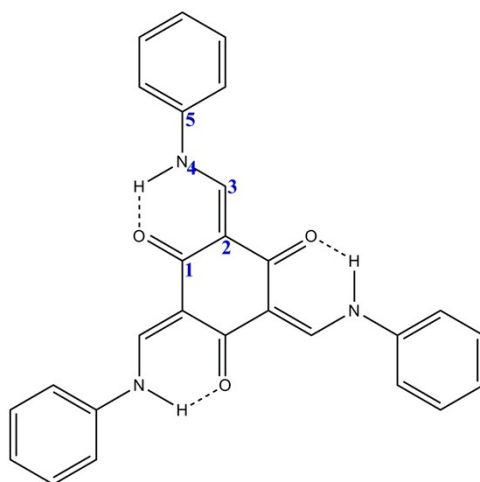


**Supporting Information for “Ab Initio Study on Photophysics of
Tris(salicylideneaniline)”**

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Scheme S1. Molecular structure showing the labeling of atoms of the *cis-kkk* isomer of the tris(*N*-salicylideneaniline).

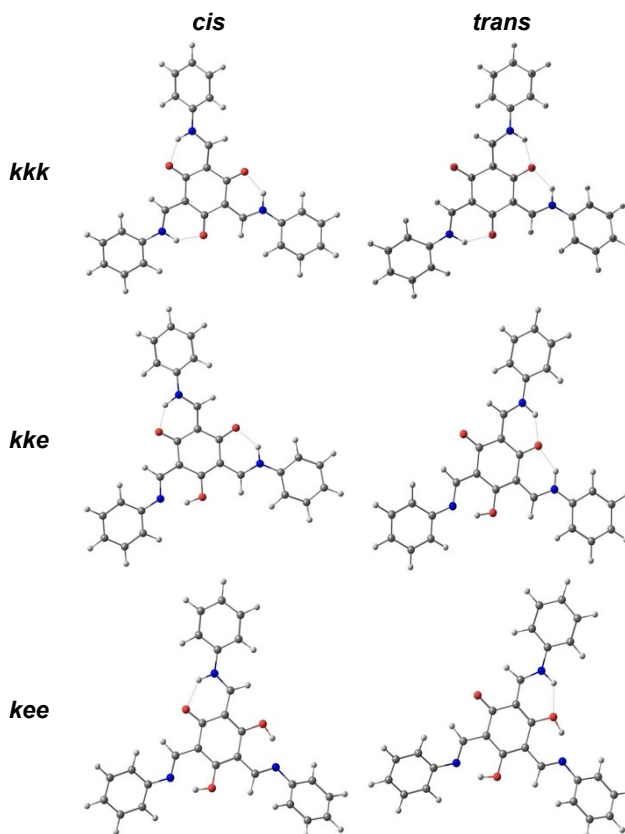


Figure S1. Photophysically relevant isomers of TSAN.

Table S1a. Vertical transition energy (ΔE), oscillator strength (f), dipole moment (μ), and leading electronic configurations of the *cis-kkk* isomer of TSAN

State	ΔE /eV	f	μ /Debye	el. config.
ADC(2)/cc-pVDZ				
S_0	0.00	-	0.00	(114a) ²
$^1\pi\pi^*$	3.37	0.97	1.67	0.86(114a-115a)
$^1\pi\pi^*$	3.37	0.97	1.68	0.86(113a-115a)
$^1n\pi^*$	3.51	0.00	0.06	0.87(105a-115a)
$^1n\pi^*$	3.82	0.00	2.31	0.47(104a-115a)-0.44(103a-115a)
$^1n\pi^*$	3.82	0.00	2.31	0.47(103a-115a)+0.44(104a-115a)
$^1\pi\pi^*$	3.94	0.00	2.70	0.60(112a-115a)+0.44(106a-115a)
ADC(2)/cc-pVTZ				
$^1\pi\pi^*$	3.30	0.90	2.03	0.87(114a-115a)
$^1\pi\pi^*$	3.30	0.90	2.03	0.87(113a-115a)
$^1n\pi^*$	3.44	0.00	0.04	0.88(105a-115a)
$^1n\pi^*$	3.77	0.00	2.30	0.57(103a-115a)+0.45(105a-117a)
$^1n\pi^*$	3.77	0.00	2.29	0.57(104a-115a)-0.45(105a-116a)
$^1\pi\pi^*$	3.88	0.00	0.03	0.58(112a-115a)-0.43(106a-115a)

Table S1b. Relevant molecular π -orbitals involved into the lowest electronic excitations of the *cis-kkk* isomers of TSAN.

