10 H   2      rH10C2  1    aH10C2N1  5  dH10C2N1C5
 11 H   4      rH11C4  3    aH11C4N3  2  dH11C4N3C2
 12 H   6      rH12C6  5    aH12C6C5  7    aH12C6C7  1
 13 H   6      rH13C6  5    aH13C6C5  7    aH13C6C7 -1
 14 H   7      rH14C7  6    aH14C7C6  8    aH14C7N8  1
 15 H   7      rH15C7  6    aH15C7C6  8    aH15C7N8 -1
 16 H   8      rH16N8  7    aH16N8C7  6  tH16N8C7C6
 17 H   8      rN17H8  7    aH17N8C7  6  tH17N8C7C6

 Variables:
      rC2N1       1.35918918         1
      rN3C2       1.32418715         2
      rC4N3       1.37189398         3
      rC5C4       1.38090767         4
      rC5N1       1.37221714         5
      rC6C5       1.48924953         6
      rC7C6       1.52559351         7
      rN8C7       1.47108355         8
      rH9N1       1.01517869         9
     rH10C2       1.07923014        10
     rH11C4       1.08004751        11
     rH12C6       1.09316825        12
     rH13C6       1.09833189        13
     rH14C7       1.09726216        14
     rH15C7       1.09293177        15
     rH16N8       1.01617569        16
     rN17H8       1.01491286        17
    aN3C2N1     111.65451590        18
    aC4N3C2     104.85638716        19
    aC6C5N1     122.47607242        20
    aC7C6C5     113.14106293        21
    aN8C7C6     109.86809141        22
    aH9N1C5     121.85185245        23
   aH10C2N1     122.65022159        24
   aH11C4N3     121.48037206        25
   aH12C6C5     108.30881450        26
   aH12C6C7     109.50595343        27
   aH13C6C5     110.82690273        28
```

```
  aH13C6C7     108.42830330        29
  aH14C7C6     109.40557884        30
  aH14C7N8     112.76741972        31
  aH15C7C6     109.24973731        32
  aH15C7N8     107.87116193        33
  aH16N8C7     109.35035548        34
  aH17N8C7     110.10237744        35
 dC4N3C2N1      -0.46747820        36
 dC5C4N1C2     179.48229583        37
 dC6C5N1C2     179.95175196        38
 tC7C6C5N1     -44.33762515        39
 tN8C7C6C5      67.26042956        40
 dH9N1C5C4    -175.10962485        41
dH10C2N1C5    -179.30307912        42
dH11C4N3C2    -179.91720709        43
tH16N8C7C6      69.98287333        44
tH17N8C7C6    -173.54422176        45
-------------------------------------------------------------
```

Table S26. UNEX Z-Matrix used for the GED+MW refinement of $N_{(3)}-H$ species. The given coordinates' values correspond to ^3G-Ib conformer. The grouping of the diffrent conformers' parameters is shown.

```
------------------------------------------------------------
 1 N
 2 C   1       rC2N1
 3 N   2       rN3C2  1     aN3C2N1
 4 C   3       rC4N3  2     aC4N3C2  1   dC4N3C2N1
 5 C   4       rC5C4  1       rC5N1  2   dC5C4N1C2  4
 6 C   5       rC6C5  1     aC6C5N1  2   dC6C5N1C2
 7 C   6       rC7C6  5     aC7C6C5  1   tC7C6C5N1
 8 N   7       rN8C7  6     aN8C7C6  5   tN8C7C6C5
 9 H   3       rH9N3  2     aH9N3C2  1   dH9N3C2N1
10 H   2      rH10C2  1    aH10C2N1  5  dH10C2N1C5
11 H   4      rH11C4  3    aH11C4N3  2  dH11C4N3C2
12 H   6      rH12C6  5    aH12C6C5  7    aH12C6C7  1
13 H   6      rH13C6  5    aH13C6C5  7    aH13C6C7 -1
14 H   7      rH14C7  6    aH14C7C6  8    aH14C7N8  1
15 H   7      rH15C7  6    aH15C7C6  8    aH15C7N8 -1
16 H   8      rH16N8  7    aH16N8C7  6  tH16N8C7C6
17 H   8      rN17H8  7    aH17N8C7  6  tH17N8C7C6

Variables:                          G-Ib G-Ic G-Vb G-Vc T-a
     rC2N1       1.32148115         101  101  101  101  101
     rN3C2       1.36066013         102  102  102  102  102
     rC4N3       1.37172969         103  103  103  103  103
     rC5C4       1.37918688         104  104  104  104  104
     rC5N1       1.37700101         105  105  105  105  105
     rC6C5       1.48976412         106  106  106  106  106
     rC7C6       1.52519130         107  107  107  107  107
     rN8C7       1.46313995         108  108  108  108  108
     rH9N3       1.00795350         109  109  109  109  109
    rH10C2       1.07929140         110  110  110  110  110
    rH11C4       1.07799804         111  111  111  111  111
    rH12C6       1.09339336         112  112  412  412  512
    rH13C6       1.09388676         113  113  413  413  513
    rH14C7       1.09773613         114  114  414  414  514
    rH15C7       1.09325483         115  115  415  415  515
    rH16N8       1.01619155         116  216  316  416  516
    rN17H8       1.01464755         117  217  317  417  517
   aN3C2N1     111.38893367         118  118  118  118  118
   aC4N3C2     107.50305617         119  119  119  119  119
   aC6C5N1     121.42722423         120  120  120  120  120
   aC7C6C5     111.18158066         121  121  421  421  121
   aN8C7C6     109.40684490         122  122  422  422  122
   aH9N3C2     126.24870326         123  123  123  123  123
  aH10C2N1     126.04998404         124  124  124  124  124
  aH11C4N3     122.50933017         125  125  125  125  125
  aH12C6C5     109.56468062         126  126  426  426  526
  aH12C6C7     109.03486035         127  127  427  427  527
  aH13C6C5     109.33459481         128  128  428  428  528
```

aH13C6C7	109.34090527	129	129	429	429	529
aH14C7C6	108.34057465	130	130	430	430	530
aH14C7N8	113.78133513	131	131	431	431	531
aH15C7C6	109.25901041	132	132	432	432	532
aH15C7N8	108.10287739	133	133	433	433	533
aH16N8C7	108.84568566	134	134	334	434	534
aH17N8C7	109.92998143	135	135	335	435	535
dC4N3C2N1	0.00296291	136	136	136	136	136
dC5C4N1C2	-179.56607856	137	137	137	137	137
dC6C5N1C2	177.71320536	138	138	138	138	138
tC7C6C5N1	-67.47462208	139	139	139	139	139
tN8C7C6C5	-62.30235123	140	140	440	440	540
dH9N3C2N1	179.38944604	141	141	141	141	141
dH10C2N1C5	179.43282065	142	142	142	142	142
dH11C4N3C2	-179.81474817	143	143	143	143	143
tH16N8C7C6	63.82182946	144	244	344	444	544
tH17N8C7C6	-179.99208694	145	245	345	445	545

2.3 Vibrational corrections for the GED refinement of histamine

Table S27. GED vibrational correction parameters for ^{1}G−IVa conformer.

At1	At2	re	l	re-ra	6*kappa
N8	H17	1.0196	0.0713	-0.0142	55.0
N8	H16	1.0208	0.0715	-0.0154	55.1
N1	H9	1.0216	0.0719	-0.0135	59.2
C2	H10	1.0890	0.0748	-0.0152	58.9
C4	H11	1.0895	0.0749	-0.0149	58.6
C6	H12	1.1007	0.0765	-0.0161	64.9
C7	H15	1.1011	0.0766	-0.0158	65.9
C6	H13	1.1062	0.0774	-0.0163	69.2
C7	H14	1.1068	0.0776	-0.0165	70.7
C2	N3	1.3246	0.0430	-0.0047	7.3
N1	C2	1.3618	0.0442	-0.0103	8.2
N3	C4	1.3698	0.0457	-0.0053	9.4
N1	C5	1.3736	0.0445	-0.0096	8.0
C4	C5	1.3888	0.0446	-0.0067	7.6
C7	N8	1.4676	0.0496	-0.0092	13.4
C5	C6	1.4943	0.0488	-0.0076	10.7
C6	C7	1.5281	0.0512	-0.0108	14.0
H16	H17	1.6231	0.1191	-0.0166	8.8
H12	H13	1.7642	0.1255	-0.0175	16.4
H14	H15	1.7758	0.1240	-0.0170	26.9
C7	H16	2.0419	0.1054	-0.0177	-0.3
C7	H17	2.0513	0.1053	-0.0182	-7.3
N8	H15	2.0892	0.1044	-0.0171	17.2
C5	H9	2.0921	0.0957	-0.0178	11.2
N8	H9	2.1043	0.2216	-0.0853	4613.8
C5	H12	2.1188	0.1074	-0.0137	2.9
C2	C4	2.1379	0.0504	-0.0082	2.8
N3	H10	2.1514	0.0945	-0.0099	18.4
C7	H13	2.1519	0.1091	-0.0152	8.9
N1	H10	2.1520	0.0963	-0.0148	18.3
C5	H13	2.1529	0.1072	-0.0097	1.0
N3	H11	2.1535	0.0977	-0.0105	17.0
C6	H15	2.1536	0.1084	-0.0163	6.4
N8	H14	2.1572	0.1020	-0.0174	23.5
C7	H12	2.1599	0.1101	-0.0160	1.6
C6	H14	2.1626	0.1081	-0.0151	13.5
C2	H9	2.1731	0.0972	-0.0046	30.5
N1	C4	2.1849	0.0501	-0.0114	2.9
C2	C5	2.2093	0.0505	-0.0116	2.9
N1	N3	2.2240	0.0492	-0.0113	3.3
C5	H11	2.2240	0.0964	-0.0106	13.4
N3	C5	2.2727	0.0510	-0.0094	3.0
H15	H17	2.3517	0.1852	-0.0073	-25.0
H14	H16	2.4008	0.1806	-0.0133	-229.3
H12	H14	2.4162	0.1705	-0.0121	-95.4
C6	N8	2.4591	0.0744	-0.0150	26.5

H14	H17	2.4701	0.1805	-0.0376	-207.4
N1	C6	2.5100	0.0676	-0.0150	11.9
C5	C7	2.5227	0.0718	-0.0182	13.3
H13	H14	2.5232	0.1785	-0.0150	-234.1
H13	H16	2.5252	0.2815	-0.0281	3114.8
H12	H15	2.5346	0.1800	-0.0162	-267.2
H9	H10	2.6209	0.1576	-0.0022	-136.0
C4	C6	2.6480	0.0683	-0.0031	8.5
H9	H16	2.6499	0.2820	-0.0676	4643.3
N8	H13	2.6785	0.1725	-0.0092	73.2
C5	H15	2.7136	0.1697	-0.0190	81.1
C7	H9	2.7228	0.2133	-0.0640	2771.9
C6	H9	2.7239	0.1440	-0.0283	104.8
C6	H16	2.7337	0.1901	-0.0285	274.5
H9	H17	2.7948	0.2686	-0.0653	4453.9
C4	H12	2.8148	0.1531	-0.0035	-78.1
N1	N8	2.8276	0.1414	-0.0590	1350.6
H11	H12	2.8519	0.2216	0.0042	-153.1
H9	H15	2.9278	0.3049	-0.0630	5082.4
H15	H16	2.9331	0.1240	-0.0150	48.4
N1	H13	2.9745	0.1659	-0.0003	-490.0
N1	C7	2.9823	0.1242	-0.0401	287.2
C5	N8	3.0166	0.1003	-0.0264	132.3
H13	H15	3.0603	0.1268	-0.0197	69.3
H9	H13	3.0736	0.2323	0.0001	-797.2
C6	H11	3.0818	0.1400	0.0012	-124.6
N1	H15	3.0947	0.2437	-0.0380	98.4
C4	H9	3.1587	0.0870	-0.0136	35.5
C2	H11	3.1771	0.0892	-0.0132	41.3
C4	H10	3.1989	0.0880	-0.0133	46.4
N3	H9	3.2190	0.0881	-0.0077	51.4
C4	H13	3.2386	0.1485	-0.0070	-520.0
C5	H10	3.2483	0.0893	-0.0169	42.0
N1	H11	3.2485	0.0882	-0.0164	44.7
C6	H17	3.3476	0.1017	-0.0102	37.2
N1	H16	3.3580	0.2527	-0.0507	-258.7
N1	H12	3.3768	0.1066	-0.0159	-12.6
N8	H12	3.4043	0.1040	-0.0181	43.9
C5	H14	3.4583	0.1046	-0.0197	32.4
C5	H16	3.4757	0.2284	-0.0302	-1916.4
N1	H17	3.6112	0.2077	-0.0292	-474.8
H13	H17	3.6341	0.1869	-0.0093	-216.7
H11	H13	3.6342	0.2221	-0.0038	-2003.5
C2	C6	3.6383	0.0630	-0.0142	9.1
H12	H16	3.6793	0.1953	-0.0286	129.6
H9	H12	3.7385	0.1594	-0.0320	62.8
N3	C6	3.7460	0.0626	-0.0074	9.5
H9	H14	3.7836	0.2222	-0.0707	2480.3
C4	H15	3.7907	0.2376	0.0088	-1639.3
C4	C7	3.7986	0.1071	-0.0005	-400.9
C5	H17	3.9051	0.1517	-0.0014	-947.7
N1	H14	4.0607	0.1351	-0.0413	228.4

N3	H12	4.1088	0.1436	-0.0055	-125.2
C2	H13	4.1146	0.1549	-0.0043	-474.0
C2	N8	4.1570	0.1514	-0.0530	1363.6
H12	H17	4.1828	0.1383	-0.0158	-65.7
H9	H11	4.1891	0.1169	-0.0178	46.7
C2	H15	4.1945	0.2590	-0.0329	-121.2
H10	H11	4.2003	0.1188	-0.0159	54.2
C2	C7	4.2585	0.1223	-0.0337	7.8
N3	H13	4.2781	0.1473	-0.0052	-473.0
C2	H12	4.3118	0.1201	-0.0124	-79.4
H11	H15	4.3329	0.2966	0.0326	-5180.1
C7	H11	4.3533	0.1741	0.0161	-1363.7
C4	N8	4.3884	0.1082	-0.0149	78.4
N3	H15	4.5707	0.2585	-0.0074	-1613.6
C6	H10	4.6129	0.1033	-0.0192	19.3
C4	H14	4.6636	0.1367	0.0029	-477.2
N3	C7	4.6797	0.1123	-0.0132	-398.9
C2	H16	4.6957	0.2685	-0.0464	-1508.2
N8	H10	4.7092	0.2041	-0.0663	1929.8
C4	H16	4.8565	0.2423	-0.0207	-4203.9
C2	H17	4.8655	0.2453	-0.0155	-2612.9
N3	N8	4.9474	0.1274	-0.0304	544.2
H10	H15	4.9511	0.3020	-0.0448	-118.4
H10	H13	5.0343	0.1919	-0.0048	-864.5
H11	H14	5.0503	0.2094	0.0239	-1869.8
C7	H10	5.0560	0.1695	-0.0439	-2.5
N8	H11	5.1770	0.1473	-0.0003	-275.5
C4	H17	5.2393	0.1878	0.0216	-3470.6
H10	H16	5.2436	0.3013	-0.0560	-87.8
H10	H17	5.2975	0.3023	-0.0303	-2420.7
C2	H14	5.3372	0.1347	-0.0317	-92.1
H10	H12	5.3553	0.1397	-0.0156	-62.4
N3	H16	5.4686	0.2594	-0.0304	-4397.3
H11	H16	5.5990	0.2608	-0.0098	-4767.5
N3	H14	5.6711	0.1330	-0.0081	-529.3
N3	H17	5.7275	0.2278	0.0118	-5017.0
H11	H17	6.0298	0.2147	0.0376	-4772.5
H10	H14	6.1565	0.1786	-0.0417	-234.4

Table S28. GED vibrational correction parameters for ^{3}G−Ib conformer.

At1	At2	re	l	re−ra	6*kappa
N3	H9	1.0129	0.0703	−0.0149	50.3
N8	H17	1.0193	0.0713	−0.0145	55.7
N8	H16	1.0205	0.0716	−0.0161	55.1
C4	H11	1.0868	0.0746	−0.0147	56.8
C2	H10	1.0891	0.0748	−0.0147	57.7
C6	H12	1.1007	0.0766	−0.0168	65.2
C6	H13	1.1021	0.0768	−0.0195	66.5
C7	H15	1.1021	0.0768	−0.0154	67.4
C7	H14	1.1072	0.0777	−0.0129	71.3
N1	C2	1.3215	0.0428	−0.0069	7.1
C2	N3	1.3640	0.0443	−0.0086	8.3
N3	C4	1.3732	0.0444	−0.0090	8.0
N1	C5	1.3762	0.0461	−0.0042	10.0
C4	C5	1.3867	0.0445	−0.0055	7.6
C7	N8	1.4595	0.0491	−0.0127	12.6
C5	C6	1.4956	0.0489	−0.0134	11.2
C6	C7	1.5262	0.0512	−0.0096	14.1
H16	H17	1.6186	0.1198	−0.0028	7.6
H14	H15	1.7800	0.1238	−0.0124	28.4
H12	H13	1.7823	0.1253	−0.0113	16.1
C7	H16	2.0233	0.1054	−0.0046	−2.9
C7	H17	2.0368	0.1059	−0.0026	−14.6
N8	H15	2.0882	0.1041	−0.0209	15.5
C2	H9	2.1266	0.0945	−0.0088	10.9
C5	H13	2.1314	0.1097	−0.0486	19.7
C5	H12	2.1329	0.1077	0.0032	4.9
C4	H9	2.1343	0.0949	−0.0095	8.9
C6	H14	2.1408	0.1085	−0.0353	18.3
C2	C5	2.1502	0.0504	−0.0119	2.9
N1	H10	2.1522	0.0943	−0.0118	18.8
N3	H10	2.1525	0.0960	−0.0143	18.2
C7	H12	2.1533	0.1103	−0.0181	4.4
C6	H15	2.1565	0.1091	0.0003	6.7
C7	H13	2.1579	0.1096	−0.0121	3.2
N3	H11	2.1634	0.0984	−0.0099	12.1
N8	H14	2.1636	0.1016	0.0004	23.2
N3	C5	2.1947	0.0497	−0.0125	2.6
C2	C4	2.2071	0.0506	−0.0118	2.9
N1	N3	2.2202	0.0490	−0.0092	3.2
C5	H11	2.2624	0.0964	−0.0094	15.8
N1	C4	2.2628	0.0515	−0.0027	3.2
H15	H17	2.3922	0.1995	0.1765	−1573.0
H14	H16	2.4267	0.1936	0.1866	−2364.4
H14	H17	2.4318	0.1896	−0.1305	227.8
C6	N8	2.4439	0.0736	−0.0298	29.4
H13	H15	2.4590	0.1795	−0.0852	61.2

H13	H14	2.4599	0.1863	0.0628	-388.1
H12	H15	2.4861	0.1832	0.1026	-476.3
C5	C7	2.4984	0.0769	-0.0241	27.5
N1	C6	2.5022	0.0689	-0.0216	15.0
H9	H10	2.5476	0.1565	-0.0095	-126.9
H9	H11	2.5609	0.1590	-0.0061	-151.0
C5	H16	2.5946	0.2568	-0.1325	4433.3
C4	C6	2.6004	0.0691	-0.0055	8.0
C6	H16	2.6478	0.2021	-0.2618	3869.6
N8	H12	2.6640	0.1849	-0.1575	1191.8
C5	H14	2.7301	0.1794	-0.1924	1030.4
C4	H12	2.7348	0.1667	-0.0047	144.1
N1	H14	2.7710	0.3398	0.1168	34870.4
H11	H12	2.7935	0.2469	-0.0225	656.5
N1	H13	2.8046	0.2545	-0.3799	31127.1
H15	H16	2.9277	0.1236	0.0035	59.3
C5	N8	2.9560	0.1591	0.1315	-1793.4
H12	H16	2.9895	0.3402	-0.5470	41133.1
H12	H14	3.0537	0.1268	-0.0285	74.0
C6	H11	3.0721	0.1424	-0.0014	-124.3
N1	C7	3.0721	0.2681	0.3459	-16461.3
C4	H16	3.0873	0.6001	-1.0389	612126.8
N1	H16	3.1026	0.6383	1.2308	-849044.9
C5	H9	3.1798	0.0855	-0.0112	38.5
N1	H9	3.1906	0.0855	-0.0085	36.2
C5	H10	3.2120	0.0881	-0.0164	45.2
C2	H11	3.2444	0.0900	-0.0135	39.1
C4	H10	3.2459	0.0892	-0.0173	41.0
C4	H13	3.3005	0.1889	0.2644	-14698.3
N1	H11	3.3301	0.0886	-0.0063	45.4
C6	H17	3.3315	0.1025	-0.0157	30.2
N8	H13	3.3922	0.1038	-0.0344	43.3
N1	H12	3.3970	0.1107	0.0276	31.0
C5	H15	3.4430	0.1049	-0.0171	46.4
H11	H16	3.5136	0.9629	-1.5993	2790804.4
C2	C6	3.5776	0.0628	-0.0222	9.7
H12	H17	3.6131	0.1912	-0.0014	-312.7
C4	C7	3.6239	0.2389	-0.3062	15239.6
N1	N8	3.6244	0.4943	0.9764	-417088.4
C4	N8	3.6419	0.4326	-0.4839	104973.4
H13	H16	3.6601	0.1906	-0.1438	910.7
N3	C6	3.6635	0.0621	-0.0157	9.3
C2	H16	3.7223	0.4810	0.6840	-190313.6
N3	H16	3.7471	0.4189	-0.4639	58573.3
H11	H13	3.8193	0.3067	0.4778	-71595.3
C5	H17	3.8560	0.1791	-0.0543	-104.1
N8	H11	3.9593	0.7419	-0.9300	683241.0
C2	H13	3.9688	0.1829	-0.2085	4063.5
C2	H14	3.9889	0.2741	-0.1393	6793.6
C4	H14	4.0010	0.3044	-0.4388	32784.3
N3	H12	4.0253	0.1496	0.0072	-70.4
N1	H15	4.0713	0.2223	0.1534	2731.0

C7	H11	4.1290	0.3970	-0.4738	59126.3
H13	H17	4.1667	0.1386	-0.0025	-75.1
C2	C7	4.2209	0.1700	0.1263	611.1
N3	H13	4.2339	0.1476	0.0830	-1696.6
H10	H11	4.2352	0.1213	-0.0171	38.6
C2	H12	4.2762	0.1209	0.0219	-55.4
N1	H17	4.3102	0.5331	0.7214	-187473.6
C2	N8	4.4659	0.3687	0.6167	-117312.2
H9	H16	4.5097	0.5182	-0.6655	171127.0
N3	N8	4.5124	0.3183	-0.0989	5339.2
N3	C7	4.5182	0.1691	-0.1721	1237.9
H10	H16	4.5486	0.6243	1.0883	-647548.9
C4	H15	4.5500	0.2047	-0.1646	945.4
C4	H17	4.5808	0.4862	-0.6821	220763.0
C6	H10	4.5878	0.1012	-0.0256	27.7
N3	H14	4.6109	0.2872	-0.3920	15356.5
C6	H9	4.6187	0.0974	-0.0106	27.2
H10	H14	4.7077	0.3353	-0.0530	21079.0
H11	H14	4.7223	0.4115	-0.5342	61705.8
H9	H12	4.8684	0.1838	0.0093	-118.7
H10	H13	4.8917	0.2350	-0.2935	12051.3
H11	H15	4.9271	0.3473	-0.2563	-1966.9
H11	H17	4.9308	0.8161	-1.0653	978698.5
C7	H10	5.1070	0.2429	0.2224	-2095.5
C2	H17	5.1520	0.4050	0.3082	-9263.9
H9	H13	5.2005	0.1816	0.1484	-5038.5
C2	H15	5.2699	0.1633	0.0507	1192.8
N3	H17	5.3257	0.3824	-0.4106	35662.3
N8	H9	5.3309	0.4083	-0.2388	24033.5
N8	H10	5.3432	0.4877	0.8681	-310319.1
H10	H12	5.3446	0.1415	0.0270	7.1
C7	H9	5.4730	0.2259	-0.2279	3732.3
N3	H15	5.5440	0.1577	-0.1033	-225.9
H9	H14	5.5914	0.3354	-0.4472	25807.7
H10	H17	5.9201	0.5525	0.5774	-90051.1
H9	H17	6.1218	0.4997	-0.5742	117125.2
H10	H15	6.1558	0.2277	0.1048	2816.9
H9	H15	6.4978	0.2063	-0.1310	-841.1

Table S29. GED vibrational correction parameters for ^{3}G−Ic conformer.

At1	At2	re	l	re−ra	6*kappa
N3	H9	1.0130	0.0703	−0.0145	50.2
N8	H17	1.0196	0.0715	−0.0161	54.7
N8	H16	1.0203	0.0716	−0.0131	55.6
C4	H11	1.0869	0.0746	−0.0149	56.9
C2	H10	1.0890	0.0748	−0.0152	57.7
C7	H14	1.0999	0.0765	−0.0191	65.1
C7	H15	1.1025	0.0769	−0.0157	67.6
C6	H12	1.1035	0.0770	−0.0156	67.0
C6	H13	1.1038	0.0770	−0.0123	67.2
N1	C2	1.3216	0.0428	−0.0036	7.1
C2	N3	1.3635	0.0442	−0.0115	8.3
N3	C4	1.3732	0.0444	−0.0102	8.0
N1	C5	1.3756	0.0461	−0.0058	10.0
C4	C5	1.3869	0.0445	−0.0082	7.6
C7	N8	1.4554	0.0489	−0.0103	12.5
C5	C6	1.4959	0.0490	−0.0040	11.2
C6	C7	1.5347	0.0523	−0.0155	16.3
H16	H17	1.6209	0.1197	−0.0163	7.7
H14	H15	1.7712	0.1247	−0.0156	19.9
H12	H13	1.7729	0.1256	−0.0244	18.4
C7	H17	2.0220	0.1055	−0.0201	−2.3
C7	H16	2.0337	0.1051	−0.0119	−5.0
N8	H14	2.0770	0.1042	−0.0279	18.8
N8	H15	2.0901	0.1040	−0.0138	16.0
C2	H9	2.1260	0.0946	−0.0115	10.9
C5	H12	2.1303	0.1077	−0.0196	7.0
C4	H9	2.1345	0.0950	−0.0113	8.9
C5	H13	2.1406	0.1091	0.0091	−17.1
C6	H14	2.1499	0.1085	−0.0187	11.2
C2	C5	2.1507	0.0504	−0.0077	2.9
N1	H10	2.1522	0.0943	−0.0086	19.0
N3	H10	2.1524	0.0959	−0.0152	18.2
N3	H11	2.1618	0.0983	−0.0148	12.1
C6	H15	2.1641	0.1088	−0.0232	15.1
C7	H13	2.1668	0.1109	−0.0223	5.0
C7	H12	2.1727	0.1104	−0.0103	9.2
N3	C5	2.1951	0.0498	−0.0140	2.6
C2	C4	2.2068	0.0505	−0.0135	2.9
N1	N3	2.2194	0.0490	−0.0129	3.3
N1	C4	2.2617	0.0515	−0.0082	3.2
C5	H11	2.2640	0.0962	−0.0104	16.4
H14	H17	2.3387	0.1980	−0.0566	−159.4
H15	H16	2.4410	0.1958	0.0205	92.0
H13	H14	2.4590	0.1868	−0.0555	−62.5
H13	H15	2.4818	0.1798	0.0089	−181.0
H12	H15	2.4868	0.1879	−0.0555	89.2

N1	C6	2.4993	0.0685	-0.0074	11.7
C5	C7	2.5070	0.0764	-0.0129	9.3
C6	N8	2.5261	0.0729	-0.0180	27.1
H9	H10	2.5474	0.1565	-0.0092	-126.2
H9	H11	2.5587	0.1589	-0.0135	-150.7
H12	H16	2.5773	0.2689	0.0189	1243.7
C4	C6	2.6037	0.0685	-0.0019	8.8
C5	H17	2.6594	0.2437	-0.0886	2354.6
C6	H16	2.6844	0.1832	-0.0450	-310.6
N1	H14	2.7341	0.2850	-0.2390	10572.3
C4	H12	2.7363	0.1672	-0.0387	70.7
C6	H17	2.7380	0.1808	0.0046	-241.3
C5	H14	2.7695	0.1878	0.0454	-717.1
H11	H12	2.8024	0.2499	-0.0445	1033.9
N8	H12	2.8345	0.1820	0.0472	-221.5
N1	H17	2.8537	0.6597	-0.6592	494822.2
N1	H13	2.8859	0.2595	0.2465	-15278.2
H14	H16	2.9262	0.1241	-0.0214	39.1
H15	H17	2.9291	0.1231	-0.0165	63.2
N1	C7	2.9919	0.2294	-0.2772	22765.9
C5	N8	2.9976	0.1478	-0.0819	1026.7
H12	H14	3.0666	0.1270	-0.0167	73.1
C6	H11	3.0797	0.1412	-0.0005	-109.9
H12	H17	3.1791	0.3090	0.1322	-9732.1
C5	H9	3.1803	0.0857	-0.0130	38.4
N1	H9	3.1899	0.0856	-0.0111	36.1
C5	H16	3.2106	0.3311	-0.1447	-11522.6
C5	H10	3.2122	0.0881	-0.0131	45.2
C2	H11	3.2435	0.0898	-0.0177	39.1
C4	H10	3.2458	0.0891	-0.0186	41.0
C4	H13	3.2467	0.2149	-0.1771	549.2
N1	H11	3.3297	0.0884	-0.0114	45.6
N1	H12	3.3904	0.1142	-0.0054	-95.3
C4	H17	3.3915	0.6148	0.6763	-404762.3
N1	N8	3.4290	0.5044	-0.5307	234833.2
C5	H15	3.4509	0.1045	-0.0132	44.4
N8	H13	3.4519	0.1043	-0.0185	37.3
C2	C6	3.5770	0.0630	-0.0043	9.0
C2	H17	3.5877	0.4514	-0.4300	117738.3
N3	C6	3.6653	0.0620	-0.0074	9.6
H13	H16	3.6948	0.1825	-0.0089	-71.9
C4	C7	3.7059	0.2233	0.2693	-24425.0
H13	H17	3.7138	0.1800	-0.0282	22.3
H11	H13	3.7220	0.3513	-0.2871	7808.6
C4	H16	3.7980	0.4920	0.3551	-29212.8
C4	N8	3.8659	0.4323	0.4850	-108062.8
N3	H17	3.8901	0.4426	0.2582	-56631.0
N1	H16	3.9558	0.6319	-0.4943	232223.9
H11	H17	4.0013	0.9341	1.2494	-1886150.5
C2	H14	4.0059	0.2724	-0.0202	2116.5
C2	H13	4.0110	0.1812	0.1042	-1942.0
H11	H16	4.0215	0.7745	0.8794	-361135.9

N3	H12	4.0243	0.1490	-0.0352	-97.3
N1	H15	4.0274	0.1974	-0.1723	5939.5
C4	H14	4.1036	0.2831	0.3173	-44802.2
C2	C7	4.1896	0.1479	-0.1065	1993.5
N3	H13	4.2153	0.1583	-0.0896	-826.7
H10	H11	4.2341	0.1211	-0.0216	38.5
C7	H11	4.2654	0.3564	0.4491	-94698.5
C2	H12	4.2718	0.1216	-0.0159	-74.5
H10	H17	4.3143	0.6075	-0.6034	346679.9
N8	H11	4.3444	0.7140	0.9426	-697377.9
C2	N8	4.3578	0.3486	-0.3098	50783.9
N3	C7	4.5612	0.1682	0.1424	-7028.8
C6	H10	4.5863	0.1013	-0.0079	26.1
C4	H15	4.6051	0.1909	0.1790	-7535.3
N3	N8	4.6094	0.3178	0.1942	-13488.7
C6	H9	4.6211	0.0973	-0.0041	28.2
N3	H14	4.6928	0.2926	0.2345	-27448.8
H10	H14	4.7010	0.3154	-0.1016	5278.6
H9	H17	4.7084	0.5548	0.4486	-180809.0
N3	H16	4.7157	0.4564	0.0630	-56212.4
C2	H16	4.7557	0.5536	-0.3517	53942.4
H11	H14	4.8605	0.3501	0.4527	-104083.8
H9	H12	4.8684	0.1836	-0.0367	-176.3
H10	H13	4.9514	0.2351	0.1556	-5348.1
H11	H15	5.0222	0.3133	0.3122	-34115.0
C7	H10	5.0510	0.2133	-0.1776	7202.5
N8	H10	5.1584	0.4760	-0.4498	146585.5
H9	H13	5.1679	0.1987	-0.1280	-1341.2
C2	H15	5.2541	0.1514	-0.0590	669.1
H10	H12	5.3390	0.1433	-0.0138	-79.6
N8	H9	5.4722	0.4152	0.3437	-53918.8
H9	H16	5.4976	0.5183	0.1940	-54701.9
C7	H9	5.5334	0.2217	0.2125	-16984.1
N3	H15	5.5756	0.1549	0.1051	-2828.4
H10	H16	5.6445	0.6668	-0.4714	175885.3
H9	H14	5.6897	0.3328	0.3079	-50965.9
H10	H15	6.1229	0.2092	-0.1062	2327.3
H9	H15	6.5419	0.2002	0.1619	-7386.9

Table S30. GED vibrational correction parameters for ^{3}G−Vb conformer.

