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

Supporting information

Salt-Induced Thermochromism of a Conjugated Polyelectrolyte

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1. Stationary absorption spectra of CPT in PBS at different concentrations

Figure S1 shows the normalized absorption spectra of CPT in PBS buffer solution at different concentrations at four temperatures (5, 25, 40 and 55°C). The shape is almost completely independent from the concentration in the investigated range.

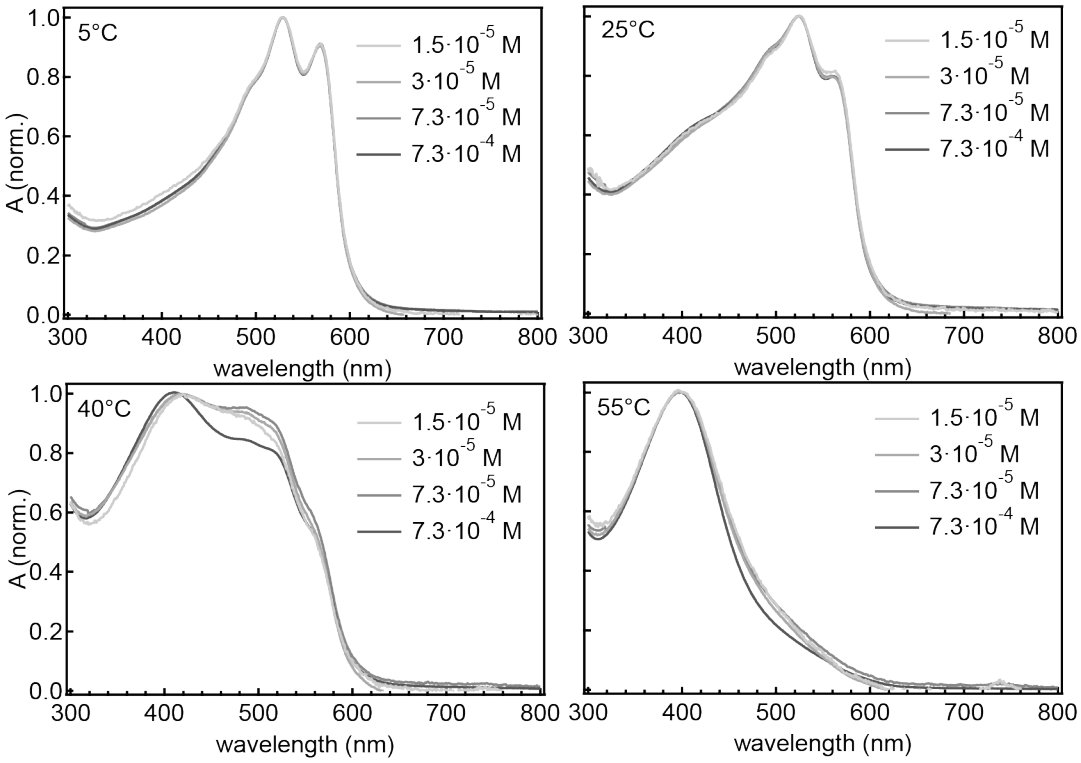

Figure S1 Normalized absorption spectra of CPT in PBS at different monomeric concentrations (from $1.5 \cdot 10^{-5}$ M to $7.3 \cdot 10^{-4}$ M) at four different temperatures (5, 25, 40 and 55°C)

2. Solvatochromism of CPT in various solvents

Figure S2 shows the stationary absorption spectra of CPT at room temperature in various solvents and solvent mixtures. The absorption is red shifted for solvents with higher refractive index, pointing to a predominant effect due to dispersion interactions.

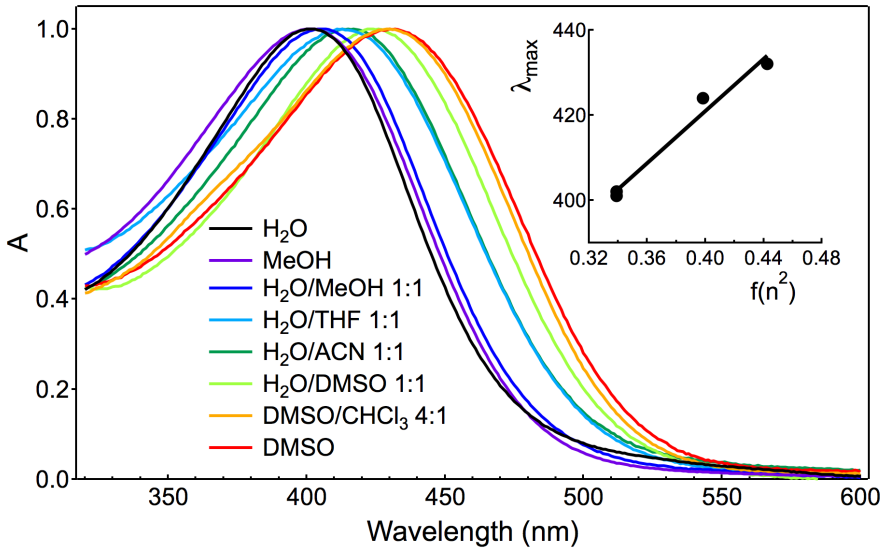

Figure S2 Normalized absorption spectra of CPT in various solvents and solvent mixtures at room temperature. The inset shows the absorption maximum as a function of the solvent Onsager refractive index function $f(n^2) = 2(n^2-1)/(2n^2+1)$, for H_2O (n=1.33), MeOH (n=1.33), H_2O/DMSO (n=1.41) and DMSO (n=1.48).

3. Stationary absorption spectra of CPT in different aqueous salt solutions

Figure S3 shows the absorption spectra of CPT at room temperature in pure water, in PBS and in different salt solutions. The main effect on the red-shifted absorption of CPT in PBS is due to the Cl^- anions present in the buffer.

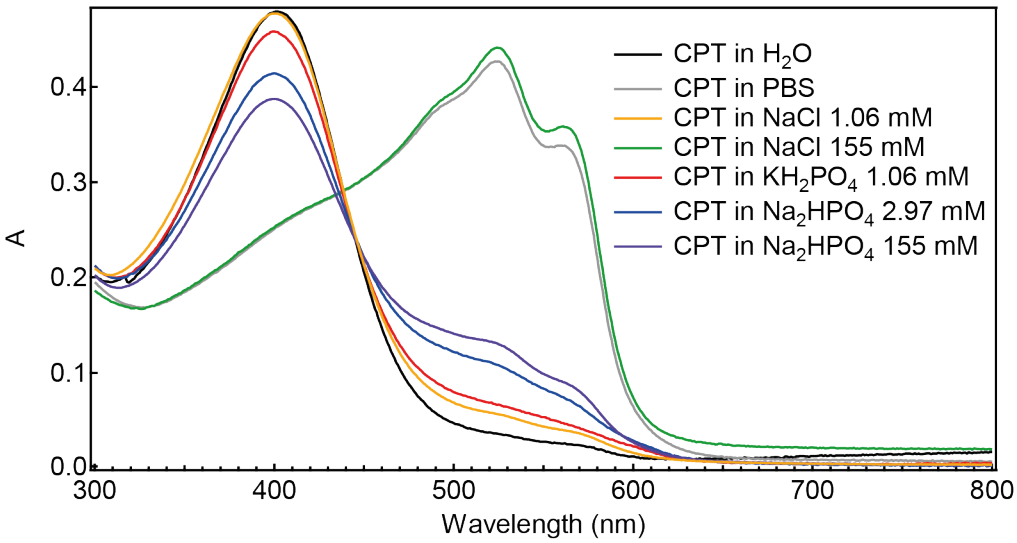

Figure S3 Absorption spectra of CPT ($7.3 \cdot 10^{-5}$ M, monomeric basis) at 25°C in water, in PBS and in different aqueous salt solutions.

4. Stationary absorption spectra of CPT in PBS for different temperature ranges

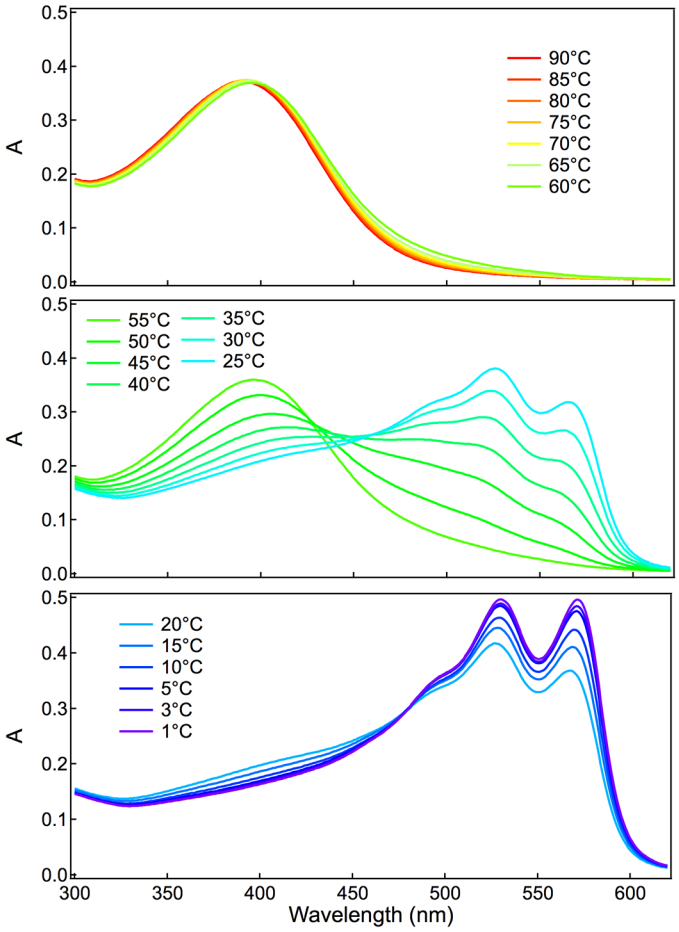

Figure S4 Absorption spectra of CPT ($7.3 \cdot 10^{-5}$ M, monomeric basis) in PBS at different temperatures between 1°C and 90°C, shown for clarity for different temperature ranges.

5. Stationary absorption spectra of CPT in PBS: increasing and decreasing temperature

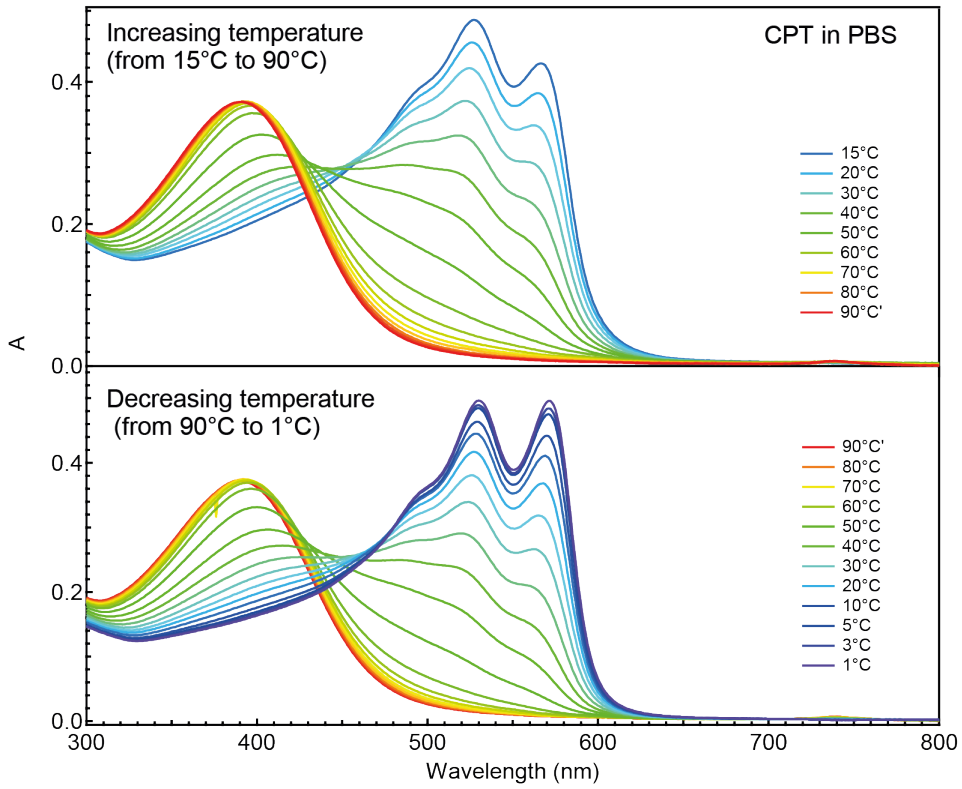

Figure S5 Absorption spectra of CPT in PBS ($7.3 \cdot 10^{-5}$ M, monomeric basis). Top: upon heating from 15 to 90°C. Bottom: upon cooling from 90 to 1°C.

6. Stationary absorption spectra of CPT in pure water, with decreasing temperature

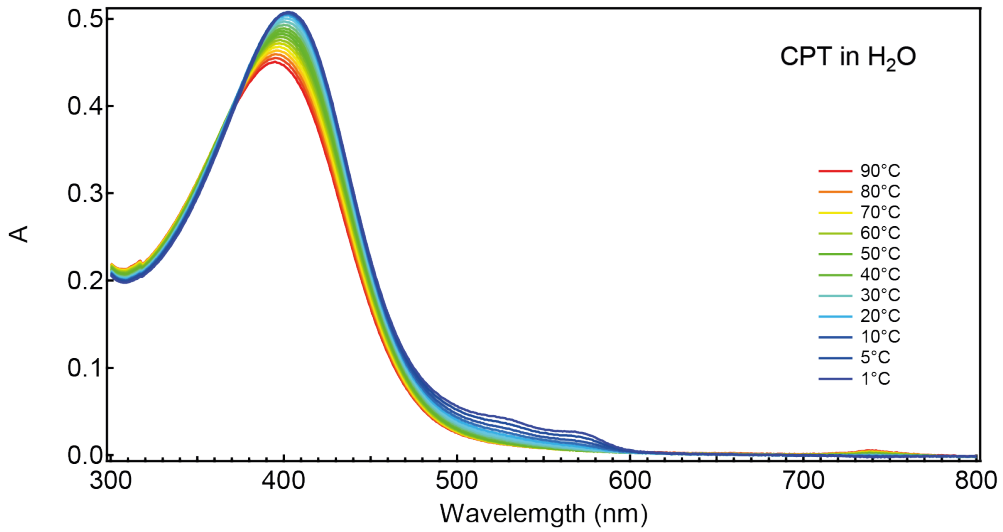

Figure S6 Absorption spectra of CPT in pure water ($7.3 \cdot 10^{-5}$ M, monomeric basis) upon decreasing temperature from 90 to 1°C.