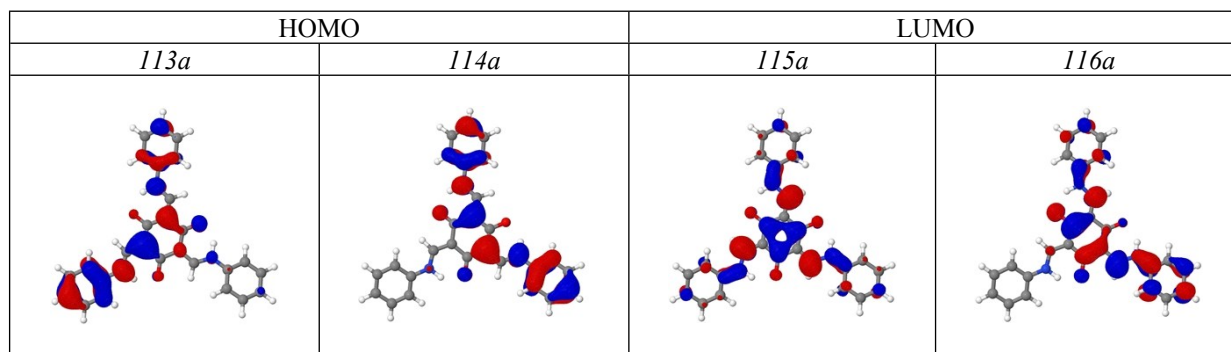


Table S1c. Vertical transition energy (ΔE), oscillator strength (f), dipole moment (μ), and leading electronic configurations of the *cis-kkk* isomer of TSAN computed with CC2/cc-pVDZ method at the MP2 equilibrium geometry of the ground state.

State	ΔE /eV	f	μ /Debye	el. config.
$^1\pi\pi^*$	3.51	0.90	96.60	0.65(114a-115a)+0.58(113a-115a)
$^1\pi\pi^*$	3.51	0.94	96.83	0.65(113a-115a)-0.59(114a-115a)
$^1n\pi^*$	3.73	0.00	0.04	0.89(105a-115a)
$^1n\pi^*$	4.08	0.00	1.75	0.61(104a-115a)+0.57(105a-116a)
$^1n\pi^*$	4.08	0.00	1.73	-0.61(103a-115a)+0.57(105a-117a)
$^1\pi\pi^*$	4.15	0.00	0.07	0.45(112a-115a)+0.38(114a-116a)

Table S2a. Vertical transition energy (ΔE), oscillator strength (f), dipole moment (μ), and leading electronic configurations of the *trans-kkk* isomer of TSAN.

State	$\Delta E/eV$	f	$\mu/Debye$	el. config.
ADC(2)/cc-pVDZ				
S_0	0.03*	-	2.22	(114a) ²
$^1\pi\pi^*$	3.24	0.75	2.39	0.76(114a-115a)
$^1\pi\pi^*$	3.43	1.07	1.17	0.35(114a-116a)-0.76(113a-115a)
$^1n\pi^*$	3.47	0.00	0.26	0.86(105a-115a)
$^1n\pi^*$	3.80	0.00	1.92	0.61(104a-115a)+0.50(105a-117a)
$^1n\pi^*$	3.82	0.00	3.97	0.52(105a-116a)-0.61(103a-115a)
$^1\pi\pi^*$	3.95	0.03	2.70	0.45(106a-115a)-0.62(112a-115a)
ADC(2)/cc-pVTZ				
S_0	0.05**	-	0.00	(114a) ²
$^1\pi\pi^*$	3.18	0.71	2.68	0.88(114a-115a)
$^1\pi\pi^*$	3.37	0.99	1.51	-0.79(113a-115a)
$^1n\pi^*$	3.40	0.01	0.20	-0.86(105a-115a)
$^1n\pi^*$	3.73	0.00	1.40	0.66(104a-115a)
$^1n\pi^*$	3.77	0.00	4.08	-0.64(103a-115a)
$^1\pi\pi^*$	3.90	0.04	3.09	0.61(112a-115a)

Relative to energy of the *cis-kkk* isomer computed at *cc-pVDZ and **cc-pVTZ, respectively.

Table S2b. Relevant molecular π -orbitals involved into the lowest electronic excitations of the *trans-kkk* isomers of TSAN.