At1	At2	re	l	re-ra	6*kappa
N3	H9	1.0129	0.0703	-0.0143	51.2
N8	H17	1.0189	0.0714	-0.0159	55.1
N8	H16	1.0212	0.0715	-0.0136	56.3
C4	H11	1.0868	0.0746	-0.0149	57.8
C2	H10	1.0888	0.0748	-0.0148	57.7
C6	H12	1.1015	0.0767	-0.0168	66.8
C6	H13	1.1024	0.0768	-0.0162	66.8
C7	H14	1.1031	0.0770	-0.0167	67.7
C7	H15	1.1108	0.0783	-0.0157	74.1
N1	C2	1.3219	0.0427	-0.0047	7.1
C2	N3	1.3622	0.0441	-0.0107	8.2
N3	C4	1.3728	0.0444	-0.0099	8.0
N1	C5	1.3772	0.0462	-0.0037	10.1
C4	C5	1.3871	0.0445	-0.0071	7.6
C7	N8	1.4567	0.0491	-0.0097	12.5
C5	C6	1.4972	0.0490	-0.0088	11.0
C6	C7	1.5287	0.0512	-0.0109	14.0
H16	H17	1.6330	0.1201	-0.0119	11.7
H14	H15	1.7745	0.1240	-0.0177	31.7
H12	H13	1.7775	0.1254	-0.0148	17.0
C7	H16	2.0164	0.1031	-0.0216	1.4
C7	H17	2.0367	0.1046	-0.0149	-6.3
N8	H14	2.0910	0.1037	-0.0134	14.0
C5	H12	2.1216	0.1071	-0.0190	4.6
C2	H9	2.1242	0.0949	-0.0109	8.5
C4	H9	2.1338	0.0948	-0.0103	6.2
C7	H13	2.1387	0.1105	-0.0184	1.9
C5	H13	2.1433	0.1079	-0.0104	-0.7
C6	H15	2.1476	0.1084	-0.0179	17.3
N1	H10	2.1522	0.0944	-0.0094	17.7
N3	H10	2.1528	0.0959	-0.0154	19.2
C6	H14	2.1544	0.1091	-0.0130	11.7
C2	C5	2.1556	0.0505	-0.0074	2.9
N3	H11	2.1612	0.0980	-0.0133	12.1
C7	H12	2.1669	0.1099	-0.0129	1.9
N8	H15	2.1685	0.1020	-0.0139	25.0
N3	C5	2.1970	0.0497	-0.0120	2.6
C2	C4	2.2069	0.0505	-0.0121	2.9
N1	H16	2.2158	0.2311	-0.1159	5287.1
N1	N3	2.2163	0.0491	-0.0111	3.2
N1	C4	2.2589	0.0515	-0.0085	3.1
C5	H11	2.2629	0.0959	-0.0108	15.3
H12	H14	2.3952	0.1721	-0.0091	-71.3
H15	H17	2.4049	0.1838	-0.0132	-417.2
H14	H17	2.4367	0.1868	-0.0084	41.0
C6	N8	2.4469	0.0734	-0.0251	29.9

H15	H16	2.4741	0.1813	-0.0240	-261.0
N1	C6	2.5161	0.0681	-0.0059	11.5
C5	C7	2.5235	0.0744	-0.0185	14.0
H13	H14	2.5361	0.1783	-0.0103	-261.8
H12	H15	2.5466	0.1841	-0.0096	-339.6
H9	H10	2.5477	0.1564	-0.0128	-128.3
H9	H11	2.5574	0.1588	-0.0111	-159.1
N8	H13	2.5707	0.1755	-0.0330	225.2
C6	H16	2.5881	0.1731	-0.0393	508.4
C4	C6	2.5958	0.0679	-0.0094	9.7
C5	H15	2.6856	0.1713	-0.0272	261.9
C4	H12	2.7077	0.1552	-0.0445	-1.0
C5	H16	2.7099	0.2130	-0.0571	1945.2
H13	H16	2.7602	0.2694	-0.0318	-206.4
H11	H12	2.7606	0.2261	-0.0627	183.2
N1	H13	2.8919	0.2058	-0.0109	1490.7
H14	H16	2.9260	0.1223	-0.0169	63.8
N1	N8	3.0070	0.1727	-0.0709	2317.1
H13	H15	3.0466	0.1278	-0.0229	62.9
N1	C7	3.0495	0.1728	-0.0158	-394.7
C6	H11	3.0631	0.1403	-0.0086	-111.0
C5	N8	3.0985	0.1146	-0.0293	151.0
N1	H15	3.1817	0.3410	0.0137	-8551.5
C5	H9	3.1818	0.0853	-0.0103	39.2
N1	H9	3.1869	0.0858	-0.0093	36.6
C5	H10	3.2165	0.0882	-0.0118	45.1
C2	H11	3.2430	0.0898	-0.0160	40.2
C4	H10	3.2462	0.0892	-0.0171	41.5
C4	H13	3.2552	0.1725	0.0178	-3201.3
N1	H11	3.3268	0.0883	-0.0117	46.6
C6	H17	3.3311	0.1024	-0.0174	13.9
N8	H12	3.3832	0.1051	-0.0232	35.8
N1	H12	3.3948	0.1073	0.0055	-3.4
C5	H14	3.4475	0.1065	-0.0195	26.9
C2	H16	3.4491	0.2404	-0.0745	4620.9
H13	H17	3.5534	0.1858	-0.0219	117.4
C2	C6	3.5892	0.0627	-0.0085	9.2
C4	H15	3.6198	0.3244	-0.0034	-1638.5
H12	H16	3.6420	0.1758	-0.0401	319.1
N3	C6	3.6649	0.0617	-0.0136	9.5
C4	C7	3.7079	0.1663	-0.0000	-2265.6
H11	H13	3.7310	0.2725	0.0419	-14493.2
N1	H17	3.7428	0.2323	-0.0691	2447.3
C5	H17	3.9384	0.1745	-0.0216	-2225.7
H10	H16	3.9969	0.2702	-0.0840	5360.8
N3	H12	4.0015	0.1438	-0.0350	-78.5
C2	H13	4.0234	0.1631	-0.0079	-115.3
C4	H16	4.0327	0.2497	-0.0215	-3118.2
H11	H15	4.1127	0.4774	0.0323	-8718.5
N1	H14	4.1158	0.1655	-0.0134	-708.0
C2	H15	4.1637	0.2824	-0.0155	1056.1
H12	H17	4.1688	0.1374	-0.0117	-51.8

N3	H13	4.2267	0.1467	0.0021	-782.3
H10	H11	4.2342	0.1211	-0.0198	40.0
C2	C7	4.2393	0.1327	-0.0161	65.6
C7	H11	4.2452	0.2671	0.0160	-6940.0
C2	H12	4.2658	0.1195	-0.0099	-59.5
C2	N8	4.2903	0.1745	-0.0369	1470.6
N3	H16	4.3569	0.2558	-0.0391	-976.9
N3	H15	4.4107	0.2849	-0.0224	-2294.0
C4	N8	4.4522	0.1611	0.0126	-3918.4
C4	H14	4.5377	0.1744	-0.0087	-1016.9
N3	C7	4.5841	0.1394	-0.0111	-1453.6
C6	H10	4.6002	0.1008	-0.0100	27.2
C6	H9	4.6181	0.0969	-0.0102	26.3
H9	H12	4.8401	0.1762	-0.0374	-156.0
H11	H14	4.8949	0.2781	0.0027	-2962.9
H11	H16	4.9363	0.2796	-0.0001	-8227.9
N8	H10	4.9431	0.2254	-0.0467	2322.1
C2	H17	4.9443	0.2655	-0.0333	-4405.6
H10	H13	4.9628	0.2066	-0.0106	32.8
H10	H15	5.0031	0.3490	-0.0094	-626.8
N3	N8	5.0241	0.1729	-0.0028	-2687.5
C7	H10	5.1099	0.1856	-0.0171	-125.9
H9	H13	5.1800	0.1794	0.0150	-2055.6
N8	H11	5.2124	0.2156	0.0378	-9502.8
C4	H17	5.2354	0.2779	0.0311	-24869.8
H9	H15	5.3030	0.3403	-0.0219	-3966.9
C2	H14	5.3066	0.1423	-0.0128	-216.8
H10	H12	5.3348	0.1392	-0.0054	-24.2
H9	H16	5.3396	0.2777	-0.0278	-3567.1
H10	H17	5.4923	0.3185	-0.0472	-1591.9
N3	H14	5.5518	0.1516	-0.0138	-1081.4
C7	H9	5.5529	0.1806	-0.0064	-2888.2
N3	H17	5.7347	0.2995	0.0132	-26865.9
H11	H17	5.9892	0.3456	0.0651	-47990.5
N8	H9	6.0248	0.2034	0.0110	-5474.9
H10	H14	6.2018	0.1895	-0.0109	-832.7
H9	H14	6.5004	0.1914	-0.0091	-2356.7
H9	H17	6.7074	0.3487	0.0298	-45072.0

Table S31. GED vibrational correction parameters for ^{3}G−Vc conformer.

At1	At2	re	l	re−ra	6*kappa
N3	H9	1.0130	0.0703	−0.0147	50.3
N8	H17	1.0202	0.0715	−0.0148	55.6
N8	H16	1.0211	0.0716	−0.0138	55.4
C4	H11	1.0868	0.0745	−0.0149	56.8
C2	H10	1.0888	0.0748	−0.0150	57.5
C7	H14	1.1028	0.0769	−0.0165	67.8
C6	H12	1.1028	0.0769	−0.0163	66.5
C7	H15	1.1030	0.0769	−0.0167	67.7
C6	H13	1.1040	0.0771	−0.0156	67.4
N1	C2	1.3223	0.0428	−0.0045	7.1
C2	N3	1.3621	0.0441	−0.0109	8.2
N3	C4	1.3727	0.0444	−0.0103	8.0
N1	C5	1.3778	0.0462	−0.0045	10.1
C4	C5	1.3873	0.0446	−0.0075	7.6
C7	N8	1.4550	0.0490	−0.0087	12.4
C5	C6	1.4954	0.0489	−0.0086	10.9
C6	C7	1.5385	0.0525	−0.0112	16.4
H16	H17	1.6106	0.1201	−0.0186	8.6
H14	H15	1.7662	0.1249	−0.0165	21.5
H12	H13	1.7725	0.1256	−0.0168	16.1
C7	H16	2.0143	0.1028	−0.0212	6.1
C7	H17	2.0207	0.1046	−0.0190	−5.5
N8	H15	2.0870	0.1042	−0.0141	17.3
N8	H14	2.0884	0.1038	−0.0145	14.6
C2	H9	2.1241	0.0948	−0.0115	10.8
C5	H12	2.1242	0.1072	−0.0181	6.4
C4	H9	2.1336	0.0948	−0.0115	9.2
C5	H13	2.1381	0.1084	−0.0074	−2.9
N1	H10	2.1524	0.0943	−0.0097	19.0
N3	H10	2.1525	0.0960	−0.0149	18.1
C2	C5	2.1551	0.0505	−0.0078	2.9
C6	H15	2.1557	0.1082	−0.0187	12.6
N3	H11	2.1613	0.0979	−0.0131	12.2
C7	H13	2.1618	0.1104	−0.0168	9.2
C6	H14	2.1644	0.1086	−0.0136	12.8
C7	H12	2.1757	0.1112	−0.0123	7.0
N3	C5	2.1965	0.0496	−0.0125	2.6
C2	C4	2.2070	0.0505	−0.0122	2.9
N1	N3	2.2172	0.0492	−0.0116	3.2
N1	C4	2.2605	0.0516	−0.0093	3.2
N1	H16	2.2628	0.2459	−0.1420	7692.4
C5	H11	2.2633	0.0960	−0.0116	15.9
H14	H17	2.3567	0.1808	−0.0426	−2.8
H12	H14	2.4253	0.1740	−0.0103	−92.7
H15	H16	2.4271	0.1809	0.0092	−281.9
N1	C6	2.5133	0.0683	−0.0057	12.2

C5	C7	2.5268	0.0756	-0.0204	12.7
C6	N8	2.5333	0.0726	-0.0212	23.8
H12	H15	2.5339	0.1851	-0.0074	-312.2
H13	H14	2.5366	0.1806	-0.0090	-208.0
H13	H17	2.5456	0.2675	-0.0094	1307.2
H9	H10	2.5471	0.1564	-0.0121	-126.7
H9	H11	2.5575	0.1588	-0.0115	-147.6
C4	C6	2.5951	0.0680	-0.0103	9.8
C6	H16	2.6492	0.1638	-0.0663	386.6
C4	H12	2.7112	0.1554	-0.0367	81.0
C5	H15	2.7184	0.1743	-0.0322	33.0
C5	H16	2.7206	0.2117	-0.0712	1427.0
C6	H17	2.7495	0.1776	-0.0028	-277.0
N8	H13	2.7521	0.1714	-0.0275	110.2
H11	H12	2.7634	0.2248	-0.0501	382.0
N1	H13	2.8414	0.1964	0.0108	85.4
H13	H16	2.9086	0.2571	-0.0852	1425.5
H14	H16	2.9216	0.1224	-0.0234	56.6
H15	H17	2.9269	0.1226	-0.0185	64.6
N1	N8	3.0544	0.1760	-0.0712	2958.1
H13	H15	3.0635	0.1272	-0.0216	67.6
C6	H11	3.0637	0.1404	-0.0108	-106.7
N1	C7	3.1016	0.1559	-0.0328	151.8
C5	N8	3.1267	0.1207	-0.0252	63.3
C5	H9	3.1814	0.0853	-0.0115	38.4
N1	H9	3.1878	0.0858	-0.0103	36.2
C5	H10	3.2161	0.0881	-0.0125	45.2
C2	H11	3.2432	0.0897	-0.0159	39.0
C4	H10	3.2462	0.0893	-0.0172	40.9
C4	H13	3.2911	0.1539	0.0031	-1735.9
N1	H15	3.3227	0.3166	-0.0283	-7284.5
N1	H11	3.3284	0.0884	-0.0126	45.5
N1	H17	3.3975	0.2811	0.0144	-7325.0
N1	H12	3.3986	0.1051	-0.0007	30.2
C2	H16	3.4225	0.2501	-0.0864	3680.9
N8	H12	3.4560	0.1046	-0.0188	37.5
C5	H14	3.4567	0.1058	-0.0200	29.0
C5	H17	3.5053	0.2213	0.0280	-3694.6
C4	H15	3.5547	0.3069	0.0013	545.8
C2	C6	3.5862	0.0627	-0.0084	9.1
C4	C7	3.6612	0.1671	0.0033	-1264.7
N3	C6	3.6627	0.0616	-0.0144	9.3
H12	H16	3.6859	0.1691	-0.0570	197.0
H12	H17	3.6872	0.1891	-0.0149	-266.2
H11	H13	3.7948	0.2409	0.0084	-6929.3
H10	H16	3.9727	0.2792	-0.0984	5032.6
H11	H15	3.9736	0.4470	0.0533	-4342.1
C4	H16	3.9779	0.2793	-0.0110	-6182.3
C2	H13	3.9989	0.1620	0.0080	-310.1
N3	H12	4.0055	0.1441	-0.0319	-49.1
N1	H14	4.1493	0.1488	-0.0249	159.8
C7	H11	4.1686	0.2627	0.0267	-4788.5

H10	H11	4.2342	0.1211	-0.0193	38.3
N3	H13	4.2410	0.1402	0.0017	-569.5
C2	H15	4.2493	0.2836	-0.0445	-1936.9
C2	C7	4.2565	0.1293	-0.0289	-67.7
C2	H12	4.2699	0.1185	-0.0125	-46.9
C2	N8	4.2797	0.1838	-0.0403	959.8
N3	H16	4.2889	0.2875	-0.0312	-4410.1
N3	H15	4.3975	0.2840	-0.0327	-1013.7
C4	N8	4.4205	0.2023	0.0199	-5785.0
C4	H14	4.5183	0.1667	-0.0056	-794.0
N3	C7	4.5555	0.1461	-0.0157	-952.1
C6	H10	4.5972	0.1008	-0.0103	28.3
C6	H9	4.6163	0.0969	-0.0118	27.1
C2	H17	4.6967	0.2893	0.0473	-9126.2
H9	H12	4.8445	0.1764	-0.0335	-93.1
H11	H14	4.8558	0.2605	0.0107	-3350.3
H11	H16	4.8657	0.3218	0.0213	-15591.0
C4	H17	4.8788	0.2259	0.0641	-4372.7
H10	H13	4.9282	0.2032	0.0090	-515.2
N8	H10	4.9307	0.2326	-0.0525	2067.7
N3	N8	4.9793	0.2103	-0.0010	-4717.8
H10	H15	5.1173	0.3431	-0.0472	-4710.6
C7	H10	5.1391	0.1785	-0.0334	-153.4
N8	H11	5.1647	0.2667	0.0503	-14290.9
H9	H13	5.2034	0.1689	0.0053	-1267.7
H9	H16	5.2525	0.3206	-0.0085	-10751.6
H9	H15	5.2651	0.3352	-0.0187	-2748.9
H10	H17	5.3208	0.3313	0.0425	-9968.2
C2	H14	5.3223	0.1369	-0.0213	-158.3
H10	H12	5.3393	0.1374	-0.0100	9.3
N3	H17	5.4598	0.2615	0.0663	-8122.3
C7	H9	5.5122	0.1875	-0.0042	-2249.0
N3	H14	5.5417	0.1518	-0.0162	-822.1
H11	H17	5.6279	0.2399	0.0766	-3035.9
N8	H9	5.9613	0.2505	0.0180	-9813.0
H10	H14	6.2244	0.1797	-0.0227	-397.2
H9	H17	6.4667	0.2774	0.0833	-9439.9
H9	H14	6.4828	0.1907	-0.0056	-2035.6

Table S32. GED vibrational correction parameters for ^{3}T−a conformer.

At1	At2	re	l	re−ra	6*kappa
N3	H9	1.0128	0.0702	−0.0149	50.3
N8	H16	1.0191	0.0714	−0.0127	55.6
N8	H17	1.0202	0.0716	−0.0140	55.5
C4	H11	1.0868	0.0746	−0.0149	56.8
C2	H10	1.0890	0.0748	−0.0148	57.7
C6	H12	1.1006	0.0766	−0.0169	65.2
C7	H14	1.1022	0.0768	−0.0174	67.1
C6	H13	1.1037	0.0771	−0.0155	67.6
C7	H15	1.1068	0.0776	−0.0153	70.9
N1	C2	1.3213	0.0427	−0.0044	7.1
C2	N3	1.3639	0.0443	−0.0105	8.3
N3	C4	1.3731	0.0444	−0.0101	8.0
N1	C5	1.3758	0.0461	−0.0045	10.0
C4	C5	1.3868	0.0445	−0.0073	7.6
C7	N8	1.4601	0.0491	−0.0096	12.7
C5	C6	1.4934	0.0486	−0.0091	10.6
C6	C7	1.5261	0.0511	−0.0113	13.9
H16	H17	1.6167	0.1195	−0.0187	6.2
H14	H15	1.7714	0.1238	−0.0155	28.5
H12	H13	1.7728	0.1250	−0.0150	15.8
C7	H17	2.0304	0.1059	−0.0210	−4.4
C7	H16	2.0382	0.1056	−0.0217	−6.7
N8	H14	2.0881	0.1047	−0.0189	17.2
C2	H9	2.1264	0.0949	−0.0110	10.7
C5	H13	2.1279	0.1095	−0.0139	−2.0
C4	H9	2.1341	0.0948	−0.0108	8.9
C5	H12	2.1426	0.1080	−0.0121	6.1
C6	H15	2.1427	0.1084	−0.0232	16.0
C6	H14	2.1474	0.1090	−0.0182	6.1
C2	C5	2.1498	0.0504	−0.0085	2.9
N1	H10	2.1520	0.0943	−0.0095	18.8
N3	H10	2.1523	0.0962	−0.0148	18.2
C7	H13	2.1530	0.1094	−0.0157	6.7
C7	H12	2.1533	0.1101	−0.0115	4.0
N3	H11	2.1625	0.0978	−0.0131	12.4
N8	H15	2.1713	0.1017	−0.0158	24.4
N3	C5	2.1944	0.0496	−0.0124	2.6
C2	C4	2.2070	0.0505	−0.0118	3.0
N1	N3	2.2201	0.0492	−0.0108	3.2
N1	C4	2.2628	0.0515	−0.0086	3.1
C5	H11	2.2634	0.0959	−0.0112	15.9
H14	H16	2.3690	0.1931	−0.0533	522.7
H15	H17	2.4271	0.1858	−0.0586	65.8
C6	N8	2.4526	0.0761	−0.0087	30.1
H15	H16	2.4608	0.1875	−0.0016	−252.1
H12	H14	2.4762	0.1833	−0.0195	−166.6

N1	C6	2.5007	0.0690	-0.0125	14.9
H13	H17	2.5027	0.2881	0.0270	1043.2
H13	H15	2.5052	0.1843	-0.0203	-117.1
C5	C7	2.5056	0.0800	-0.0265	24.8
H9	H10	2.5471	0.1565	-0.0124	-127.1
H9	H11	2.5595	0.1589	-0.0113	-149.8
C4	C6	2.5976	0.0686	-0.0053	8.4
N8	H12	2.6728	0.1820	0.0083	-171.7
C5	H15	2.6848	0.1789	-0.0470	397.4
N8	H13	2.6883	0.1792	-0.0097	-45.5
C6	H17	2.6993	0.2020	0.0331	-1024.6
N1	H15	2.7458	0.2980	-0.0667	12912.5
C5	H14	2.7499	0.1830	-0.0224	68.4
C4	H12	2.7502	0.1616	-0.0212	123.7
N1	H13	2.7841	0.2103	-0.0294	982.3
H11	H12	2.8125	0.2349	-0.0306	694.9
H14	H17	2.9306	0.1242	-0.0206	52.7
H12	H17	3.0519	0.3154	0.0993	-13773.7
H12	H15	3.0547	0.1266	-0.0197	75.4
H13	H14	3.0577	0.1270	-0.0186	71.3
C6	H11	3.0708	0.1415	-0.0014	-118.0
N1	C7	3.1010	0.1985	-0.0197	3160.0
C5	H9	3.1794	0.0852	-0.0111	38.5
N1	H9	3.1903	0.0859	-0.0093	36.1
C5	H10	3.2115	0.0881	-0.0130	45.2
C2	H11	3.2440	0.0895	-0.0156	39.2
C4	H10	3.2457	0.0894	-0.0167	41.0
C4	H13	3.3091	0.1555	0.0276	-2093.1
N1	H11	3.3304	0.0884	-0.0120	45.4
C6	H16	3.3387	0.1020	-0.0052	41.8
N1	H12	3.4030	0.1059	0.0037	22.4
N1	H14	3.4348	0.3419	0.0349	-4302.1
C4	H14	3.5284	0.3339	-0.0362	-3037.3
C2	C6	3.5753	0.0626	-0.0125	9.2
H12	H16	3.6046	0.1930	0.0025	-454.4
C4	C7	3.6164	0.1824	-0.0216	-2441.7
H13	H16	3.6254	0.1923	0.0193	-635.2
N3	C6	3.6608	0.0615	-0.0129	8.8
C5	N8	3.7846	0.0756	-0.0118	22.3
H11	H13	3.8374	0.2454	0.0562	-9088.9
H11	H14	3.8890	0.4980	-0.0099	-26299.4
C4	H15	3.9246	0.2603	-0.0248	-7447.7
C2	H15	3.9334	0.2683	-0.0754	4746.9
C2	H13	3.9568	0.1686	-0.0158	-124.1
N3	H12	4.0390	0.1471	-0.0169	-71.5
C5	H17	4.0669	0.1851	0.0128	-373.1
C7	H11	4.1119	0.2947	-0.0019	-11966.1
H10	H11	4.2344	0.1211	-0.0191	38.6
N3	H13	4.2350	0.1402	0.0080	-596.9
C2	C7	4.2400	0.1516	-0.0353	689.2
C2	H12	4.2858	0.1187	-0.0028	-49.9
C2	H14	4.3400	0.3012	-0.0112	-891.1

N3	H14	4.4239	0.2988	-0.0487	-1350.4
N1	N8	4.4497	0.1721	-0.0169	1403.6
N3	C7	4.5204	0.1518	-0.0388	-1056.7
N3	H15	4.5309	0.2676	-0.0552	-2933.9
C5	H16	4.5330	0.1220	-0.0203	-74.5
N1	H17	4.5832	0.2629	-0.0390	-3317.6
C6	H10	4.5857	0.1010	-0.0152	27.7
C6	H9	4.6158	0.0967	-0.0088	26.9
H11	H15	4.6419	0.3319	0.0058	-25062.2
H10	H15	4.6585	0.3169	-0.0832	9638.0
C4	N8	4.8589	0.1600	0.0028	-2052.7
H10	H13	4.8761	0.2123	-0.0232	-49.5
H9	H12	4.8830	0.1799	-0.0158	-123.2
N1	H16	5.0573	0.2492	-0.0152	2216.8
C7	H10	5.1313	0.2063	-0.0347	1672.3
N8	H11	5.1849	0.2847	0.0244	-11143.6
H9	H13	5.2040	0.1682	0.0186	-1383.4
H10	H14	5.2340	0.3649	0.0019	-2450.6
C4	H17	5.2703	0.1978	0.0598	-516.2
H9	H14	5.2781	0.3531	-0.0467	-3840.7
H10	H12	5.3534	0.1379	-0.0001	9.1
C7	H9	5.4720	0.1952	-0.0316	-2640.7
H9	H15	5.5030	0.3038	-0.0441	-7769.8
C4	H16	5.5939	0.2269	-0.0181	-4004.5
C2	N8	5.6445	0.1352	-0.0158	120.2
H11	H17	5.6822	0.2832	0.1080	-6087.8
C2	H17	5.8620	0.2388	-0.0171	-3881.9
N3	N8	5.8880	0.1283	-0.0102	-951.6
H11	H16	5.9419	0.3692	0.0038	-20593.4
C2	H16	6.2291	0.2148	-0.0281	93.8
N3	H17	6.2434	0.1885	0.0265	-356.5
N8	H10	6.5377	0.1955	-0.0163	319.1
N3	H16	6.5414	0.2053	-0.0332	-2944.0
H10	H17	6.7049	0.2950	-0.0331	-7395.2
N8	H9	6.8341	0.1744	0.0012	-2633.9
H10	H16	7.0529	0.2875	-0.0252	983.9
H9	H17	7.2276	0.2028	0.0457	-88.6
H9	H16	7.4733	0.2595	-0.0245	-7371.9

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3 Results of the GED+MW refinement

3.1 Cartesian coordinates of the refined structures

Table S33. Cartesian coordinates of ^{1}G−IVa conformer obtained from GED+MW refinement

N	At	X	Y	Z
1	N	0.461698845158	−0.836137379986	0.164523881958
2	C	1.784600236745	−1.071775866119	−0.032528609923
3	N	2.456668230333	0.054128136423	−0.167711377480
4	C	1.504868498229	1.035777369661	−0.059397387931
5	C	0.237087757377	0.520298039683	0.146073508552
6	C	−1.117584588380	1.109794387012	0.333108096928
7	C	−2.201951688756	0.390155570040	−0.462395066915
8	N	−2.397360703899	−0.965397114913	0.068915700098
9	H	−0.299876739064	−1.504062601535	0.227157502321
10	H	2.199261701597	−2.066846389766	−0.069170777377
11	H	1.763122630287	2.081640900103	−0.132442770663
12	H	−1.362864811489	1.075100323803	1.397657463592
13	H	−1.124522127442	2.170230845391	0.048402841929
14	H	−3.121039680088	0.987899427539	−0.448201996769
15	H	−1.884042686881	0.299326961128	−1.503951323551
16	H	−2.834282660445	−0.908110361960	0.984375907044
17	H	−3.039754881952	−1.482221963725	−0.522404874292

Table S34. Cartesian coordinates of ^{3}G−Ib conformer obtained from GED+MW refinement

N	At	X	Y	Z
1	N	0.838696227344	−1.110052686420	−0.273842537063
2	C	2.000523691933	−0.568742319790	−0.599780494241
3	N	2.126389841587	0.689828350531	−0.100559970410
4	C	0.975297853170	0.975231635713	0.582990876205
5	C	0.184426505414	−0.153508837748	0.474604753694
6	C	−1.197279797242	−0.381471357974	1.008610536672
7	C	−2.246556634617	−0.446735691254	−0.093113806586
8	N	−2.304016153033	0.830955422051	−0.788284907227
9	H	2.922222180989	1.296607345836	−0.208471683166
10	H	2.777737908165	−1.038166976440	−1.180117181950
11	H	0.814229452552	1.919235299498	1.077270006642
12	H	−1.219636841935	−1.315318049509	1.575933534384
13	H	−1.453252497021	0.423176303743	1.703167670749
14	H	−2.009869360874	−1.296482729441	−0.746302396589
15	H	−3.226857910967	−0.635109400008	0.352971540923
16	H	−1.411556288007	0.995441318757	−1.247246267717
17	H	−3.001515333025	0.792899545975	−1.524208145055

Table S35. Cartesian coordinates of ^{3}G−Ic conformer obtained from GED+MW refinement

N	At	X	Y	Z
1	N	0.814115991512	−1.117763822680	−0.177511552180
2	C	1.985389930589	−0.638932613144	−0.561104482610
3	N	2.152421340505	0.652944933848	−0.171749942808
4	C	1.018621886968	1.026851191435	0.498108114800
5	C	0.195652737316	−0.084121673049	0.494351885972
6	C	−1.181813914086	−0.237225957821	1.061409933118
7	C	−2.248566351723	−0.440353691107	−0.018894724188
8	N	−2.383635370277	0.643320797890	−0.973584423987
9	H	2.962470446403	1.225950135909	−0.340946189534
10	H	2.740311549197	−1.176507152132	−1.110920523676
11	H	0.897064275726	2.010971724663	0.920591131877
12	H	−1.197831316267	−1.083425266088	1.756281654515
13	H	−1.433274153888	0.649090872997	1.652665917333
14	H	−2.011674777372	−1.351349646859	−0.572904392914
15	H	−3.220149894092	−0.600324022722	0.457038473744
16	H	−2.593490263130	1.508811558387	−0.486547475821
17	H	−1.495377450434	0.787180841678	−1.444300295125

Table S36. Cartesian coordinates of ^{3}G−Vb conformer obtained from GED+MW refinement

N	At	X	Y	Z
1	N	0.485505719997	−0.938818773359	0.295892008533
2	C	1.767687735565	−1.079353652295	0.002061903933
3	N	2.354821860147	0.117560870588	−0.257105424882
4	C	1.392930559435	1.082145623959	−0.129289270202
5	C	0.231717793201	0.416291667474	0.217511548505
6	C	−1.125627934287	1.001065444900	0.476215465451
7	C	−2.201883581289	0.437230195121	−0.443963855778
8	N	−2.532446917925	−0.916662567715	−0.034904539795
9	H	3.321290306366	0.266642770392	−0.495359099095
10	H	2.311601905565	−2.008784388587	−0.031236712336
11	H	1.601485547566	2.127812225191	−0.285964784960
12	H	−1.393377762728	0.803198027352	1.517266313705
13	H	−1.099127058828	2.086307309891	0.341150068672
14	H	−3.102449616427	1.051448149661	−0.353876868424
15	H	−1.846416412978	0.518568867442	−1.481806073114
16	H	−1.680656719515	−1.471806328983	−0.016358191513
17	H	−3.162007031469	−1.341607753843	−0.706765811870

Table S37. Cartesian coordinates of ^{3}G−Vc conformer obtained from GED+MW refinement

N	At	X	Y	Z
1	N	0.533482103291	−0.928854676288	0.426885939630
2	C	1.793995855894	−1.049516997590	0.041829378112
3	N	2.314632244318	0.143071879902	−0.346742597207
4	C	1.331559261143	1.084349603010	−0.209616371439
5	C	0.225881204129	0.409078535758	0.274966869299
6	C	−1.134256872786	0.961448918781	0.575726019390