7. Resonance Raman spectra

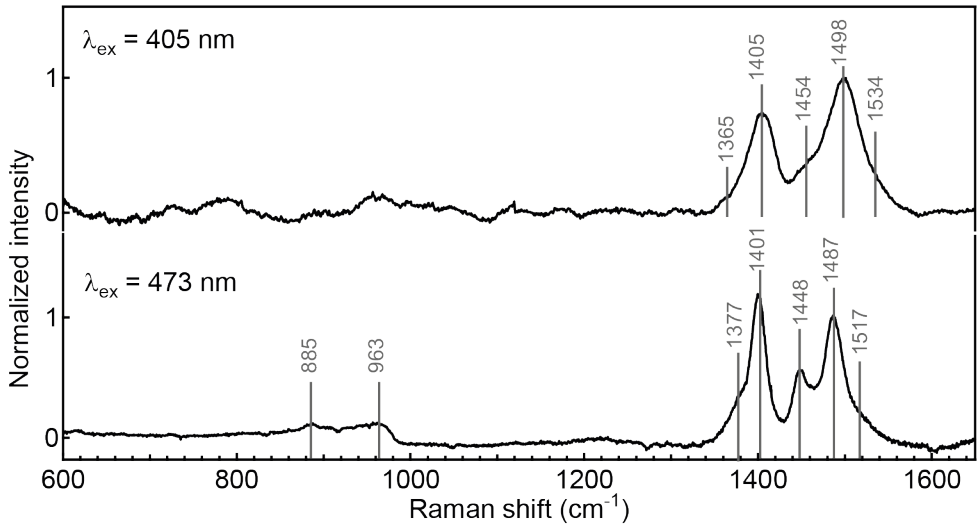

Figure S7 Experimental Resonance Raman spectra of CPT in PBS solution ($1.5 \cdot 10^{-4}$ M, monomeric basis) at room temperature excited at 405 nm and 473 nm. They are shown over an extended range compared to the main text.

8. Computed Raman spectra and coordinates for the optimized and scan structures

8.1 Computed Raman Spectra

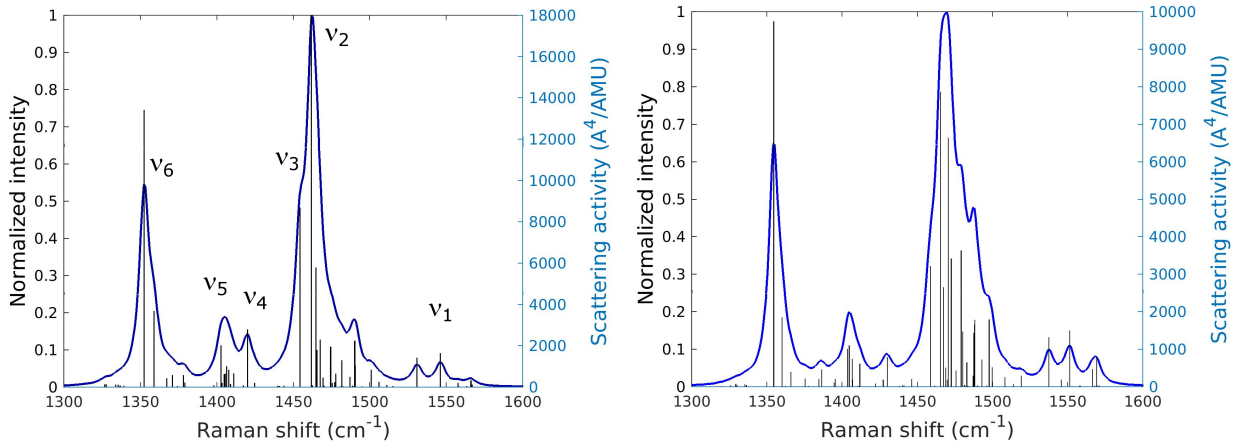

Figure S8.1: Raman spectra featuring both individual and convoluted (4 cm^{-1}) vibrational modes of CPT scan at θ=0° (left) and θ=20° (right), computed at the B3LYP-D3(BJ)/6-31G* level, applying the 0.97 scaling factor for B3LYP.

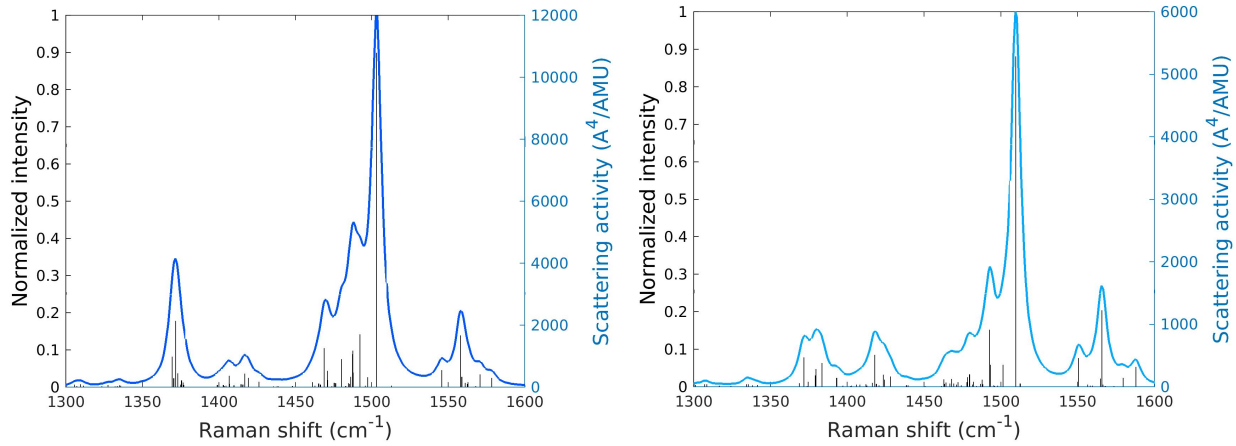

Figure S8.2: Raman spectra featuring both individual and convoluted (4 cm^{-1}) vibrational modes of CPT scan at θ=40° (left) and θ=60° (right), computed at the B3LYP-D3(BJ)/6-31G* level, applying the 0.97 scaling factor for B3LYP.

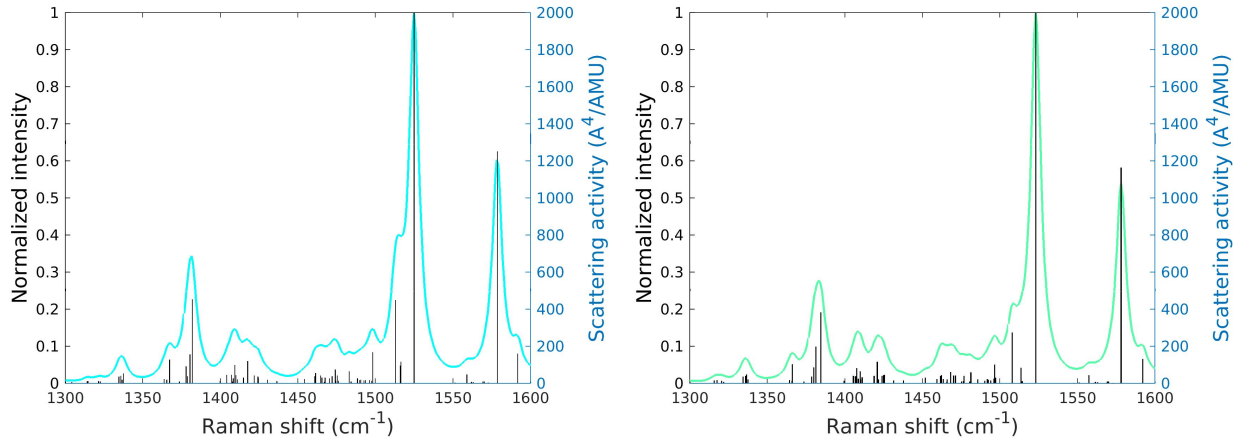

Figure S8.3: Raman spectra featuring both individual and convoluted (4 cm^{-1}) vibrational modes of CPT scan at θ=80° (left) and θ=90° (right), computed at the B3LYP-D3(BJ)/6-31G* level, applying the 0.97 scaling factor for B3LYP.

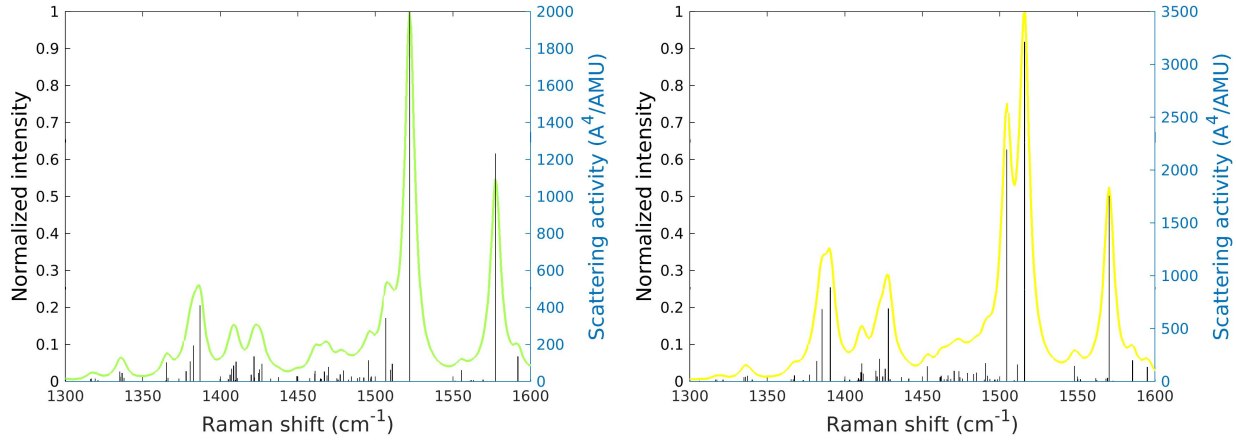

Figure S8.4: Raman spectra featuring both individual and convoluted (4 cm^{-1}) vibrational modes of CPT scan at θ=100° (left) and θ=120° (right), computed at the B3LYP-D3(BJ)/6-31G* level, applying the 0.97 scaling factor for B3LYP.

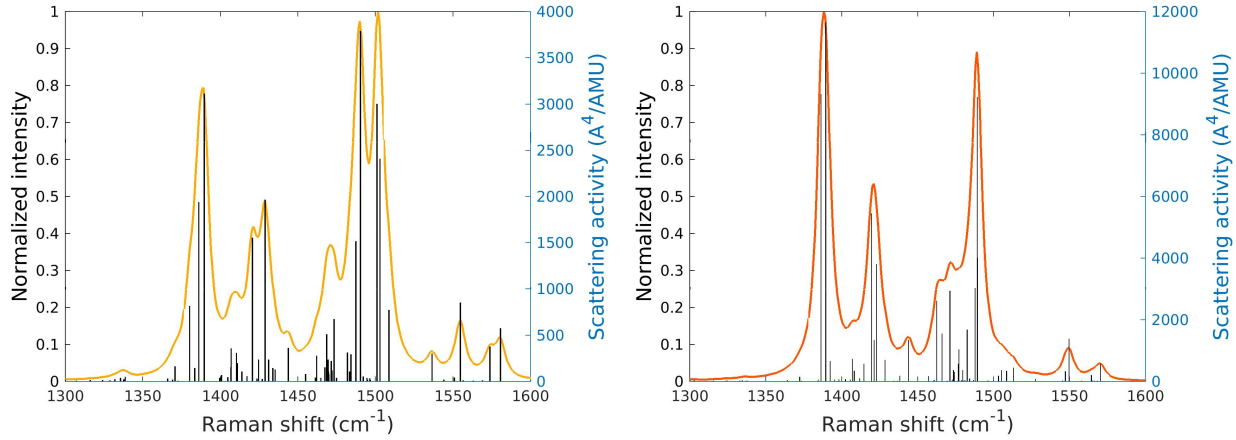

Figure S8.5: Raman spectra featuring both individual and convoluted (4 cm^{-1}) vibrational modes of CPT scan at θ=140° (left) and θ=160° (right), computed at the B3LYP-D3(BJ)/6-31G* level, applying the 0.97 scaling factor for B3LYP.

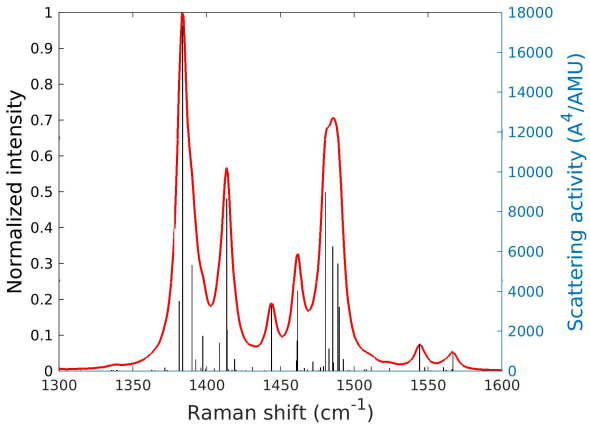

Figure S8.6: Raman spectrum featuring both individual and convoluted (4 cm^{-1}) vibrational modes of CPT scan at θ=180°, computed at the B3LYP-D3(BJ)/6-31G* level, applying the 0.97 scaling factor for B3LYP.

8.2 Optimized structures

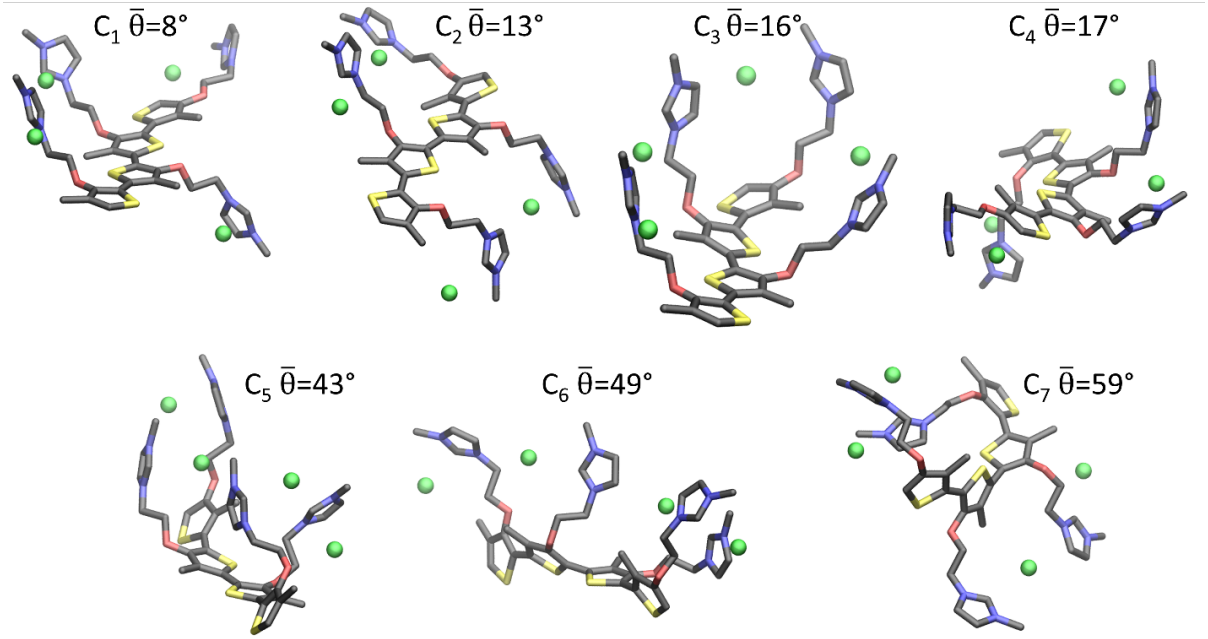

Figure S8.7: 3D representations of geometries optimized at the B3LYP-D3(BJ)/6-31G*. Starting geometries were randomly generated with seven distinct θ dihedral angles. Only the mean dihedral angle, mapped in the [0,90] range, is shown.