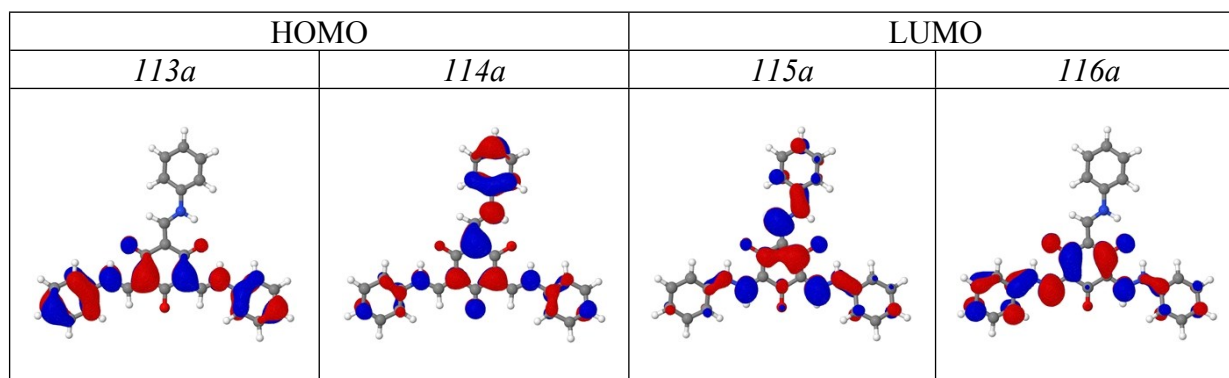


Table S2c. Vertical transition energy (ΔE), oscillator strength (f), dipole moment (μ), and leading electronic configurations of the *trans-kkk* isomer of TSAN computed with CC2/cc-pVDZ method at the MP2/cc-pVDZ equilibrium geometry of the ground state.

State	$\Delta E/eV$	f	$\mu/Debye$	el. config.
$^1\pi\pi^*$	3.38	0.96	2.48	0.87(114a-115a)
$^1\pi\pi^*$	3.58	1.32	1.50	0.78(113a-115a)
$^1n\pi^*$	3.69	0.00	0.60	-0.78(105a-115a)
$^1n\pi^*$	4.05	0.00	1.42	0.61(104a-115a)+0.49(105a-117a)
$^1n\pi^*$	4.07	0.00	3.17	0.60(103a-115a)+0.54(105a-116a)
$^1\pi\pi^*$	4.15	0.02	5.48	0.74(114a-115a)

Table S3. Adiabatic energy of the fluorescing state ($E(S_1)$), vertical transition energy (ΔE), oscillator strength (f), and dipole moments ($\mu(S_1)$ and $\mu(S_0)$), computed with ADC(2)/cc-pVDZ method at the equilibrium geometry of the S_1 state.

Isomer	$E(S_1)/\text{eV}$	$\Delta E/\text{eV}$	f	$\mu(S_1)/\text{Debye}$	$\mu(S_0)/\text{Debye}$
<i>cis-kkk</i>	3.16	2.93	0.88	1.48	1.11
<i>trans-kkk</i>	3.05	2.81	0.68	1.38	1.43
<i>cis-kke</i>	2.92	2.26	0.53	6.55	6.50
<i>trans-kke</i>	2.96	2.20	0.54	5.16	8.81
<i>cis-kee</i>	2.70	2.02	0.10	6.62	6.07
<i>trans-kee</i>	2.70	1.80	0.13	5.22	7.18

Table S4. Vertical transition energy (ΔE) and oscillator strength (f) computed with ADC(2)/cc-pVTZ method at the equilibrium geometry of the S_1 state obtained at ADC(2)/cc-pVDZ level.

Isomer	$\Delta E/\text{eV}$	f
<i>cis-kkk</i>	2.82	0.84
<i>trans-kkk</i>	2.71	0.65
<i>cis-kke</i>	2.18	0.49
<i>trans-kke</i>	2.11	0.51
<i>cis-kee</i>	1.95	0.08
<i>trans-kee</i>	1.72	0.11

Table S5. Vertical transition energy (ΔE) and oscillator strength (f) computed with CC(2)/cc-pVDZ method at the equilibrium geometry of the S_1 state obtained at ADC(2)/cc-pVDZ level.