7	C	−2.205266015204	0.450595408160	−0.396078417020
8	N	−2.501320255704	−0.965790892648	−0.303287423397
9	H	3.253951584233	0.304612561729	−0.670492903802
10	H	2.368101226126	−1.961162108289	0.031028510938
11	H	1.490793912547	2.122764053090	−0.450136241973
12	H	−1.407957153644	0.683943158098	1.598405711398
13	H	−1.106927580147	2.054840877254	0.532611953341
14	H	−3.133161290355	1.005198061784	−0.230521157281
15	H	−1.878035487527	0.667008648049	−1.417101468492
16	H	−1.625002811698	−1.481392579415	−0.308682386704
17	H	−2.922092191322	−1.157378118853	0.600124357639

Table S38. Cartesian coordinates of ^{3}T−a conformer obtained from GED+MW refinement

N	At	X	Y	Z
1	N	0.913090234142	−1.074819373854	0.233044006839
2	C	2.178272986251	−0.868990598491	−0.092000526995
3	N	2.443271297369	0.452821233949	−0.267302378800
4	C	1.278538482724	1.136069327787	−0.044603942574
5	C	0.334047146445	0.176281086157	0.267847344180
6	C	−1.117046044038	0.362763713357	0.586280611117
7	C	−2.041163410960	−0.180320638446	−0.493769799139
8	N	−3.429956816775	0.011611829591	−0.100270042207
9	H	3.333538752645	0.854793235447	−0.509806412071
10	H	2.934533533728	−1.628056886260	−0.205743660221
11	H	1.216588223833	2.209410472467	−0.119579391243
12	H	−1.361748243138	−0.113169232353	1.539377755245
13	H	−1.319357067359	1.430741085883	0.723708575459
14	H	−1.869493716166	0.377271510204	−1.418972662402
15	H	−1.768418488035	−1.224872233770	−0.690007000451
16	H	−4.047881543921	−0.321535449143	−0.832569012877
17	H	−3.628047949853	−0.554989113079	0.718579902583

3.2 All internal geometrical parameters of refined structures

Table S39. Refined geometrical parameters of ^{1}G−IVa conformer

No.	Type	i	j	k	l	a-Value	g-Value	e-Value	Error
1	stretch	1	2	0	0	1.36840	1.36983	1.35810	0.00357
2	stretch	1	5	0	0	1.38463	1.38607	1.37503	0.00331
3	stretch	1	9	0	0	1.02841	1.03350	1.01491	0.00376
4	stretch	2	3	0	0	1.32288	1.32429	1.31818	0.00329
5	stretch	2	10	0	0	1.09383	1.09902	1.07863	0.00375
6	stretch	3	4	0	0	1.37690	1.37842	1.37160	0.00332
7	stretch	4	5	0	0	1.39061	1.39205	1.38391	0.00334
8	stretch	4	11	0	0	1.09465	1.09985	1.07975	0.00375
9	stretch	5	6	0	0	1.49677	1.49837	1.48917	0.00317
10	stretch	6	7	0	0	1.53611	1.53782	1.52531	0.00333
11	stretch	6	12	0	0	1.10909	1.11445	1.09299	0.00378
12	stretch	6	13	0	0	1.11431	1.11977	1.09801	0.00378
13	stretch	7	8	0	0	1.47821	1.47989	1.46901	0.00321
14	stretch	7	14	0	0	1.11296	1.11845	1.09646	0.00378
15	stretch	7	15	0	0	1.10857	1.11394	1.09277	0.00378
16	stretch	8	16	0	0	1.03140	1.03643	1.01600	0.00376
17	stretch	8	17	0	0	1.02881	1.03382	1.01461	0.00376
18	bend	2	1	5	0			109.16746	0.35665
19	bend	2	1	9	0			128.73420	0.41557
20	bend	1	2	3	0			111.30384	0.19935
21	bend	1	2	10	0			122.64711	0.21775
22	bend	5	1	9	0			121.83433	0.21756
23	bend	1	5	4	0			102.69687	0.44052
24	bend	1	5	6	0			122.50778	0.19957
25	bend	3	2	10	0			126.04902	0.29419
26	bend	2	3	4	0			104.44219	0.18744
27	bend	3	4	5	0			112.38602	0.36853
28	bend	3	4	11	0			121.46096	0.21785
29	bend	5	4	11	0			126.15302	0.42966
30	bend	4	5	6	0			134.79300	0.48098
31	bend	5	6	7	0			113.23119	0.16710
32	bend	5	6	12	0			108.29481	0.21785
33	bend	5	6	13	0			110.82351	0.21797
34	bend	7	6	12	0			109.47836	0.21771
35	bend	7	6	13	0			108.41710	0.21797
36	bend	6	7	8	0			109.95597	0.20216
37	bend	6	7	14	0			109.38767	0.21797
38	bend	6	7	15	0			109.23769	0.21792
39	bend	12	6	13	0			106.36660	0.50549
40	bend	8	7	14	0			112.75981	0.21790
41	bend	8	7	15	0			107.86212	0.21792
42	bend	7	8	16	0			109.33336	0.21777
43	bend	7	8	17	0			110.08856	0.21779
44	bend	14	7	15	0			107.54820	0.49027
45	bend	16	8	17	0			106.35434	0.29416
46	torsion	3	2	1	5			0.64672	0.20134

47	torsion	10	2	1	5	-179.30239	0.21806
48	torsion	2	1	5	4	-0.52799	0.21587
49	torsion	2	1	5	6	179.95402	0.21004
50	torsion	3	2	1	9	174.74198	0.29356
51	torsion	10	2	1	9	-5.20713	0.39929
52	torsion	1	2	3	4	-0.45145	0.21748
53	torsion	4	5	1	9	-175.10794	0.21805
54	torsion	6	5	1	9	5.37407	0.36740
55	torsion	1	5	4	3	0.26401	0.26474
56	torsion	1	5	4	11	-179.71034	0.25953
57	torsion	1	5	6	7	-44.33694	0.21514
58	torsion	1	5	6	12	77.27117	0.39774
59	torsion	1	5	6	13	-166.41616	0.41181
60	torsion	4	3	2	10	179.49555	0.28084
61	torsion	2	3	4	5	0.10487	0.26678
62	torsion	2	3	4	11	-179.91941	0.21806
63	torsion	3	4	5	6	179.69121	0.28361
64	torsion	6	5	4	11	-0.28314	0.39710
65	torsion	4	5	6	7	136.32567	0.45241
66	torsion	4	5	6	12	-102.06622	0.55334
67	torsion	4	5	6	13	14.24645	0.58378
68	torsion	5	6	7	8	67.28939	0.20804
69	torsion	5	6	7	14	-168.37049	0.39571
70	torsion	5	6	7	15	-50.89649	0.38326
71	torsion	8	7	6	12	-53.65209	0.40937
72	torsion	14	7	6	12	70.68803	0.53516
73	torsion	15	7	6	12	-171.83797	0.51537
74	torsion	8	7	6	13	-169.29739	0.38720
75	torsion	14	7	6	13	-44.95727	0.50790
76	torsion	15	7	6	13	72.51673	0.50878
77	torsion	6	7	8	16	69.96954	0.21785
78	torsion	6	7	8	17	-173.54008	0.21779
79	torsion	16	8	7	14	-52.39599	0.41375
80	torsion	17	8	7	14	64.09439	0.41311
81	torsion	16	8	7	15	-170.99825	0.38205
82	torsion	17	8	7	15	-54.50788	0.38251
83	o.o.p	9	2	1	5	-4.60284	0.26041
84	o.o.p	10	1	2	3	0.04285	0.24983
85	o.o.p	11	3	4	5	-0.02070	0.29392

Table S40. Refined geometrical parameters of ^{3}G−Ib conformer

No.	Type	i	j	k	l	a-Value	g-Value	e-Value	Error
1	stretch	1	2	0	0	1.32943	1.33082	1.32253	0.00219
2	stretch	1	5	0	0	1.38377	1.38531	1.37957	0.00297
3	stretch	2	3	0	0	1.36840	1.36985	1.35980	0.00286
4	stretch	2	10	0	0	1.09230	1.09749	1.07760	0.00361
5	stretch	3	4	0	0	1.37784	1.37928	1.36884	0.00316
6	stretch	3	9	0	0	1.02147	1.02638	1.00657	0.00348
7	stretch	4	5	0	0	1.38799	1.38942	1.38249	0.00274
8	stretch	4	11	0	0	1.09238	1.09755	1.07768	0.00361
9	stretch	5	6	0	0	1.51215	1.51374	1.49875	0.00260
10	stretch	6	7	0	0	1.53244	1.53416	1.52284	0.00243
11	stretch	6	12	0	0	1.10970	1.11507	1.09290	0.00374
12	stretch	6	13	0	0	1.11284	1.11823	1.09334	0.00375
13	stretch	7	8	0	0	1.46840	1.47005	1.45570	0.00211
14	stretch	7	14	0	0	1.11051	1.11601	1.09761	0.00375
15	stretch	7	15	0	0	1.10877	1.11417	1.09337	0.00375
16	stretch	8	16	0	0	1.03305	1.03809	1.01695	0.00375
17	stretch	8	17	0	0	1.02916	1.03417	1.01466	0.00373
18	bend	2	1	5	0			105.45843	0.18031
19	bend	1	2	3	0			111.69486	0.16320
20	bend	1	2	10	0			126.01750	0.21732
21	bend	1	5	4	0			109.71419	0.22264
22	bend	1	5	6	0			121.67224	0.19415
23	bend	3	2	10	0			122.28609	0.27049
24	bend	2	3	4	0			107.36584	0.16743
25	bend	2	3	9	0			126.28255	0.21757
26	bend	4	3	9	0			126.35025	0.27325
27	bend	3	4	5	0			105.76440	0.25516
28	bend	3	4	11	0			122.50386	0.21720
29	bend	5	4	11	0			131.73128	0.33293
30	bend	4	5	6	0			128.58243	0.27936
31	bend	5	6	7	0			112.57952	0.13838
32	bend	5	6	12	0			109.49848	0.21748
33	bend	5	6	13	0			109.28347	0.21759
34	bend	7	6	12	0			108.95568	0.21766
35	bend	7	6	13	0			109.25770	0.21735
36	bend	6	7	8	0			109.57704	0.16961
37	bend	6	7	14	0			108.36893	0.21782
38	bend	6	7	15	0			109.26796	0.21789
39	bend	12	6	13	0			107.11533	0.48567
40	bend	8	7	14	0			113.81788	0.21770
41	bend	8	7	15	0			108.09930	0.21771
42	bend	7	8	16	0			108.83539	0.21641
43	bend	7	8	17	0			109.91207	0.21717
44	bend	14	7	15	0			107.62300	0.47161
45	bend	16	8	17	0			106.37991	0.29231
46	torsion	3	2	1	5			-0.10766	0.17790

47	torsion	10	2	1	5	179.44661	0.21755
48	torsion	2	1	5	4	0.37505	0.20054
49	torsion	2	1	5	6	178.50896	0.17947
50	torsion	1	2	3	4	-0.19841	0.21527
51	torsion	1	2	3	9	179.39768	0.21786
52	torsion	1	5	4	3	-0.49346	0.24100
53	torsion	1	5	4	11	179.75615	0.27197
54	torsion	1	5	6	7	-67.79028	0.16852
55	torsion	1	5	6	12	53.57223	0.37556
56	torsion	1	5	6	13	170.61419	0.36493
57	torsion	4	3	2	10	-179.77196	0.25729
58	torsion	9	3	2	10	-0.17587	0.34738
59	torsion	2	3	4	5	0.41510	0.23883
60	torsion	2	3	4	11	-179.80577	0.21788
61	torsion	5	4	3	9	-179.18063	0.25062
62	torsion	11	4	3	9	0.59849	0.37649
63	torsion	3	4	5	6	-178.46174	0.22002
64	torsion	6	5	4	11	1.78787	0.36352
65	torsion	4	5	6	7	109.96227	0.29792
66	torsion	4	5	6	12	-128.67522	0.42820
67	torsion	4	5	6	13	-11.63326	0.45735
68	torsion	5	6	7	8	-62.92874	0.19401
69	torsion	5	6	7	14	61.80114	0.37957
70	torsion	5	6	7	15	178.80247	0.36562
71	torsion	8	7	6	12	175.40003	0.36467
72	torsion	14	7	6	12	-59.87009	0.49891
73	torsion	15	7	6	12	57.13124	0.47068
74	torsion	8	7	6	13	58.68143	0.39999
75	torsion	14	7	6	13	-176.58869	0.50610
76	torsion	15	7	6	13	-59.58735	0.51397
77	torsion	6	7	8	16	63.83052	0.21769
78	torsion	6	7	8	17	179.96444	0.21617
79	torsion	16	8	7	14	-57.67577	0.40592
80	torsion	17	8	7	14	58.45815	0.40203
81	torsion	16	8	7	15	-177.17676	0.37541
82	torsion	17	8	7	15	-61.04285	0.37666
83	o.o.p	10	1	2	3	-0.36052	0.22798
84	o.o.p	9	2	3	4	-0.32560	0.24739
85	o.o.p	11	3	4	5	-0.18628	0.27339

Table S41. Refined geometrical parameters of ^{3}G−Ic conformer

No.	Type	i	j	k	l	a-Value	g-Value	e-Value	Error
1	stretch	1	2	0	0	1.32584	1.32722	1.32224	0.00219
2	stretch	1	5	0	0	1.38504	1.38658	1.37924	0.00297
3	stretch	2	3	0	0	1.37107	1.37251	1.35957	0.00286
4	stretch	2	10	0	0	1.09279	1.09798	1.07759	0.00361
5	stretch	3	4	0	0	1.37915	1.38059	1.36895	0.00316
6	stretch	3	9	0	0	1.02105	1.02596	1.00655	0.00348
7	stretch	4	5	0	0	1.39079	1.39222	1.38259	0.00274
8	stretch	4	11	0	0	1.09275	1.09791	1.07785	0.00361
9	stretch	5	6	0	0	1.50147	1.50307	1.49747	0.00260
10	stretch	6	7	0	0	1.54726	1.54904	1.53176	0.00243
11	stretch	6	12	0	0	1.11066	1.11607	1.09506	0.00374
12	stretch	6	13	0	0	1.10700	1.11242	1.09470	0.00375
13	stretch	7	8	0	0	1.46083	1.46247	1.45053	0.00211
14	stretch	7	14	0	0	1.11133	1.11668	1.09223	0.00375
15	stretch	7	15	0	0	1.10935	1.11476	1.09365	0.00375
16	stretch	8	16	0	0	1.02815	1.03320	1.01505	0.00378
17	stretch	8	17	0	0	1.03162	1.03665	1.01552	0.00379
18	bend	2	1	5	0			105.49392	0.18033
19	bend	1	2	3	0			111.70658	0.16320
20	bend	1	2	10	0			126.01139	0.21732
21	bend	1	5	4	0			109.67063	0.22250
22	bend	1	5	6	0			121.35333	0.19415
23	bend	3	2	10	0			122.28153	0.27050
24	bend	2	3	4	0			107.33235	0.16743
25	bend	2	3	9	0			126.27512	0.21757
26	bend	4	3	9	0			126.39177	0.27325
27	bend	3	4	5	0			105.79445	0.25516
28	bend	3	4	11	0			122.31593	0.21720
29	bend	5	4	11	0			131.88242	0.33291
30	bend	4	5	6	0			128.95169	0.27933
31	bend	5	6	7	0			112.77436	0.13838
32	bend	5	6	12	0			109.43591	0.21748
33	bend	5	6	13	0			109.45374	0.21759
34	bend	7	6	12	0			109.56465	0.21766
35	bend	7	6	13	0			109.16660	0.21735
36	bend	6	7	8	0			115.46526	0.16961
37	bend	6	7	14	0			108.49944	0.21782
38	bend	6	7	15	0			109.33984	0.21789
39	bend	12	6	13	0			106.23390	0.48991
40	bend	8	7	14	0			108.02799	0.21770
41	bend	8	7	15	0			108.23855	0.21771
42	bend	7	8	16	0			109.90529	0.21641
43	bend	7	8	17	0			109.23617	0.21717
44	bend	14	7	15	0			106.94265	0.51811
45	bend	16	8	17	0			106.40670	0.29378
46	torsion	3	2	1	5			-0.09016	0.17802

47	torsion	10	2	1	5	179.65510	0.21755
48	torsion	2	1	5	4	0.35003	0.20058
49	torsion	2	1	5	6	178.70752	0.17947
50	torsion	1	2	3	4	-0.20208	0.21527
51	torsion	1	2	3	9	179.49555	0.21786
52	torsion	1	5	4	3	-0.47055	0.24107
53	torsion	1	5	4	11	-179.48374	0.27330
54	torsion	1	5	6	7	-65.05597	0.16852
55	torsion	1	5	6	12	57.17106	0.37898
56	torsion	1	5	6	13	173.21343	0.36687
57	torsion	4	3	2	10	-179.95835	0.25731
58	torsion	9	3	2	10	-0.26072	0.34744
59	torsion	2	3	4	5	0.40334	0.23890
60	torsion	2	3	4	11	179.53400	0.21788
61	torsion	5	4	3	9	-179.29384	0.25076
62	torsion	11	4	3	9	-0.16318	0.37665
63	torsion	3	4	5	6	-178.66685	0.22132
64	torsion	6	5	4	11	2.31997	0.36622
65	torsion	4	5	6	7	112.95509	0.29918
66	torsion	4	5	6	12	-124.81788	0.43147
67	torsion	4	5	6	13	-8.77551	0.46011
68	torsion	5	6	7	8	-60.77788	0.19401
69	torsion	5	6	7	14	60.60818	0.39832
70	torsion	5	6	7	15	176.91011	0.40476
71	torsion	8	7	6	12	177.06751	0.36884
72	torsion	14	7	6	12	-61.54643	0.51710
73	torsion	15	7	6	12	54.75550	0.50278
74	torsion	8	7	6	13	61.11492	0.40143
75	torsion	14	7	6	13	-177.49903	0.52080
76	torsion	15	7	6	13	-61.19709	0.54530
77	torsion	6	7	8	16	-57.67884	0.21774
78	torsion	6	7	8	17	58.71359	0.21802
79	torsion	16	8	7	14	-179.31866	0.40784
80	torsion	17	8	7	14	-62.92623	0.40819
81	torsion	16	8	7	15	65.21894	0.41474
82	torsion	17	8	7	15	-178.38863	0.41481
83	o.o.p	10	1	2	3	-0.20606	0.22805
84	o.o.p	9	2	3	4	-0.24376	0.24742
85	o.o.p	11	3	4	5	-0.73468	0.27400

Table S42. Refined geometrical parameters of ^{3}G−Vb conformer

No.	Type	i	j	k	l	a-Value	g-Value	e-Value	Error
1	stretch	1	2	0	0	1.32760	1.32898	1.32290	0.00219
2	stretch	1	5	0	0	1.38460	1.38614	1.38090	0.00297
3	stretch	2	3	0	0	1.36882	1.37026	1.35812	0.00286
4	stretch	2	10	0	0	1.09220	1.09739	1.07740	0.00361
5	stretch	3	4	0	0	1.37811	1.37955	1.36821	0.00316
6	stretch	3	9	0	0	1.02080	1.02571	1.00650	0.00348
7	stretch	4	5	0	0	1.38987	1.39130	1.38277	0.00274
8	stretch	4	11	0	0	1.09261	1.09777	1.07771	0.00361
9	stretch	5	6	0	0	1.50923	1.51083	1.50043	0.00260
10	stretch	6	7	0	0	1.53503	1.53675	1.52413	0.00243
11	stretch	6	12	0	0	1.10979	1.11517	1.09299	0.00380
12	stretch	6	13	0	0	1.11014	1.11553	1.09394	0.00379
13	stretch	7	8	0	0	1.46216	1.46382	1.45246	0.00211
14	stretch	7	14	0	0	1.11050	1.11592	1.09380	0.00380
15	stretch	7	15	0	0	1.11574	1.12131	1.10004	0.00380
16	stretch	8	16	0	0	1.03049	1.03552	1.01689	0.00381
17	stretch	8	17	0	0	1.02996	1.03499	1.01406	0.00381
18	bend	2	1	5	0			105.65050	0.18043
19	bend	1	2	3	0			111.57799	0.16320
20	bend	1	2	10	0			126.00144	0.21732
21	bend	1	5	4	0			109.41711	0.22154
22	bend	1	5	6	0			122.61107	0.19415
23	bend	3	2	10	0			122.41965	0.27049
24	bend	2	3	4	0			107.43115	0.16743
25	bend	2	3	9	0			126.21557	0.21757
26	bend	4	3	9	0			126.35276	0.27326
27	bend	3	4	5	0			105.92226	0.25501
28	bend	3	4	11	0			122.30370	0.21720
29	bend	5	4	11	0			131.77372	0.33282
30	bend	4	5	6	0			127.97108	0.27912
31	bend	5	6	7	0			112.98752	0.14655
32	bend	5	6	12	0			108.37778	0.21786
33	bend	5	6	13	0			110.08647	0.21797
34	bend	7	6	12	0			109.57835	0.21777
35	bend	7	6	13	0			108.03294	0.21798
36	bend	6	7	8	0			109.60375	0.19633
37	bend	6	7	14	0			108.90092	0.21803
38	bend	6	7	15	0			108.30451	0.21790
39	bend	12	6	13	0			107.64563	0.48993
40	bend	8	7	14	0			108.23170	0.21790
41	bend	8	7	15	0			114.09030	0.21793
42	bend	7	8	16	0			108.86707	0.21806
43	bend	7	8	17	0			110.20107	0.21806
44	bend	14	7	15	0			107.59197	0.48084
45	bend	16	8	17	0			107.65864	0.29490
46	torsion	3	2	1	5			0.22517	0.17819

47	torsion	10	2	1	5	179.88116	0.21755
48	torsion	2	1	5	4	-0.03814	0.20078
49	torsion	2	1	5	6	179.67109	0.17947
50	torsion	1	2	3	4	-0.32830	0.21527
51	torsion	1	2	3	9	179.42480	0.21786
52	torsion	1	5	4	3	-0.15540	0.24118
53	torsion	1	5	4	11	-179.94788	0.27291
54	torsion	1	5	6	7	-58.12850	0.16852
55	torsion	1	5	6	12	63.50603	0.37326
56	torsion	1	5	6	13	-179.00389	0.37230
57	torsion	4	3	2	10	-179.99862	0.17819
58	torsion	9	3	2	10	-0.24552	0.34787
59	torsion	2	3	4	5	0.28483	0.23973
60	torsion	2	3	4	11	-179.89826	0.21788
61	torsion	5	4	3	9	-179.46783	0.25102
62	torsion	11	4	3	9	0.34907	0.37671
63	torsion	3	4	5	6	-179.84469	0.21715
64	torsion	6	5	4	11	0.36282	0.36136
65	torsion	4	5	6	7	121.52363	0.29507
66	torsion	4	5	6	12	-116.84184	0.43342
67	torsion	4	5	6	13	0.64824	0.45612
68	torsion	5	6	7	8	73.94273	0.20903
69	torsion	5	6	7	14	-167.82899	0.37494
70	torsion	5	6	7	15	-51.10111	0.39432
71	torsion	8	7	6	12	-47.01258	0.40773
72	torsion	14	7	6	12	71.21569	0.52083
73	torsion	15	7	6	12	-172.05643	0.51713
74	torsion	8	7	6	13	-164.02199	0.37479
75	torsion	14	7	6	13	-45.79372	0.47966
76	torsion	15	7	6	13	70.93416	0.51170
77	torsion	6	7	8	16	-55.17668	0.21807
78	torsion	6	7	8	17	-173.03728	0.21807
79	torsion	16	8	7	14	-173.82006	0.38039
80	torsion	17	8	7	14	68.31934	0.38038
81	torsion	16	8	7	15	66.45417	0.41166
82	torsion	17	8	7	15	-51.40643	0.41166
83	o.o.p	10	1	2	3	-0.27830	0.22817
84	o.o.p	9	2	3	4	-0.19920	0.24761
85	o.o.p	11	3	4	5	-0.15476	0.27456

Table S43. Refined geometrical parameters of ^{3}G−Vc conformer

No.	Type	i	j	k	l	a-Value	g-Value	e-Value	Error
1	stretch	1	2	0	0	1.32803	1.32941	1.32353	0.00219
2	stretch	1	5	0	0	1.38572	1.38726	1.38122	0.00297
3	stretch	2	3	0	0	1.36896	1.37039	1.35806	0.00286
4	stretch	2	10	0	0	1.09241	1.09760	1.07741	0.00361
5	stretch	3	4	0	0	1.37823	1.37967	1.36793	0.00316
6	stretch	3	9	0	0	1.02129	1.02620	1.00659	0.00348
7	stretch	4	5	0	0	1.39073	1.39217	1.38323	0.00274
8	stretch	4	11	0	0	1.09263	1.09778	1.07773	0.00361
9	stretch	5	6	0	0	1.50711	1.50871	1.49851	0.00260
10	stretch	6	7	0	0	1.54497	1.54676	1.53377	0.00243
11	stretch	6	12	0	0	1.11074	1.11614	1.09444	0.00380
12	stretch	6	13	0	0	1.11018	1.11561	1.09458	0.00379
13	stretch	7	8	0	0	1.45867	1.46032	1.44997	0.00211
14	stretch	7	14	0	0	1.11011	1.11552	1.09361	0.00380
15	stretch	7	15	0	0	1.11050	1.11591	1.09380	0.00380
16	stretch	8	16	0	0	1.03056	1.03560	1.01676	0.00380
17	stretch	8	17	0	0	1.02964	1.03468	1.01484	0.00380
18	bend	2	1	5	0			105.56971	0.18036
19	bend	1	2	3	0			111.61079	0.16320
20	bend	1	2	10	0			125.98302	0.21732
21	bend	1	5	4	0			109.47530	0.22164
22	bend	1	5	6	0			122.48800	0.19415
23	bend	3	2	10	0			122.40501	0.27049
24	bend	2	3	4	0			107.46185	0.16743
25	bend	2	3	9	0			126.20681	0.21757
26	bend	4	3	9	0			126.33024	0.27325
27	bend	3	4	5	0			105.88162	0.25492
28	bend	3	4	11	0			122.30632	0.21720
29	bend	5	4	11	0			131.80964	0.33274
30	bend	4	5	6	0			128.01675	0.27877
31	bend	5	6	7	0			112.57323	0.14655
32	bend	5	6	12	0			108.72763	0.21786
33	bend	5	6	13	0			109.73336	0.21797
34	bend	7	6	12	0			109.44976	0.21777
35	bend	7	6	13	0			108.97690	0.21798
36	bend	6	7	8	0			115.30177	0.19633
37	bend	6	7	14	0			109.12597	0.21803
38	bend	6	7	15	0			108.46006	0.21790
39	bend	12	6	13	0			107.23756	0.48821
40	bend	8	7	14	0			108.20732	0.21790
41	bend	8	7	15	0			108.30606	0.21793
42	bend	7	8	16	0			108.60491	0.21776
43	bend	7	8	17	0			109.02844	0.21789
44	bend	14	7	15	0			107.14617	0.52634
45	bend	16	8	17	0			105.44640	0.29518
46	torsion	3	2	1	5			0.16745	0.17805

47	torsion	10	2	1	5	179.77901	0.21755
48	torsion	2	1	5	4	0.00177	0.22835
49	torsion	2	1	5	6	178.49698	0.17947
50	torsion	1	2	3	4	-0.27444	0.21527
51	torsion	1	2	3	9	179.36240	0.21786
52	torsion	1	5	4	3	-0.16351	0.24107
53	torsion	1	5	4	11	-179.59027	0.27309
54	torsion	1	5	6	7	-67.05740	0.16852
55	torsion	1	5	6	12	54.38895	0.37207
56	torsion	1	5	6	13	171.39158	0.37097
57	torsion	4	3	2	10	-179.90214	0.25779
58	torsion	9	3	2	10	-0.26530	0.34782
59	torsion	2	3	4	5	0.25854	0.23952
60	torsion	2	3	4	11	179.75301	0.21788
61	torsion	5	4	3	9	-179.37772	0.25094
62	torsion	11	4	3	9	0.11674	0.37667
63	torsion	3	4	5	6	-178.55236	0.21752
64	torsion	6	5	4	11	2.02089	0.36172
65	torsion	4	5	6	7	111.14175	0.29599
66	torsion	4	5	6	12	-127.41190	0.43301
67	torsion	4	5	6	13	-10.40927	0.45558
68	torsion	5	6	7	8	67.01658	0.20903
69	torsion	5	6	7	14	-170.99536	0.41265
70	torsion	5	6	7	15	-54.58952	0.41184
71	torsion	8	7	6	12	-54.01779	0.40553
72	torsion	14	7	6	12	67.97027	0.54853
73	torsion	15	7	6	12	-175.62389	0.52853
74	torsion	8	7	6	13	-171.00326	0.37588
75	torsion	14	7	6	13	-49.01519	0.50869
76	torsion	15	7	6	13	67.39065	0.52674
77	torsion	6	7	8	16	-48.66273	0.21804
78	torsion	6	7	8	17	65.75367	0.21803