8.3 Coordinates of dihedral scan

Geometries optimized at the B3LYP-D3(BJ)/6-31G(d) level with all three θ=∠SCCS angles frozen at the angle corresponding to output name (20.log means θ =20°)

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118
0.log  Energy: -3690946.1754128 Ha
C          -6.62434       -4.03393       -0.60993
C          -5.85475       -2.84884       -0.87374
C          -5.81208       -5.09500       -0.33044
C          -4.47748       -3.01951       -0.84969
S          -4.12988       -4.69263       -0.40317
H          -6.11017       -6.10894       -0.10072
C          -8.12473       -4.07866       -0.64489
H          -8.56524       -3.80644        0.32525
H          -8.47344       -5.08700       -0.88788
H          -8.50926       -3.39218       -1.40768
O          -6.47801       -1.65901       -1.15097
C          -7.08687       -1.01516       -0.02598
C          -8.22872       -0.17191       -0.59023
H          -6.35188       -0.37445        0.47807
H          -7.45821       -1.75618        0.69119
N          -9.03313        0.39014        0.50300
H          -8.87387       -0.79954       -1.20981
H          -7.84477        0.66334       -1.17991
C          -9.71515       -0.35825        1.38153
N         -10.27945        0.46488        2.27134
C          -9.95629        1.77551        1.94484
C          -9.16769        1.73146        0.83329
H          -8.65856        2.49131        0.25017
H         -10.31134        2.60973        2.52842
H          -9.73224       -1.45847        1.48776
C         -11.06064       -0.00628        3.41639
H         -10.87290       -1.08118        3.52052
H         -12.12382        0.18672        3.24895
H         -10.72720        0.51972        4.31385
C          -3.26681       -0.79221       -1.46113
C          -1.90493       -0.33910       -1.48926
C          -3.36770       -2.08847       -0.97449
C          -0.93938       -1.27529       -1.15834
S          -1.76129       -2.74531       -0.65969
C          -4.35691        0.08601       -2.01243
H          -4.92584        0.61928       -1.24171
H          -5.07803       -0.49095       -2.58865
H          -3.91014        0.84131       -2.66503
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C          -2.03304        3.26819       -1.55774
H          -1.11236        1.95567       -0.09306
H          -2.86021        1.67641       -0.34798
N          -2.70856        4.25100       -0.70054
H          -2.63485        3.14385       -2.46020
H          -1.04858        3.66445       -1.81056
C          -4.04050        4.36927       -0.60639
N          -4.30758        5.30530        0.31186
C          -3.11129        5.79372        0.81752
C          -2.10260        5.12910        0.18638
H          -1.02079        5.16662        0.26490
H          -3.08811        6.56399        1.57162
H          -4.81661        3.79436       -1.12503
C          -5.65689        5.72617        0.69488
H          -6.36829        5.05605        0.20131
H          -5.82113        6.75973        0.37910
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C	2.90086	-2.01595	-0.62336
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C	1.24629	0.95728	-2.25986
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H	2.16870	1.18941	-2.80072
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H	3.15030	1.55404	-0.20165
N	5.20587	3.19378	-0.13149
H	4.80217	2.33434	-1.99416
H	6.11113	1.56744	-1.05178
C	4.21758	4.08695	0.00860
N	4.59430	4.98118	0.92847
C	5.86249	4.64949	1.38519
C	6.24791	3.52115	0.72327
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H	6.36780	5.23916	2.13312
H	3.22520	4.07398	-0.45436
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H	4.16454	7.03988	0.98473
H	3.74373	6.12327	2.46072
H	2.74842	5.93224	0.98514
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C	6.15828	-3.59948	0.35437
C	4.05089	-2.68574	-0.04177
C	5.42288	-4.46323	1.11158
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C	6.06334	-1.77179	-1.41769
H	5.38433	-1.57072	-2.24527
H	6.93184	-2.32040	-1.79990
H	6.42878	-0.80981	-1.04172
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N	10.57858	-1.78950	0.71825
H	9.62806	-2.72919	-0.87594
H	10.11629	-3.80799	0.43945
C	10.79160	-0.61308	0.11683
N	11.53066	0.15295	0.92829
C	11.74937	-0.53751	2.11000
C	11.15442	-1.75433	1.98066
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H	12.31103	-0.10582	2.92254
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H	12.36310	1.69145	-0.23841
H	12.36769	1.96668	1.52133
H	10.82063	2.07101	0.60090
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Cl	1.08129	4.31700	-0.30023
Cl	8.40559	0.98616	0.15093

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20.log Energy: -3690927.6898623 Ha
C          -4.90789       -4.93108        0.95826
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C          -3.38524       -3.12227        0.64771
S          -2.62441       -4.13369        1.87995
H          -3.87974       -6.16137        2.45922
C          -6.11722       -5.76797        0.65468
H          -7.00135       -5.47743        1.23919
H          -5.91444       -6.82079        0.87314
H          -6.37716       -5.68641       -0.40696
O          -5.45713       -3.16942       -0.64714
C          -6.68361       -2.64923       -0.10962
C          -7.57490       -2.33485       -1.31070
H          -6.48348       -1.73846        0.46714
H          -7.15664       -3.38006        0.55425
N          -8.94581       -2.04298       -0.86878
H          -7.59521       -3.19666       -1.98337
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C         -10.85837       -1.01984       -0.48806
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H         -11.70241       -0.35301       -0.41534
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H         -11.47450       -3.67284        1.51112
H         -12.72571       -3.25215        0.28215
H         -12.32663       -2.09698        1.58647
C          -2.97479       -0.80145       -0.47603
C          -1.84035        0.04897       -0.69952
C          -2.62348       -1.98208        0.15670
C          -0.61218       -0.46002       -0.30961
S          -0.88121       -2.04020        0.41462
C          -4.34123       -0.40382       -0.95305
H          -4.99328       -0.05711       -0.14150
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H          -8.26849        5.15666       -0.97387
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S          2.01558       -1.22343       -0.28292
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H          2.35366        3.31998        0.81271
N          3.31611        5.78805        0.64124
H          2.97735        4.78330       -1.15285
H          4.65823        4.77973       -0.59827
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C          3.47385        7.31402        2.22839
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H          3.77128        8.01866        2.98854
H          1.12224        5.90010        0.44150
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H          1.06680        8.94348        2.11304
H          0.97790        7.77768        3.46797
H          0.09190        7.44226        1.94438
C          5.87609        0.05355        0.01156
C          6.99511       -0.81096       -0.23269
C          4.68990       -0.51635       -0.41295
C          6.67569       -2.02176       -0.78725
S          4.96724       -2.13507       -1.05289
H          7.32537       -2.84707       -1.04336
C          6.04460        1.35305        0.74009
H          6.02298        2.21119        0.05949
H          7.00237        1.36023        1.26707
H          5.24516        1.48683        1.47623
O          8.24575       -0.37658        0.11766
C          9.29536       -1.29080       -0.17188
C         10.54720       -0.72356        0.49278
H          9.44054       -1.38105       -1.25664
H          9.08620       -2.29360        0.21034
N         11.73617       -1.48196        0.10942
H         10.45001       -0.75181        1.58113
H         10.70272        0.31705        0.19600
C         12.08206       -2.68124        0.61276
N         13.15901       -3.12474       -0.05888
C         13.40652       -2.25659       -1.11345
C         12.52297       -1.23156       -1.01041
H         12.38921       -0.34395       -1.60711
H         14.19304       -2.44484       -1.82605
H         11.68293       -3.11654        1.51054
C         13.65962       -4.49107        0.06025
H         13.93692       -4.69393        1.09705
H         14.53907       -4.59741       -0.57591
H         12.85074       -5.16139       -0.25263
Cl        -9.32610       -4.91537        2.14599
Cl        -7.30756        1.23781       -2.22709
Cl        -0.99238        5.67333        0.42283
Cl        10.30121       -4.47382       -0.29519

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40.log Energy: -3690959.4860809 Ha
C         -6.79200       -3.71230       -0.22063
C         -5.90841       -2.58171       -0.07514
C         -6.20670       -4.85101        0.25983
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C	-8.13596	-3.67018	-0.89182
H	-8.94587	-3.31283	-0.24071
H	-8.41866	-4.66996	-1.23469
H	-8.10173	-3.01491	-1.77083
O	-6.18038	-1.33786	-0.57712
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C	-7.92397	0.13477	-1.21845
H	-7.04240	0.01002	0.73949
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N	-9.07950	0.90131	-0.73896
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H	-7.17984	0.84253	-1.58793
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C	-10.32322	2.48729	0.14830
C	-9.09092	2.24270	-0.38131
H	-8.20391	2.85133	-0.51426
H	-10.75512	3.39103	0.54734
H	-10.53126	-0.72604	-0.43499
C	-12.37032	1.02928	0.64084
H	-13.12740	1.39410	-0.05883
H	-12.47859	1.53928	1.60049
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C	-3.37665	-0.78606	1.19877
C	-2.00679	-0.36197	1.22742
C	-3.50511	-2.04962	0.65726
C	-1.09827	-1.28015	0.73599
S	-1.94348	-2.71858	0.20052
C	-4.49469	0.03377	1.76800
H	-4.13028	0.63244	2.60941
H	-5.29688	-0.61730	2.12740
H	-4.92015	0.72091	1.02594
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C	-1.18435	1.99774	-0.34418
H	-1.59798	2.85083	1.59144
H	-3.01597	2.07052	0.82730
N	-1.60788	3.14739	-1.15524
H	-1.39567	1.08412	-0.90459
H	-0.11293	2.09038	-0.16676
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C	-1.69859	5.14639	-2.07602
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H	0.08819	4.43913	-0.90907
H	-1.53919	6.14715	-2.44380
H	-3.66013	2.58505	-1.62500
C	-4.08968	4.99802	-2.95203
H	-4.95525	4.46675	-2.54283
H	-4.01161	4.84790	-4.03236
H	-4.17293	6.06427	-2.73337
C	1.26447	-0.75726	1.57267
C	2.60763	-0.96903	1.12066
C	0.34414	-1.19641	0.64028
C	2.72824	-1.56150	-0.12056
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H          4.66081        0.83532        2.85206
H          3.18373        1.34561        1.98966
N          5.28711        2.47383        0.76813
H          4.36597        0.86660       -0.20597
H          5.84944        0.47138        0.70303
C          4.39900        3.46713        0.63915
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C          6.35393        4.35384        1.19595
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H          7.37040        2.34618        1.27991
H          7.05012        5.14168        1.43530
H          3.31689        3.38403        0.48072
C          4.35570        5.92316        0.90559
H          4.63334        6.49343        0.01499
H          4.65578        6.47008        1.80184
H          3.27696        5.74101        0.92804
C          5.04956       -2.59146       -0.38343
C          5.96018       -2.87720       -1.45790
C          3.92678       -1.93406       -0.84490
C          5.54713       -2.45169       -2.69030
S          4.00156       -1.67379       -2.58781
H          6.04013       -2.60630       -3.63942
C          5.28129       -3.06138        1.02138
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H          4.33193       -3.24107        1.53109
O          7.10335       -3.63002       -1.27661
C          8.19002       -2.94337       -0.66618
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H          8.78496       -3.69651       -0.14010
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H         12.96642       -1.30926        0.49562
H          9.49953        0.43246       -1.18271
C         11.64987        1.20875        0.43928
H         11.65059        2.02642       -0.28460
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118
60.log Energy: -3690958.6247551 Ha
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C         -6.38402       -2.16281       -0.85668
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S         -5.79515       -4.47985        0.10124
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C	-7.42928	1.19887	-1.61786
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H	-8.22401	-0.48935	-0.52157
N	-8.46469	2.10420	-1.10457
H	-7.73581	0.84677	-2.60556
H	-6.49523	1.75853	-1.68466
C	-9.77529	1.82068	-1.12857
N	-10.41705	2.78976	-0.46626
C	-9.48984	3.71689	-0.00996
C	-8.25848	3.28432	-0.40288
H	-7.25329	3.64949	-0.22792
H	-9.78750	4.58630	0.55392
H	-10.27045	0.89468	-1.46503
C	-11.86226	2.78616	-0.23099
H	-12.35575	3.48318	-0.91399
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H	-12.21644	1.76103	-0.39328
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H	-3.50478	4.88939	-1.22399
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C	0.13663	-2.45718	3.18273
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O	3.00608	-2.34980	2.40427
C	3.48963	-1.08581	2.88833
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H          6.21647        3.03162        4.56539
H          5.65936        1.05957        0.87455
C          6.15626        3.64858        1.79335
H          6.74292        3.47631        0.88767
H          6.65921        4.37403        2.43478
H          5.14026        3.97456        1.55170
C          4.72002       -2.64537       -0.38375
C          5.89345       -1.96093       -0.84354
C          3.60784       -1.83604       -0.46926
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S          3.98956       -0.26394       -1.14326
H          6.37616        0.07981       -1.58024
C          4.74265       -4.03036        0.18906
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H          5.32541       -4.70681       -0.44510
H          3.72709       -4.41982        0.28867
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C          8.52591       -1.70761       -2.49757
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N          9.56513       -0.70379       -2.74343
H          7.62006       -1.38904       -3.01536
H          8.85023       -2.65877       -2.92569
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C         10.92520       -0.87193       -2.51764
H         11.35136       -1.84122       -2.31508
H         12.52823        0.66856       -2.53922
H          8.35817        1.04377       -3.10712
C         10.58836        2.71846       -2.92090
H         10.24769        3.11399       -3.88017
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H          9.95826        3.08739       -2.10436
Cl       -11.58145       -0.66878       -0.90232
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Cl         8.08842        1.83901       -0.64766

118
80.log Energy: -3690940.0238810 Ha
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C         -7.25828       -1.60360        4.14464
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H         -7.90393       -1.63491        5.01220
C         -8.30263       -3.51809        2.80575
H         -8.99967       -3.28556        1.99000
H         -8.88983       -3.71405        3.70768
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C         -6.70746       -3.49912       -1.18464
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N	-9.41445	-3.27706	-3.51837
C	-8.63554	-2.21704	-3.96418
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H	-6.62877	-1.57390	-3.25861
H	-8.96105	-1.57718	-4.76824
H	-9.12962	-4.72557	-1.94949
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C	-4.36245	-0.44112	1.75203
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H	-6.52110	0.71822	0.62634
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H	-3.36598	3.28925	0.28558
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H	-3.95282	3.48544	-2.13490
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C	1.60033	0.92400	0.67422
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H	-1.16352	2.29013	2.27289
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H	0.48008	2.26268	2.94919
O	2.51947	1.84586	1.09864
C	3.91436	1.62754	0.93299
C	4.34586	2.19241	-0.42546
H	4.18226	0.57719	1.02338
H	4.39228	2.16451	1.75556
N	5.72768	1.83391	-0.75945
H	4.23923	3.28176	-0.43716
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N	7.84164	1.38973	-0.57023