Isomer	$\Delta E/\text{eV}$	f
<i>cis-kkk</i>	3.12	1.16
<i>trans-kkk</i>	2.98	0.90
<i>cis-kke</i>	2.55	0.83
<i>trans-kke</i>	2.51	0.88
<i>cis-kee</i>	2.25	0.17
<i>trans-kee</i>	2.06	0.23

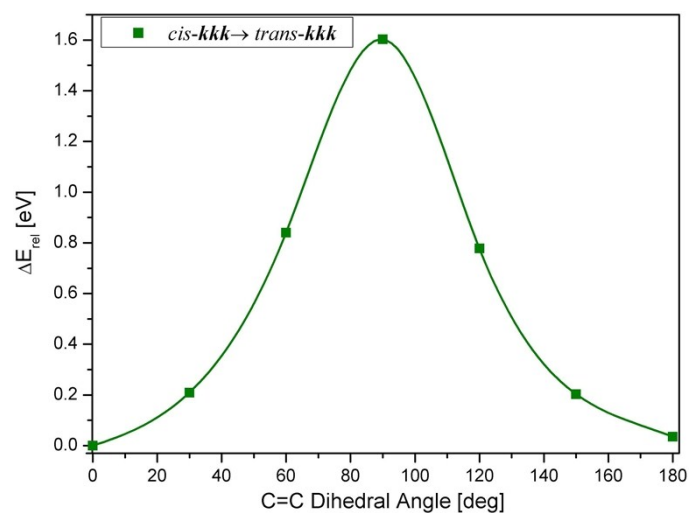


Figure S2. Minimum-energy profile for the ground state rotamerization of TSAN computed at MP2/cc-pVDZ level of theory.

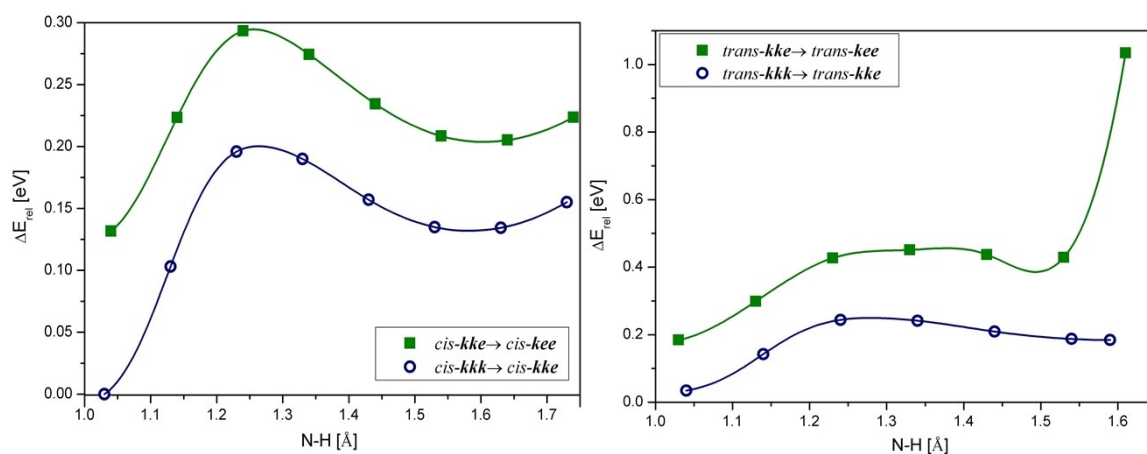


Figure S3. Minimum energy profiles for hydrogen transfer in the ground state of TSAN obtained at MP2/cc-pVDZ level of theory.

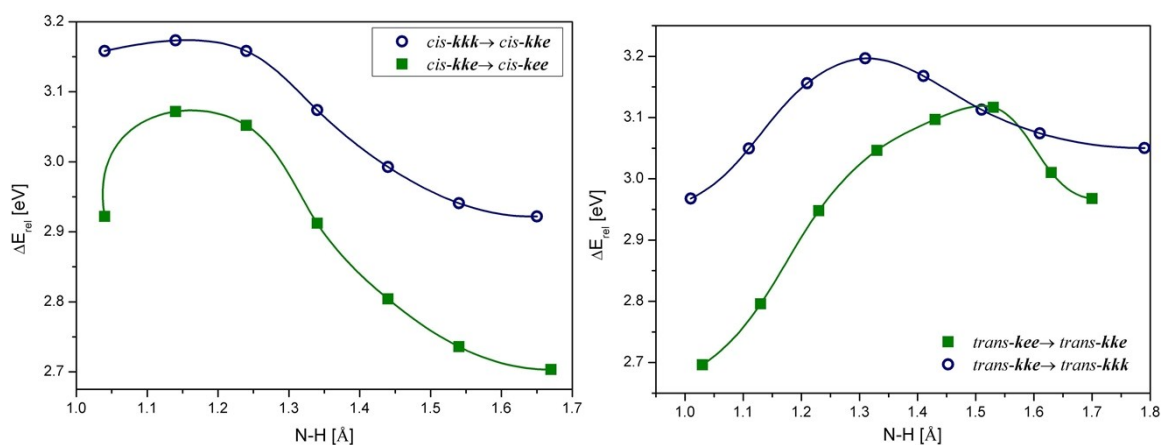


Figure S4. Minimum-energy profiles for hydrogen transfer in the S_1 state of TSAN computed at ADC(2)/cc-pVDZ level of theory.