79	torsion	16	8	7	14	-171.14297	0.41664
80	torsion	17	8	7	14	-56.72657	0.41738
81	torsion	16	8	7	15	73.02640	0.41387
82	torsion	17	8	7	15	-172.55720	0.41303
83	o.o.p	10	1	2	3	-0.31432	0.22815
84	o.o.p	9	2	3	4	-0.29303	0.24763
85	o.o.p	11	3	4	5	-0.42728	0.27442

Table S44. Refined geometrical parameters of ^{3}T−a conformer

No.	Type	i	j	k	l	a-Value	g-Value	e-Value	Error
1	stretch	1	2	0	0	1.32679	1.32817	1.32239	0.00219
2	stretch	1	5	0	0	1.38354	1.38508	1.37904	0.00297
3	stretch	2	3	0	0	1.36996	1.37141	1.35946	0.00286
4	stretch	2	10	0	0	1.09232	1.09751	1.07752	0.00361
5	stretch	3	4	0	0	1.37869	1.38013	1.36859	0.00316
6	stretch	3	9	0	0	1.02136	1.02626	1.00646	0.00348
7	stretch	4	5	0	0	1.38965	1.39108	1.38235	0.00274
8	stretch	4	11	0	0	1.09264	1.09780	1.07774	0.00361
9	stretch	5	6	0	0	1.50638	1.50796	1.49728	0.00260
10	stretch	6	7	0	0	1.53296	1.53467	1.52166	0.00243
11	stretch	6	12	0	0	1.10996	1.11533	1.09306	0.00380
12	stretch	6	13	0	0	1.11112	1.11655	1.09562	0.00380
13	stretch	7	8	0	0	1.46577	1.46742	1.45617	0.00211
14	stretch	7	14	0	0	1.11119	1.11658	1.09379	0.00380
15	stretch	7	15	0	0	1.11256	1.11805	1.09726	0.00380
16	stretch	8	16	0	0	1.02714	1.03216	1.01444	0.00380
17	stretch	8	17	0	0	1.02928	1.03433	1.01528	0.00380
18	bend	2	1	5	0			105.46912	0.18036
19	bend	1	2	3	0			111.68668	0.16320
20	bend	1	2	10	0			126.00038	0.21732
21	bend	1	5	4	0			109.71299	0.22267
22	bend	1	5	6	0			121.68817	0.19415
23	bend	3	2	10	0			122.31157	0.27049
24	bend	2	3	4	0			107.36953	0.16743
25	bend	2	3	9	0			126.28654	0.21757
26	bend	4	3	9	0			126.34266	0.27325
27	bend	3	4	5	0			105.76139	0.25518
28	bend	3	4	11	0			122.33031	0.21720
29	bend	5	4	11	0			131.90787	0.33294
30	bend	4	5	6	0			128.59202	0.27975
31	bend	5	6	7	0			113.15197	0.13838
32	bend	5	6	12	0			110.37573	0.21805
33	bend	5	6	13	0			109.08915	0.21806
34	bend	7	6	12	0			109.11958	0.21806
35	bend	7	6	13	0			108.95261	0.21806
36	bend	6	7	8	0			109.89899	0.16961
37	bend	6	7	14	0			108.85208	0.21806
38	bend	6	7	15	0			108.40546	0.21806
39	bend	12	6	13	0			105.88547	0.49405
40	bend	8	7	14	0			108.12394	0.21805
41	bend	8	7	15	0			114.25953	0.21806
42	bend	7	8	16	0			110.03467	0.21806
43	bend	7	8	17	0			109.29743	0.21806
44	bend	14	7	15	0			107.15755	0.47912
45	bend	16	8	17	0			106.26565	0.29457
46	torsion	3	2	1	5			0.04831	0.17789

47	torsion	10	2	1	5	179.62902	0.21755
48	torsion	2	1	5	4	0.06435	0.20054
49	torsion	2	1	5	6	179.19083	0.17947
50	torsion	1	2	3	4	-0.14272	0.21527
51	torsion	1	2	3	9	179.46786	0.21786
52	torsion	1	5	4	3	-0.14871	0.24099
53	torsion	1	5	4	11	-179.90606	0.27329
54	torsion	1	5	6	7	-67.98857	0.16852
55	torsion	1	5	6	12	54.61524	0.39131
56	torsion	1	5	6	13	170.56038	0.36196
57	torsion	4	3	2	10	-179.74137	0.25738
58	torsion	9	3	2	10	-0.13079	0.34748
59	torsion	2	3	4	5	0.17292	0.23883
60	torsion	2	3	4	11	179.95920	0.21788
61	torsion	5	4	3	9	-179.43738	0.25055
62	torsion	11	4	3	9	0.34890	0.37645
63	torsion	3	4	5	6	-179.19772	0.21991
64	torsion	6	5	4	11	1.04493	0.36478
65	torsion	4	5	6	7	110.95931	0.29711
66	torsion	4	5	6	12	-126.43688	0.44134
67	torsion	4	5	6	13	-10.49174	0.45597
68	torsion	5	6	7	8	178.79791	0.21805
69	torsion	5	6	7	14	-62.96169	0.37960
70	torsion	5	6	7	15	53.27924	0.39696
71	torsion	8	7	6	12	55.49839	0.40256
72	torsion	14	7	6	12	173.73880	0.51373
73	torsion	15	7	6	12	-70.02027	0.51574
74	torsion	8	7	6	13	-59.67420	0.39679
75	torsion	14	7	6	13	58.56621	0.49892
76	torsion	15	7	6	13	174.80714	0.52278
77	torsion	6	7	8	16	178.11507	0.21807
78	torsion	6	7	8	17	-65.55353	0.21807
79	torsion	16	8	7	14	59.42561	0.37815
80	torsion	17	8	7	14	175.75700	0.37817
81	torsion	16	8	7	15	-59.78196	0.41167
82	torsion	17	8	7	15	56.54944	0.41164
83	o.o.p	10	1	2	3	-0.33921	0.22802
84	o.o.p	9	2	3	4	-0.31390	0.24738
85	o.o.p	11	3	4	5	-0.18059	0.27391

3.3 Correlation matrix of GED+MW refinement

Table S45. Matrix of correlation for the regularized GED+MW refinement. Parameters 1000 and 2000 are the scale factors for LD and SD, respectively. The defenition of all other parameters can be found in Tab. S25 and S26

1000	1.0000							
2000	0.2762	1.0000						
1	0.0440	0.0689	1.0000					
2	-0.0909	-0.1319	-0.0262	1.0000				
3	-0.0052	-0.0105	-0.0270	-0.1531	1.0000			
4	0.0831	0.0774	-0.0617	0.0291	-0.1440	1.0000		
5	-0.0343	-0.0326	-0.0326	-0.0599	-0.2263	-0.1580	1.0000	
6	0.0071	-0.0030	-0.0930	-0.0636	-0.0233	-0.1745	-0.1431	1.0000
7	0.0807	0.0737	-0.0630	-0.1059	-0.0607	-0.0520	-0.1385	-0.2438
8	0.0623	0.0866	0.0035	-0.1329	-0.1176	-0.0418	-0.2013	-0.1478
9	-0.0079	-0.0026	-0.0010	-0.0117	-0.0127	-0.0102	-0.0143	-0.0102
10	-0.0081	0.0115	0.0007	-0.0263	-0.0242	-0.0152	-0.0331	-0.0195
11	0.0000	0.0220	0.0029	-0.0251	-0.0230	-0.0148	-0.0341	-0.0167
12	-0.0122	0.0009	0.0006	-0.0046	-0.0063	-0.0039	-0.0120	-0.0087
13	-0.0119	0.0045	0.0024	-0.0137	-0.0131	-0.0054	-0.0237	-0.0085
14	-0.0067	0.0084	-0.0042	-0.0049	-0.0020	-0.0030	-0.0045	-0.0106
15	-0.0162	-0.0039	0.0019	-0.0042	-0.0076	-0.0033	-0.0121	-0.0064
16	-0.0062	-0.0115	-0.0012	-0.0008	-0.0063	-0.0054	-0.0154	-0.0082
17	-0.0067	-0.0100	-0.0019	-0.0070	-0.0101	-0.0098	-0.0211	-0.0123
101	-0.1731	-0.3150	-0.1318	-0.4621	0.0473	0.0098	0.1033	0.0095
102	0.0181	0.0396	-0.1057	-0.0129	-0.0185	-0.0282	-0.0557	0.0585
103	0.0756	0.1040	-0.1447	0.0123	-0.0886	-0.0333	-0.0490	0.0773
104	0.0777	0.1483	-0.0419	0.0587	0.0329	-0.1535	-0.0824	-0.0021
105	-0.0688	-0.0846	-0.0725	-0.0024	-0.1198	-0.0078	-0.1365	0.0642
106	0.0473	0.0922	0.0644	0.0818	0.1070	0.1028	-0.0239	-0.1732
107	0.2027	0.1663	0.0686	-0.0413	0.0231	0.1019	0.1163	-0.0076
108	-0.0468	-0.0738	0.0941	0.0754	0.0355	0.0019	0.1623	-0.1495
109	-0.0344	-0.0210	-0.0029	-0.0065	-0.0065	-0.0146	0.0197	-0.0052
110	-0.0230	0.0208	-0.0019	-0.0120	0.0013	-0.0103	0.0248	-0.0085
111	-0.0026	0.0397	0.0078	-0.0089	0.0064	-0.0052	0.0244	-0.0005
112	-0.0219	-0.0034	0.0042	0.0046	0.0020	-0.0015	0.0125	0.0028
113	-0.0157	0.0025	0.0038	0.0060	0.0033	-0.0033	0.0105	-0.0002
114	-0.0243	-0.0044	0.0058	0.0049	0.0009	0.0022	0.0108	-0.0019
115	-0.0289	-0.0069	-0.0000	0.0078	0.0006	0.0017	0.0093	0.0031
116	-0.0100	-0.0150	0.0023	0.0096	0.0015	0.0014	-0.0002	0.0019
117	-0.0166	-0.0225	0.0060	0.0055	0.0018	0.0014	0.0025	0.0052
216	-0.0042	-0.0075	-0.0000	0.0055	0.0010	0.0008	0.0006	0.0002
217	-0.0032	-0.0064	-0.0005	0.0050	0.0018	0.0021	-0.0002	0.0000
412	-0.0047	0.0006	-0.0001	0.0021	0.0024	-0.0018	0.0026	0.0012
413	-0.0075	-0.0019	0.0027	0.0008	0.0053	0.0004	0.0037	0.0012
414	-0.0094	-0.0038	0.0010	0.0029	0.0013	0.0002	0.0023	0.0020
415	-0.0080	-0.0021	0.0009	0.0024	0.0026	-0.0005	0.0020	0.0002
416	-0.0031	-0.0048	0.0007	0.0021	0.0023	0.0013	0.0004	-0.0004
417	-0.0038	-0.0057	0.0012	0.0034	0.0016	-0.0003	0.0001	0.0020
316	-0.0007	-0.0016	-0.0001	0.0011	0.0004	0.0004	-0.0001	-0.0001
317	-0.0006	-0.0009	-0.0004	0.0007	0.0003	0.0003	0.0001	-0.0001
512	-0.0015	0.0024	-0.0011	0.0007	0.0009	0.0002	0.0019	-0.0009

513	-0.0023	0.0019	-0.0008	0.0010	0.0010	0.0004	0.0016	-0.0010
514	-0.0050	-0.0008	-0.0004	0.0017	0.0003	0.0007	0.0013	-0.0008
515	-0.0015	0.0033	-0.0005	0.0005	0.0010	0.0004	0.0019	-0.0014
516	-0.0015	-0.0023	-0.0010	0.0018	0.0008	0.0004	0.0002	-0.0003
517	-0.0015	-0.0031	-0.0004	0.0026	0.0008	0.0009	-0.0000	-0.0001
18	0.0446	0.0672	-0.0426	-0.1291	0.0899	0.1628	0.1746	0.0181
19	-0.0437	-0.0253	0.0344	-0.2835	-0.1056	0.1742	0.0152	0.0634
20	-0.0573	-0.0391	-0.0840	0.0228	0.0119	0.0389	-0.0169	-0.1055
21	-0.0731	-0.0729	-0.1619	0.0755	0.0882	-0.1238	0.0862	-0.3080
22	-0.0346	-0.0444	-0.0350	-0.0229	-0.0136	-0.0374	-0.0834	-0.1094
23	-0.0081	-0.0101	0.0057	-0.0106	-0.0155	-0.0067	-0.0224	-0.0046
24	0.0023	0.0018	-0.0079	0.0068	0.0098	-0.0021	0.0143	-0.0033
25	-0.0058	-0.0068	0.0047	-0.0058	-0.0077	0.0018	-0.0094	0.0022
26	-0.0125	-0.0081	0.0012	-0.0096	-0.0109	-0.0029	-0.0155	-0.0068
27	-0.0056	-0.0066	0.0051	-0.0115	-0.0094	-0.0103	-0.0182	-0.0076
28	-0.0068	-0.0021	-0.0016	-0.0067	-0.0065	-0.0029	-0.0073	-0.0048
29	-0.0056	0.0003	0.0003	-0.0087	-0.0065	-0.0033	-0.0082	-0.0030
30	-0.0028	0.0022	-0.0033	-0.0038	-0.0013	-0.0022	0.0012	-0.0033
31	-0.0046	0.0015	0.0023	-0.0106	-0.0089	-0.0028	-0.0109	-0.0023
32	-0.0046	-0.0026	-0.0024	-0.0067	-0.0045	-0.0095	-0.0066	-0.0099
33	-0.0136	-0.0091	-0.0009	-0.0068	-0.0086	-0.0059	-0.0087	-0.0056
34	-0.0161	-0.0147	0.0029	-0.0082	-0.0124	-0.0057	-0.0185	-0.0048
35	-0.0151	-0.0105	0.0025	-0.0098	-0.0121	-0.0043	-0.0166	-0.0037
118	0.0686	0.1338	0.0103	0.1302	0.1000	0.0137	-0.0984	-0.0091
119	0.0022	0.0161	0.0551	0.0216	-0.0723	-0.0418	-0.0327	0.0689
120	-0.0449	-0.0310	-0.0139	0.0152	-0.0081	0.1012	-0.0307	0.0491
121	-0.0555	-0.0398	0.0272	0.0243	-0.0090	-0.0255	-0.0169	0.0800
122	-0.1007	-0.1315	0.0582	0.0350	0.0112	0.0166	-0.0269	0.0749
123	-0.0084	-0.0103	0.0055	-0.0003	-0.0007	0.0003	0.0021	0.0017
124	0.0092	0.0108	-0.0073	0.0014	-0.0019	-0.0007	-0.0023	-0.0005
125	-0.0094	-0.0045	-0.0097	-0.0043	0.0011	-0.0041	0.0002	-0.0073
126	-0.0096	-0.0086	-0.0038	-0.0033	-0.0029	-0.0103	0.0065	0.0041
127	-0.0076	-0.0020	-0.0009	-0.0027	-0.0019	-0.0052	0.0032	0.0018
128	-0.0103	-0.0074	-0.0000	-0.0029	-0.0019	-0.0090	0.0051	0.0025
129	-0.0078	-0.0093	0.0013	-0.0014	-0.0011	-0.0129	0.0059	0.0005
130	-0.0070	-0.0012	0.0023	-0.0033	-0.0038	-0.0024	0.0054	0.0031
131	-0.0168	-0.0111	0.0020	-0.0034	-0.0055	-0.0019	0.0066	0.0016
132	-0.0061	0.0010	-0.0014	-0.0046	-0.0021	-0.0010	0.0053	0.0006
133	-0.0268	-0.0215	0.0016	-0.0011	-0.0056	-0.0010	0.0040	0.0002
134	-0.0377	-0.0415	0.0101	0.0041	-0.0039	-0.0010	0.0028	0.0051
135	-0.0346	-0.0344	0.0057	0.0029	-0.0037	-0.0033	0.0020	0.0031
421	-0.0561	-0.0573	0.0320	0.0404	-0.0485	-0.0506	-0.0137	0.0769
422	-0.0414	-0.0440	0.0250	0.0136	0.0061	-0.0141	-0.0069	0.0308
426	-0.0036	-0.0047	0.0002	-0.0007	0.0007	-0.0023	0.0026	0.0024
427	-0.0022	-0.0038	0.0010	-0.0003	0.0023	-0.0030	0.0020	0.0007
428	-0.0038	-0.0030	-0.0000	-0.0005	0.0004	-0.0014	0.0011	0.0012
429	-0.0026	-0.0002	-0.0000	-0.0009	0.0007	-0.0008	0.0010	0.0003
430	-0.0021	0.0003	-0.0003	-0.0008	-0.0002	-0.0007	0.0011	0.0007
431	-0.0079	-0.0059	0.0008	-0.0005	0.0009	-0.0001	0.0010	0.0001
432	-0.0038	-0.0029	0.0011	0.0002	0.0005	-0.0027	0.0012	0.0019
433	-0.0067	-0.0054	0.0012	-0.0001	0.0003	-0.0013	0.0014	0.0013
434	-0.0078	-0.0087	0.0027	0.0011	0.0022	-0.0014	0.0007	0.0018

435	-0.0071	-0.0074	0.0019	0.0007	0.0016	-0.0006	0.0007	0.0012
334	-0.0019	-0.0018	-0.0002	0.0003	-0.0001	-0.0002	-0.0001	-0.0001
335	-0.0018	-0.0013	-0.0003	0.0000	-0.0002	-0.0001	0.0000	-0.0000
526	-0.0007	-0.0001	-0.0014	-0.0011	-0.0008	-0.0005	0.0016	0.0007
527	-0.0011	-0.0009	-0.0006	-0.0005	-0.0002	-0.0007	0.0007	-0.0004
528	-0.0018	-0.0005	-0.0010	-0.0010	-0.0004	-0.0001	0.0008	-0.0000
529	-0.0011	-0.0001	-0.0005	-0.0007	-0.0002	-0.0004	0.0006	-0.0005
530	-0.0011	0.0001	-0.0004	-0.0007	-0.0004	-0.0002	0.0007	-0.0004
531	-0.0043	-0.0024	-0.0006	-0.0004	-0.0010	0.0000	0.0004	-0.0002
532	-0.0011	-0.0003	-0.0004	-0.0008	-0.0002	-0.0004	0.0006	-0.0007
533	-0.0008	0.0018	-0.0006	-0.0012	-0.0004	-0.0001	0.0009	-0.0004
534	-0.0046	-0.0033	-0.0006	0.0001	-0.0006	-0.0004	0.0001	-0.0001
535	-0.0048	-0.0042	-0.0004	0.0005	-0.0004	-0.0002	-0.0001	-0.0001
36	-0.0028	-0.0018	0.0079	-0.0090	-0.0103	-0.0006	-0.0184	0.0038
37	-0.0028	0.0013	0.0101	-0.0135	-0.0133	0.0105	-0.0235	0.0149
38	0.0089	0.0061	-0.0336	0.0371	0.0391	-0.0160	0.0660	-0.0310
39	0.0095	0.0056	-0.0073	0.0178	0.0214	0.0021	0.0374	0.0050
40	-0.0028	0.0015	-0.0645	0.0469	0.0476	-0.0296	0.0822	-0.0601
41	0.0009	0.0004	-0.0003	0.0017	0.0018	0.0012	0.0025	0.0010
42	-0.0003	-0.0002	0.0009	-0.0008	-0.0011	0.0003	-0.0016	0.0004
43	-0.0001	-0.0004	0.0006	-0.0003	-0.0005	0.0004	-0.0007	0.0004
44	-0.0019	-0.0032	-0.0061	0.0025	0.0036	-0.0056	0.0040	-0.0055
45	0.0013	0.0015	0.0069	-0.0062	-0.0076	0.0032	-0.0121	0.0031
136	-0.0203	-0.0262	0.0153	-0.0035	0.0043	0.0054	0.0037	-0.0041
137	0.0054	-0.0102	0.0008	-0.0135	0.0027	0.0291	0.0084	-0.0271
138	0.0689	0.0988	-0.0512	0.0281	-0.0196	-0.0370	-0.0066	0.0443
139	0.0128	0.0328	-0.0314	0.0080	0.0095	-0.0264	-0.0324	-0.0025
140	-0.0025	0.0105	-0.0187	-0.0044	0.0105	-0.0030	-0.0264	-0.0306
141	-0.0042	-0.0049	0.0033	0.0002	0.0000	-0.0006	0.0004	0.0011
142	-0.0036	-0.0022	0.0017	0.0007	0.0002	-0.0024	-0.0012	0.0013
143	0.0019	0.0004	-0.0005	-0.0006	-0.0001	0.0021	0.0009	-0.0018
144	-0.0070	-0.0075	0.0031	0.0012	-0.0004	-0.0026	-0.0004	0.0024
145	0.0065	0.0038	-0.0010	-0.0022	0.0011	0.0040	0.0014	-0.0012
244	-0.0019	-0.0008	-0.0003	-0.0004	0.0003	0.0012	-0.0002	-0.0001
245	0.0017	0.0004	0.0003	0.0001	0.0002	-0.0004	-0.0002	0.0001
440	-0.0039	-0.0028	0.0039	0.0094	-0.0176	-0.0116	-0.0004	0.0200
444	-0.0004	0.0003	-0.0006	-0.0002	-0.0007	0.0005	-0.0000	-0.0005
445	0.0004	-0.0008	0.0004	0.0008	-0.0008	-0.0009	-0.0001	0.0015
344	0.0003	0.0004	0.0001	-0.0001	-0.0000	0.0001	0.0000	0.0001
345	-0.0003	-0.0002	-0.0000	0.0001	-0.0000	-0.0000	-0.0000	0.0000
540	-0.0001	0.0001	0.0006	0.0001	0.0001	-0.0007	0.0001	-0.0002
544	-0.0009	-0.0008	-0.0001	0.0001	-0.0001	-0.0001	0.0000	-0.0000
545	0.0008	0.0009	0.0001	-0.0001	-0.0001	0.0002	0.0000	0.0001

	1000	2000	1	2	3	4	5	6
7	1.0000							
8	-0.1669	1.0000						
9	-0.0094	-0.0170	1.0000					
10	-0.0204	-0.0330	-0.0156	1.0000				
11	-0.0201	-0.0367	-0.0165	-0.0282	1.0000			
12	-0.0141	-0.0135	-0.0058	-0.0135	-0.0135	1.0000		

13	-0.0172	-0.0273	-0.0053	-0.0159	-0.0157	-0.0132	1.0000	
14	-0.0104	-0.0077	-0.0045	-0.0130	-0.0123	-0.0118	-0.0130	1.0000
15	-0.0143	-0.0140	-0.0059	-0.0134	-0.0132	-0.0138	-0.0130	-0.0115
16	-0.0158	-0.0160	-0.0213	-0.0120	-0.0112	-0.0071	-0.0060	-0.0051
17	-0.0184	-0.0213	-0.0221	-0.0141	-0.0127	-0.0060	-0.0065	-0.0052
101	0.0230	0.0491	0.0091	0.0118	0.0053	0.0156	0.0172	0.0123
102	-0.0105	0.0484	0.0011	-0.0005	-0.0004	-0.0030	-0.0027	-0.0035
103	0.0276	-0.0012	0.0017	0.0072	0.0079	0.0032	0.0077	0.0038
104	0.0985	0.0421	-0.0032	-0.0090	-0.0113	-0.0101	-0.0127	-0.0118
105	0.0721	0.1087	0.0084	0.0194	0.0203	0.0113	0.0138	0.0107
106	-0.0527	-0.0772	-0.0023	0.0059	0.0030	0.0013	0.0038	0.0044
107	-0.2595	0.0866	0.0012	-0.0046	-0.0002	-0.0019	-0.0046	-0.0028
108	0.1318	-0.3656	0.0074	0.0221	0.0268	0.0206	0.0264	0.0188
109	0.0026	0.0155	-0.0631	-0.0237	-0.0241	-0.0075	-0.0031	-0.0060
110	0.0059	0.0221	-0.0249	-0.0385	-0.0368	-0.0269	-0.0257	-0.0262
111	0.0055	0.0225	-0.0188	-0.0348	-0.0333	-0.0266	-0.0276	-0.0261
112	0.0020	0.0118	-0.0070	-0.0193	-0.0184	-0.0184	-0.0195	-0.0189
113	0.0028	0.0089	-0.0075	-0.0189	-0.0186	-0.0184	-0.0187	-0.0186
114	-0.0006	0.0102	-0.0072	-0.0183	-0.0179	-0.0183	-0.0181	-0.0181
115	-0.0007	0.0034	-0.0070	-0.0174	-0.0163	-0.0182	-0.0187	-0.0192
116	0.0004	0.0015	-0.0195	-0.0067	-0.0064	-0.0051	-0.0040	-0.0040
117	0.0002	0.0053	-0.0176	-0.0060	-0.0052	-0.0037	-0.0035	-0.0030
216	-0.0003	-0.0003	-0.0125	-0.0037	-0.0033	-0.0027	-0.0019	-0.0021
217	-0.0009	-0.0006	-0.0120	-0.0037	-0.0034	-0.0028	-0.0021	-0.0023
412	0.0020	-0.0001	-0.0022	-0.0054	-0.0052	-0.0051	-0.0054	-0.0052
413	-0.0003	0.0017	-0.0021	-0.0057	-0.0056	-0.0053	-0.0058	-0.0055
414	0.0002	0.0009	-0.0017	-0.0048	-0.0045	-0.0051	-0.0054	-0.0053
415	0.0007	0.0002	-0.0021	-0.0051	-0.0051	-0.0050	-0.0051	-0.0050
416	-0.0009	-0.0001	-0.0061	-0.0020	-0.0020	-0.0015	-0.0011	-0.0011
417	0.0005	-0.0007	-0.0060	-0.0022	-0.0020	-0.0016	-0.0014	-0.0014
316	-0.0001	-0.0001	-0.0025	-0.0007	-0.0007	-0.0006	-0.0004	-0.0004
317	-0.0001	-0.0001	-0.0024	-0.0008	-0.0006	-0.0005	-0.0004	-0.0005
512	0.0002	0.0008	-0.0016	-0.0037	-0.0035	-0.0036	-0.0037	-0.0037
513	-0.0000	0.0008	-0.0015	-0.0036	-0.0034	-0.0036	-0.0036	-0.0037
514	-0.0004	0.0007	-0.0015	-0.0035	-0.0033	-0.0036	-0.0035	-0.0036
515	-0.0001	0.0007	-0.0015	-0.0036	-0.0035	-0.0036	-0.0036	-0.0037
516	-0.0003	-0.0001	-0.0064	-0.0020	-0.0015	-0.0012	-0.0009	-0.0010
517	-0.0004	-0.0004	-0.0065	-0.0019	-0.0017	-0.0014	-0.0010	-0.0011
18	-0.0176	0.0144	0.0027	0.0096	0.0114	0.0008	0.0037	-0.0060
19	-0.0692	-0.1362	-0.0139	-0.0251	-0.0241	-0.0122	-0.0213	-0.0106
20	-0.0814	0.0286	0.0052	0.0023	0.0039	-0.0001	0.0020	-0.0053
21	-0.1543	0.1453	0.0092	0.0182	0.0203	0.0085	0.0170	-0.0084
22	-0.1448	-0.0939	-0.0005	-0.0077	-0.0106	-0.0040	-0.0103	-0.0047
23	-0.0103	-0.0216	-0.0032	-0.0078	-0.0078	-0.0023	-0.0039	-0.0017
24	0.0020	0.0138	0.0018	0.0034	0.0044	0.0011	0.0020	0.0003
25	-0.0002	-0.0074	-0.0012	-0.0030	-0.0026	-0.0008	-0.0015	-0.0007
26	-0.0091	-0.0159	-0.0013	-0.0037	-0.0034	-0.0025	-0.0035	-0.0021
27	-0.0102	-0.0186	-0.0018	-0.0043	-0.0040	-0.0031	-0.0043	-0.0024
28	-0.0062	-0.0097	-0.0007	-0.0024	-0.0020	-0.0019	-0.0026	-0.0017
29	-0.0062	-0.0104	-0.0010	-0.0025	-0.0023	-0.0014	-0.0023	-0.0014
30	-0.0043	-0.0015	-0.0002	-0.0009	-0.0004	-0.0013	-0.0010	-0.0015
31	-0.0075	-0.0137	-0.0016	-0.0033	-0.0033	-0.0023	-0.0027	-0.0014

32	-0.0099	-0.0074	-0.0013	-0.0030	-0.0024	-0.0021	-0.0021	-0.0017
33	-0.0092	-0.0101	-0.0016	-0.0032	-0.0027	-0.0021	-0.0022	-0.0014
34	-0.0104	-0.0175	-0.0024	-0.0061	-0.0058	-0.0018	-0.0031	-0.0014
35	-0.0074	-0.0161	-0.0021	-0.0058	-0.0053	-0.0010	-0.0028	-0.0012
118	0.0031	-0.0712	-0.0023	-0.0033	-0.0068	-0.0035	-0.0069	-0.0042
119	0.0203	0.0340	0.0070	0.0066	0.0057	0.0045	0.0010	0.0028
120	-0.0098	-0.0187	-0.0006	0.0011	-0.0008	0.0030	0.0016	0.0028
121	0.0225	-0.0319	0.0019	-0.0040	-0.0055	-0.0019	-0.0054	-0.0027
122	0.0156	0.0172	0.0086	-0.0007	-0.0035	0.0028	-0.0020	0.0045
123	-0.0009	0.0057	-0.0001	-0.0003	-0.0007	0.0000	-0.0002	0.0005
124	0.0010	-0.0076	-0.0002	0.0007	0.0009	0.0002	0.0008	-0.0001
125	0.0015	0.0007	-0.0020	-0.0021	-0.0005	-0.0007	-0.0008	-0.0011
126	0.0056	0.0010	-0.0015	-0.0031	-0.0018	-0.0020	-0.0023	-0.0023
127	0.0033	0.0010	-0.0007	-0.0018	-0.0012	-0.0014	-0.0016	-0.0018
128	0.0045	0.0030	-0.0010	-0.0025	-0.0017	-0.0018	-0.0021	-0.0022
129	0.0058	0.0051	-0.0013	-0.0030	-0.0021	-0.0020	-0.0026	-0.0023
130	0.0021	0.0013	-0.0008	-0.0018	-0.0016	-0.0017	-0.0015	-0.0016
131	-0.0003	0.0032	-0.0008	-0.0019	-0.0011	-0.0016	-0.0014	-0.0015
132	-0.0011	-0.0002	-0.0001	-0.0009	-0.0002	-0.0009	-0.0014	-0.0019
133	-0.0019	0.0041	-0.0006	-0.0014	-0.0003	-0.0011	-0.0008	-0.0009
134	-0.0011	0.0081	0.0013	-0.0006	-0.0001	-0.0006	-0.0009	0.0000
135	-0.0003	0.0072	0.0004	-0.0012	-0.0003	-0.0007	-0.0009	-0.0003
421	0.0353	0.0137	0.0032	-0.0030	-0.0027	-0.0016	-0.0041	-0.0011
422	0.0128	0.0032	-0.0011	-0.0045	-0.0062	-0.0021	-0.0037	-0.0015
426	0.0016	0.0001	-0.0004	-0.0013	-0.0009	-0.0009	-0.0012	-0.0010
427	0.0013	0.0001	-0.0006	-0.0012	-0.0010	-0.0009	-0.0011	-0.0010
428	0.0012	-0.0001	-0.0002	-0.0008	-0.0005	-0.0006	-0.0007	-0.0008
429	0.0004	-0.0005	-0.0002	-0.0006	-0.0004	-0.0004	-0.0005	-0.0005
430	0.0004	-0.0005	-0.0000	-0.0004	-0.0002	-0.0004	-0.0006	-0.0006
431	-0.0006	0.0003	-0.0004	-0.0007	-0.0006	-0.0005	-0.0005	-0.0004
432	0.0014	-0.0001	-0.0001	-0.0009	-0.0006	-0.0006	-0.0009	-0.0008
433	0.0001	0.0004	-0.0002	-0.0008	-0.0006	-0.0006	-0.0008	-0.0006
434	0.0000	0.0007	-0.0001	-0.0008	-0.0007	-0.0006	-0.0008	-0.0005
435	-0.0004	0.0005	-0.0001	-0.0006	-0.0005	-0.0005	-0.0006	-0.0004