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H          9.69728        0.46719       -0.61524
H          8.97490        0.71166        1.02791
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H          7.86451       -3.99002        0.37868
H          7.27942       -2.85777        1.63144
C         10.15584       -2.46672       -0.00470
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C         10.94144       -1.48194        1.81808
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H          8.98039       -1.61935        2.88656
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H         13.11471       -2.50353       -0.21565
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Cl       -10.35699       -3.00390       -0.45098
Cl        -5.22178        4.93039        0.89824
Cl         6.87882       -0.12012        2.59309
Cl        10.02185       -0.94129       -2.66635

118
90.log Energy: -3690940.0825468 Ha
C         -7.32976        2.36593       -3.11076
C         -6.25681        2.04626       -2.21225
C         -7.40861        1.43546       -4.11065
C         -5.56992        0.89446       -2.51128
S         -6.21807        0.17589       -3.96951
H         -8.11498        1.41441       -4.92987
C         -8.21658        3.56483       -2.93877
H         -8.83577        3.48673       -2.03538
H         -8.88263        3.68305       -3.79845
H         -7.61626        4.47709       -2.84080
O         -5.91647        2.85105       -1.14998
C         -6.61467        2.52980        0.05304
C         -6.27235        3.64594        1.03655
H         -6.27743        1.55741        0.43554
H         -7.69937        2.50726       -0.09859
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H	-8.50871	5.09122	1.96550
C	-10.17281	4.02006	3.95228
H	-10.23610	5.08438	4.19021
H	-10.44163	3.43660	4.83361
H	-10.82208	3.78282	3.10194
C	-4.48674	-0.58175	-0.73745
C	-3.17046	-0.86300	-0.24602
C	-4.44784	0.32826	-1.76951
C	-2.15114	-0.22140	-0.90775
S	-2.80451	0.80951	-2.15762
C	-5.72326	-1.22759	-0.18552
H	-5.73032	-2.30870	-0.37835
H	-6.61944	-0.79389	-0.63612
H	-5.77765	-1.09617	0.90236
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C	-2.71134	-3.05070	0.46198
C	-2.74813	-3.84611	1.76438
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H	-3.48796	-3.43111	-0.21005
N	-2.68112	-5.27778	1.47853
H	-3.69356	-3.65132	2.27317
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C	0.16577	-1.22529	-1.20689
C	1.49924	-1.05662	-0.69847
C	-0.72056	-0.34294	-0.63904
C	1.62526	-0.06895	0.25933
S	0.06834	0.71436	0.50507
C	-0.17454	-2.23917	-2.25837
H	-1.23333	-2.18325	-2.52180
H	0.04581	-3.25840	-1.91742
H	0.42100	-2.07496	-3.16345
O	2.44065	-1.90108	-1.22411
C	3.82592	-1.57126	-1.17097
C	4.45833	-2.38404	-0.03616
H	3.99102	-0.50513	-1.03289
H	4.24291	-1.84983	-2.14224
N	5.84018	-1.98242	0.24222
H	4.43078	-3.45268	-0.27160
H	3.89320	-2.21531	0.87989
C	6.76397	-1.65611	-0.67391
N	7.89092	-1.33271	-0.03097
C	7.69338	-1.44848	1.33602
C	6.40465	-1.85696	1.50641
H	5.82740	-2.03893	2.39686
H	8.47209	-1.14590	2.02812
H	6.60815	-1.53203	-1.73576

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C          9.10853       -0.85082       -0.68915
H          9.68205       -1.70086       -1.06873
H          9.69071       -0.31037        0.06244
H          8.79888       -0.19956       -1.51017
C          3.67190        1.41603        0.61235
C          4.70363        1.60950        1.59662
C          2.78383        0.43846        0.99245
C          4.58235        0.81834        2.70476
S          3.19109       -0.21160        2.58588
H          5.22799        0.80441        3.57158
C          3.61485        2.18953       -0.66953
H          2.64108        2.07119       -1.15163
H          4.39228        1.85331       -1.37032
H          3.78518        3.25377       -0.47357
O          5.70153        2.53241        1.41876
C          6.87216        2.01777        0.76233
C          7.37298        3.14218       -0.14066
H          6.62242        1.15771        0.13678
H          7.62148        1.72678        1.50917
N          8.72933        2.86419       -0.63149
H          7.38503        4.08852        0.40680
H          6.72672        3.22791       -1.01379
C          9.81067        2.74549        0.15181
N         10.85592        2.43208       -0.62157
C         10.42573        2.34547       -1.93899
C          9.08862        2.60888       -1.94589
H          8.34129        2.54630       -2.72278
H         11.10123        2.09221       -2.73986
H          9.83152        2.76821        1.23236
C         12.19020        2.12428       -0.10409
H         12.76418        3.04354        0.03796
H         12.69920        1.48338       -0.82545
H         12.05781        1.59123        0.84360
Cl        -9.98575        3.51692        0.55026
Cl        -5.36497       -5.15646       -0.45998
Cl         6.45320        0.75755       -2.58936
Cl        10.16418        0.62786        2.35164

118
100.log      Energy: -3690940.0178192 Ha
C         -7.19400       -2.44436        3.09576
C         -6.08101       -2.07971        2.26717
C         -7.54166       -1.40315        3.91271
C         -5.62717       -0.79321        2.43101
S         -6.55493        0.01035        3.67858
H         -8.34217       -1.38113        4.64022
C         -7.85906       -3.78836        3.03007
H         -8.33752       -3.95501        2.05594
H         -8.62387       -3.88317        3.80643
H         -7.12478       -4.59036        3.17040
O         -5.50160       -2.95701        1.38026
C         -6.05328       -2.86820        0.06594
C         -5.39704       -3.99144       -0.73269
H         -5.82050       -1.88887       -0.37337
H         -7.13823       -3.02120        0.07264
N         -6.05591       -4.12854       -2.03101
H         -5.52284       -4.93179       -0.19344
H         -4.32889       -3.81295       -0.88321
C         -7.01375       -5.03348       -2.29045
N         -7.56019       -4.74261       -3.48239
C         -7.01138       -3.55096       -3.93834
C         -6.07123       -3.16696       -3.03658
H         -5.40856       -2.31705       -3.01748
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H	-7.33422	-3.09820	-4.86174
H	-7.21575	-5.91096	-1.70506
C	-8.78743	-5.37168	-3.96333
H	-8.62740	-6.44339	-4.10257
H	-9.06011	-4.92051	-4.91801
H	-9.55953	-5.19790	-3.20504
C	-4.58354	0.71376	0.65667
C	-3.27139	1.08186	0.21598
C	-4.52216	-0.16366	1.71631
C	-2.23648	0.53984	0.94030
S	-2.86603	-0.51218	2.18539
C	-5.83883	1.22958	0.01741
H	-5.97388	2.30374	0.20095
H	-6.71459	0.70136	0.40280
H	-5.79783	1.09706	-1.07041
O	-3.05982	1.89410	-0.87379
C	-2.94593	3.27736	-0.53423
C	-2.87999	4.02053	-1.86630
H	-2.03317	3.44360	0.05439
H	-3.81816	3.62880	0.02793
N	-2.99642	5.46059	-1.64766
H	-3.72292	3.70862	-2.48529
H	-1.95218	3.80735	-2.40453
C	-4.14333	6.14729	-1.78908
N	-3.95547	7.38815	-1.30836
C	-2.69463	7.44827	-0.72850
C	-2.09326	6.24972	-0.94145
H	-1.11355	5.88846	-0.67449
H	-2.34372	8.33890	-0.23289
H	-5.00259	5.81427	-2.34053
C	-5.05444	8.32380	-1.08660
H	-5.54311	8.55500	-2.03588
H	-4.65122	9.24112	-0.65613
H	-5.76287	7.84088	-0.40432
C	0.08569	1.47462	1.41536
C	1.41928	1.37352	0.89250
C	-0.80950	0.72189	0.69364
C	1.53673	0.57343	-0.22656
S	-0.02570	-0.13069	-0.61566
C	-0.25139	2.30395	2.61856
H	-1.32093	2.25405	2.83557
H	0.02710	3.35350	2.46584
H	0.29880	1.95629	3.50046
O	2.38807	2.08791	1.54809
C	3.73445	1.61174	1.57165
C	4.57987	2.62279	0.79073
H	3.82683	0.61413	1.14724
H	4.03746	1.55956	2.62164
N	5.93297	2.13524	0.50894
H	4.64090	3.57312	1.33038
H	4.10541	2.80128	-0.17358
C	6.71710	1.44613	1.35094
N	7.86579	1.17570	0.72138
C	7.82498	1.69838	-0.56147
C	6.61002	2.30083	-0.69364
H	6.15073	2.80185	-1.52886
H	8.63753	1.50827	-1.25515
H	6.44071	1.05143	2.31776
C	8.95480	0.37715	1.29075
H	9.56708	1.00419	1.94459
H	9.55569	0.00788	0.45527
H	8.49823	-0.43839	1.85727
C	3.48977	-0.90429	-0.93451

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C          4.58723       -0.86503       -1.86442
C          2.70261        0.21790       -1.03157
C          4.61292        0.24549       -2.66139
S          3.28443        1.30229       -2.29968
H          5.33126        0.47869       -3.43463
C          3.28708       -2.02437        0.03991
H          2.28413       -1.98947        0.47199
H          4.01848       -1.96544        0.85814
H          3.42208       -2.98929       -0.46085
O          5.51013       -1.87642       -1.92968
C          6.65168       -1.69422       -1.07461
C          6.97471       -3.07526       -0.50936
H          6.41483       -1.02746       -0.24192
H          7.48818       -1.28228       -1.65286
N          8.29455       -3.08983        0.13508
H          6.96648       -3.82156       -1.30832
H          6.24207       -3.34036        0.25230
C          9.45179       -2.86166       -0.50171
N         10.43899       -2.88983        0.40033
C          9.89292       -3.14331        1.65151
C          8.54505       -3.26126        1.48785
H          7.73487       -3.35292        2.19553
H         10.50608       -3.20060        2.53616
H          9.57477       -2.57161       -1.53620
C         11.83654       -2.58464        0.08965
H         12.35548       -3.48443       -0.25063
H         12.31524       -2.20611        0.99401
H         11.83734       -1.81075       -0.68546
Cl        -9.10416       -4.52146       -0.63604
Cl        -5.86979        5.15572        0.00707
Cl         6.02042       -1.37480        2.43474
Cl        10.18110       -0.26834       -1.98389

118
c1_120.log   Energy: -3690941.5774877 Ha
C         -7.06827       -2.88987        2.59253
C         -5.88554       -2.38076        1.96623
C         -7.92973       -1.86801        2.88862
C         -5.87689       -1.02235        1.74236
S         -7.33433       -0.30829        2.40123
H         -8.90460       -1.94598        3.35135
C         -7.29223       -4.35307        2.84172
H         -7.31308       -4.91888        1.90112
H         -8.23827       -4.52029        3.36471
H         -6.48267       -4.77149        3.45122
O         -4.82827       -3.19525        1.63437
C         -4.80241       -3.56294        0.25406
C         -3.59899       -4.49042        0.10491
H         -4.68730       -2.66825       -0.37222
H         -5.71263       -4.10355       -0.02866
N         -3.63883       -5.14975       -1.19980
H         -3.65216       -5.26427        0.87246
H         -2.65332       -3.95258        0.21252
C         -4.14643       -6.37661       -1.40013
N         -4.25011       -6.58155       -2.72320
C         -3.89862       -5.40879       -3.37903
C         -3.51450       -4.51465       -2.43129
H         -3.15656       -3.50103       -2.51191
H         -3.94504       -5.32717       -4.45285
H         -4.32962       -7.10807       -0.63539
C         -4.98138       -7.71016       -3.29313
H         -4.48729       -8.64800       -3.02849
H         -4.99657       -7.60353       -4.37834
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H	-5.99477	-7.68239	-2.87631
C	-4.84556	0.65095	0.10872
C	-3.56195	1.23115	-0.13442
C	-4.79645	-0.24598	1.15614
C	-2.56172	0.84315	0.72913
S	-3.18504	-0.34149	1.85671
C	-6.05480	0.99981	-0.70810
H	-6.42446	2.00557	-0.46692
H	-6.86346	0.28517	-0.53849
H	-5.80096	1.00043	-1.77417
O	-3.33695	2.08712	-1.18788
C	-3.45809	3.46587	-0.82976
C	-3.40219	4.23754	-2.14598
H	-2.63007	3.75468	-0.16773
H	-4.41495	3.66769	-0.33562
N	-3.74785	5.63998	-1.92204
H	-4.13885	3.81732	-2.83281
H	-2.41459	4.17675	-2.61136
C	-4.97778	6.14682	-2.11222
N	-5.00460	7.39221	-1.60926
C	-3.79347	7.63650	-0.97489
C	-3.00677	6.54704	-1.17068
H	-1.99533	6.33536	-0.86408
H	-3.60464	8.56313	-0.45752
H	-5.75601	5.68951	-2.69416
C	-6.24292	8.14546	-1.42965
H	-6.71152	8.32846	-2.39937
H	-6.00587	9.09953	-0.95758
H	-6.90264	7.54012	-0.79777
C	-0.31729	1.61506	1.66757
C	1.03477	1.75284	1.21785
C	-1.15369	1.19617	0.65505
C	1.23534	1.46087	-0.11557
S	-0.27280	0.94939	-0.84457
C	-0.72602	1.89906	3.08359
H	-1.81207	1.97425	3.17230
H	-0.27514	2.83319	3.43418
H	-0.38738	1.10556	3.76131
O	1.99291	2.19033	2.09917
C	3.21468	1.44510	2.17329
C	4.30451	2.47999	2.46513
H	3.43685	0.92352	1.24351
H	3.13569	0.69130	2.96443
N	5.63942	1.99328	2.10809
H	4.29997	2.79265	3.51345
H	4.11109	3.35429	1.84372
C	6.19749	0.84828	2.52575
N	7.39307	0.72792	1.93966
C	7.60864	1.81292	1.10486
C	6.50574	2.60574	1.21034
H	6.24407	3.53003	0.72372
H	8.49832	1.85618	0.48444
H	5.73353	0.10190	3.14922
C	8.27570	-0.43155	2.08648
H	8.79526	-0.38007	3.04722
H	8.99744	-0.39623	1.26578
H	7.64847	-1.32431	2.03140
C	3.21601	0.47236	-1.38324
C	4.48342	0.92041	-1.89454
C	2.48111	1.51539	-0.86851
C	4.69320	2.26708	-1.78513
S	3.33786	3.04997	-1.03743
H	5.55992	2.82150	-2.11612