334	-0.0001	0.0000	0.0000	-0.0000	0.0001	-0.0000	-0.0000	-0.0000
335	-0.0001	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000
526	0.0006	-0.0005	-0.0002	-0.0005	-0.0002	-0.0004	-0.0004	-0.0004
527	0.0001	0.0001	-0.0002	-0.0003	-0.0001	-0.0002	-0.0002	-0.0003
528	0.0002	-0.0001	-0.0002	-0.0003	-0.0001	-0.0002	-0.0002	-0.0003
529	-0.0001	0.0001	-0.0001	-0.0002	-0.0001	-0.0002	-0.0001	-0.0002
530	-0.0000	-0.0000	-0.0001	-0.0002	-0.0001	-0.0002	-0.0002	-0.0002
531	-0.0004	0.0000	-0.0002	-0.0002	-0.0001	-0.0001	-0.0000	-0.0001
532	0.0001	0.0002	-0.0002	-0.0002	-0.0001	-0.0002	-0.0002	-0.0003
533	-0.0002	-0.0001	-0.0002	-0.0002	-0.0002	-0.0001	-0.0002	-0.0003
534	-0.0003	0.0001	0.0000	-0.0002	0.0001	-0.0000	-0.0000	-0.0001
535	-0.0003	0.0000	-0.0001	-0.0001	0.0001	-0.0001	-0.0000	-0.0001
36	-0.0102	-0.0199	-0.0009	-0.0023	-0.0031	-0.0036	-0.0029	-0.0002
37	-0.0100	-0.0273	-0.0018	-0.0040	-0.0051	-0.0059	-0.0039	-0.0009
38	0.0296	0.0742	0.0040	0.0094	0.0119	0.0136	0.0102	0.0015
39	0.0346	0.0407	0.0032	0.0072	0.0091	0.0092	0.0061	0.0024
40	-0.0256	0.0685	0.0069	0.0147	0.0153	0.0024	0.0096	-0.0007
41	0.0021	0.0025	0.0006	0.0011	0.0012	0.0005	0.0004	0.0002

42	-0.0004	-0.0015	-0.0002	-0.0004	-0.0004	-0.0002	-0.0002	-0.0000
43	-0.0003	-0.0005	-0.0001	-0.0002	-0.0002	-0.0002	-0.0000	-0.0000
44	-0.0019	0.0032	0.0006	0.0005	0.0012	0.0009	0.0001	-0.0004
45	-0.0016	-0.0103	-0.0015	-0.0031	-0.0036	-0.0013	-0.0016	-0.0003
136	-0.0015	0.0161	0.0002	-0.0009	-0.0018	-0.0008	-0.0014	0.0001
137	-0.0205	0.0133	0.0011	0.0032	0.0041	0.0021	0.0034	0.0028
138	0.0154	-0.0706	0.0005	0.0021	0.0037	0.0009	0.0004	-0.0021
139	0.0269	-0.0219	-0.0024	-0.0001	0.0002	-0.0018	-0.0015	-0.0032
140	0.0126	0.0062	-0.0029	0.0012	0.0008	0.0001	0.0016	0.0005
141	0.0005	0.0028	-0.0001	-0.0005	-0.0005	-0.0002	-0.0003	-0.0001
142	0.0022	0.0016	-0.0005	-0.0007	-0.0008	-0.0004	-0.0005	-0.0003
143	-0.0021	-0.0001	0.0001	0.0003	0.0005	0.0002	0.0003	0.0002
144	0.0026	0.0015	0.0003	-0.0002	-0.0005	-0.0002	-0.0004	-0.0001
145	-0.0032	-0.0013	0.0009	0.0008	0.0010	0.0006	0.0006	0.0005
244	-0.0008	-0.0006	0.0003	0.0003	0.0001	0.0002	0.0002	0.0002
245	0.0004	0.0007	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001
440	0.0077	-0.0000	0.0006	0.0002	-0.0003	0.0000	0.0002	0.0005
444	-0.0004	-0.0001	0.0001	0.0002	0.0002	0.0001	0.0002	0.0001
445	0.0006	0.0003	0.0002	-0.0001	0.0001	-0.0001	-0.0002	-0.0002
344	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000
345	-0.0000	-0.0001	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000
540	-0.0002	0.0001	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000
544	-0.0000	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000
545	-0.0000	0.0001	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0000

	7	8	9	10	11	12	13	14
15	1.0000							
16	-0.0073	1.0000						
17	-0.0062	-0.0248	1.0000					
101	0.0181	0.0128	0.0151	1.0000				
102	-0.0035	0.0012	0.0020	-0.3516	1.0000			
103	0.0020	0.0031	0.0054	-0.1199	-0.3648	1.0000		
104	-0.0076	-0.0018	-0.0032	-0.0407	-0.1866	-0.1852	1.0000	
105	0.0106	0.0046	0.0063	0.0919	-0.1613	-0.2912	-0.3723	1.0000
106	0.0010	0.0018	0.0057	-0.2357	0.1716	0.1992	-0.1766	-0.2025
107	-0.0036	0.0006	-0.0024	-0.0960	-0.1213	0.0015	0.0946	0.0064
108	0.0189	0.0086	0.0105	0.2895	-0.1016	-0.1231	-0.0813	-0.0828
109	-0.0080	-0.0493	-0.0500	0.0157	-0.0132	-0.0034	-0.0233	0.0158
110	-0.0267	-0.0158	-0.0161	0.0132	-0.0212	-0.0076	-0.0225	0.0226
111	-0.0256	-0.0169	-0.0186	0.0010	-0.0347	0.0053	-0.0418	0.0277
112	-0.0182	-0.0078	-0.0075	0.0162	-0.0203	0.0118	-0.0289	0.0155
113	-0.0183	-0.0075	-0.0068	0.0140	-0.0145	0.0060	-0.0251	0.0158
114	-0.0183	-0.0070	-0.0061	0.0190	-0.0184	0.0063	-0.0244	0.0152
115	-0.0184	-0.0085	-0.0076	0.0247	-0.0102	0.0008	-0.0148	0.0118
116	-0.0053	-0.0208	-0.0207	0.0104	-0.0056	0.0004	-0.0026	0.0024
117	-0.0036	-0.0196	-0.0203	0.0110	-0.0088	0.0047	-0.0190	0.0062
216	-0.0028	-0.0133	-0.0134	0.0072	-0.0017	-0.0011	0.0008	0.0003
217	-0.0030	-0.0129	-0.0128	0.0073	0.0002	-0.0019	0.0016	-0.0008
412	-0.0051	-0.0023	-0.0023	0.0051	0.0009	-0.0059	0.0003	0.0005
413	-0.0052	-0.0025	-0.0025	0.0079	-0.0014	-0.0080	0.0039	-0.0063
414	-0.0050	-0.0024	-0.0022	0.0071	-0.0013	-0.0029	-0.0020	0.0006

415	-0.0050	-0.0021	-0.0019	0.0074	0.0005	-0.0063	0.0016	-0.0016
416	-0.0015	-0.0064	-0.0064	0.0054	-0.0005	-0.0037	0.0042	-0.0032
417	-0.0016	-0.0067	-0.0067	0.0035	0.0013	-0.0041	0.0018	-0.0024
316	-0.0006	-0.0026	-0.0026	0.0017	-0.0001	-0.0003	0.0003	-0.0001
317	-0.0005	-0.0026	-0.0027	0.0017	-0.0000	-0.0003	0.0004	-0.0001
512	-0.0036	-0.0016	-0.0014	0.0041	-0.0016	-0.0005	-0.0016	0.0026
513	-0.0036	-0.0015	-0.0013	0.0044	-0.0015	-0.0002	-0.0019	0.0021
514	-0.0037	-0.0015	-0.0012	0.0056	-0.0016	-0.0012	-0.0010	0.0024
515	-0.0036	-0.0013	-0.0011	0.0034	-0.0015	-0.0005	-0.0028	0.0027
516	-0.0012	-0.0069	-0.0071	0.0043	0.0000	-0.0009	0.0010	-0.0003
517	-0.0015	-0.0069	-0.0069	0.0040	-0.0001	-0.0009	0.0008	-0.0002
18	0.0010	0.0059	0.0065	0.0268	-0.0437	-0.0526	-0.0073	-0.0465
19	-0.0131	-0.0033	-0.0069	0.1206	0.0159	-0.0112	0.0390	-0.0797
20	0.0023	-0.0041	-0.0037	0.0171	0.0126	-0.0170	0.0662	-0.0538
21	0.0128	0.0043	0.0029	0.0024	0.0134	0.0157	0.0119	-0.0340
22	-0.0026	-0.0077	-0.0116	0.0235	0.0092	0.0173	0.0306	-0.0049
23	-0.0023	-0.0033	-0.0041	0.0038	0.0002	0.0038	-0.0040	0.0102
24	0.0011	0.0009	0.0008	-0.0019	-0.0001	-0.0023	0.0015	-0.0026
25	-0.0009	-0.0008	-0.0009	0.0050	-0.0003	0.0015	-0.0001	0.0011
26	-0.0022	-0.0012	-0.0016	0.0036	-0.0000	0.0020	-0.0063	0.0088
27	-0.0030	-0.0021	-0.0024	0.0013	0.0001	0.0086	-0.0142	0.0083
28	-0.0017	-0.0010	-0.0011	-0.0001	-0.0005	0.0003	-0.0033	0.0069
29	-0.0014	-0.0006	-0.0010	0.0010	0.0001	0.0024	-0.0042	0.0038
30	-0.0013	-0.0007	-0.0005	-0.0016	-0.0005	0.0001	-0.0033	0.0031
31	-0.0024	-0.0012	-0.0012	-0.0004	0.0001	0.0017	-0.0050	0.0059
32	-0.0021	-0.0013	-0.0014	-0.0004	-0.0001	0.0026	-0.0053	0.0064
33	-0.0022	-0.0012	-0.0013	0.0043	-0.0004	-0.0000	-0.0016	0.0069
34	-0.0020	-0.0026	-0.0033	0.0074	0.0001	0.0033	-0.0024	0.0061
35	-0.0010	-0.0014	-0.0027	0.0076	0.0001	0.0027	-0.0016	0.0054
118	-0.0040	-0.0023	-0.0036	-0.0660	-0.4152	0.0395	0.0954	0.2549
119	0.0056	0.0026	0.0001	0.0833	-0.3272	0.0695	0.3121	0.0495
120	0.0021	-0.0001	0.0007	0.0132	-0.0027	-0.0224	0.1540	-0.1322
121	-0.0017	0.0004	-0.0024	-0.0089	0.0900	0.0270	-0.0760	-0.1068
122	0.0036	0.0018	-0.0012	-0.0065	0.0028	0.0239	-0.0330	-0.0845
123	0.0001	0.0002	0.0001	0.0022	-0.0109	0.0079	-0.0077	0.0006
124	0.0000	-0.0001	0.0002	-0.0021	0.0130	-0.0079	0.0086	0.0028
125	-0.0009	-0.0008	-0.0011	0.0080	0.0064	-0.0058	0.0150	-0.0084
126	-0.0019	-0.0008	-0.0013	-0.0041	-0.0023	-0.0035	-0.0054	0.0119
127	-0.0014	-0.0002	-0.0003	-0.0062	-0.0001	-0.0026	-0.0064	0.0055
128	-0.0017	-0.0004	-0.0007	-0.0058	-0.0036	0.0017	-0.0129	0.0088
129	-0.0020	-0.0006	-0.0007	-0.0095	-0.0061	0.0031	-0.0162	0.0122
130	-0.0016	0.0001	0.0002	-0.0078	-0.0047	0.0001	-0.0118	0.0087
131	-0.0017	0.0001	0.0002	-0.0016	-0.0091	0.0020	-0.0112	0.0096
132	-0.0011	-0.0001	-0.0001	-0.0025	-0.0036	0.0013	-0.0071	0.0044
133	-0.0014	0.0001	0.0002	0.0061	-0.0089	0.0011	-0.0061	0.0062
134	-0.0007	0.0004	0.0005	0.0071	-0.0180	0.0085	-0.0219	0.0112
135	-0.0007	-0.0001	-0.0004	0.0082	-0.0144	0.0075	-0.0144	0.0074
421	-0.0013	-0.0002	-0.0028	-0.0578	0.0289	0.0713	-0.1644	0.0524
422	-0.0017	-0.0013	-0.0027	0.0012	0.0244	-0.0148	-0.0120	-0.0430
426	-0.0009	-0.0006	-0.0008	-0.0001	-0.0003	-0.0058	0.0028	0.0003
427	-0.0009	-0.0006	-0.0007	-0.0003	0.0005	-0.0061	0.0033	-0.0022
428	-0.0006	-0.0003	-0.0004	0.0001	0.0008	-0.0030	0.0001	-0.0005

429	-0.0004	-0.0001	-0.0002	-0.0002	0.0011	-0.0031	0.0011	-0.0018
430	-0.0004	-0.0001	-0.0001	-0.0011	0.0005	-0.0014	-0.0011	0.0003
431	-0.0005	-0.0001	-0.0001	0.0035	-0.0001	-0.0055	0.0050	-0.0037
432	-0.0006	-0.0004	-0.0005	-0.0014	0.0014	-0.0032	-0.0012	-0.0007
433	-0.0006	-0.0003	-0.0003	0.0013	-0.0001	-0.0042	0.0017	-0.0017
434	-0.0006	-0.0005	-0.0006	0.0030	0.0001	-0.0054	0.0038	-0.0051
435	-0.0005	-0.0004	-0.0004	0.0029	-0.0004	-0.0046	0.0037	-0.0039
334	-0.0000	-0.0000	-0.0000	0.0008	-0.0001	-0.0000	0.0002	-0.0001
335	-0.0000	-0.0000	-0.0000	0.0008	-0.0001	-0.0003	0.0003	0.0001
526	-0.0004	-0.0002	-0.0002	-0.0008	-0.0008	-0.0018	0.0005	0.0030
527	-0.0003	-0.0001	-0.0001	-0.0003	-0.0004	-0.0005	-0.0004	0.0011
528	-0.0002	-0.0000	-0.0001	0.0002	-0.0004	-0.0006	-0.0003	0.0011
529	-0.0002	0.0000	0.0000	-0.0003	-0.0002	-0.0003	-0.0005	0.0006
530	-0.0002	0.0000	0.0000	-0.0005	-0.0003	-0.0007	-0.0004	0.0010
531	-0.0002	0.0001	0.0001	0.0014	-0.0003	-0.0009	0.0005	0.0005
532	-0.0002	0.0000	0.0000	-0.0002	-0.0003	-0.0003	-0.0008	0.0009
533	-0.0002	0.0001	0.0001	-0.0009	-0.0001	-0.0005	-0.0007	0.0006
534	-0.0001	0.0000	-0.0001	0.0019	-0.0002	-0.0007	0.0007	0.0003
535	-0.0001	-0.0000	-0.0000	0.0021	-0.0003	-0.0004	0.0005	0.0001
36	-0.0038	-0.0029	-0.0019	0.0024	0.0006	0.0043	-0.0044	0.0033
37	-0.0058	-0.0048	-0.0027	0.0032	0.0010	0.0050	-0.0063	0.0018
38	0.0141	0.0109	0.0069	-0.0128	-0.0016	-0.0135	0.0158	-0.0078
39	0.0090	0.0078	0.0048	-0.0027	-0.0026	-0.0073	0.0097	-0.0110
40	0.0038	0.0011	0.0033	-0.0241	0.0022	-0.0206	0.0125	0.0056
41	0.0006	0.0006	0.0006	-0.0002	-0.0001	-0.0006	0.0007	-0.0011
42	-0.0002	-0.0002	-0.0001	0.0002	-0.0000	0.0003	-0.0002	0.0003
43	-0.0002	-0.0002	-0.0001	0.0002	-0.0000	0.0000	-0.0001	0.0001
44	0.0010	0.0002	-0.0007	-0.0003	0.0005	0.0007	-0.0006	0.0002
45	-0.0013	-0.0012	-0.0008	0.0014	0.0001	0.0025	-0.0014	0.0013
136	-0.0005	0.0001	0.0002	0.0056	-0.0262	0.0169	-0.0165	-0.0091
137	0.0020	0.0011	0.0017	0.0300	-0.0475	0.0289	0.0081	-0.0042
138	0.0000	-0.0012	-0.0017	-0.0551	0.1131	-0.0610	0.0199	0.0494
139	-0.0021	-0.0024	-0.0020	-0.0118	0.0879	-0.0761	0.0676	-0.0161
140	0.0003	-0.0004	0.0003	0.0156	0.0280	-0.0218	0.0467	-0.0283
141	-0.0001	-0.0001	-0.0001	-0.0001	-0.0044	0.0030	-0.0041	-0.0003
142	-0.0003	-0.0003	-0.0004	-0.0013	0.0002	-0.0003	-0.0002	-0.0020
143	0.0001	0.0000	0.0001	0.0018	-0.0027	0.0018	0.0005	0.0006
144	-0.0001	0.0003	0.0003	-0.0019	-0.0010	0.0008	-0.0068	0.0020
145	0.0005	0.0007	0.0007	0.0020	0.0013	-0.0011	0.0006	0.0002
244	0.0002	0.0004	0.0004	0.0007	0.0008	-0.0009	0.0006	-0.0012
245	-0.0001	-0.0002	-0.0002	-0.0005	0.0002	0.0006	-0.0005	0.0001
440	0.0001	0.0007	0.0004	-0.0214	0.0038	0.0223	-0.0472	0.0315
444	0.0001	0.0001	0.0002	0.0000	-0.0006	0.0011	-0.0007	0.0012
445	-0.0001	-0.0002	-0.0003	-0.0013	0.0002	0.0013	-0.0029	0.0017
344	0.0000	0.0000	0.0000	-0.0001	-0.0000	-0.0001	0.0001	0.0001
345	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0001	0.0000	-0.0000
540	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0001	0.0001	-0.0003
544	0.0000	0.0000	0.0000	0.0001	-0.0000	-0.0002	0.0000	0.0001
545	-0.0000	-0.0000	0.0000	-0.0002	0.0000	-0.0000	0.0001	0.0001

	15	16	17	101	102	103	104	105

106	1.0000							
107	-0.4817	1.0000						
108	-0.3155	-0.0532	1.0000					
109	-0.0066	-0.0277	-0.0354	1.0000				
110	0.0031	-0.0440	-0.0170	-0.0828	1.0000			
111	0.0087	-0.0528	-0.0252	-0.0624	-0.1017	1.0000		
112	0.0067	-0.0326	-0.0049	-0.0155	-0.0476	-0.0518	1.0000	
113	0.0047	-0.0249	0.0055	-0.0143	-0.0461	-0.0476	-0.0354	1.0000
114	0.0020	-0.0228	0.0026	-0.0161	-0.0467	-0.0479	-0.0348	-0.0334
115	0.0017	-0.0215	0.0118	-0.0111	-0.0415	-0.0413	-0.0324	-0.0315
116	-0.0025	-0.0104	-0.0052	-0.0454	-0.0131	-0.0186	-0.0095	-0.0094
117	0.0104	-0.0324	-0.0226	-0.0658	-0.0300	-0.0331	-0.0115	-0.0087
216	-0.0030	-0.0007	0.0009	-0.0305	-0.0073	-0.0078	-0.0041	-0.0045
217	-0.0013	-0.0003	0.0013	-0.0327	-0.0104	-0.0096	-0.0043	-0.0042
412	0.0021	-0.0106	0.0046	-0.0021	-0.0128	-0.0115	-0.0062	-0.0070
413	-0.0011	-0.0121	0.0007	-0.0010	-0.0138	-0.0132	-0.0053	-0.0062
414	-0.0011	-0.0093	0.0027	-0.0018	-0.0115	-0.0112	-0.0069	-0.0072
415	0.0007	-0.0103	0.0049	-0.0018	-0.0124	-0.0108	-0.0057	-0.0067
416	-0.0009	-0.0017	-0.0004	-0.0150	-0.0052	-0.0048	-0.0010	-0.0014
417	-0.0007	-0.0068	-0.0009	-0.0146	-0.0051	-0.0049	-0.0008	-0.0013
316	-0.0005	0.0002	0.0005	-0.0065	-0.0018	-0.0018	-0.0008	-0.0008
317	-0.0002	-0.0001	0.0004	-0.0065	-0.0020	-0.0021	-0.0008	-0.0008
512	0.0000	-0.0005	0.0047	-0.0027	-0.0090	-0.0087	-0.0061	-0.0061
513	-0.0006	-0.0004	0.0052	-0.0024	-0.0088	-0.0084	-0.0059	-0.0059
514	-0.0005	-0.0013	0.0043	-0.0025	-0.0088	-0.0081	-0.0058	-0.0059
515	-0.0005	-0.0002	0.0053	-0.0025	-0.0089	-0.0085	-0.0059	-0.0060
516	-0.0007	-0.0003	0.0011	-0.0173	-0.0050	-0.0052	-0.0018	-0.0017
517	-0.0012	0.0003	0.0013	-0.0170	-0.0047	-0.0047	-0.0019	-0.0020
18	0.1283	-0.0290	-0.0834	-0.0094	-0.0100	-0.0020	-0.0041	-0.0040
19	0.1358	-0.0595	-0.0807	-0.0155	-0.0205	-0.0135	-0.0163	-0.0115
20	-0.0177	0.0254	0.0128	0.0098	0.0049	-0.0015	-0.0020	0.0002
21	0.0947	-0.0001	-0.0285	-0.0050	-0.0057	-0.0055	-0.0070	-0.0057
22	0.0878	-0.0134	0.0113	0.0153	0.0114	-0.0019	-0.0016	0.0008
23	0.0053	-0.0043	0.0035	0.0013	-0.0004	-0.0009	-0.0020	-0.0019
24	0.0007	0.0017	-0.0045	-0.0015	-0.0016	-0.0008	0.0002	0.0003
25	-0.0003	-0.0036	0.0008	0.0005	-0.0000	0.0002	-0.0007	-0.0005
26	0.0022	-0.0040	0.0022	0.0008	-0.0017	-0.0018	-0.0021	-0.0020
27	-0.0017	-0.0012	0.0082	0.0007	-0.0014	-0.0013	-0.0028	-0.0027
28	0.0032	-0.0030	-0.0007	0.0006	-0.0016	-0.0018	-0.0021	-0.0018
29	0.0000	-0.0029	0.0024	-0.0007	-0.0022	-0.0018	-0.0013	-0.0011
30	0.0019	-0.0020	-0.0019	-0.0009	-0.0019	-0.0011	-0.0013	-0.0012
31	0.0005	-0.0023	0.0028	-0.0009	-0.0025	-0.0021	-0.0015	-0.0015
32	0.0040	-0.0018	0.0006	-0.0021	-0.0036	-0.0024	-0.0020	-0.0019
33	0.0035	-0.0053	-0.0019	-0.0019	-0.0034	-0.0016	-0.0017	-0.0015
34	0.0020	-0.0051	0.0026	0.0008	-0.0009	-0.0007	-0.0015	-0.0011
35	0.0023	-0.0063	0.0023	0.0005	-0.0015	-0.0017	-0.0012	-0.0008
118	-0.0367	0.0902	0.0000	0.0092	0.0200	0.0138	0.0001	-0.0014
119	0.0833	-0.0570	-0.1848	0.0068	-0.0009	-0.0277	-0.0021	0.0043
120	-0.0819	-0.0286	0.0206	0.0137	0.0203	0.0249	0.0090	0.0079
121	-0.1333	-0.0989	0.1113	-0.0107	-0.0113	-0.0016	0.0082	0.0080
122	0.1094	-0.3401	-0.1669	-0.0001	-0.0120	-0.0352	-0.0340	-0.0260
123	-0.0008	-0.0099	-0.0143	-0.0013	-0.0017	-0.0077	-0.0032	-0.0017

124	0.0002	0.0156	0.0179	-0.0004	0.0024	0.0107	0.0036	0.0021
125	-0.0032	0.0029	0.0063	0.0038	0.0003	0.0059	0.0006	-0.0003
126	0.0120	-0.0218	-0.0190	-0.0024	-0.0061	-0.0041	-0.0064	-0.0058
127	0.0073	-0.0200	-0.0132	-0.0013	-0.0041	-0.0026	-0.0046	-0.0047
128	0.0076	-0.0234	-0.0182	-0.0026	-0.0056	-0.0052	-0.0066	-0.0059
129	0.0092	-0.0249	-0.0228	-0.0041	-0.0073	-0.0066	-0.0085	-0.0075
130	0.0040	-0.0163	-0.0155	-0.0021	-0.0040	-0.0046	-0.0049	-0.0045
131	0.0011	-0.0140	-0.0191	-0.0045	-0.0058	-0.0057	-0.0053	-0.0041
132	-0.0002	-0.0058	-0.0066	-0.0014	-0.0024	-0.0018	-0.0027	-0.0021
133	0.0001	-0.0160	-0.0191	-0.0050	-0.0057	-0.0040	-0.0044	-0.0032
134	0.0060	-0.0335	-0.0362	-0.0106	-0.0113	-0.0154	-0.0079	-0.0048
135	0.0021	-0.0274	-0.0277	-0.0027	-0.0048	-0.0101	-0.0065	-0.0043
421	-0.0868	-0.1198	-0.0097	-0.0180	-0.0038	-0.0160	-0.0070	-0.0001
422	-0.0287	-0.1036	-0.0100	0.0041	-0.0085	-0.0056	0.0156	0.0109
426	0.0022	-0.0085	-0.0069	0.0003	-0.0028	-0.0018	0.0000	-0.0004
427	0.0014	-0.0080	-0.0046	0.0006	-0.0026	-0.0011	0.0007	-0.0001
428	0.0003	-0.0068	-0.0028	0.0003	-0.0016	-0.0008	0.0003	-0.0001
429	0.0004	-0.0054	-0.0014	0.0003	-0.0013	-0.0005	0.0006	0.0002
430	0.0001	-0.0043	-0.0015	0.0002	-0.0008	-0.0004	-0.0001	-0.0002
431	-0.0001	-0.0068	-0.0044	0.0002	-0.0021	-0.0007	0.0010	0.0005
432	-0.0003	-0.0091	-0.0033	0.0004	-0.0018	-0.0012	0.0005	0.0001
433	-0.0005	-0.0077	-0.0050	0.0002	-0.0021	-0.0012	0.0005	0.0002
434	-0.0008	-0.0097	-0.0054	0.0014	-0.0017	-0.0011	0.0015	0.0008
435	-0.0007	-0.0069	-0.0047	0.0010	-0.0015	-0.0009	0.0011	0.0006
334	-0.0004	-0.0005	-0.0003	0.0000	-0.0000	0.0002	-0.0001	-0.0000
335	-0.0000	-0.0006	-0.0005	-0.0000	-0.0002	-0.0000	-0.0000	0.0000
526	0.0018	-0.0009	-0.0028	-0.0006	-0.0011	-0.0006	-0.0008	-0.0007
527	-0.0002	-0.0005	-0.0011	-0.0005	-0.0007	-0.0001	-0.0005	-0.0005
528	0.0001	-0.0008	-0.0012	-0.0004	-0.0008	-0.0003	-0.0004	-0.0004
529	-0.0003	-0.0006	-0.0007	-0.0004	-0.0006	-0.0002	-0.0003	-0.0003
530	0.0000	-0.0006	-0.0009	-0.0004	-0.0007	-0.0002	-0.0003	-0.0003
531	-0.0003	-0.0017	-0.0015	-0.0006	-0.0008	-0.0000	-0.0002	-0.0002
532	-0.0003	-0.0005	-0.0007	-0.0004	-0.0007	-0.0002	-0.0003	-0.0004
533	-0.0003	-0.0006	-0.0006	-0.0006	-0.0008	-0.0005	-0.0002	-0.0003
534	-0.0002	-0.0014	-0.0012	-0.0003	-0.0006	-0.0002	-0.0001	-0.0000
535	-0.0006	-0.0012	-0.0010	-0.0001	-0.0002	0.0003	-0.0001	-0.0001
36	-0.0019	0.0002	0.0081	0.0025	0.0014	-0.0002	-0.0004	-0.0004
37	-0.0099	0.0041	0.0120	0.0028	0.0021	0.0003	-0.0003	-0.0002
38	0.0159	-0.0035	-0.0301	-0.0078	-0.0056	-0.0011	0.0004	0.0009
39	-0.0059	-0.0019	-0.0122	-0.0034	-0.0019	0.0011	0.0017	0.0017
40	0.0434	0.0074	-0.0427	-0.0011	-0.0022	-0.0030	-0.0033	-0.0026
41	-0.0006	0.0003	-0.0006	0.0004	0.0005	0.0004	0.0002	0.0002
42	-0.0001	-0.0002	0.0005	0.0002	0.0002	0.0000	-0.0000	-0.0000
43	-0.0001	-0.0001	0.0001	0.0000	0.0001	0.0001	0.0000	0.0000
44	0.0013	0.0011	-0.0019	-0.0003	-0.0008	-0.0007	-0.0007	-0.0003
45	-0.0009	-0.0013	0.0050	0.0011	0.0010	0.0002	-0.0001	-0.0001
136	0.0094	-0.0388	-0.0396	-0.0015	-0.0044	-0.0127	-0.0080	-0.0052
137	-0.0149	0.0631	-0.0025	-0.0098	0.0014	-0.0033	0.0024	0.0074
138	-0.0415	0.1111	0.1376	0.0004	0.0089	0.0364	0.0238	0.0157
139	0.0371	-0.0383	0.0468	0.0352	0.0147	0.0356	0.0053	-0.0095
140	0.0165	-0.0227	0.0254	0.0284	0.0188	0.0261	0.0052	-0.0031
141	0.0010	-0.0091	-0.0076	0.0013	0.0001	-0.0034	-0.0018	-0.0013

142	0.0023	-0.0117	-0.0050	0.0051	0.0024	-0.0005	-0.0015	-0.0019
143	-0.0031	0.0091	0.0028	-0.0013	0.0004	0.0005	0.0007	0.0010
144	0.0051	-0.0154	-0.0096	-0.0010	-0.0028	-0.0042	-0.0023	-0.0021
145	0.0013	0.0096	0.0042	-0.0109	-0.0074	-0.0012	0.0021	0.0028
244	0.0008	0.0001	-0.0005	-0.0020	-0.0017	-0.0007	0.0003	0.0006
245	0.0008	-0.0010	-0.0004	-0.0000	0.0000	0.0002	-0.0004	-0.0003
440	-0.0129	-0.0134	-0.0040	-0.0078	0.0009	-0.0034	-0.0054	-0.0025
444	-0.0004	0.0026	0.0002	-0.0004	0.0003	0.0001	-0.0004	-0.0002
445	-0.0007	-0.0017	-0.0005	-0.0001	0.0000	-0.0003	-0.0004	-0.0002
344	0.0001	-0.0000	0.0001	-0.0001	-0.0000	-0.0000	0.0000	0.0000
345	-0.0001	0.0000	-0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
540	0.0002	-0.0002	0.0001	-0.0002	-0.0000	0.0001	0.0001	0.0001
544	-0.0001	0.0000	-0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
545	0.0002	-0.0001	0.0002	-0.0001	-0.0001	-0.0001	0.0000	0.0000

	106	107	108	109	110	111	112	113
114	1.0000							
115	-0.0313	1.0000						
116	-0.0089	-0.0099	1.0000					
117	-0.0086	-0.0067	-0.0165	1.0000				
216	-0.0043	-0.0051	-0.0148	-0.0080	1.0000			
217	-0.0042	-0.0050	-0.0114	-0.0137	-0.0080	1.0000		
412	-0.0064	-0.0076	-0.0015	0.0001	-0.0011	-0.0012	1.0000	
413	-0.0057	-0.0073	-0.0009	0.0013	-0.0009	-0.0011	-0.0055	1.0000
414	-0.0071	-0.0082	-0.0018	-0.0004	-0.0011	-0.0013	-0.0036	-0.0047
415	-0.0063	-0.0075	-0.0014	0.0005	-0.0010	-0.0011	-0.0050	-0.0056
416	-0.0013	-0.0022	-0.0062	-0.0050	-0.0042	-0.0040	-0.0015	-0.0024
417	-0.0010	-0.0021	-0.0061	-0.0049	-0.0042	-0.0041	-0.0024	-0.0030
316	-0.0008	-0.0010	-0.0027	-0.0024	-0.0018	-0.0017	-0.0002	-0.0002
317	-0.0007	-0.0010	-0.0027	-0.0025	-0.0017	-0.0017	-0.0002	-0.0002
512	-0.0060	-0.0061	-0.0016	-0.0011	-0.0009	-0.0010	-0.0017	-0.0017
513	-0.0059	-0.0060	-0.0016	-0.0010	-0.0009	-0.0009	-0.0017	-0.0017
514	-0.0060	-0.0061	-0.0016	-0.0009	-0.0009	-0.0010	-0.0016	-0.0016
515	-0.0061	-0.0060	-0.0014	-0.0008	-0.0008	-0.0008	-0.0017	-0.0017
516	-0.0017	-0.0022	-0.0070	-0.0065	-0.0046	-0.0044	-0.0006	-0.0005
517	-0.0020	-0.0025	-0.0071	-0.0064	-0.0046	-0.0044	-0.0006	-0.0006
18	-0.0062	-0.0076	0.0018	0.0062	-0.0005	-0.0003	-0.0000	0.0014
19	-0.0166	-0.0123	0.0016	0.0011	0.0004	0.0016	0.0006	0.0009
20	-0.0021	-0.0011	-0.0005	-0.0021	0.0001	-0.0002	0.0001	0.0001
21	-0.0080	-0.0069	-0.0007	-0.0011	0.0003	0.0007	-0.0005	-0.0008
22	0.0009	0.0022	0.0001	-0.0036	0.0009	0.0010	0.0002	-0.0021
23	-0.0015	-0.0013	-0.0003	-0.0007	-0.0001	0.0000	-0.0007	-0.0008
24	0.0004	0.0002	0.0002	-0.0000	0.0000	0.0000	0.0001	0.0002
25	-0.0006	-0.0007	-0.0001	-0.0002	-0.0001	-0.0001	-0.0002	-0.0002
26	-0.0021	-0.0022	-0.0004	-0.0004	-0.0002	-0.0001	-0.0007	-0.0007
27	-0.0022	-0.0022	-0.0003	-0.0006	-0.0001	-0.0000	-0.0008	-0.0009
28	-0.0017	-0.0021	-0.0001	-0.0003	-0.0001	-0.0000	-0.0007	-0.0007
29	-0.0011	-0.0013	0.0003	0.0000	0.0001	0.0001	-0.0004	-0.0005
30	-0.0011	-0.0017	0.0002	0.0002	0.0001	0.0001	-0.0004	-0.0004
31	-0.0016	-0.0014	0.0002	0.0002	0.0001	0.0002	-0.0005	-0.0006
32	-0.0015	-0.0015	0.0001	-0.0002	0.0001	0.0002	-0.0006	-0.0006

33	-0.0016	-0.0018	-0.0000	-0.0001	-0.0000	0.0001	-0.0005	-0.0004
34	-0.0010	-0.0013	-0.0001	-0.0005	-0.0000	0.0000	-0.0004	-0.0005
35	-0.0007	-0.0010	0.0001	-0.0004	0.0001	0.0001	-0.0003	-0.0004
118	-0.0026	-0.0025	-0.0000	0.0043	-0.0014	-0.0013	0.0030	0.0087
119	0.0045	0.0052	0.0027	-0.0117	0.0027	0.0024	-0.0004	-0.0096
120	0.0076	0.0053	-0.0058	0.0224	-0.0040	0.0019	-0.0002	0.0032
121	0.0093	-0.0228	0.0253	-0.0101	0.0004	0.0038	-0.0030	-0.0029
122	-0.0145	-0.0069	-0.0067	-0.0557	0.0052	0.0037	0.0117	0.0206
123	-0.0022	-0.0002	-0.0028	-0.0013	0.0001	0.0008	0.0011	0.0011
124	0.0022	0.0003	0.0036	0.0015	-0.0002	-0.0010	-0.0006	0.0003
125	0.0010	-0.0019	-0.0026	0.0077	-0.0015	-0.0001	-0.0017	-0.0021
126	-0.0037	-0.0043	-0.0013	-0.0023	-0.0003	-0.0001	-0.0013	-0.0000
127	-0.0034	-0.0032	-0.0010	-0.0019	0.0000	-0.0000	-0.0006	0.0003
128	-0.0044	-0.0040	-0.0013	-0.0029	0.0000	0.0001	-0.0004	0.0006
129	-0.0057	-0.0042	-0.0014	-0.0042	0.0001	0.0001	-0.0004	0.0009
130	-0.0045	-0.0037	-0.0011	-0.0004	-0.0005	0.0004	-0.0000	0.0006
131	-0.0051	-0.0039	-0.0006	-0.0011	-0.0003	0.0003	0.0003	0.0009
132	-0.0025	-0.0032	0.0003	0.0003	-0.0002	0.0001	-0.0002	-0.0002
133	-0.0043	-0.0031	-0.0003	-0.0020	-0.0001	-0.0001	0.0006	0.0012
134	-0.0057	-0.0020	0.0002	-0.0150	0.0023	0.0002	0.0023	0.0036
135	-0.0045	-0.0027	-0.0043	-0.0038	-0.0009	0.0012	0.0016	0.0027
421	-0.0049	0.0052	0.0022	-0.0047	0.0031	0.0009	0.0027	0.0073
422	0.0120	0.0077	0.0066	0.0133	0.0022	0.0010	-0.0196	-0.0264
426	0.0002	-0.0007	0.0005	0.0011	-0.0000	-0.0000	-0.0025	-0.0036
427	0.0006	-0.0005	0.0006	0.0016	-0.0000	0.0000	-0.0030	-0.0041
428	0.0002	-0.0005	0.0004	0.0009	0.0000	-0.0000	-0.0018	-0.0022
429	0.0003	-0.0003	0.0004	0.0010	0.0001	0.0001	-0.0016	-0.0019
430	-0.0001	-0.0007	0.0003	0.0005	0.0000	0.0000	-0.0009	-0.0011
431	0.0005	-0.0003	0.0005	0.0015	0.0000	0.0000	-0.0017	-0.0030
432	0.0003	-0.0004	0.0005	0.0012	0.0001	0.0000	-0.0022	-0.0028
433	0.0002	-0.0005	0.0005	0.0012	0.0000	0.0000	-0.0016	-0.0028
434	0.0011	0.0001	0.0007	0.0017	0.0001	0.0000	-0.0024	-0.0043
435	0.0008	0.0000	0.0005	0.0013	0.0000	0.0000	-0.0017	-0.0033
334	-0.0000	-0.0001	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000
335	-0.0000	-0.0001	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000
526	-0.0005	-0.0007	-0.0000	-0.0001	-0.0001	-0.0000	-0.0003	-0.0002
527	-0.0004	-0.0005	-0.0000	0.0000	-0.0000	-0.0000	-0.0002	-0.0001
528	-0.0003	-0.0005	0.0000	0.0000	-0.0000	-0.0000	-0.0002	-0.0001
529	-0.0003	-0.0004	0.0000	0.0001	-0.0000	-0.0000	-0.0001	-0.0001
530	-0.0004	-0.0005	0.0000	0.0001	-0.0000	-0.0000	-0.0001	-0.0001
531	-0.0003	-0.0004	0.0000	0.0002	-0.0000	-0.0000	-0.0000	0.0000
532	-0.0004	-0.0004	0.0000	0.0001	-0.0000	-0.0000	-0.0001	-0.0001
533	-0.0004	-0.0004	0.0001	0.0002	0.0000	0.0000	-0.0001	-0.0001
534	-0.0001	-0.0003	0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000
535	-0.0001	-0.0003	-0.0000	0.0000	-0.0001	-0.0001	-0.0000	0.0000
36	-0.0004	-0.0000	-0.0001	-0.0003	0.0000	0.0000	-0.0002	-0.0004
37	0.0000	-0.0001	0.0001	-0.0002	0.0002	0.0001	-0.0001	-0.0004
38	0.0007	-0.0000	0.0004	0.0007	-0.0002	-0.0001	0.0003	0.0010
39	0.0016	0.0010	0.0002	0.0007	-0.0003	-0.0004	0.0005	0.0010
40	-0.0029	-0.0034	-0.0004	-0.0007	-0.0003	0.0000	-0.0007	-0.0003
41	0.0001	0.0001	-0.0001	-0.0000	-0.0001	-0.0001	0.0001	0.0001
42	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000

43	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000
44	0.0001	-0.0003	0.0001	-0.0003	0.0000	0.0001	-0.0001	-0.0001
45	-0.0002	0.0000	-0.0001	-0.0001	0.0000	-0.0000	-0.0000	-0.0002
136	-0.0058	0.0000	-0.0020	-0.0041	0.0005	0.0005	-0.0017	-0.0005
137	-0.0010	0.0062	0.0062	0.0048	0.0002	-0.0010	-0.0009	0.0022
138	0.0186	-0.0050	0.0145	0.0060	-0.0005	-0.0015	0.0054	0.0004
139	0.0086	-0.0052	-0.0177	0.0004	-0.0025	-0.0012	0.0039	-0.0031
140	0.0058	0.0042	-0.0178	0.0156	-0.0034	-0.0007	-0.0032	-0.0016
141	-0.0011	-0.0006	-0.0028	0.0004	-0.0002	0.0005	-0.0001	0.0002
142	-0.0007	-0.0012	-0.0050	0.0025	-0.0009	0.0007	-0.0002	-0.0002
143	0.0001	0.0005	0.0015	0.0011	0.0000	-0.0003	0.0000	0.0001
144	-0.0013	-0.0005	-0.0015	-0.0058	0.0010	0.0006	0.0004	0.0010
145	0.0014	0.0023	0.0109	-0.0094	0.0033	-0.0026	0.0000	-0.0004
244	0.0003	0.0006	0.0029	-0.0044	0.0021	-0.0014	0.0001	0.0001
245	-0.0002	-0.0002	0.0002	0.0007	-0.0004	-0.0003	-0.0000	0.0000
440	-0.0044	0.0003	-0.0008	-0.0044	0.0006	0.0002	0.0055	0.0089
444	-0.0003	-0.0001	-0.0001	-0.0004	-0.0000	0.0000	0.0008	0.0010
445	-0.0003	-0.0001	-0.0001	-0.0003	-0.0000	-0.0000	0.0001	0.0001
344	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000
345	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
540	0.0000	0.0000	-0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
544	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000
545	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000

	114	115	116	117	216	217	412	413
414	1.0000							
415	-0.0035	1.0000						
416	-0.0011	-0.0016	1.0000					
417	-0.0018	-0.0023	-0.0026	1.0000				
316	-0.0002	-0.0002	-0.0008	-0.0008	1.0000			
317	-0.0002	-0.0002	-0.0008	-0.0008	-0.0003	1.0000		
512	-0.0017	-0.0016	-0.0005	-0.0005	-0.0002	-0.0002	1.0000	
513	-0.0016	-0.0016	-0.0004	-0.0005	-0.0002	-0.0002	-0.0012	1.0000
514	-0.0016	-0.0016	-0.0005	-0.0005	-0.0002	-0.0002	-0.0012	-0.0012
515	-0.0016	-0.0017	-0.0004	-0.0004	-0.0002	-0.0002	-0.0012	-0.0012
516	-0.0006	-0.0005	-0.0022	-0.0022	-0.0009	-0.0009	-0.0004	-0.0004
517	-0.0006	-0.0006	-0.0022	-0.0022	-0.0009	-0.0009	-0.0005	-0.0005
18	-0.0003	0.0003	0.0008	0.0021	-0.0001	-0.0004	-0.0025	-0.0023
19	-0.0014	0.0007	0.0016	0.0032	0.0003	0.0002	-0.0026	-0.0025
20	-0.0005	0.0004	0.0002	0.0000	0.0000	0.0000	-0.0001	-0.0000
21	-0.0016	-0.0007	0.0005	0.0004	0.0001	0.0003	-0.0006	-0.0006
22	-0.0007	0.0002	0.0001	-0.0009	0.0002	0.0003	0.0011	0.0009
23	-0.0006	-0.0005	-0.0001	-0.0003	0.0000	0.0001	-0.0002	-0.0002
24	0.0001	0.0001	0.0001	0.0001	0.0000	-0.0001	-0.0000	0.0000
25	-0.0003	-0.0002	-0.0000	-0.0001	-0.0000	-0.0000	-0.0001	-0.0001
26	-0.0007	-0.0006	-0.0001	-0.0002	-0.0000	0.0000	-0.0003	-0.0003
27	-0.0008	-0.0007	-0.0001	-0.0002	-0.0000	0.0000	-0.0004	-0.0004
28	-0.0007	-0.0005	-0.0000	-0.0002	0.0000	0.0000	-0.0004	-0.0003
29	-0.0004	-0.0003	0.0001	0.0000	0.0000	0.0000	-0.0002	-0.0002
30	-0.0005	-0.0003	0.0001	-0.0000	0.0000	-0.0000	-0.0003	-0.0003
31	-0.0004	-0.0005	0.0000	-0.0000	0.0000	0.0000	-0.0003	-0.0003

32	-0.0005	-0.0005	0.0000	-0.0001	0.0000	0.0000	-0.0003	-0.0003
33	-0.0005	-0.0005	0.0000	-0.0001	0.0000	0.0000	-0.0003	-0.0003
34	-0.0005	-0.0003	-0.0000	-0.0002	0.0000	0.0000	-0.0002	-0.0001
35	-0.0004	-0.0003	0.0000	-0.0001	0.0000	-0.0000	-0.0001	-0.0001
118	0.0020	0.0035	0.0027	0.0023	-0.0003	-0.0003	-0.0007	-0.0007
119	-0.0013	-0.0011	-0.0025	-0.0013	0.0006	0.0003	0.0019	0.0018
120	-0.0027	0.0016	0.0029	-0.0018	-0.0001	-0.0001	0.0003	0.0004
121	0.0041	-0.0035	-0.0028	0.0018	0.0004	0.0002	-0.0003	0.0003
122	0.0128	0.0122	0.0066	0.0098	0.0010	0.0010	0.0026	0.0027
123	0.0006	0.0011	0.0004	0.0007	0.0001	0.0001	0.0001	0.0001
124	-0.0003	-0.0005	-0.0000	-0.0004	-0.0001	-0.0001	-0.0001	-0.0001
125	-0.0009	-0.0016	-0.0009	-0.0008	-0.0001	-0.0002	-0.0006	-0.0005
126	-0.0005	-0.0005	0.0003	0.0001	0.0000	-0.0000	-0.0009	-0.0006
127	-0.0002	-0.0003	0.0003	0.0003	0.0000	0.0000	-0.0005	-0.0005
128	-0.0001	0.0001	0.0005	0.0005	0.0001	0.0000	-0.0007	-0.0005
129	-0.0001	0.0002	0.0006	0.0007	0.0001	0.0001	-0.0008	-0.0006
130	-0.0001	0.0001	0.0004	0.0006	0.0001	0.0001	-0.0005	-0.0004
131	-0.0001	0.0004	0.0005	0.0007	0.0000	0.0001	-0.0005	-0.0005
132	-0.0006	-0.0002	0.0002	0.0002	0.0000	-0.0000	-0.0004	-0.0004
133	-0.0001	0.0005	0.0005	0.0007	0.0000	0.0000	-0.0004	-0.0004
134	0.0012	0.0025	0.0015	0.0019	0.0002	0.0002	0.0001	0.0001
135	0.0008	0.0018	0.0010	0.0013	0.0001	0.0001	-0.0001	-0.0001
421	-0.0188	0.0108	0.0142	-0.0055	0.0004	0.0003	0.0002	0.0005
422	-0.0162	-0.0174	-0.0040	-0.0145	0.0002	0.0001	0.0000	0.0001
426	-0.0018	-0.0022	-0.0009	-0.0015	-0.0000	-0.0000	-0.0003	-0.0002
427	-0.0017	-0.0028	-0.0012	-0.0017	-0.0000	-0.0000	-0.0003	-0.0002
428	-0.0012	-0.0016	-0.0005	-0.0010	-0.0000	-0.0000	-0.0002	-0.0002
429	-0.0008	-0.0016	-0.0005	-0.0009	0.0000	-0.0000	-0.0001	-0.0001
430	-0.0007	-0.0009	-0.0002	-0.0005	0.0000	-0.0000	-0.0001	-0.0001
431	-0.0011	-0.0019	-0.0009	-0.0011	-0.0000	-0.0000	-0.0001	-0.0001
432	-0.0016	-0.0020	-0.0005	-0.0014	0.0000	-0.0000	-0.0002	-0.0002
433	-0.0014	-0.0016	-0.0007	-0.0011	0.0000	-0.0000	-0.0002	-0.0002
434	-0.0019	-0.0024	-0.0012	-0.0017	-0.0000	-0.0000	-0.0001	-0.0001
435	-0.0014	-0.0017	-0.0009	-0.0012	-0.0000	-0.0000	-0.0001	-0.0001
334	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000
335	-0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000
526	-0.0002	-0.0002	-0.0000	-0.0001	-0.0000	-0.0000	-0.0002	-0.0001
527	-0.0001	-0.0001	-0.0000	-0.0000	-0.0000	-0.0000	-0.0001	-0.0001
528	-0.0001	-0.0001	0.0000	-0.0000	-0.0000	-0.0000	-0.0001	-0.0001
529	-0.0001	-0.0001	0.0000	0.0000	0.0000	-0.0000	-0.0001	-0.0001
530	-0.0001	-0.0001	0.0000	0.0000	0.0000	-0.0000	-0.0001	-0.0001
531	-0.0001	-0.0001	0.0000	0.0000	-0.0000	-0.0000	-0.0001	-0.0001
532	-0.0001	-0.0001	-0.0000	0.0000	-0.0000	-0.0000	-0.0001	-0.0001
533	-0.0001	-0.0001	0.0000	0.0000	0.0000	0.0000	-0.0001	-0.0001
534	-0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000
535	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000
36	-0.0002	-0.0002	-0.0001	-0.0001	0.0000	0.0001	0.0000	0.0000
37	-0.0002	-0.0001	-0.0000	-0.0000	0.0000	0.0001	0.0001	0.0000
38	0.0004	0.0005	0.0002	0.0004	-0.0000	-0.0002	-0.0002	-0.0001
39	0.0007	0.0005	0.0001	0.0003	-0.0001	-0.0002	-0.0001	-0.0000
40	-0.0008	-0.0004	0.0002	-0.0001	0.0000	0.0000	-0.0004	-0.0003
41	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000

42	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000
43	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000
44	-0.0001	0.0000	0.0001	-0.0000	0.0000	-0.0000	-0.0001	-0.0000
45	-0.0001	-0.0001	-0.0001	-0.0001	0.0000	0.0000	0.0000	0.0000
136	0.0006	-0.0017	-0.0001	-0.0002	0.0002	0.0002	0.0002	0.0001
137	0.0019	-0.0012	0.0000	-0.0000	-0.0001	-0.0000	0.0004	0.0003
138	-0.0051	0.0067	0.0014	0.0001	-0.0003	-0.0006	-0.0010	-0.0006
139	-0.0007	0.0028	-0.0025	0.0010	-0.0005	-0.0005	-0.0011	-0.0010
140	-0.0009	-0.0033	-0.0012	-0.0020	-0.0004	-0.0004	-0.0003	-0.0005
141	0.0002	-0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
142	0.0001	-0.0002	-0.0001	-0.0000	-0.0000	-0.0000	-0.0001	-0.0000
143	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000
144	0.0005	0.0005	0.0004	0.0005	0.0001	0.0001	0.0000	0.0001
145	-0.0001	-0.0000	0.0001	-0.0000	0.0001	0.0001	0.0001	0.0001
244	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0001	0.0000
245	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000
440	-0.0017	0.0074	0.0055	0.0018	0.0001	0.0001	0.0002	0.0002
444	0.0004	0.0008	0.0003	0.0005	0.0000	0.0000	0.0000	0.0000
445	-0.0003	0.0002	0.0002	-0.0001	-0.0000	-0.0000	-0.0000	-0.0000
344	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000
345	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000
540	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
544	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000
545	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000

	414	415	416	417	316	317	512	513
514	1.0000							
515	-0.0012	1.0000						
516	-0.0004	-0.0004	1.0000					
517	-0.0005	-0.0004	-0.0024	1.0000				
18	-0.0017	-0.0027	-0.0009	-0.0005	1.0000			
19	-0.0022	-0.0026	0.0005	0.0005	-0.2533	1.0000		
20	-0.0001	0.0001	0.0003	-0.0000	-0.0198	0.0276	1.0000	
21	-0.0008	-0.0009	0.0009	0.0003	-0.0708	0.1419	-0.2993	1.0000
22	0.0011	0.0012	0.0009	0.0006	0.0120	-0.0142	-0.1014	-0.1843
23	-0.0002	-0.0001	0.0002	0.0000	0.0130	-0.0103	0.0012	0.0148
24	0.0000	0.0000	-0.0002	-0.0000	-0.0083	0.0085	-0.0063	-0.0221
25	-0.0001	-0.0001	-0.0000	-0.0000	0.0050	-0.0067	0.0056	0.0183
26	-0.0004	-0.0003	0.0001	-0.0000	0.0052	-0.0107	-0.0031	0.0038
27	-0.0003	-0.0004	0.0001	-0.0000	0.0075	-0.0107	0.0080	0.0168
28	-0.0003	-0.0003	0.0000	-0.0000	0.0015	-0.0077	-0.0035	0.0002
29	-0.0002	-0.0002	0.0000	0.0001	0.0007	-0.0083	0.0026	0.0079
30	-0.0002	-0.0003	-0.0000	0.0000	-0.0035	-0.0029	-0.0022	-0.0039
31	-0.0003	-0.0003	0.0001	0.0001	0.0023	-0.0105	0.0035	0.0139
32	-0.0002	-0.0003	0.0000	0.0001	0.0015	-0.0040	-0.0017	-0.0043
33	-0.0003	-0.0002	0.0000	0.0000	0.0031	-0.0071	-0.0007	0.0015
34	-0.0002	-0.0001	0.0001	0.0000	0.0095	-0.0085	0.0014	0.0117
35	-0.0001	-0.0001	-0.0000	0.0001	0.0072	-0.0097	0.0028	0.0116
118	-0.0005	-0.0013	-0.0008	-0.0007	0.0843	0.1808	-0.0022	0.0698
119	0.0025	0.0024	0.0010	0.0013	0.0734	0.0496	-0.0111	-0.0256
120	0.0004	0.0006	-0.0004	-0.0004	-0.0542	-0.0638	-0.0809	-0.0251

121	0.0004	0.0004	0.0009	0.0010	0.0335	0.0747	-0.0036	-0.0183
122	0.0031	0.0030	0.0028	0.0028	0.0621	0.0331	-0.0276	-0.0134
123	0.0001	0.0002	0.0003	0.0002	0.0036	-0.0044	-0.0008	-0.0021
124	-0.0002	-0.0001	-0.0003	-0.0003	-0.0049	0.0039	0.0009	0.0020
125	-0.0005	-0.0004	-0.0006	-0.0004	-0.0070	-0.0041	0.0035	0.0037
126	-0.0005	-0.0005	-0.0000	-0.0000	-0.0004	-0.0049	0.0008	-0.0020
127	-0.0004	-0.0005	0.0001	0.0001	-0.0001	-0.0022	-0.0002	-0.0018
128	-0.0004	-0.0005	0.0001	0.0001	0.0012	-0.0036	0.0015	-0.0023
129	-0.0005	-0.0005	0.0002	0.0002	0.0045	-0.0027	0.0034	-0.0009
130	-0.0005	-0.0005	0.0002	0.0001	-0.0005	-0.0057	-0.0023	-0.0050
131	-0.0006	-0.0005	0.0001	0.0001	-0.0011	-0.0094	-0.0014	-0.0049
132	-0.0004	-0.0004	-0.0000	0.0000	-0.0051	-0.0069	-0.0000	-0.0029
133	-0.0005	-0.0003	0.0000	0.0001	0.0005	-0.0080	-0.0003	-0.0032
134	-0.0000	0.0002	0.0006	0.0005	0.0104	-0.0044	-0.0023	-0.0037
135	-0.0001	0.0001	0.0002	0.0002	0.0064	-0.0042	0.0002	-0.0022
421	0.0005	0.0008	0.0010	0.0012	0.0206	0.0018	0.0023	-0.0315
422	0.0003	0.0001	0.0005	0.0005	0.0236	0.0234	0.0034	-0.0089
426	-0.0002	-0.0002	-0.0000	-0.0000	0.0017	0.0004	-0.0007	-0.0002
427	-0.0002	-0.0002	-0.0000	-0.0000	0.0027	0.0023	0.0008	0.0006
428	-0.0001	-0.0001	-0.0000	-0.0000	0.0006	0.0001	-0.0002	-0.0004
429	-0.0001	-0.0001	-0.0000	0.0000	0.0001	0.0005	0.0002	-0.0002
430	-0.0001	-0.0001	-0.0000	0.0000	-0.0006	-0.0006	-0.0001	-0.0006
431	-0.0002	-0.0001	-0.0000	-0.0000	0.0017	0.0008	0.0003	-0.0002
432	-0.0001	-0.0002	-0.0000	0.0000	0.0018	0.0014	0.0005	-0.0004
433	-0.0002	-0.0001	-0.0000	-0.0000	0.0018	0.0006	0.0003	-0.0005
434	-0.0001	-0.0001	-0.0000	-0.0000	0.0040	0.0032	0.0007	0.0003
435	-0.0001	-0.0001	-0.0000	-0.0000	0.0030	0.0022	0.0003	0.0002
334	-0.0000	-0.0000	-0.0000	-0.0000	0.0001	0.0000	0.0002	0.0002
335	-0.0000	-0.0000	-0.0000	-0.0000	-0.0001	-0.0001	0.0001	0.0001
526	-0.0001	-0.0001	-0.0000	-0.0000	-0.0012	-0.0018	-0.0010	-0.0004
527	-0.0001	-0.0001	-0.0000	-0.0000	-0.0006	-0.0009	0.0001	-0.0000
528	-0.0001	-0.0001	-0.0000	-0.0000	-0.0011	-0.0014	-0.0003	-0.0003
529	-0.0001	-0.0001	-0.0000	-0.0000	-0.0008	-0.0009	0.0002	-0.0001
530	-0.0001	-0.0001	-0.0000	-0.0000	-0.0008	-0.0010	-0.0001	-0.0003
531	-0.0001	-0.0001	-0.0000	-0.0000	-0.0006	-0.0011	0.0001	-0.0004
532	-0.0001	-0.0001	-0.0000	-0.0000	-0.0009	-0.0011	0.0002	-0.0003
533	-0.0001	-0.0001	0.0000	0.0000	-0.0013	-0.0013	0.0001	-0.0004
534	-0.0001	-0.0000	-0.0001	-0.0000	-0.0001	-0.0002	0.0004	0.0003
535	-0.0001	-0.0000	-0.0000	-0.0000	0.0000	-0.0002	0.0003	0.0001
36	0.0000	0.0000	0.0001	0.0000	0.0082	-0.0102	0.0084	0.0336
37	0.0001	0.0001	0.0002	0.0001	0.0087	-0.0189	0.0102	0.0573
38	-0.0001	-0.0001	-0.0005	-0.0001	-0.0247	0.0476	-0.0347	-0.1460
39	0.0000	-0.0000	-0.0006	-0.0003	-0.0156	0.0183	0.0051	-0.0300
40	-0.0004	-0.0003	0.0001	-0.0000	-0.0366	0.0595	-0.1031	-0.2519
41	0.0000	0.0000	-0.0000	-0.0000	-0.0012	0.0013	-0.0001	-0.0021
42	-0.0000	-0.0000	0.0000	0.0000	0.0009	-0.0009	0.0008	0.0030
43	-0.0000	-0.0000	0.0000	0.0000	0.0004	-0.0002	0.0006	0.0022
44	0.0000	0.0000	-0.0001	0.0000	-0.0027	0.0042	-0.0060	-0.0182
45	0.0000	0.0000	0.0001	0.0000	0.0069	-0.0071	0.0056	0.0218
136	0.0002	0.0001	0.0006	0.0004	0.0068	-0.0123	-0.0037	-0.0052
137	0.0003	0.0005	-0.0002	-0.0002	-0.0236	-0.0414	-0.0061	-0.0019
138	-0.0008	-0.0006	-0.0015	-0.0011	-0.0036	0.0635	0.0123	0.0182

139	-0.0010	-0.0013	-0.0012	-0.0013	0.0072	0.0574	0.0092	0.0179
140	-0.0003	-0.0005	-0.0011	-0.0010	-0.0119	0.0059	0.0065	0.0089
141	0.0000	0.0000	0.0001	0.0001	0.0025	-0.0006	-0.0003	-0.0011
142	-0.0000	-0.0001	-0.0000	-0.0000	0.0026	0.0020	0.0004	-0.0007
143	-0.0000	0.0000	-0.0001	-0.0000	-0.0021	-0.0024	-0.0002	0.0004
144	0.0001	0.0001	0.0003	0.0002	0.0043	0.0019	-0.0003	-0.0012
145	0.0001	0.0001	0.0002	0.0002	-0.0018	-0.0013	-0.0010	0.0007
244	0.0000	0.0000	0.0001	0.0001	-0.0001	0.0006	-0.0004	0.0002
245	-0.0000	-0.0000	-0.0000	-0.0000	0.0005	0.0000	0.0000	-0.0001
440	0.0001	0.0002	0.0004	0.0003	0.0002	-0.0052	-0.0001	-0.0094
444	0.0000	0.0000	0.0000	0.0000	-0.0010	-0.0009	-0.0001	-0.0000
445	-0.0000	0.0000	-0.0000	-0.0000	0.0006	0.0002	-0.0002	-0.0002
344	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0001	-0.0001	-0.0001
345	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
540	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0007	-0.0000
544	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0001	0.0001	0.0001
545	-0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0001	-0.0002	-0.0002

	514	515	516	517	18	19	20	21