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C          2.83457       -0.97630       -1.33586
H          1.76462       -1.10079       -1.15783
H          3.37711       -1.47581       -0.52135
H          3.09614       -1.46945       -2.27819
O          5.39478        0.04502       -2.42753
C          6.36627       -0.44754       -1.48686
C          6.45391       -1.95416       -1.72133
H          6.03704       -0.27401       -0.45981
H          7.33082        0.04612       -1.65541
N          7.59151       -2.54202       -1.00200
H          6.56830       -2.16536       -2.78802
H          5.55302       -2.43853       -1.34661
C          8.87801       -2.27302       -1.26321
N          9.63344       -2.93276       -0.37828
C          8.79967       -3.63587        0.48118
C          7.51679       -3.38571        0.09587
H          6.56372       -3.63314        0.54011
H          9.19306       -4.23223        1.28828
H          9.25133       -1.56619       -1.98810
C         11.08655       -2.78898       -0.27980
H         11.58235       -3.41851       -1.02305
H         11.39472       -3.09465        0.72093
H         11.32059       -1.73061       -0.43928
Cl        -6.77485       -6.34764       -0.67161
Cl        -6.65491        4.87924       -0.41361
Cl         5.00186       -1.79588        1.52952
Cl        10.05254        0.50581       -0.84914

118
c1_140.log   Energy: -3690953.7499917 Ha
C          6.51479       -4.92975       -0.22131
C          5.47990       -3.94961       -0.33630
C          7.71829       -4.33840        0.05425
C          5.88601       -2.64389       -0.11708
S          7.61421       -2.61008        0.18518
H          8.67034       -4.82794        0.21061
C          6.25501       -6.39778       -0.39347
H          5.43197       -6.73048        0.24867
H          7.14508       -6.98645       -0.15397
H          5.95978       -6.62348       -1.42484
O          4.21909       -4.31069       -0.72611
C          3.15239       -4.16185        0.22722
C          1.88188       -4.30753       -0.60681
H          3.19826       -3.17816        0.70568
H          3.19115       -4.95778        0.97787
N          0.71443       -3.71011        0.05421
H          1.67095       -5.36837       -0.75677
H          2.01190       -3.79447       -1.56080
C         -0.05831       -4.35048        0.94240
N         -1.04398       -3.51562        1.29993
C         -0.89688       -2.30851        0.62981
C          0.21574       -2.42999       -0.14948
H          0.69417       -1.72792       -0.81395
H         -1.62788       -1.52172        0.73814
H          0.16674       -5.38510        1.27635
C         -2.08668       -3.82646        2.27793
H         -2.16019       -4.91081        2.36867
H         -3.02740       -3.39419        1.92950
H         -1.82068       -3.39703        3.24794
C          5.09826       -0.29103        0.53453
C          4.05449        0.59838        0.14510
C          5.06534       -1.45617       -0.21109
C          3.25178        0.17820       -0.89791
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S	3.80159	-1.39680	-1.43886
C	6.03513	0.03400	1.66020
H	6.84368	0.69994	1.33062
H	6.47883	-0.86939	2.08450
H	5.49159	0.56313	2.45005
O	3.77429	1.74105	0.85795
C	4.44313	2.90645	0.36198
C	4.23014	3.98330	1.42329
H	4.00507	3.20744	-0.59932
H	5.51710	2.72735	0.23957
N	5.06988	5.14476	1.13826
H	4.52535	3.58653	2.39628
H	3.18466	4.29878	1.47897
C	6.28876	5.33664	1.67089
N	6.86411	6.37670	1.04614
C	6.03468	6.78067	0.00835
C	4.91390	6.01560	0.06426
H	4.02103	6.01626	-0.53963
H	6.31530	7.57801	-0.66058
H	6.67559	4.83324	2.53734
C	8.27528	6.71678	1.20979
H	8.47356	6.99270	2.24798
H	8.50808	7.56166	0.56080
H	8.85688	5.82960	0.93487
C	1.16542	0.39952	-2.34867
C	-0.16785	0.88451	-2.19869
C	1.94981	0.70236	-1.24621
C	-0.41787	1.57905	-1.03252
S	1.01843	1.58584	-0.03232
C	1.59770	-0.38047	-3.55844
H	2.65111	-0.20477	-3.79294
H	0.99165	-0.09526	-4.42261
H	1.47228	-1.46251	-3.41681
O	-1.12675	0.63948	-3.15934
C	-2.20829	-0.18298	-2.70154
C	-3.34079	-0.00607	-3.72127
H	-2.54830	0.13212	-1.71195
H	-1.87499	-1.22592	-2.63229
N	-4.65659	0.11341	-3.08345
H	-3.37727	-0.82019	-4.44998
H	-3.16369	0.92663	-4.25666
C	-5.20521	-0.77576	-2.24204
N	-6.40394	-0.31514	-1.87160
C	-6.63141	0.91258	-2.47012
C	-5.53238	1.18037	-3.23125
H	-5.28184	2.02969	-3.84496
H	-7.52504	1.47912	-2.22853
H	-4.73638	-1.66412	-1.84720
C	-7.32436	-1.00860	-0.96574
H	-7.89264	-1.75464	-1.52824
H	-8.00096	-0.25482	-0.55396
H	-6.72267	-1.48101	-0.18786
C	-2.36951	2.03998	0.55904
C	-3.66843	2.64802	0.48339
C	-1.67399	2.18160	-0.62379
C	-3.95305	3.23763	-0.71642
S	-2.62665	3.07230	-1.81892
H	-4.86292	3.74705	-1.00061
C	-1.94697	1.26618	1.77180
H	-0.96504	0.80863	1.64032
H	-2.67699	0.47159	1.96410
H	-1.90793	1.91186	2.65659
O	-4.53113	2.56947	1.54463

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C         -5.69500        1.76722        1.30106
C         -5.98142        1.06616        2.62521
H         -5.47833        1.01039        0.54448
H         -6.53792        2.38353        0.96852
N         -7.19625        0.24707        2.53536
H         -6.10197        1.79185        3.43402
H         -5.15656        0.39300        2.85653
C         -8.43170        0.72511        2.33500
N         -9.27251       -0.31022        2.23113
C         -8.54501       -1.48653        2.34781
C         -7.24086       -1.13868        2.53376
H         -6.33300       -1.72098        2.58299
H         -9.01834       -2.45271        2.28129
H         -8.70075        1.75950        2.19749
C        -10.68488       -0.17760        1.86909
H        -11.26075        0.19105        2.72130
H        -11.05754       -1.15948        1.57569
H        -10.74095        0.52034        1.02638
Cl         1.42816       -7.05935        1.29452
Cl         7.89414        3.31862        0.83118
Cl        -4.30933       -1.47810        0.78231
Cl        -9.03688        1.99618       -0.33235

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c1_180.log   Energy: -3690931.7221064 Ha
C          8.14830        1.55630       -0.22976
C          6.75839        1.25670       -0.38333
C          8.30945        2.76213        0.39698
C          5.87982        2.20668        0.11444
S          6.80832        3.53341        0.80173
H          9.24080        3.25303        0.64519
C          9.25126        0.65627       -0.70646
H          9.38558       -0.21720       -0.05322
H         10.20162        1.19662       -0.74524
H          9.02868        0.27900       -1.71120
O          6.30987        0.12583       -1.02617
C          6.33070       -1.06350       -0.22460
C          5.84943       -2.17539       -1.15243
H          5.64545       -0.95824        0.62528
H          7.33892       -1.27231        0.15297
N          5.76269       -3.44060       -0.42059
H          6.53737       -2.28809       -1.99408
H          4.85641       -1.94584       -1.54204
C          6.80686       -3.99319        0.21393
N          6.35694       -5.06435        0.87743
C          4.99334       -5.20759        0.65436
C          4.61863       -4.18208       -0.15903
H          3.64142       -3.95227       -0.55336
H          4.39274       -5.99743        1.07511
H          7.83453       -3.57584        0.30735
C          7.21707       -5.88234        1.73124
H          8.16211       -5.34768        1.85890
H          7.39161       -6.85694        1.26773
H          6.73522       -6.01732        2.70204
C          3.51771        3.03212        0.68290
C          2.18319        2.56853        0.51157
C          4.43764        2.15322        0.12557
C          2.03747        1.35538       -0.13945
S          3.62494        0.76348       -0.59878
C          3.81986        4.30676        1.41785
H          4.16193        5.10421        0.74844
H          4.58631        4.15406        2.18453
H          2.91823        4.67252        1.91347
```

O	1.09314	3.25872	0.99235
C	0.68613	4.34763	0.15210
C	-0.51259	4.97124	0.86114
H	0.39814	3.96738	-0.83656
H	1.47822	5.09468	0.03837
N	-0.97656	6.15027	0.13537
H	-0.21977	5.28510	1.86490
H	-1.33495	4.25606	0.94668
C	-0.61451	7.41150	0.42974
N	-1.06499	8.21782	-0.54808
C	-1.60494	7.42742	-1.55535
C	-1.55451	6.13903	-1.13098
H	-1.88110	5.22244	-1.59507
H	-1.98145	7.85781	-2.46911
H	-0.20936	7.73657	1.36973
C	-0.65112	9.61201	-0.67246
H	-0.98560	10.17920	0.19946
H	-1.10393	10.03252	-1.57116
H	0.44307	9.62306	-0.73420
C	0.63260	-0.57970	-1.05542
C	-0.74310	-0.93725	-1.12167
C	0.82037	0.64078	-0.41931
C	-1.63430	-0.03154	-0.57287
S	-0.72780	1.32358	0.08574
C	1.70267	-1.46623	-1.62639
H	2.33758	-0.92766	-2.33831
H	1.24701	-2.30794	-2.15277
H	2.35004	-1.87159	-0.83953
O	-1.16337	-2.11151	-1.71007
C	-1.11460	-3.24300	-0.83365
C	-1.74250	-4.38694	-1.62579
H	-1.70048	-3.04078	0.07126
H	-0.08860	-3.49769	-0.54495
N	-1.82937	-5.58427	-0.79078
H	-1.13477	-4.62431	-2.50089
H	-2.74599	-4.11664	-1.95955
C	-0.91409	-6.56059	-0.76184
N	-1.20524	-7.38486	0.25266
C	-2.31076	-6.88514	0.92626
C	-2.70389	-5.75801	0.27481
H	-3.51610	-5.07195	0.45565
H	-2.71596	-7.38045	1.79368
H	-0.08012	-6.66066	-1.43327
C	-0.30430	-8.44222	0.70925
H	-0.22195	-9.22048	-0.05287
H	-0.71127	-8.87270	1.62451
H	0.67102	-7.97872	0.89357
C	-3.97777	0.73411	0.11728
C	-5.32246	0.24385	0.02328
C	-3.07145	-0.12981	-0.47911
C	-5.45564	-0.95751	-0.61896
S	-3.91070	-1.52608	-1.16751
H	-6.35343	-1.52778	-0.82532
C	-3.66874	2.03630	0.80171
H	-2.97752	1.90417	1.64224
H	-4.59090	2.47798	1.18620
H	-3.20940	2.75760	0.11370
O	-6.33711	0.98553	0.57283
C	-7.59967	0.34079	0.52821
C	-8.63751	1.34151	1.02312
H	-7.60321	-0.55907	1.15580
H	-7.84600	0.01044	-0.48468
N	-9.93996	0.67991	1.14758

H	-8.72838	2.18730	0.33610
H	-8.36899	1.73201	2.00731
C	-10.64067	0.16777	0.12135
N	-11.70329	-0.48186	0.61725
C	-11.62498	-0.46643	2.00111
C	-10.52497	0.25844	2.33516
H	-10.11304	0.52632	3.29448
H	-12.35929	-0.96305	2.61429
H	-10.42126	0.30351	-0.92233
C	-12.55921	-1.34827	-0.19232
H	-13.04724	-0.76161	-0.97354
H	-13.31635	-1.79087	0.45553
H	-11.90983	-2.11235	-0.63668
Cl	9.45784	-2.67604	1.11630
Cl	2.01891	7.58959	0.05799
Cl	1.59944	-5.55787	0.10298
Cl	-9.33040	-2.07919	-0.95339

8.4 Coordinates of optimized structures

geometries optimized at the B3LYP-D3(BJ)/6-31G(d) level

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C_1 ($\bar{\theta} = 8°$) CPT conformer Energy: -3690932.0224324 Ha

C	8.24678	1.00435	-0.12105
C	6.84041	0.80110	-0.27800
C	8.49188	2.23561	0.42417
C	6.03083	1.84056	0.15150
S	7.04843	3.14330	0.75122
H	9.45462	2.66978	0.65796
C	9.28005	-0.01049	-0.51507
H	9.31208	-0.85942	0.18211
H	10.27587	0.44133	-0.54372
H	9.05684	-0.41611	-1.50862
O	6.31636	-0.32129	-0.87556
C	6.17955	-1.45880	-0.01226
C	5.65513	-2.57131	-0.91534
H	5.45587	-1.24473	0.78389
H	7.14104	-1.73463	0.43800
N	5.40359	-3.78657	-0.13823
H	6.38088	-2.78766	-1.70331
H	4.71396	-2.27334	-1.38038
C	6.34214	-4.39444	0.60176
N	5.75475	-5.41198	1.24230
C	4.40995	-5.46267	0.89682
C	4.18871	-4.43585	0.03073
H	3.27103	-4.14878	-0.45862
H	3.71758	-6.19711	1.27476
H	7.39425	-4.05732	0.75635
C	6.47019	-6.27566	2.17953
H	7.45881	-5.84068	2.34507
H	6.56594	-7.28265	1.76501
H	5.92257	-6.31708	3.12379
C	3.72525	2.83590	0.67596
C	2.36513	2.49038	0.44195
C	4.58922	1.89805	0.12626
C	2.14430	1.31851	-0.25949
S	3.69314	0.60625	-0.67900
C	4.09957	4.06319	1.45650
H	4.44142	4.88049	0.81047
H	4.88774	3.85030	2.18495
H	3.22686	4.43339	1.99998
O	1.31862	3.25180	0.91284

C	1.01657	4.37329	0.07184
C	-0.12652	5.10850	0.76496
H	0.70569	4.02097	-0.92047
H	1.87457	5.04523	-0.03294
N	-0.46316	6.32258	0.02573
H	0.18161	5.39898	1.77115
H	-1.01565	4.47655	0.84158
C	0.02130	7.54331	0.31428
N	-0.32953	8.38085	-0.67731
C	-0.93701	7.64044	-1.68383
C	-1.02487	6.35806	-1.24752
H	-1.43952	5.47545	-1.70707
H	-1.25667	8.09824	-2.60591
H	0.45835	7.83202	1.25185
C	0.23108	9.72190	-0.81384
H	-0.02881	10.32407	0.05983
H	-0.18613	10.18562	-1.70852
H	1.31923	9.61422	-0.88770
C	0.61366	-0.45185	-1.29593
C	-0.77771	-0.74518	-1.32737
C	0.88232	0.70280	-0.57277
C	-1.60209	0.14108	-0.65754
S	-0.61190	1.40776	0.05459
C	1.61382	-1.34041	-1.97850
H	2.31163	-0.76822	-2.59819
H	1.09207	-2.05277	-2.62245
H	2.20474	-1.91408	-1.25321
O	-1.27132	-1.84517	-1.99674
C	-1.32005	-3.02649	-1.18936
C	-2.01578	-4.07502	-2.05364
H	-1.90700	-2.83656	-0.28276
H	-0.32058	-3.36756	-0.89690
N	-2.27194	-5.28077	-1.26651
H	-1.39498	-4.34827	-2.90910
H	-2.96863	-3.69009	-2.42179
C	-1.44395	-6.32922	-1.18341
N	-1.89439	-7.14971	-0.22573
C	-3.01609	-6.57720	0.35696
C	-3.25453	-5.40628	-0.29251
H	-4.02154	-4.65854	-0.16606
H	-3.54071	-7.05795	1.16660
H	-0.55455	-6.47637	-1.77023
C	-1.13051	-8.29122	0.27633
H	-1.05129	-9.05919	-0.49648
H	-1.64956	-8.70128	1.14305
H	-0.13814	-7.91849	0.55317
C	-3.86926	0.84945	0.29698
C	-5.24446	0.46685	0.15423
C	-3.03809	0.09254	-0.51438
C	-5.47182	-0.55196	-0.73131
S	-3.98211	-1.06992	-1.45645
H	-6.40787	-1.02129	-1.01007
C	-3.45505	1.93745	1.24759
H	-2.65105	1.61141	1.91603
H	-4.30954	2.23850	1.85820
H	-3.09373	2.82868	0.71754
O	-6.19248	1.11632	0.90365
C	-7.48421	0.53927	0.80756
C	-8.44569	1.44815	1.56456
H	-7.49426	-0.47176	1.23338
H	-7.80316	0.43726	-0.23352
N	-9.77095	0.82275	1.62091
H	-8.52884	2.42468	1.07963