22	1.0000							
23	-0.0056	1.0000						
24	-0.0011	0.0029	1.0000					
25	0.0045	-0.0022	0.0021	1.0000				
26	-0.0047	-0.0025	0.0012	-0.0009	1.0000			
27	-0.0032	-0.0031	0.0014	-0.0012	-0.0026	1.0000		
28	-0.0027	-0.0016	0.0007	-0.0006	-0.0019	-0.0017	1.0000	
29	-0.0015	-0.0010	0.0005	-0.0005	-0.0011	-0.0014	-0.0009	1.0000
30	0.0006	-0.0001	-0.0003	-0.0001	-0.0005	-0.0006	-0.0006	-0.0005
31	-0.0011	-0.0017	0.0010	-0.0008	-0.0015	-0.0019	-0.0011	-0.0011
32	-0.0037	-0.0014	0.0002	-0.0004	-0.0012	-0.0018	-0.0011	-0.0008
33	-0.0023	-0.0017	0.0006	-0.0007	-0.0016	-0.0017	-0.0012	-0.0009
34	-0.0048	-0.0038	0.0019	-0.0016	-0.0019	-0.0023	-0.0012	-0.0010
35	-0.0033	-0.0032	0.0017	-0.0015	-0.0017	-0.0018	-0.0010	-0.0010
118	0.0065	-0.0013	0.0031	-0.0009	-0.0010	-0.0020	-0.0001	-0.0022
119	-0.0016	0.0011	-0.0002	0.0013	0.0000	0.0007	0.0004	-0.0005
120	-0.0494	0.0026	0.0009	0.0005	0.0046	0.0087	0.0018	0.0018
121	-0.0305	-0.0041	0.0017	0.0003	-0.0025	0.0008	-0.0024	-0.0009
122	-0.0893	-0.0045	0.0028	0.0003	0.0015	0.0018	0.0023	0.0019
123	-0.0044	-0.0004	0.0003	-0.0000	-0.0001	-0.0002	-0.0000	0.0000
124	0.0051	0.0006	-0.0004	0.0001	0.0003	0.0006	0.0002	0.0001
125	0.0082	0.0004	-0.0008	-0.0005	-0.0002	-0.0006	-0.0007	-0.0007
126	0.0049	-0.0020	-0.0003	-0.0006	-0.0018	-0.0024	-0.0019	-0.0009
127	0.0030	-0.0009	-0.0001	-0.0003	-0.0010	-0.0013	-0.0010	-0.0007
128	0.0031	-0.0015	-0.0002	-0.0004	-0.0016	-0.0021	-0.0014	-0.0008
129	0.0038	-0.0021	-0.0001	-0.0005	-0.0016	-0.0028	-0.0017	-0.0008
130	0.0013	-0.0011	0.0002	-0.0002	-0.0016	-0.0011	-0.0012	-0.0006
131	0.0024	-0.0010	0.0000	-0.0004	-0.0016	-0.0012	-0.0013	-0.0007
132	0.0024	-0.0002	-0.0002	-0.0003	-0.0007	-0.0007	-0.0009	-0.0007
133	0.0031	-0.0006	-0.0001	-0.0005	-0.0011	-0.0008	-0.0009	-0.0007
134	-0.0038	-0.0019	0.0004	-0.0005	-0.0013	-0.0015	-0.0009	-0.0002
135	-0.0013	-0.0012	-0.0000	-0.0004	-0.0010	-0.0011	-0.0007	-0.0003

421	-0.0409	-0.0038	0.0008	0.0002	-0.0016	0.0004	-0.0009	0.0003
422	-0.0288	-0.0024	0.0012	0.0002	-0.0006	-0.0007	0.0001	-0.0001
426	0.0001	-0.0010	0.0000	-0.0003	-0.0008	-0.0010	-0.0008	-0.0003
427	0.0002	-0.0009	0.0001	-0.0002	-0.0006	-0.0010	-0.0006	-0.0003
428	0.0003	-0.0005	-0.0000	-0.0002	-0.0006	-0.0006	-0.0005	-0.0002
429	0.0003	-0.0001	-0.0000	-0.0001	-0.0002	-0.0002	-0.0002	-0.0002
430	0.0004	-0.0001	-0.0000	-0.0001	-0.0003	-0.0003	-0.0003	-0.0002
431	0.0003	-0.0003	0.0001	-0.0001	-0.0004	-0.0003	-0.0003	-0.0002
432	-0.0005	-0.0005	0.0000	-0.0001	-0.0004	-0.0006	-0.0005	-0.0003
433	-0.0003	-0.0004	0.0000	-0.0001	-0.0005	-0.0005	-0.0004	-0.0003
434	-0.0017	-0.0006	0.0001	-0.0001	-0.0004	-0.0006	-0.0003	-0.0001
435	-0.0011	-0.0005	0.0001	-0.0001	-0.0003	-0.0004	-0.0002	-0.0001
334	0.0003	-0.0000	-0.0000	-0.0000	-0.0000	-0.0001	-0.0000	-0.0000
335	0.0003	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000
526	0.0012	-0.0004	-0.0001	-0.0001	-0.0004	-0.0003	-0.0004	-0.0002
527	0.0010	-0.0002	-0.0001	-0.0001	-0.0002	-0.0003	-0.0002	-0.0001
528	0.0009	-0.0001	-0.0001	-0.0001	-0.0003	-0.0002	-0.0002	-0.0001
529	0.0009	-0.0000	-0.0000	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001
530	0.0009	-0.0000	-0.0000	-0.0001	-0.0002	-0.0001	-0.0002	-0.0001
531	0.0010	0.0000	-0.0000	-0.0001	-0.0002	-0.0000	-0.0001	-0.0001
532	0.0011	-0.0001	-0.0000	-0.0001	-0.0002	-0.0002	-0.0002	-0.0001
533	0.0007	0.0001	-0.0000	-0.0000	-0.0001	0.0000	-0.0001	-0.0002
534	0.0007	0.0000	-0.0001	-0.0000	-0.0001	-0.0000	-0.0001	-0.0001
535	0.0007	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001
36	-0.0024	-0.0020	0.0018	-0.0008	-0.0013	-0.0024	-0.0009	-0.0010
37	0.0018	-0.0031	0.0028	-0.0015	-0.0022	-0.0035	-0.0014	-0.0014
38	-0.0001	0.0078	-0.0069	0.0037	0.0051	0.0090	0.0029	0.0035
39	0.0155	0.0055	-0.0037	0.0014	0.0038	0.0049	0.0026	0.0018
40	-0.0538	0.0094	-0.0113	0.0094	0.0034	0.0084	0.0005	0.0037
41	0.0006	0.0006	-0.0003	0.0002	0.0002	0.0004	0.0002	0.0001
42	0.0003	-0.0003	0.0004	-0.0002	-0.0001	-0.0002	-0.0001	-0.0001
43	0.0007	-0.0002	0.0002	-0.0002	-0.0000	-0.0001	-0.0000	-0.0000
44	-0.0063	0.0008	-0.0020	0.0014	0.0003	0.0003	0.0001	0.0001
45	0.0027	-0.0024	0.0027	-0.0019	-0.0010	-0.0012	-0.0006	-0.0005
136	-0.0083	-0.0012	0.0009	-0.0001	-0.0006	-0.0013	-0.0002	-0.0000
137	0.0013	0.0018	-0.0005	-0.0003	0.0014	0.0011	0.0011	0.0008
138	0.0153	0.0014	-0.0016	0.0005	0.0001	0.0034	-0.0017	-0.0007
139	0.0298	0.0007	-0.0005	-0.0001	-0.0005	-0.0016	-0.0007	-0.0008
140	0.0227	0.0033	-0.0006	0.0004	0.0014	0.0001	0.0012	0.0000
141	-0.0018	-0.0003	0.0001	-0.0000	-0.0001	-0.0002	-0.0001	-0.0000
142	-0.0005	-0.0002	0.0001	0.0000	-0.0002	-0.0002	-0.0001	-0.0001
143	0.0003	0.0002	-0.0001	-0.0001	0.0002	0.0002	0.0001	0.0001
144	-0.0014	-0.0005	0.0002	0.0000	-0.0003	-0.0004	-0.0002	0.0000
145	-0.0001	0.0001	-0.0001	-0.0001	0.0002	0.0002	0.0001	0.0000
244	0.0000	0.0001	0.0000	0.0001	0.0001	0.0002	0.0001	0.0000
245	-0.0000	-0.0002	0.0000	-0.0000	-0.0001	-0.0002	-0.0001	-0.0000
440	-0.0088	-0.0004	0.0002	0.0003	-0.0004	0.0007	0.0000	0.0003
444	0.0005	0.0002	-0.0000	0.0000	0.0001	0.0002	0.0001	0.0000
445	-0.0006	-0.0002	-0.0000	-0.0001	-0.0001	-0.0001	-0.0001	-0.0000
344	-0.0001	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000
345	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000
540	-0.0001	0.0000	-0.0000	0.0001	0.0001	0.0000	0.0001	0.0000

544	0.0001	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
545	-0.0001	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000

	22	23	24	25	26	27	28	29
30	1.0000							
31	-0.0006	1.0000						
32	-0.0008	-0.0011	1.0000					
33	-0.0007	-0.0012	-0.0014	1.0000				
34	-0.0003	-0.0014	-0.0011	-0.0015	1.0000			
35	-0.0001	-0.0011	-0.0007	-0.0012	-0.0026	1.0000		
118	-0.0004	-0.0030	0.0010	0.0009	-0.0009	-0.0019	1.0000	
119	-0.0001	0.0010	0.0014	0.0013	0.0003	-0.0010	-0.4065	1.0000
120	0.0021	0.0018	0.0032	0.0027	0.0021	0.0017	-0.0698	-0.0245
121	-0.0006	-0.0012	-0.0012	-0.0019	-0.0018	-0.0029	-0.0532	0.0211
122	0.0041	0.0014	0.0014	0.0027	-0.0019	-0.0014	0.0090	-0.0201
123	0.0003	-0.0001	-0.0001	-0.0001	-0.0003	-0.0002	0.0055	-0.0091
124	-0.0002	0.0002	0.0003	0.0000	0.0004	0.0003	-0.0092	0.0149
125	-0.0008	-0.0004	-0.0009	-0.0009	-0.0003	-0.0005	0.0053	0.0083
126	-0.0010	-0.0010	-0.0021	-0.0019	-0.0014	-0.0011	0.0054	0.0006
127	-0.0009	-0.0008	-0.0011	-0.0010	-0.0006	-0.0005	0.0020	0.0009
128	-0.0009	-0.0009	-0.0017	-0.0014	-0.0010	-0.0008	0.0037	-0.0011
129	-0.0009	-0.0010	-0.0021	-0.0016	-0.0014	-0.0008	0.0065	0.0006
130	-0.0007	-0.0010	-0.0010	-0.0011	-0.0006	-0.0004	0.0003	0.0010
131	-0.0008	-0.0010	-0.0011	-0.0015	-0.0008	-0.0007	0.0020	0.0005
132	-0.0010	-0.0006	-0.0007	-0.0008	-0.0004	-0.0004	-0.0012	-0.0004
133	-0.0007	-0.0007	-0.0009	-0.0014	-0.0008	-0.0007	0.0030	-0.0003
134	0.0000	-0.0004	-0.0009	-0.0011	-0.0014	-0.0009	0.0085	-0.0108
135	-0.0002	-0.0003	-0.0008	-0.0010	-0.0011	-0.0009	0.0062	-0.0073
421	0.0007	0.0003	-0.0009	-0.0013	-0.0021	-0.0024	-0.0754	0.0628
422	0.0008	-0.0004	-0.0005	-0.0001	-0.0011	-0.0012	0.0105	-0.0240
426	-0.0003	-0.0004	-0.0008	-0.0007	-0.0006	-0.0004	0.0057	-0.0036
427	-0.0003	-0.0004	-0.0007	-0.0005	-0.0005	-0.0003	0.0066	-0.0039
428	-0.0003	-0.0003	-0.0004	-0.0004	-0.0003	-0.0003	0.0026	-0.0018
429	-0.0002	-0.0002	-0.0002	-0.0002	-0.0001	-0.0001	0.0021	-0.0019
430	-0.0003	-0.0002	-0.0002	-0.0002	-0.0001	-0.0001	0.0006	-0.0007
431	-0.0002	-0.0003	-0.0003	-0.0004	-0.0003	-0.0002	0.0055	-0.0046
432	-0.0003	-0.0003	-0.0004	-0.0004	-0.0004	-0.0003	0.0030	-0.0016
433	-0.0002	-0.0003	-0.0004	-0.0004	-0.0004	-0.0003	0.0045	-0.0034
434	-0.0001	-0.0002	-0.0004	-0.0003	-0.0004	-0.0003	0.0069	-0.0066
435	-0.0001	-0.0002	-0.0002	-0.0003	-0.0003	-0.0002	0.0056	-0.0053
334	-0.0000	-0.0000	-0.0000	-0.0001	-0.0001	-0.0000	0.0002	0.0001
335	-0.0000	-0.0000	-0.0000	-0.0001	-0.0000	-0.0001	0.0001	-0.0000
526	-0.0002	-0.0002	-0.0004	-0.0004	-0.0002	-0.0002	0.0004	0.0007
527	-0.0002	-0.0001	-0.0002	-0.0002	-0.0001	-0.0001	0.0002	0.0010
528	-0.0002	-0.0001	-0.0002	-0.0002	-0.0001	-0.0001	0.0001	0.0001
529	-0.0001	-0.0001	-0.0001	-0.0001	-0.0000	-0.0001	0.0000	0.0006
530	-0.0001	-0.0001	-0.0001	-0.0002	-0.0001	-0.0001	-0.0000	0.0008
531	-0.0001	-0.0001	-0.0001	-0.0002	-0.0001	-0.0001	0.0003	0.0004
532	-0.0001	-0.0001	-0.0002	-0.0002	-0.0001	-0.0001	-0.0001	0.0007
533	-0.0002	-0.0002	-0.0001	-0.0001	0.0000	-0.0000	-0.0003	0.0004
534	-0.0001	-0.0000	-0.0001	-0.0002	-0.0001	-0.0001	0.0002	0.0002

535	-0.0001	-0.0000	-0.0001	-0.0002	-0.0001	-0.0001	0.0003	0.0002
36	-0.0005	-0.0021	-0.0012	-0.0012	-0.0016	-0.0006	-0.0060	-0.0015
37	-0.0013	-0.0032	-0.0017	-0.0019	-0.0025	-0.0008	-0.0094	-0.0040
38	0.0021	0.0079	0.0040	0.0045	0.0063	0.0024	0.0251	0.0061
39	0.0021	0.0044	0.0036	0.0035	0.0041	0.0012	0.0059	0.0043
40	-0.0024	0.0052	-0.0010	0.0010	0.0071	0.0081	0.0367	-0.0024
41	0.0001	0.0003	0.0003	0.0003	0.0005	0.0003	0.0002	-0.0001
42	-0.0000	-0.0002	-0.0001	-0.0001	-0.0002	-0.0001	-0.0004	0.0000
43	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001	-0.0000	-0.0003	0.0002
44	-0.0000	0.0007	-0.0000	0.0002	0.0004	0.0002	0.0027	-0.0009
45	0.0000	-0.0010	-0.0003	-0.0006	-0.0016	-0.0013	-0.0028	0.0002
136	0.0006	-0.0003	-0.0003	0.0001	-0.0007	-0.0002	0.0118	-0.0275
137	0.0008	0.0011	0.0010	0.0010	0.0009	0.0008	-0.0087	-0.0188
138	-0.0024	-0.0001	0.0004	-0.0012	0.0008	-0.0005	-0.0357	0.1178
139	-0.0015	-0.0008	-0.0005	-0.0002	0.0006	0.0005	0.0118	0.0295
140	0.0001	0.0004	0.0009	0.0014	0.0020	0.0013	-0.0022	0.0010
141	0.0001	-0.0001	-0.0001	-0.0001	-0.0002	-0.0001	0.0029	-0.0038
142	0.0000	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001	0.0027	-0.0016
143	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001	-0.0016	0.0010
144	0.0001	-0.0001	-0.0002	-0.0001	-0.0002	-0.0001	0.0028	-0.0034
145	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	-0.0014	-0.0016
244	0.0000	0.0000	0.0001	0.0001	0.0001	0.0001	-0.0002	-0.0010
245	0.0000	-0.0000	-0.0001	-0.0001	-0.0001	-0.0000	0.0002	0.0005
440	0.0002	0.0001	0.0002	-0.0003	-0.0001	-0.0003	-0.0258	0.0276
444	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001	-0.0014	0.0011
445	-0.0000	-0.0000	-0.0001	-0.0001	-0.0001	-0.0001	-0.0008	0.0015
344	0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000
345	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
540	0.0000	0.0001	-0.0000	0.0000	0.0000	0.0000	-0.0001	0.0002
544	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000
545	-0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0001

	30	31	32	33	34	35	118	119
120	1.0000							
121	-0.0118	1.0000						
122	-0.0378	-0.3134	1.0000					
123	0.0024	0.0136	-0.0085	1.0000				
124	-0.0059	-0.0172	0.0119	0.0054	1.0000			
125	-0.0066	0.0175	0.0193	0.0015	-0.0009	1.0000		
126	0.0067	-0.0015	-0.0213	-0.0002	0.0004	-0.0031	1.0000	
127	0.0046	0.0193	-0.0230	0.0003	0.0000	-0.0018	-0.0049	1.0000
128	0.0089	0.0028	-0.0259	-0.0008	0.0011	-0.0015	-0.0065	-0.0044
129	0.0115	0.0232	-0.0292	-0.0013	0.0017	-0.0014	-0.0077	-0.0053
130	0.0050	-0.0206	-0.0151	-0.0010	0.0011	0.0002	-0.0033	-0.0022
131	0.0067	-0.0158	-0.0013	-0.0018	0.0015	0.0003	-0.0027	-0.0013
132	0.0039	-0.0132	0.0060	-0.0001	0.0000	-0.0007	-0.0012	-0.0008
133	0.0065	0.0072	0.0003	-0.0014	0.0011	-0.0000	-0.0021	-0.0014
134	0.0188	0.0007	-0.0426	-0.0049	0.0051	0.0069	-0.0031	-0.0018
135	0.0066	0.0128	-0.0260	-0.0049	0.0054	0.0014	-0.0032	-0.0017
421	-0.2779	0.3344	0.1087	-0.0042	-0.0077	0.0238	0.0041	0.0063
422	-0.0860	0.0751	0.1008	0.0050	-0.0034	-0.0007	0.0062	0.0061

426	0.0007	-0.0015	0.0118	0.0006	-0.0000	-0.0015	-0.0019	-0.0005
427	0.0038	-0.0040	0.0120	0.0008	-0.0000	-0.0018	-0.0013	-0.0004
428	-0.0003	0.0004	0.0083	0.0005	-0.0002	-0.0010	-0.0009	-0.0003
429	0.0012	-0.0019	0.0065	0.0006	-0.0003	-0.0009	-0.0002	-0.0002
430	-0.0006	0.0009	0.0053	0.0004	-0.0002	-0.0005	-0.0003	-0.0002
431	0.0038	-0.0036	0.0098	0.0005	0.0000	-0.0014	-0.0001	0.0001
432	-0.0025	0.0036	0.0111	0.0006	-0.0003	-0.0009	-0.0006	-0.0001
433	0.0002	0.0015	0.0111	0.0004	-0.0000	-0.0010	-0.0004	-0.0000
434	0.0012	0.0001	0.0134	0.0006	0.0002	-0.0012	-0.0001	0.0004
435	0.0018	-0.0006	0.0103	0.0004	0.0002	-0.0009	0.0000	0.0003
334	0.0002	0.0003	0.0005	0.0000	-0.0000	-0.0002	-0.0002	-0.0001
335	0.0001	-0.0000	0.0005	0.0000	-0.0000	-0.0001	-0.0001	-0.0000
526	0.0004	-0.0014	0.0017	0.0001	-0.0001	-0.0005	-0.0013	-0.0005
527	0.0006	0.0004	0.0018	0.0001	-0.0001	-0.0004	-0.0006	-0.0003
528	0.0006	-0.0002	0.0018	0.0001	-0.0001	-0.0004	-0.0006	-0.0003
529	0.0005	0.0004	0.0016	0.0001	-0.0001	-0.0003	-0.0003	-0.0002
530	0.0005	0.0002	0.0017	0.0001	-0.0001	-0.0003	-0.0003	-0.0002
531	0.0005	0.0003	0.0020	0.0001	-0.0001	-0.0004	-0.0002	-0.0002
532	0.0007	0.0003	0.0018	0.0001	-0.0001	-0.0003	-0.0004	-0.0003
533	0.0003	0.0004	0.0018	0.0001	-0.0001	-0.0003	-0.0001	-0.0002
534	0.0004	0.0002	0.0013	0.0001	-0.0001	-0.0004	-0.0002	-0.0001
535	0.0005	0.0003	0.0013	0.0000	-0.0001	-0.0003	-0.0003	-0.0001
36	0.0001	-0.0030	-0.0051	-0.0004	0.0006	0.0008	0.0002	0.0000
37	-0.0006	-0.0021	-0.0041	-0.0002	0.0005	0.0011	0.0002	0.0001
38	-0.0006	0.0081	0.0145	0.0007	-0.0011	-0.0033	-0.0012	-0.0003
39	-0.0001	0.0088	0.0122	0.0008	-0.0012	-0.0032	0.0001	0.0002
40	-0.0016	-0.0039	0.0046	-0.0005	-0.0004	0.0011	-0.0032	-0.0018
41	-0.0002	0.0004	0.0005	0.0001	-0.0001	0.0000	0.0002	0.0001
42	-0.0001	-0.0002	-0.0003	-0.0000	0.0000	0.0001	0.0000	0.0000
43	0.0000	0.0001	-0.0001	0.0000	-0.0000	0.0000	0.0000	0.0000
44	0.0015	0.0009	0.0001	-0.0000	0.0001	-0.0005	-0.0008	-0.0002
45	-0.0011	-0.0012	-0.0026	-0.0002	0.0003	0.0005	0.0004	0.0001
136	0.0198	0.0782	-0.0209	-0.0062	0.0081	0.0028	-0.0004	-0.0012
137	0.0167	0.0317	0.1439	-0.0070	0.0054	0.0063	0.0133	0.0140
138	-0.0850	-0.4540	0.0294	0.0240	-0.0321	-0.0016	-0.0016	0.0049
139	-0.0145	0.2521	-0.2040	0.0188	-0.0139	-0.0298	-0.0263	-0.0331
140	-0.0317	0.4592	-0.0197	0.0057	-0.0018	-0.0249	-0.0091	-0.0175
141	0.0006	0.0124	-0.0075	-0.0024	0.0031	-0.0003	-0.0006	-0.0005
142	-0.0029	0.0232	-0.0153	-0.0015	0.0026	-0.0030	-0.0018	-0.0019
143	0.0004	-0.0079	0.0171	-0.0003	-0.0002	0.0010	0.0015	0.0016
144	0.0045	0.0066	-0.0301	-0.0009	0.0014	0.0010	-0.0020	-0.0020
145	0.0130	-0.0364	0.0103	0.0033	-0.0047	0.0058	0.0021	0.0021
244	0.0047	0.0028	-0.0003	0.0006	-0.0008	0.0012	0.0004	0.0001
245	0.0000	0.0003	-0.0017	0.0001	-0.0001	-0.0001	-0.0004	-0.0003
440	-0.0659	0.0831	0.0058	-0.0026	-0.0019	0.0087	0.0003	0.0006
444	-0.0001	0.0006	-0.0025	-0.0002	0.0000	0.0003	0.0001	-0.0000
445	-0.0040	0.0057	0.0014	-0.0001	-0.0001	0.0003	-0.0002	-0.0000
344	-0.0001	-0.0001	-0.0001	-0.0000	0.0000	0.0000	0.0000	0.0000
345	-0.0000	0.0001	0.0001	0.0000	-0.0000	0.0000	0.0000	0.0000
540	-0.0002	-0.0001	-0.0000	0.0000	-0.0000	0.0000	0.0001	0.0000
544	0.0001	0.0000	0.0002	0.0000	-0.0000	0.0000	0.0000	0.0000
545	-0.0001	-0.0001	-0.0002	-0.0000	0.0000	0.0000	0.0001	0.0000

	120	121	122	123	124	125	126	127
128	1.0000							
129	-0.0068	1.0000						
130	-0.0032	-0.0034	1.0000					
131	-0.0026	-0.0029	-0.0032	1.0000				
132	-0.0013	-0.0012	-0.0015	-0.0021	1.0000			
133	-0.0022	-0.0027	-0.0021	-0.0035	-0.0017	1.0000		
134	-0.0039	-0.0057	-0.0026	-0.0042	-0.0007	-0.0045	1.0000	
135	-0.0035	-0.0045	-0.0025	-0.0035	-0.0008	-0.0034	-0.0088	1.0000
421	0.0044	0.0018	0.0045	-0.0013	0.0020	-0.0039	-0.0120	-0.0076
422	0.0089	0.0106	0.0084	0.0096	0.0044	0.0088	0.0172	0.0138
426	-0.0008	-0.0009	-0.0002	-0.0001	-0.0002	0.0002	0.0011	0.0008
427	-0.0004	-0.0006	0.0001	0.0004	-0.0001	0.0006	0.0019	0.0015
428	-0.0004	-0.0003	-0.0000	0.0000	-0.0002	0.0002	0.0010	0.0007
429	0.0001	0.0002	0.0001	0.0002	-0.0002	0.0003	0.0014	0.0010
430	-0.0001	-0.0001	-0.0001	-0.0001	-0.0003	-0.0000	0.0007	0.0005
431	0.0002	0.0005	0.0002	0.0002	-0.0001	0.0002	0.0016	0.0011
432	-0.0000	-0.0001	0.0002	0.0003	-0.0001	0.0003	0.0013	0.0010
433	0.0001	0.0001	0.0001	0.0000	-0.0002	0.0001	0.0011	0.0008
434	0.0005	0.0006	0.0006	0.0007	0.0002	0.0008	0.0020	0.0015
435	0.0004	0.0005	0.0005	0.0005	0.0001	0.0005	0.0014	0.0011
334	-0.0001	-0.0001	-0.0000	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001
335	-0.0001	-0.0000	-0.0000	-0.0001	-0.0001	-0.0001	-0.0000	-0.0001
526	-0.0008	-0.0009	-0.0005	-0.0006	-0.0003	-0.0004	-0.0003	-0.0003
527	-0.0005	-0.0006	-0.0003	-0.0004	-0.0002	-0.0003	-0.0001	-0.0001
528	-0.0005	-0.0004	-0.0003	-0.0004	-0.0003	-0.0003	-0.0001	-0.0001
529	-0.0003	-0.0003	-0.0002	-0.0003	-0.0002	-0.0003	-0.0000	-0.0000
530	-0.0002	-0.0003	-0.0002	-0.0003	-0.0002	-0.0003	-0.0000	-0.0001
531	-0.0002	-0.0001	-0.0002	-0.0004	-0.0003	-0.0004	-0.0001	-0.0001
532	-0.0003	-0.0004	-0.0003	-0.0003	-0.0002	-0.0003	-0.0000	-0.0001
533	-0.0001	-0.0001	-0.0002	-0.0003	-0.0003	-0.0002	0.0002	0.0001
534	-0.0001	-0.0001	-0.0000	-0.0002	-0.0002	-0.0003	-0.0001	-0.0002
535	-0.0002	-0.0002	-0.0001	-0.0002	-0.0001	-0.0003	-0.0002	-0.0002
36	0.0001	-0.0002	-0.0002	0.0001	0.0003	0.0003	-0.0005	-0.0001
37	-0.0001	0.0000	-0.0003	0.0002	0.0003	0.0004	-0.0004	-0.0000
38	-0.0003	-0.0003	0.0005	-0.0005	-0.0011	-0.0010	0.0015	0.0002
39	0.0006	0.0007	0.0015	0.0006	-0.0003	-0.0002	0.0020	0.0007
40	-0.0022	-0.0018	-0.0030	-0.0031	-0.0018	-0.0019	-0.0015	-0.0008
41	0.0002	0.0002	0.0001	0.0001	0.0000	0.0001	0.0002	0.0001
42	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000
43	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000
44	-0.0005	-0.0007	0.0002	-0.0000	-0.0002	-0.0001	-0.0003	-0.0004
45	0.0002	0.0001	-0.0001	0.0000	0.0001	0.0001	-0.0002	-0.0000
136	-0.0022	-0.0045	-0.0012	-0.0020	0.0005	-0.0024	-0.0079	-0.0061
137	0.0107	0.0111	0.0037	-0.0050	-0.0019	-0.0047	-0.0037	-0.0007
138	0.0060	0.0149	0.0006	0.0040	-0.0043	0.0085	0.0222	0.0228
139	-0.0201	-0.0235	0.0010	0.0194	0.0081	0.0121	0.0215	0.0081
140	-0.0076	-0.0118	0.0064	0.0151	0.0079	0.0069	0.0206	0.0030
141	-0.0009	-0.0011	-0.0007	-0.0007	0.0000	-0.0004	-0.0016	-0.0027
142	-0.0018	-0.0019	-0.0009	0.0001	0.0004	0.0003	0.0009	-0.0023

143	0.0013	0.0015	0.0004	-0.0005	-0.0004	-0.0004	0.0002	0.0007
144	-0.0021	-0.0028	-0.0009	-0.0002	0.0004	-0.0003	-0.0043	-0.0024
145	0.0020	0.0020	0.0017	0.0003	-0.0003	-0.0005	-0.0037	0.0050
244	0.0002	0.0002	0.0005	0.0003	0.0001	-0.0001	-0.0015	0.0019
245	-0.0004	-0.0005	-0.0001	-0.0001	0.0000	-0.0001	0.0000	-0.0003
440	-0.0005	-0.0014	-0.0010	-0.0028	-0.0001	-0.0031	-0.0076	-0.0054
444	-0.0001	-0.0001	-0.0001	-0.0002	-0.0001	-0.0003	-0.0006	-0.0005
445	-0.0001	-0.0003	-0.0000	-0.0002	-0.0001	-0.0002	-0.0005	-0.0003
344	0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000
345	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000
540	0.0001	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
544	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
545	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000

	128	129	130	131	132	133	134	135
421	1.0000							
422	-0.3201	1.0000						
426	-0.0043	-0.0161	1.0000					
427	0.0118	-0.0160	-0.0027	1.0000				
428	-0.0048	-0.0119	-0.0015	-0.0016	1.0000			
429	0.0064	-0.0086	-0.0011	-0.0014	-0.0008	1.0000		
430	-0.0044	-0.0063	-0.0007	-0.0007	-0.0005	-0.0005	1.0000	
431	0.0138	-0.0095	-0.0016	-0.0019	-0.0010	-0.0010	-0.0005	1.0000
432	-0.0152	-0.0178	-0.0019	-0.0020	-0.0013	-0.0010	-0.0007	-0.0011
433	-0.0061	-0.0131	-0.0017	-0.0017	-0.0010	-0.0008	-0.0005	-0.0013
434	-0.0022	-0.0195	-0.0024	-0.0027	-0.0015	-0.0012	-0.0007	-0.0019
435	0.0016	-0.0133	-0.0018	-0.0020	-0.0010	-0.0009	-0.0005	-0.0015
334	0.0002	0.0002	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000
335	0.0000	0.0001	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000
526	-0.0003	0.0003	-0.0005	-0.0003	-0.0002	-0.0001	-0.0001	-0.0001
527	0.0007	0.0005	-0.0002	-0.0002	-0.0001	-0.0001	-0.0001	-0.0001
528	0.0003	0.0004	-0.0002	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001
529	0.0007	0.0005	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001
530	0.0006	0.0005	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001
531	0.0005	0.0005	-0.0000	0.0000	-0.0001	-0.0001	-0.0001	-0.0001
532	0.0006	0.0005	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001
533	0.0009	0.0005	0.0000	0.0000	-0.0000	-0.0001	-0.0001	-0.0001
534	0.0002	0.0004	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0001
535	0.0002	0.0004	-0.0001	-0.0000	-0.0001	-0.0000	-0.0000	-0.0001
36	-0.0018	-0.0022	-0.0001	-0.0002	-0.0000	-0.0000	0.0000	-0.0001
37	0.0002	-0.0018	-0.0001	-0.0001	-0.0001	-0.0000	-0.0000	-0.0001
38	0.0030	0.0064	0.0001	0.0003	0.0001	0.0000	-0.0001	0.0002
39	0.0073	0.0060	0.0005	0.0004	0.0003	0.0001	0.0001	0.0003
40	-0.0099	0.0006	-0.0010	-0.0003	-0.0006	-0.0003	-0.0005	-0.0002
41	0.0004	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
42	-0.0001	-0.0001	-0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000
43	0.0001	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44	-0.0004	0.0002	-0.0003	-0.0002	-0.0001	-0.0000	-0.0000	0.0000
45	-0.0005	-0.0010	0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000
136	0.0424	0.0006	-0.0001	-0.0013	-0.0003	-0.0008	-0.0000	-0.0005
137	0.0500	0.0048	0.0013	-0.0002	-0.0000	-0.0007	0.0001	-0.0001

138	-0.2513	-0.0249	-0.0019	0.0044	0.0003	0.0031	-0.0007	0.0025
139	0.0559	0.0392	-0.0005	0.0004	0.0013	0.0015	0.0007	-0.0009
140	-0.0045	-0.0240	0.0001	-0.0014	-0.0013	-0.0017	-0.0009	-0.0009
141	0.0037	0.0011	0.0001	-0.0000	0.0001	0.0000	0.0001	0.0001
142	0.0086	0.0017	0.0000	-0.0001	0.0000	-0.0001	0.0000	-0.0001
143	-0.0017	-0.0003	0.0001	0.0001	0.0000	0.0000	-0.0000	0.0000
144	0.0021	0.0047	0.0003	0.0004	0.0003	0.0003	0.0002	0.0005
145	-0.0048	-0.0037	-0.0004	-0.0003	-0.0002	-0.0001	-0.0001	-0.0003
244	-0.0023	-0.0005	0.0001	0.0001	0.0001	0.0000	0.0000	0.0001
245	0.0001	0.0003	-0.0001	-0.0001	-0.0000	0.0000	0.0000	0.0000
440	-0.3228	-0.0440	0.0028	0.0077	0.0014	0.0040	0.0002	0.0066
444	-0.0009	0.0054	0.0006	0.0008	0.0004	0.0004	0.0002	0.0005
445	-0.0211	-0.0045	-0.0001	0.0002	-0.0001	0.0001	-0.0001	0.0003
344	-0.0001	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000
345	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000
540	-0.0001	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
544	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
545	-0.0001	-0.0001	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000

	421	422	426	427	428	429	430	431
432	1.0000							
433	-0.0014	1.0000						
434	-0.0019	-0.0019	1.0000					
435	-0.0014	-0.0014	-0.0022	1.0000				
334	-0.0000	-0.0000	-0.0000	-0.0000	1.0000			
335	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	1.0000		
526	-0.0002	-0.0002	-0.0001	-0.0001	-0.0000	-0.0000	1.0000	
527	-0.0001	-0.0001	-0.0001	-0.0000	-0.0000	-0.0000	-0.0001	1.0000
528	-0.0001	-0.0001	-0.0000	-0.0000	-0.0000	-0.0000	-0.0001	-0.0001
529	-0.0001	-0.0001	-0.0000	-0.0000	-0.0000	-0.0000	-0.0001	-0.0001
530	-0.0001	-0.0001	-0.0000	-0.0000	-0.0000	-0.0000	-0.0001	-0.0001
531	-0.0000	-0.0001	0.0000	-0.0000	-0.0000	-0.0000	-0.0001	-0.0001
532	-0.0001	-0.0001	-0.0000	-0.0000	-0.0000	-0.0000	-0.0001	-0.0001
533	-0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000
534	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000
535	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0001	-0.0000
36	-0.0001	-0.0001	-0.0003	-0.0002	0.0000	0.0000	0.0001	0.0001
37	-0.0000	-0.0000	-0.0002	-0.0001	0.0000	0.0000	0.0001	0.0001
38	0.0002	0.0002	0.0007	0.0005	-0.0001	-0.0001	-0.0003	-0.0003
39	0.0004	0.0003	0.0006	0.0005	-0.0001	-0.0001	-0.0000	-0.0002
40	-0.0005	-0.0005	0.0001	0.0000	0.0000	-0.0000	-0.0009	-0.0002
41	0.0000	0.0000	0.0001	0.0000	-0.0000	-0.0000	0.0000	0.0000
42	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000
43	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000
44	-0.0001	-0.0001	-0.0001	-0.0001	-0.0000	-0.0000	-0.0001	-0.0001
45	-0.0000	-0.0000	-0.0001	-0.0001	0.0000	0.0000	0.0001	0.0001
136	-0.0002	0.0003	-0.0002	-0.0000	0.0000	0.0001	0.0003	0.0001
137	0.0005	0.0012	0.0011	0.0011	-0.0002	-0.0000	0.0006	0.0000
138	-0.0012	-0.0024	-0.0005	-0.0006	-0.0001	-0.0003	-0.0020	-0.0005
139	0.0021	-0.0008	-0.0009	-0.0015	-0.0001	-0.0000	-0.0008	-0.0006
140	-0.0015	-0.0004	-0.0007	-0.0002	-0.0001	-0.0000	0.0008	-0.0000

141	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
142	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
143	-0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000
144	0.0004	0.0005	0.0006	0.0005	0.0000	0.0000	-0.0000	0.0000
145	-0.0003	-0.0003	-0.0005	-0.0004	-0.0000	-0.0000	-0.0000	-0.0000
244	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
245	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000
440	-0.0003	0.0014	0.0042	0.0039	0.0001	-0.0000	-0.0001	0.0002
444	0.0005	0.0004	0.0007	0.0005	0.0000	-0.0000	0.0000	0.0000
445	-0.0003	-0.0001	-0.0000	0.0000	-0.0000	-0.0000	-0.0001	-0.0000
344	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000
345	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
540	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000
544	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000
545	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000

	432	433	434	435	334	335	526	527
528	1.0000							
529	-0.0001	1.0000						
530	-0.0001	-0.0000	1.0000					
531	-0.0001	-0.0001	-0.0001	1.0000				
532	-0.0001	-0.0001	-0.0001	-0.0001	1.0000			
533	-0.0000	-0.0000	-0.0001	-0.0001	-0.0000	1.0000		
534	-0.0000	-0.0000	-0.0000	-0.0001	-0.0000	-0.0000	1.0000	
535	-0.0001	-0.0000	-0.0000	-0.0001	-0.0000	-0.0000	-0.0000	1.0000
36	0.0001	0.0001	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001
37	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0000
38	-0.0002	-0.0002	-0.0002	-0.0003	-0.0002	-0.0003	-0.0003	-0.0002
39	-0.0001	-0.0002	-0.0001	-0.0002	-0.0001	-0.0002	-0.0003	-0.0001
40	-0.0004	-0.0002	-0.0003	-0.0003	-0.0002	-0.0003	-0.0001	-0.0000
41	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000
42	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44	-0.0001	-0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001	-0.0000
45	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
136	0.0003	0.0001	0.0002	0.0003	0.0001	0.0002	0.0003	0.0002
137	0.0001	-0.0000	0.0001	-0.0001	-0.0000	0.0001	-0.0001	-0.0002
138	-0.0010	-0.0005	-0.0006	-0.0008	-0.0004	-0.0007	-0.0008	-0.0005
139	-0.0006	-0.0004	-0.0005	-0.0002	-0.0006	-0.0004	-0.0001	-0.0002
140	-0.0000	-0.0002	-0.0001	-0.0001	-0.0003	-0.0003	-0.0001	-0.0001
141	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
142	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
143	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000
144	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0001	0.0000
145	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000
244	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000
245	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000
440	0.0000	0.0001	0.0001	-0.0000	0.0001	0.0001	0.0000	0.0000
444	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000
445	-0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000
344	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000

345	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
540	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000
544	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
545	0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000

	528	529	530	531	532	533	534	535
36	1.0000							
37	-0.0086	1.0000						
38	0.0207	0.0346	1.0000					
39	0.0114	0.0200	-0.0442	1.0000				
40	0.0096	0.0151	-0.0422	-0.0066	1.0000			
41	0.0006	0.0011	-0.0024	-0.0017	-0.0008	1.0000		
42	-0.0003	-0.0006	0.0014	0.0008	0.0013	0.0001	1.0000	
43	-0.0003	-0.0006	0.0013	0.0008	0.0008	0.0001	-0.0000	1.0000
44	0.0017	0.0030	-0.0068	-0.0036	-0.0074	-0.0002	0.0003	0.0002
45	-0.0020	-0.0036	0.0083	0.0047	0.0104	0.0004	-0.0004	-0.0002
136	-0.0012	-0.0011	0.0030	0.0027	0.0008	0.0001	-0.0001	0.0000
137	0.0012	0.0013	-0.0039	-0.0039	0.0033	-0.0002	0.0000	0.0000
138	0.0021	0.0023	-0.0068	-0.0047	-0.0108	-0.0003	0.0002	0.0001
139	0.0001	-0.0007	0.0016	-0.0023	0.0051	-0.0001	0.0000	-0.0001
140	0.0006	-0.0004	-0.0010	-0.0042	0.0105	-0.0003	0.0000	0.0000
141	-0.0002	-0.0002	0.0006	0.0006	0.0000	0.0000	-0.0000	-0.0000
142	-0.0002	-0.0003	0.0007	0.0007	0.0002	0.0000	-0.0000	-0.0000
143	0.0002	0.0003	-0.0006	-0.0006	0.0001	-0.0000	0.0000	-0.0000
144	-0.0003	-0.0004	0.0010	0.0011	-0.0003	0.0001	-0.0000	0.0000
145	0.0001	0.0002	-0.0004	-0.0005	0.0000	-0.0000	0.0000	-0.0000
244	0.0000	-0.0000	0.0000	-0.0000	0.0001	-0.0000	-0.0000	0.0000
245	-0.0001	-0.0000	0.0001	0.0001	0.0001	0.0000	-0.0000	0.0000
440	-0.0001	0.0001	0.0002	0.0018	-0.0053	0.0000	0.0000	0.0000
444	0.0001	0.0001	-0.0002	-0.0002	-0.0000	-0.0000	0.0000	0.0000
445	-0.0000	0.0000	0.0000	0.0001	-0.0002	0.0000	-0.0000	-0.0000
344	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000
345	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000
540	0.0000	0.0002	-0.0001	-0.0002	0.0002	-0.0000	0.0000	0.0000
544	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000
545	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000

	36	37	38	39	40	41	42	43
44	1.0000							
45	0.0021	1.0000						
136	0.0001	-0.0007	1.0000					
137	0.0002	0.0001	-0.0293	1.0000				
138	-0.0005	0.0019	0.1116	0.1279	1.0000			
139	0.0001	0.0005	0.0522	0.2671	-0.1634	1.0000		
140	0.0007	0.0000	-0.0075	0.0865	0.0981	-0.3174	1.0000	
141	-0.0000	-0.0001	-0.0041	-0.0010	0.0184	0.0026	-0.0048	1.0000
142	0.0000	-0.0001	-0.0021	0.0112	0.0144	-0.0279	-0.0226	-0.0022
143	-0.0000	0.0001	-0.0005	-0.0119	0.0008	0.0262	0.0135	0.0005
144	-0.0000	-0.0001	-0.0019	0.0105	0.0070	-0.0200	-0.0089	-0.0010
145	-0.0000	0.0001	0.0022	-0.0136	-0.0196	0.0349	0.0336	0.0040

244	0.0001	-0.0000	-0.0001	-0.0016	-0.0007	0.0026	0.0029	0.0006
245	-0.0000	-0.0000	-0.0003	0.0003	0.0011	-0.0008	-0.0008	0.0000
440	0.0001	0.0000	0.0127	0.0147	-0.0720	0.0110	0.0057	0.0008
444	0.0000	0.0000	0.0005	0.0003	-0.0017	-0.0010	0.0007	0.0000
445	-0.0001	0.0000	0.0007	0.0010	-0.0045	0.0006	0.0005	0.0001
344	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000
345	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000
540	0.0000	0.0000	0.0001	-0.0001	0.0001	-0.0000	-0.0002	-0.0000
544	-0.0000	0.0000	0.0001	0.0000	-0.0002	-0.0001	-0.0000	0.0000
545	0.0000	-0.0000	-0.0000	0.0001	0.0001	0.0001	0.0001	-0.0000

	44	45	136	137	138	139	140	141
142	1.0000							
143	0.0021	1.0000						
144	-0.0020	0.0019	1.0000					
145	0.0081	-0.0027	0.0020	1.0000				
244	0.0012	-0.0002	-0.0004	-0.0048	1.0000			
245	0.0000	-0.0000	0.0004	-0.0003	0.0002	1.0000		
440	0.0022	-0.0004	-0.0006	-0.0005	-0.0006	0.0000	1.0000	
444	0.0000	-0.0000	-0.0001	0.0001	-0.0000	0.0000	-0.0016	1.0000
445	0.0002	-0.0000	0.0000	-0.0001	-0.0000	-0.0000	-0.0054	-0.0000
344	-0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000
345	0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000
540	-0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0001	0.0000
544	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000
545	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000

	142	143	144	145	244	245	440	444
445	1.0000							
344	0.0000	1.0000						
345	0.0000	0.0000	1.0000					
540	0.0000	0.0000	-0.0000	1.0000				
544	0.0000	0.0000	-0.0000	-0.0000	1.0000			
545	0.0000	-0.0000	-0.0000	0.0000	0.0000	1.0000		

	445	344	345	540	544	545

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4 Wigner-Kirkwood transmission coefficient

Let us consider that the Eyring-Polanyi equation is in the following form:[1]

$$\tau^{-1} = \chi \frac{kT}{h} \exp\left(-\frac{\Delta G^{\ddagger}}{kT}\right) . \tag{1}$$

The first order Wigner-Kirkwood transmission coefficient conventionally has a form:[2]

$$\chi = 1 + \frac{1}{24}\left(\frac{h\nu_{TS}}{kT}\right)^2 . \tag{2}$$

However, it is possible to give non-strict derivation of this coefficient in the form $\chi = \exp\left(\frac{1}{24}\left(\frac{h\nu_{TS}}{kT}\right)^2\right)$. Obviously, the eq. 2 can be derived from it as the first two terms of the Taylor expansion.
The $\Delta G^{\ddagger}$ at the ideal gas – rigid rotor – harmonic oscillator approximation has all the terms that correspond to all degrees of freedom excluding the vibrational energy for the imaginary frequency. Therefore it is possible to say that this degree of freedom is described in the classical approximation only by the electronic energies diffrencies. Thus it becomes possible to make a quantum correction $\Delta G_{TS,quant}$ to the $\Delta G^{\ddagger}$. The first order Wigner-Kirkwood correction to the Helmholz free energy F for a system with single degree of freedom is given by the equation:[3]

$$\Delta F_{quant} = \frac{\hbar^2}{24kT\mu}\left\langle \frac{d^2V}{dx^2} \right\rangle_x , \tag{3}$$

where V is the potential energy function, μ is the reduced mass of the particle and x is the coordinate. Let us approximate the barrier by the inverted parabola:

$$V_{TS}(x) = -\frac{\mu\omega_{TS}^2 x^2}{2} + E_{BH} , \tag{4}$$

where $\omega = 2\pi\nu$ - angular frequency. Thus, $\left\langle \frac{d^2V}{dx^2} \right\rangle_x = -\mu\omega_{TS}^2$ and the eq. 5 is transformed into:

$$\Delta F_{quant} = -\frac{(\hbar\omega_{TS})^2}{24kT} . \tag{5}$$

In the ideal gas approximation $G = F + nRT$, therefore the $\Delta F_{quant} = \Delta G_{quant}$.[1] The substitution of the $\Delta G_{TS,quant}$ into the eq. 1 that lacks χ gives:

$$\tau^{-1} = \frac{kT}{h}\exp\left(-\frac{\Delta G_0^{\ddagger} + \Delta G_{TS}}{kT}\right) = \frac{kT}{h}\exp\left(-\frac{\Delta G_0^{\ddagger}}{kT}\right)\underbrace{\exp\left(\frac{1}{24}\left(\frac{\hbar\omega_{TS}}{kT}\right)^2\right)}_{\chi} .$$

Q.E.D.

5 The explanation of the low-temperature estimation formula

Let us consider a simplest model (see Fig. 1).

- A trial energy levels are given. They are described by the one-dimensional harmonic oscillator model with the frequency ν_{ES}.
- The population on these levels is given by the Boltzmann distribution. Therefore for the n-th level

$$w_n = \frac{\exp\left(-\frac{E_n}{kT}\right)}{z_{HO}} , \tag{6}$$

where w_n - is the population, $E_n = h\nu_{ES}(n+1/2)$, and z_{HO} - is the harmonic oscillator partition function:[3]

$$z_{HO} = \frac{\exp\left(-\frac{h\nu_{ES}}{kT}\right)}{1-\exp\left(-\frac{h\nu_{ES}}{kT}\right)} .$$

- A barrier is approximated by the inverted parabola potential (see Eq. 4) with the height of E_{BH} and the curvature that corresponds to the imaginary frequency with the absolute value ν_{TS}.
- The height of the barrier is sufficient for the application of quasi-classical tunneling probability formula:[4,5]

$$p(E) = \exp\left(\frac{4\pi\sqrt{2\mu}}{h}\int_{x_1}^{x_2} dx\sqrt{V(x)-E}\right) ,$$

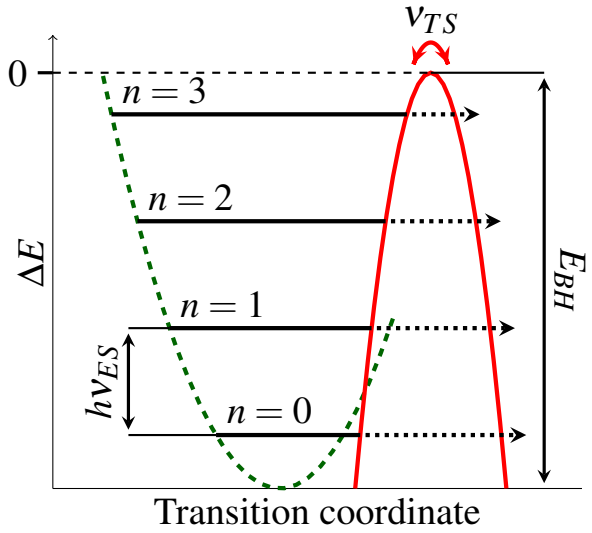
where E is the full energy of the system, μ is the reduced mass, V - potential function, x - tunneling coordinate. In the case of the inverted parabola this expression takes the form:

$$p(E) = \exp\left(2\pi\frac{\Delta E}{h\nu_{TS}}\right) , \tag{7}$$

where $\Delta E = E - E_{BH}$.

- The frequency of system stumbling to the barrier is ν_{ES}.

Figure 1. The illustration of the model used



The passing of the system trough the barrier in this model at at the temperature T can be described as the first-order reaction with the half-time given as:[4]

$$\tau_T^{-1} = \nu_{ES}\langle p\rangle_T = \nu_{ES}\sum_{n=0}^{\infty} p(E_n)w_n = \nu_{ES}\exp\left(\pi\left(\frac{\nu_{ES}}{\nu_{TS}}-\frac{2E_{BH}}{h\nu_{TS}}\right)\right)\left(\frac{\exp\left(-\frac{h\nu_{ES}}{kT}\right)}{1-\exp\left(\frac{2\pi\nu_{ES}}{\nu_{TS}}-\frac{h\nu_{ES}}{kT}\right)}\right) . \tag{8}$$

During the summation a condition for the convergence of the row appears: $\frac{2\pi\nu_{ES}}{\nu_{TS}} - \frac{h\nu_{ES}}{kT} < 0$. It can be rewritten as: $T < T_{cr} = \frac{h\nu_{TS}}{2\pi K}$. In the final equation 8 this condition still can be seen because if $T = T_{cr}$ the denominator turns to zero.
If the $T \to 0K$ then:

$$\tau_T^{-1} \xrightarrow[T\to 0]{} \nu_{ES}\exp\left(\pi\left(\frac{\nu_{ES}}{\nu_{TS}}-\frac{2E_{BH}}{h\nu_{TS}}\right)\right) = \tau_0^{-1} .$$

Therefore τ_0^{-1} - is the half-time of the system tunneling at the lowest-energy level.
In the general case of the inverted parabola barrier an analytic expression exists that cover both cases of tunneling and over-the-barrier reflection:[6]

$$p(E) = \frac{1}{1+\exp\left(-2\pi\frac{\Delta E}{h\nu_{TS}}\right)} \,. \tag{9}$$

This expression transforms to the eq. 7 if $\Delta E \to -\infty$. But, unfortunately it cannot be averaged over the temperature yielding the elementary function as the result.
To check the applicability of the experession 8 a set of numerical tests were made. The results of the analytic formula 8 were compared to those obtained numerically for the model with the usage of Eq. 9 to describe tunneling probability (see Tab. S46).

Table S46. The numerical tests of the equation 8 (**Appr.**) compared with the model having the tunneling described by the eq. 9 (**Ex.**). $T_{cr} = 23$ K, $\tau_\infty^{-1} = \nu_{ES} = \nu_{TS} = 100\ \text{cm}^{-1} = 3.0 \cdot 10^{12}$ Hz

	τ_T^{-1}, [Hz]							
E_{BH}	100 cm^{-1}		500 cm^{-1}		1000 cm^{-1}		1500 cm^{-1}	
T[K]	Ex.	Appr.	Ex.	Appr.	Ex.	Appr.	Ex.	Appr.
0.0	$1.2{\cdot}10^{11}$	$1.3{\cdot}10^{11}$	1.6	1.6	$3.6{\cdot}10^{-14}$	$3.6{\cdot}10^{-14}$	$8.1{\cdot}10^{-28}$	$8.1{\cdot}10^{-28}$
5.0	$1.2{\cdot}10^{11}$	$1.3{\cdot}10^{11}$	1.6	1.6	$3.6{\cdot}10^{-14}$	$3.6{\cdot}10^{-14}$	$8.1{\cdot}10^{-28}$	$8.1{\cdot}10^{-28}$
10.0	$1.2{\cdot}10^{11}$	$1.3{\cdot}10^{11}$	1.6	1.6	$3.6{\cdot}10^{-14}$	$3.6{\cdot}10^{-14}$	$8.1{\cdot}10^{-28}$	$8.1{\cdot}10^{-28}$
15.0	$1.2{\cdot}10^{11}$	$1.3{\cdot}10^{11}$	1.6	1.6	$3.7{\cdot}10^{-14}$	$3.7{\cdot}10^{-14}$	$8.4{\cdot}10^{-28}$	$8.4{\cdot}10^{-28}$
20.0	$1.2{\cdot}10^{11}$	$2.2{\cdot}10^{11}$	2.5	2.6	$5.8{\cdot}10^{-14}$	$6.0{\cdot}10^{-14}$	$1.3{\cdot}10^{-27}$	$1.4{\cdot}10^{-27}$
25.0	$1.3{\cdot}10^{11}$		28.2		$9.6{\cdot}10^{-12}$		$3.1{\cdot}10^{-24}$	

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