```
H         -8.11095        1.60774        2.59198
C        -10.53899        0.55744        0.55049
N        -11.60641       -0.14311        0.95864
C        -11.46849       -0.41161        2.31144
C        -10.32287        0.19000        2.72758
H         -9.85833        0.24221        3.69878
H        -12.19754       -0.99587        2.84893
H        -10.35620        0.89006       -0.45548
C        -12.53671       -0.79183        0.03509
H        -13.05332       -0.03782       -0.56272
H        -13.26587       -1.35590        0.61724
H        -11.93875       -1.44928       -0.60796
Cl         9.09004       -3.24754        1.48217
Cl         2.68049        7.46395       -0.01876
Cl         1.07149       -5.59561       -0.05654
Cl        -9.38583       -1.46083       -1.04902


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C2 (θ̄ = 13°) CPT conformer   Energy: -3690940.6535491 Ha
C         -6.02080        4.70040       -0.08513
C         -5.00448        3.72515        0.15373
C         -5.46882        5.84937       -0.58491
C         -3.71337        4.10874       -0.17451
S         -3.74596        5.76217       -0.76958
H         -5.98492        6.76048       -0.85633
C         -7.47802        4.46409        0.18872
H         -7.93360        3.79061       -0.55040
H         -8.03287        5.40673        0.17300
H         -7.61177        4.00255        1.17398
O         -5.27112        2.50687        0.73605
C         -5.75336        1.49755       -0.15890
C         -6.03835        0.29388        0.73474
H         -4.98284        1.24541       -0.89779
H         -6.65915        1.82729       -0.68219
N         -6.46910       -0.85134       -0.06956
H         -6.81663        0.54105        1.46113
H         -5.13727        0.00100        1.27597
C         -7.51257       -0.80689       -0.90985
N         -7.57078       -1.98354       -1.54461
C         -6.54535       -2.80488       -1.09312
C         -5.84929       -2.08934       -0.16705
H         -4.98576       -2.38181        0.40929
H         -6.37757       -3.80950       -1.44550
H         -8.15767        0.07530       -1.13728
C         -8.56505       -2.27505       -2.57569
H         -9.09283       -1.34448       -2.79990
H         -9.26836       -3.03124       -2.21699
H         -8.05957       -2.63883       -3.47316
C         -1.22676        3.58600       -0.52938
C         -0.33837        2.51173       -0.24276
C         -2.50935        3.32014       -0.06749
C         -0.88988        1.42006        0.40434
S         -2.58696        1.74039        0.71847
C         -0.76773        4.80729       -1.27102
H         -0.58769        5.65794       -0.59944
H         -1.49274        5.10887       -2.03298
H          0.17677        4.58784       -1.77769
O          0.98590        2.53131       -0.62106
C          1.81951        3.27229        0.28137
C          3.16593        3.44569       -0.41905
H          1.94226        2.71777        1.22025
H          1.36295        4.24491        0.50281
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N	4.00685	4.35853	0.36749
H	3.01147	3.87619	-1.41181
H	3.70634	2.50268	-0.52367
C	3.64744	5.61696	0.65906
N	4.56962	6.12674	1.48180
C	5.55057	5.17129	1.71272
C	5.19589	4.05427	1.01526
H	5.66676	3.08793	0.88306
H	6.39964	5.36977	2.34697
H	2.69592	6.13600	0.42323
C	4.46277	7.46591	2.06485
H	3.43280	7.80718	1.91064
H	5.17117	8.14401	1.58134
H	4.67897	7.40537	3.13372
C	-0.75711	-0.93007	1.40694
C	0.17906	-1.99727	1.44279
C	-0.25309	0.17046	0.72154
C	1.38138	-1.77052	0.80027
S	1.38305	-0.14470	0.13754
C	-2.11459	-1.05766	2.03637
H	-2.34819	-0.20491	2.68205
H	-2.15393	-1.96701	2.64152
H	-2.90475	-1.12479	1.27782
O	-0.09372	-3.18658	2.08974
C	-0.65974	-4.17876	1.23031
C	-0.75818	-5.43956	2.08456
H	0.00032	-4.35311	0.37114
H	-1.65077	-3.88860	0.86329
N	-1.26274	-6.55486	1.28451
H	-1.44380	-5.28157	2.91908
H	0.22331	-5.70613	2.48342
C	-2.54255	-6.94682	1.23777
N	-2.66907	-7.87162	0.27581
C	-1.44598	-8.01218	-0.36418
C	-0.56427	-7.19157	0.26597
H	0.48419	-7.00406	0.09852
H	-1.31821	-8.68457	-1.19693
H	-3.32620	-6.60754	1.89044
C	-3.96265	-8.35241	-0.20558
H	-4.49747	-8.85499	0.60329
H	-3.79087	-9.05808	-1.01884
H	-4.52527	-7.47757	-0.54962
C	3.54513	-2.65296	-0.23469
C	4.49345	-3.69675	0.03280
C	2.50968	-2.66351	0.68437
C	4.19360	-4.49273	1.09924
S	2.71131	-3.98811	1.84633
H	4.75034	-5.34405	1.46347
C	3.68395	-1.73214	-1.41409
H	2.70942	-1.49213	-1.84773
H	4.28457	-2.22113	-2.18946
H	4.17572	-0.78600	-1.15237
O	5.60211	-3.91141	-0.76725
C	6.63199	-2.94619	-0.59948
C	7.42761	-2.96301	-1.90511
H	7.27820	-3.21124	0.24984
H	6.22077	-1.94648	-0.41503
N	8.50398	-1.96463	-1.87230
H	6.76514	-2.74043	-2.74459
H	7.88052	-3.94175	-2.07450
C	8.28244	-0.65022	-1.73277
N	9.46735	-0.03619	-1.65445
C	10.47728	-0.97970	-1.75574

C	9.87107	-2.19388	-1.88827
H	10.28243	-3.18507	-1.99350
H	11.52038	-0.70820	-1.72410
H	7.31843	-0.13720	-1.57196
C	9.61232	1.40981	-1.45175
H	8.63661	1.79578	-1.14152
H	9.93642	1.88435	-2.38097
H	10.35011	1.58487	-0.66643
Cl	-9.03589	1.66576	-1.99277
Cl	1.00636	7.14356	0.99210
Cl	-4.05774	-4.90422	0.07141
Cl	6.07136	1.10486	-0.47280

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C_3 ($\bar{\theta} = 16°$) CPT conformer Energy: -3690957.1900174 Ha

C	-8.41501	-1.17773	0.08189
C	-7.09019	-0.97314	-0.41894
C	-8.61695	-2.49826	0.37638
C	-6.29645	-2.10651	-0.49373
S	-7.22562	-3.49198	0.06532
H	-9.51709	-2.95476	0.76506
C	-9.41476	-0.07205	0.25252
H	-9.18000	0.55559	1.12435
H	-10.42196	-0.47688	0.38692
H	-9.41789	0.57850	-0.62945
O	-6.63805	0.25321	-0.84223
C	-6.17095	1.11456	0.21035
C	-5.84026	2.43964	-0.47078
H	-5.26827	0.69075	0.66743
H	-6.93598	1.24562	0.98564
N	-5.27226	3.37878	0.49934
H	-6.74198	2.87281	-0.91082
H	-5.10353	2.29235	-1.26208
C	-5.91284	3.76039	1.61462
N	-5.07193	4.52334	2.32289
C	-3.86668	4.64130	1.64236
C	-3.99143	3.91724	0.49661
H	-3.26696	3.76245	-0.28648
H	-3.01692	5.20284	1.99674
H	-6.90042	3.39653	1.96883
C	-5.41590	5.08286	3.62831
H	-6.33366	4.59762	3.96886
H	-5.56614	6.16267	3.54832
H	-4.60643	4.87636	4.33174
C	-4.00965	-3.22831	-0.80975
C	-2.70821	-2.83873	-1.23506
C	-4.91647	-2.18128	-0.90807
C	-2.58044	-1.53294	-1.67285
S	-4.14614	-0.75076	-1.58962
C	-4.30199	-4.61529	-0.31223
H	-5.09746	-5.09388	-0.89393
H	-4.62455	-4.61831	0.73604
H	-3.40797	-5.23806	-0.40839
O	-1.63062	-3.71067	-1.18100
C	-0.95505	-3.69191	0.07177
C	0.21983	-4.66057	-0.07170
H	-1.63348	-4.01874	0.87195
H	-0.60238	-2.68179	0.31022
N	0.72911	-5.07530	1.24165
H	1.04039	-4.20807	-0.62889
H	-0.11483	-5.55281	-0.60759
C	1.93539	-4.79053	1.75872

N	2.00133	-5.34419	2.97754
C	0.81082	-5.99665	3.24594
C	0.01085	-5.82970	2.15798
H	-0.98807	-6.17880	1.95079
H	0.64442	-6.51776	4.17525
H	2.77241	-4.24303	1.30629
C	3.15928	-5.26987	3.87871
H	3.96800	-4.75938	3.34438
H	3.46099	-6.28448	4.14767
H	2.87683	-4.71375	4.77572
C	-1.16443	0.53043	-2.19413
C	0.18541	0.81357	-2.54961
C	-1.39056	-0.83565	-2.08890
C	1.00498	-0.28716	-2.70688
S	0.07310	-1.74800	-2.46523
C	-2.13857	1.63668	-1.90552
H	-2.92172	1.69880	-2.67165
H	-1.61590	2.59605	-1.87291
H	-2.62939	1.48609	-0.93850
O	0.65067	2.10005	-2.65691
C	1.32922	2.54534	-1.47437
C	1.89980	3.91588	-1.80574
H	2.13458	1.84639	-1.21881
H	0.62456	2.63645	-0.64056
N	2.79617	4.34282	-0.72701
H	1.09092	4.64300	-1.88728
H	2.47620	3.87772	-2.73203
C	2.40266	5.03325	0.35060
N	3.45748	5.13793	1.17320
C	4.54979	4.49066	0.60965
C	4.12949	3.98476	-0.58157
H	4.67153	3.40193	-1.30936
H	5.52689	4.41181	1.06529
H	1.36308	5.33719	0.52338
C	3.44311	5.83003	2.45678
H	4.08398	6.71431	2.41298
H	3.80389	5.15655	3.23745
H	2.41859	6.12980	2.68017
C	3.38525	-1.11520	-2.33191
C	4.71767	-0.68843	-2.64773
C	2.43840	-0.28783	-2.90754
C	4.78287	0.40134	-3.47136
S	3.19963	0.96790	-3.88445
H	5.67201	0.90451	-3.82366
C	3.11095	-2.30025	-1.45116
H	2.36921	-2.05824	-0.68175
H	4.01774	-2.64217	-0.94939
H	2.72173	-3.14421	-2.03593
O	5.82530	-1.29524	-2.10474
C	6.13531	-0.76789	-0.80970
C	7.26534	-1.62721	-0.25722
H	5.26952	-0.84497	-0.14107
H	6.42769	0.28801	-0.88813
N	7.70221	-1.08554	1.03640
H	8.11581	-1.63654	-0.94376
H	6.90968	-2.64377	-0.08510
C	8.24114	0.13079	1.19901
N	8.41813	0.33468	2.50886
C	7.97915	-0.78526	3.20127
C	7.51971	-1.67610	2.27752
H	7.01462	-2.62903	2.36321
H	8.02350	-0.83958	4.27700
H	8.36655	0.90587	0.44397

C	8.91848	1.58878	3.07295
H	8.67788	2.38632	2.36169
H	9.99706	1.52599	3.24023
H	8.40986	1.77050	4.02165
Cl	-8.28608	2.26440	2.97102
Cl	4.93674	-3.67199	1.42538
Cl	-0.78406	4.84017	0.26256
Cl	7.38625	2.91967	0.13199

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C_4 ($\bar{\theta} = 17°$) CPT conformer Energy: -3690933.8286243 Ha

C	7.51499	-1.72921	-2.11835
C	6.24232	-1.51976	-1.50419
C	8.11457	-0.52920	-2.39212
C	5.88679	-0.19895	-1.29385
S	7.16076	0.83961	-1.91386
H	9.07793	-0.36753	-2.85695
C	8.07638	-3.09063	-2.41238
H	8.31885	-3.64491	-1.49652
H	8.98739	-3.01287	-3.01281
H	7.34921	-3.69437	-2.96771
O	5.40604	-2.56270	-1.16801
C	5.67831	-3.11249	0.12494
C	4.66707	-4.24018	0.30700
H	5.53975	-2.34239	0.89504
H	6.69406	-3.51640	0.18963
N	4.94437	-4.96096	1.54833
H	4.75448	-4.94583	-0.52119
H	3.64428	-3.85604	0.33494
C	5.69102	-6.07387	1.62426
N	5.91639	-6.34481	2.92018
C	5.38720	-5.31253	3.68402
C	4.77802	-4.44888	2.83069
H	4.23578	-3.53391	3.00686
H	5.48588	-5.29715	4.75729
H	5.96727	-6.69795	0.79492
C	6.89067	-7.33875	3.36268
H	6.58814	-8.33309	3.02610
H	6.93394	-7.32382	4.45233
H	7.85518	-7.06484	2.91941
C	4.35778	1.57128	-0.24912
C	3.01865	1.64569	0.24697
C	4.66574	0.29873	-0.70272
C	2.30235	0.46822	0.19724
S	3.29663	-0.80337	-0.48500
C	5.25424	2.77487	-0.25457
H	5.26603	3.27439	-1.23388
H	6.28171	2.51370	0.01602
H	4.88424	3.50184	0.47476
O	2.48419	2.81968	0.71973
C	1.94055	3.65710	-0.30681
C	1.64091	4.99778	0.36232
H	1.02173	3.21107	-0.70901
H	2.66403	3.77760	-1.12355
N	1.29031	5.99198	-0.65983
H	2.52952	5.34332	0.89690
H	0.80241	4.93266	1.05920
C	2.12204	6.35000	-1.64766
N	1.46127	7.18256	-2.45833
C	0.17551	7.37004	-1.96694
C	0.06360	6.61672	-0.83527
H	-0.74400	6.45141	-0.13079

H	-0.53415	8.01279	-2.46272
H	3.12215	5.93566	-1.88597
C	2.04310	7.72057	-3.68918
H	2.93450	7.12542	-3.91607
H	2.30642	8.77296	-3.55294
H	1.31591	7.62346	-4.49831
C	0.19889	0.74182	1.62295
C	-1.15302	0.29560	1.58168
C	0.92421	0.23849	0.55993
C	-1.49313	-0.54977	0.54092
S	-0.07003	-0.79614	-0.46260
C	0.72198	1.59261	2.74215
H	1.79657	1.44823	2.87213
H	0.20693	1.33276	3.67326
H	0.56055	2.65984	2.55404
O	-2.06791	0.67362	2.54269
C	-2.66832	1.93903	2.25806
C	-3.62369	2.20384	3.41716
H	-3.22671	1.88893	1.31509
H	-1.92425	2.73825	2.17734
N	-4.40658	3.41182	3.14903
H	-3.07522	2.34470	4.35083
H	-4.31418	1.36744	3.54308
C	-3.99962	4.65909	3.41394
N	-4.86741	5.51499	2.86093
C	-5.83099	4.78899	2.17712
C	-5.54303	3.47097	2.35434
H	-6.03074	2.57670	1.99975
H	-6.63020	5.27394	1.64049
H	-3.10742	4.92926	3.95158
C	-4.63973	6.95834	2.78622
H	-4.67399	7.39588	3.78642
H	-5.42321	7.39974	2.16986
H	-3.65327	7.10691	2.33315
C	-3.18409	-1.89709	-0.82629
C	-4.56969	-2.25825	-0.73844
C	-2.78202	-1.13953	0.26128
C	-5.21840	-1.79332	0.37363
S	-4.12597	-0.90641	1.38948
H	-6.25305	-1.92485	0.66707
C	-2.33405	-2.31513	-1.99290
H	-1.89284	-1.45298	-2.50623
H	-2.94193	-2.86521	-2.71472
H	-1.50683	-2.96513	-1.68402
O	-5.12287	-3.00673	-1.74592
C	-6.52487	-3.17544	-1.62523
C	-6.95642	-4.16272	-2.70355
H	-7.04726	-2.21843	-1.74715
H	-6.80088	-3.55309	-0.63668
N	-8.41990	-4.25830	-2.72417
H	-6.53324	-5.15431	-2.52160
H	-6.63210	-3.83220	-3.69275
C	-9.17239	-4.71686	-1.70972
N	-10.46230	-4.52320	-2.01851
C	-10.53143	-3.84030	-3.22256
C	-9.25718	-3.67338	-3.66541
H	-8.86833	-3.21207	-4.55857
H	-11.47512	-3.54584	-3.65210
H	-8.80761	-5.19651	-0.81924
C	-11.54923	-4.69788	-1.05574
H	-11.60423	-5.74300	-0.74351
H	-12.48595	-4.41248	-1.53531
H	-11.32109	-4.05214	-0.19874

Cl	8.22928	-5.49000	0.79271
Cl	4.42493	4.96983	-3.14668
Cl	-1.66029	5.40432	1.87740
Cl	-9.08461	-2.95955	0.50382

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C_5 ($\bar{\theta} = 43°$) CPT conformer Energy: -3690972.5496232 Ha

C	-8.20650	0.22379	1.90025
C	-6.93753	0.15511	1.21989
C	-8.73403	1.48168	1.85923
C	-6.54235	1.35562	0.65672
S	-7.73398	2.60773	0.99887
H	-9.66619	1.81235	2.29785
C	-8.82107	-0.97103	2.56639
H	-8.99049	-1.77656	1.84334
H	-9.77644	-0.71312	3.03244
H	-8.15598	-1.37716	3.33747
O	-6.32378	-1.06018	1.22710
C	-4.90614	-1.20976	1.11794
C	-4.23628	-0.59592	2.35573
H	-4.52593	-0.76621	0.19879
H	-4.73031	-2.28466	1.07006
N	-2.77773	-0.74164	2.32964
H	-4.60032	-1.09603	3.25569
H	-4.46727	0.46864	2.43285
C	-2.08752	-1.64931	3.03258
N	-0.78617	-1.51078	2.75137
C	-0.64084	-0.53434	1.77744
C	-1.88678	-0.04969	1.51209
H	-2.21631	0.72971	0.84861
H	0.33978	-0.27688	1.39966
H	-2.50868	-2.35254	3.72808
C	0.24944	-2.44644	3.19104
H	0.24548	-2.50464	4.28234
H	1.21389	-2.07421	2.84104
H	0.00475	-3.42325	2.76180
C	-5.03261	1.10305	-1.36476
C	-3.68174	1.42554	-1.72288
C	-5.36215	1.63863	-0.13924
C	-3.02081	2.27038	-0.83774
S	-4.09257	2.66359	0.50274
C	-5.99203	0.31455	-2.20443
H	-5.89475	-0.76978	-2.04990
H	-5.81754	0.51825	-3.26642
H	-7.01761	0.60131	-1.95655
O	-3.05878	0.98624	-2.86006
C	-2.97401	-0.44244	-3.04775
C	-1.81786	-1.03103	-2.22398
H	-2.79096	-0.57561	-4.11637
H	-3.89779	-0.96046	-2.77948
N	-1.78490	-2.48410	-2.34545
H	-1.94205	-0.79101	-1.16623
H	-0.85697	-0.63034	-2.54967
C	-2.30947	-3.34581	-1.45483
N	-2.22623	-4.57794	-1.97142
C	-1.74152	-4.49062	-3.26580
C	-1.45949	-3.18293	-3.50426
H	-1.04766	-2.68857	-4.36916
H	-1.63594	-5.36299	-3.89021
H	-2.58253	-3.14794	-0.42614
C	-2.87657	-5.73809	-1.36286
H	-2.73436	-5.68099	-0.28101

H	-2.42490	-6.64510	-1.76971
H	-3.94360	-5.67906	-1.59666
C	-0.89921	3.31679	0.13368
C	0.48925	3.36833	-0.19048
C	-1.63494	2.67517	-0.85739
C	0.83225	2.80037	-1.39731
S	-0.59879	2.20881	-2.20617
C	-1.40739	3.86200	1.43808
H	-2.21225	4.59077	1.29516
H	-0.58744	4.36115	1.95990
H	-1.79480	3.07014	2.09045
O	1.39880	3.92602	0.67981
C	2.34341	3.00946	1.23939
C	3.63257	3.80450	1.45276
H	2.53627	2.17190	0.56855
H	1.95089	2.59900	2.17773
N	4.78973	2.91439	1.58670
H	3.57248	4.46081	2.32585
H	3.80282	4.41740	0.56768
C	4.86281	1.84372	2.38880
N	6.03308	1.23599	2.17406
C	6.73553	1.92558	1.19870
C	5.95121	2.97684	0.82742
H	6.09315	3.74275	0.08363
H	7.68411	1.54308	0.83614
H	4.08066	1.47436	3.03017
C	6.44764	-0.01744	2.81104
H	5.56935	-0.66384	2.86302
H	6.84076	0.18937	3.81000
H	7.22555	-0.46034	2.18271
C	2.80236	1.32528	-2.03411
C	4.19084	1.47774	-2.37318
C	2.17641	2.54570	-1.89739
C	4.59429	2.77643	-2.52063
S	3.27868	3.87445	-2.24494
H	5.57746	3.12627	-2.80206
C	2.17225	-0.01684	-1.80689
H	2.49854	-0.44721	-0.85196
H	2.44374	-0.70531	-2.61557
H	1.08529	0.06071	-1.76971
O	5.02530	0.40238	-2.54632
C	5.46191	-0.23341	-1.33243
C	5.35899	-1.73677	-1.58400
H	4.82829	0.04584	-0.48442
H	6.50038	0.04156	-1.11817
N	5.95140	-2.50418	-0.48681
H	5.88828	-1.99470	-2.50421
H	4.31691	-2.04275	-1.68695
C	7.23365	-2.88522	-0.42756
N	7.44089	-3.49701	0.74294
C	6.26528	-3.44331	1.48007
C	5.32790	-2.82228	0.71265
H	4.31228	-2.51057	0.92724
H	6.20343	-3.85499	2.47438
H	7.97428	-2.71969	-1.19005
C	8.76489	-3.85892	1.24537
H	9.26073	-4.52453	0.53581
H	8.64502	-4.37425	2.19880
H	9.33801	-2.93293	1.36160
Cl	-2.41687	-4.15221	1.76210
Cl	-5.03126	-3.03828	-1.90860
Cl	2.98640	-0.54429	1.70329
Cl	8.82736	-0.53680	0.26309

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C_6 ($\bar{\theta} = 49°$) CPT conformer Energy: -3690966.9531361 Ha

C	8.01707	-2.55875	0.71263
C	6.79408	-1.85488	0.41652
C	7.90691	-3.88146	0.38167
C	5.78922	-2.64963	-0.10132
S	6.35423	-4.30391	-0.26388
H	8.66492	-4.64425	0.49946
C	9.21787	-1.95012	1.38001
H	9.86707	-1.39090	0.69266
H	9.82773	-2.73031	1.84534
H	8.90431	-1.25506	2.16826
O	6.56807	-0.54467	0.74690
C	7.41150	0.42643	0.11754
C	7.23131	1.71099	0.92143
H	7.09364	0.58794	-0.91798
H	8.45863	0.11069	0.10824
N	8.02503	2.78380	0.30997
H	7.56734	1.56431	1.95126
H	6.18622	2.02944	0.91880
C	9.35862	2.73699	0.18165
N	9.73997	3.80167	-0.53192
C	8.61905	4.55287	-0.86000
C	7.53600	3.91082	-0.33662
H	6.47122	4.11234	-0.36164
H	8.69271	5.46232	-1.43442
H	10.03990	1.90732	0.43800
C	11.12704	4.03584	-0.93768
H	11.58191	4.80145	-0.30325
H	11.13861	4.36467	-1.97890
H	11.65980	3.08302	-0.84127
C	3.87889	-1.28330	-1.13755
C	2.45113	-1.34115	-1.17056
C	4.40610	-2.31628	-0.38922
C	1.88283	-2.38211	-0.46126
S	3.14036	-3.34795	0.27147
C	4.66259	-0.24227	-1.87680
H	4.76521	0.67971	-1.29088
H	4.15459	0.01734	-2.81128
H	5.66304	-0.61393	-2.11367
O	1.68414	-0.45727	-1.90036
C	1.45778	0.80800	-1.28201
C	0.47273	0.66318	-0.11027
H	1.02764	1.44784	-2.05674
H	2.40357	1.25319	-0.95166
N	0.23098	1.95997	0.53640
H	0.86473	-0.03615	0.63126
H	-0.48986	0.28646	-0.45765
C	1.19603	2.83744	0.84538
N	0.61918	3.90341	1.41007
C	-0.75114	3.69602	1.47376
C	-0.99942	2.47354	0.92335
H	-1.94240	1.94940	0.79727
H	-1.42601	4.42314	1.89556
H	2.27288	2.77320	0.63174
C	1.36564	5.08573	1.84446
H	1.32831	5.16795	2.93362
H	0.92466	5.97643	1.39132
H	2.39923	4.96985	1.50681
C	-0.22488	-2.82814	0.90546
C	-1.63711	-2.85811	0.68756

C	0.46658	-2.63556	-0.27659
C	-2.02759	-2.71008	-0.62831
S	-0.62020	-2.53711	-1.64901
C	0.38151	-2.91006	2.27622
H	1.30145	-2.32205	2.34009
H	0.63833	-3.94229	2.54376
H	-0.33010	-2.54969	3.02473
O	-2.49805	-2.99532	1.75283
C	-3.47502	-1.96374	1.91186
C	-4.73245	-2.64829	2.45055
H	-3.70389	-1.47229	0.96644
H	-3.09388	-1.20109	2.60204
N	-5.92227	-1.81468	2.25335
H	-4.63765	-2.90513	3.50956
H	-4.88855	-3.56561	1.88324
C	-6.03432	-0.52029	2.58220
N	-7.23722	-0.09018	2.19082
C	-7.92074	-1.12987	1.58153
C	-7.09174	-2.21151	1.61792
H	-7.20935	-3.21179	1.23636
H	-8.89255	-0.95505	1.13177
H	-5.26093	0.10089	3.00245
C	-7.71300	1.28948	2.32728
H	-6.86981	1.94825	2.11170
H	-8.08553	1.45025	3.34257
H	-8.51971	1.42896	1.60219
C	-4.00475	-1.52489	-1.71567
C	-5.39821	-1.77832	-1.96158
C	-3.38443	-2.61634	-1.14933
C	-5.81085	-3.03722	-1.62197
S	-4.49754	-3.97202	-0.98052
H	-6.79992	-3.45507	-1.74550
C	-3.36444	-0.19901	-2.00403
H	-3.61683	0.53256	-1.22488
H	-3.71661	0.18626	-2.96716
H	-2.27715	-0.28766	-2.05137
O	-6.22598	-0.82830	-2.50324
C	-6.72413	0.14244	-1.56620
C	-6.65991	1.48597	-2.29003
H	-6.10464	0.17735	-0.66453
H	-7.75874	-0.09287	-1.29254
N	-7.36314	2.53363	-1.54586
H	-7.12642	1.39599	-3.27395
H	-5.62548	1.80514	-2.42387
C	-8.67362	2.79065	-1.64567
N	-8.98345	3.75934	-0.77780
C	-7.84256	4.08236	-0.05559
C	-6.82345	3.31717	-0.53488
H	-5.79642	3.19165	-0.21207
H	-7.86190	4.82517	0.72533
H	-9.36324	2.29491	-2.30616
C	-10.35437	4.15455	-0.45860
H	-10.86548	4.48378	-1.36568
H	-10.32005	4.97859	0.25470
H	-10.85873	3.27987	-0.03384
Cl	11.41484	0.49687	-0.26781
Cl	4.19249	3.37276	0.02407
Cl	-4.32273	1.63583	1.05673
Cl	-10.12980	0.72339	-0.17431

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C_7 ($\bar{\theta} = 59°$) CPT conformer Energy: -3690951.4706891 Ha

C	-0.08176	-6.94349	-0.82814
C	-0.18432	-5.59478	-0.35558
C	-1.32089	-7.46065	-1.09806
C	-1.47769	-5.11153	-0.27565
S	-2.60996	-6.33972	-0.79181
H	-1.55122	-8.45997	-1.44331
C	1.22693	-7.66765	-0.95831
H	1.81262	-7.29567	-1.80899
H	1.07250	-8.74026	-1.10597
H	1.83817	-7.52521	-0.06041
O	0.89965	-4.88753	0.11313
C	1.69872	-4.17424	-0.83218
C	2.34852	-3.04476	-0.03065
H	1.07685	-3.76281	-1.63380
H	2.45358	-4.83846	-1.27334
N	2.91822	-1.99261	-0.87558
H	3.15557	-3.42575	0.60323
H	1.57705	-2.57983	0.58358
C	3.84468	-2.18837	-1.82250
N	4.33171	-1.00040	-2.19734
C	3.75163	-0.00822	-1.41726
C	2.86764	-0.63074	-0.58967
H	2.19320	-0.24039	0.15355
H	4.07639	1.01985	-1.49778
H	4.15055	-3.13991	-2.21652
C	5.43101	-0.81444	-3.14384
H	5.92916	0.12701	-2.89035
H	5.04896	-0.78660	-4.16819
H	6.12526	-1.64773	-3.01550
C	-2.71324	-3.34911	1.13826
C	-2.70264	-1.91349	1.25101
C	-1.87594	-3.77340	0.12860
C	-1.90204	-1.26526	0.33986
S	-1.14138	-2.42595	-0.71818
C	-3.49064	-4.24254	2.05625
H	-4.51451	-4.39455	1.68457
H	-3.55320	-3.79412	3.05349
H	-3.01059	-5.22175	2.13993
O	-3.35895	-1.22326	2.24143
C	-4.76505	-1.06583	2.01681
C	-5.01340	-0.06947	0.87375
H	-5.17498	-0.68567	2.95558
H	-5.22682	-2.03612	1.79604
N	-6.43857	-0.04812	0.51724
H	-4.44585	-0.37455	-0.00694
H	-4.71684	0.94825	1.13267
C	-7.14281	-1.15249	0.23364
N	-8.40291	-0.78268	-0.01590
C	-8.50349	0.59744	0.09957
C	-7.26597	1.06301	0.43542
H	-6.86980	2.06178	0.57282
H	-9.43269	1.11777	-0.06903
H	-6.81522	-2.21444	0.25675
C	-9.46477	-1.74152	-0.32723
H	-9.79969	-1.60261	-1.35847
H	-10.30235	-1.58833	0.35737
H	-9.04989	-2.74588	-0.19243
C	-1.59148	1.09133	-0.62694
C	-0.61659	2.12774	-0.48951
C	-1.39781	0.10017	0.30340
C	0.32133	1.94878	0.50571
S	-0.04866	0.46886	1.37102
C	-2.65227	1.10519	-1.68639

H	-3.04616	0.09897	-1.85386
H	-2.24682	1.48080	-2.63170
H	-3.48297	1.75982	-1.38991
O	-0.59157	3.20822	-1.35045
C	-1.28144	4.33258	-0.81109
C	-1.53816	5.27857	-1.98246
H	-0.67332	4.82429	-0.04041
H	-2.23156	4.01295	-0.36430
N	-2.43269	6.36318	-1.55384
H	-2.01299	4.73140	-2.79990
H	-0.61278	5.72426	-2.35181
C	-3.67453	6.14335	-1.10033
N	-4.17321	7.30848	-0.67607
C	-3.22992	8.30588	-0.86996
C	-2.13244	7.70914	-1.41728
H	-1.17893	8.11426	-1.71664
H	-3.41885	9.33354	-0.60359
H	-4.17490	5.16858	-0.95887
C	-5.49834	7.43638	-0.06138
H	-5.84517	6.42893	0.18427
H	-6.18778	7.92047	-0.75718
H	-5.41115	8.02998	0.85055
C	2.42388	2.64224	1.78506
C	3.66439	3.29836	1.48726
C	1.55863	2.67243	0.70690
C	3.74095	3.81412	0.22308
S	2.28453	3.52025	-0.66262
H	4.58549	4.28730	-0.25601
C	2.17383	1.98772	3.11415
H	2.81271	2.44387	3.87465
H	2.40894	0.91481	3.09198
H	1.13013	2.08419	3.42665
O	4.65588	3.37197	2.43846
C	5.90205	2.78538	2.05552
C	5.82436	1.26323	2.23371
H	6.65170	3.22077	2.72219
H	6.16052	3.00065	1.01340
N	7.03589	0.62819	1.72150
H	4.98831	0.87413	1.64915
H	5.67876	0.99135	3.28328
C	7.07129	-0.16147	0.63930
N	8.34915	-0.40494	0.33946
C	9.15846	0.29582	1.21700
C	8.33870	0.94278	2.08802
H	8.55894	1.57880	2.92942
H	10.23344	0.26201	1.14627
H	6.23110	-0.64209	0.16347
C	8.77517	-1.14825	-0.84398
H	8.10895	-2.00952	-0.95392
H	9.80394	-1.48034	-0.69549
H	8.70750	-0.48369	-1.70979
Cl	5.96195	-3.13245	-0.19093
Cl	-6.83965	-4.21907	0.56972
Cl	-5.03369	3.64614	0.16544
Cl	6.49279	1.98819	-1.33925

9. Dihedral angle dependance

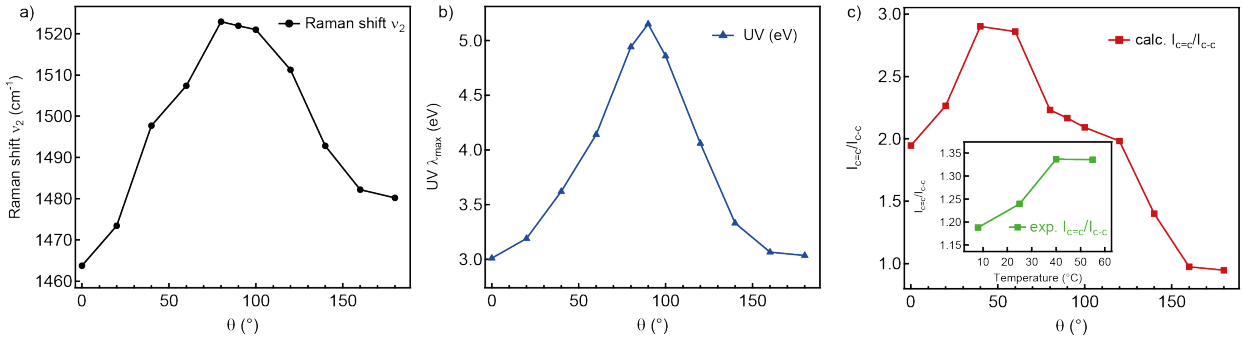

Figure S9: Dihedral angle dependence (a) of the computed ν_2 band maximum, (b) of the vertical excitation energies (computed at the CAM-B3LYP/6-311G*level) and (c) of the computed $\frac{I_{\nu\,\mathrm{c{=}c}}}{I_{\nu\,\mathrm{c-c}}}$ Raman intensity ratio. The inset shows the experimental $\frac{I_{\nu\,\mathrm{c{=}c}}}{I_{\nu\,\mathrm{c-c}}}$ ratio as a function of temperature.

10. TA spectra at the different excitation wavelengths

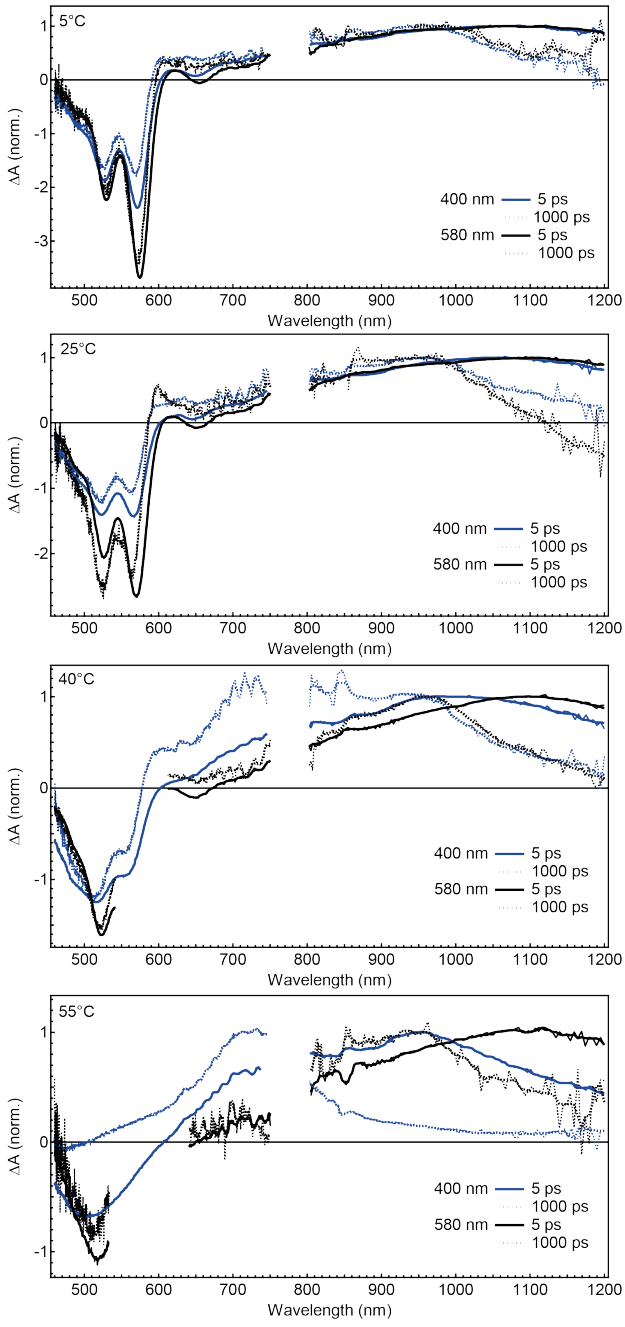

Figure S10. Normalized TA spectra for CPT at different temperatures, compared at 5 ps and 1000 ps after photoexcitation at 400 nm or 580 nm.

11. Dynamic Light Scattering (DLS) measurements

DLS measurements were performed on a DelsaMax Pro Beckman Coulter instrument at room temperature. Each result indicated in the following table is the average value over 5 measurements.

Table S1 DLS results for different concentrations of CPT in PBS

Monomeric concentration (M)	Diameter (nm)
$1.5 \cdot 10^{-5}$ (sonicated for 1h)	137.0
$1.5 \cdot 10^{-5}$	152.2
$7.5 \cdot 10^{-5}$	121.8
$1.5 \cdot 10^{-4}$	122.3

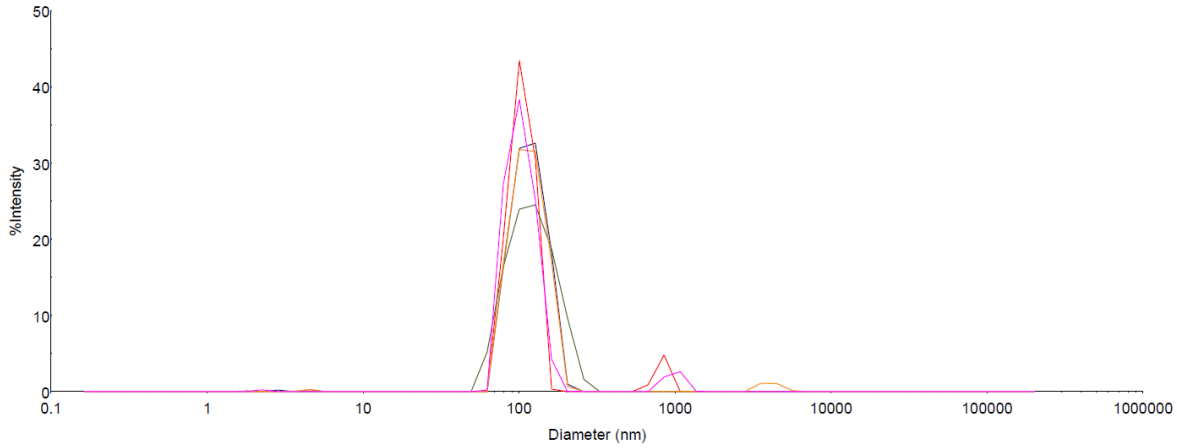

Figure S11 Size distribution of CPT in PBS ($1.5 \cdot 10^{-4}$ M, monomeric basis) obtained by the DLS measurement.

12. Fluence dependence of polaron formation

Figure S11 shows the TA dynamics probed in the GSB obtained for CPT at 5°C with 400 nm excitation with two different laser fluences. The dynamics and long-lived offset (related to polaron yield) are independent of the excitation intensity, and the signal amplitude scales linearly with fluence. This shows that exciton-exciton anihiliation does not play a role in polaron formation within the investigated fluence range.

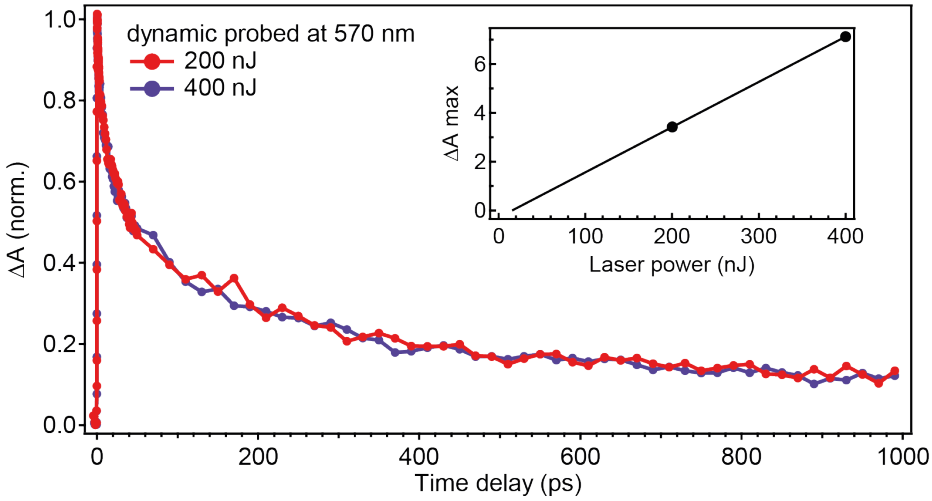

Figure S12 Transient absorption dynamics for CPT ($1.5 \cdot 10^{-4}$ M on a monomeric unit basis in PBS) at 5°C with 400 nm excitation, probed at 570 nm (GSB) and recorded with two excitation fluences. The maximum signal amplitude as a function of pulse energy is shown in the inset.