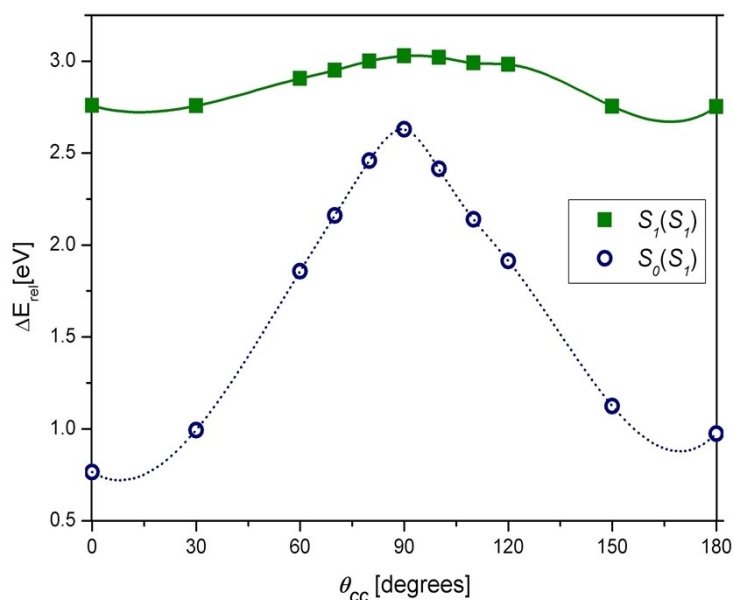


Figure S5. Minimum energy profiles for *cis-kee* \rightarrow *trans-kee* reaction of the TSAN in the ground (S_0) and first excited singlet state (S_1) computed at MP2/ADC(2)/cc-pVDZ level of theory, respectively. Symbols connected by solid line denote energy profile optimized in the S_1 state, while dashed lines denotes vertical energy of the S_0 .

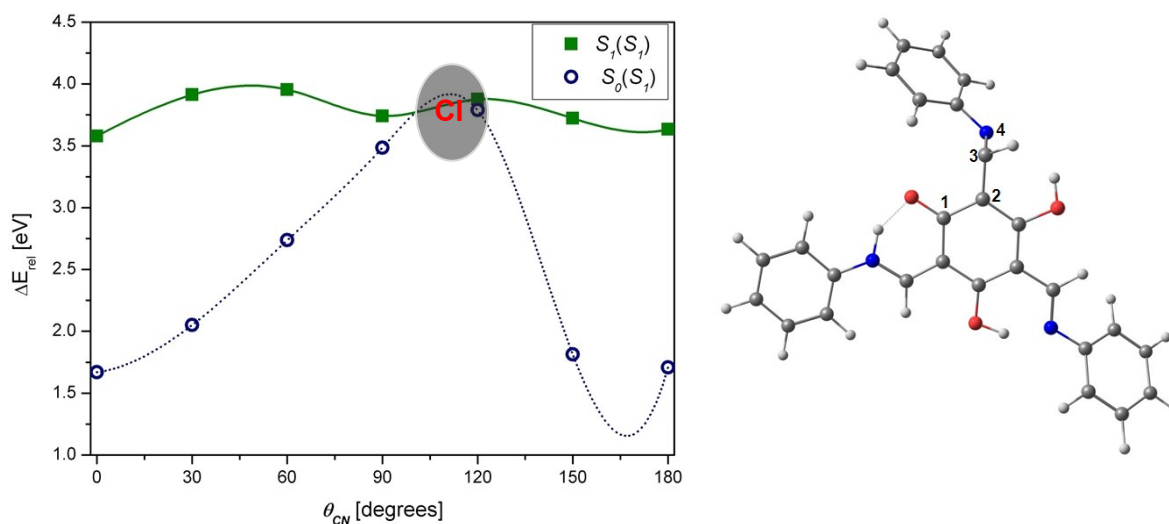


Figure S6. Minimum energy profiles for the C=N twist of the *kee* isomer of TSAN computed keeping $C_1C_2=C_3N_4$ twist angle equal to 90° in the ground (S_0) and first excited singlet state (S_1). Symbols connected by solid line denote energy profile optimized in the S_1 state, while dashed lines denotes vertical energy of the ground state computed along the minimum reaction path in the S_1 state. Molecular structure of *kee* for which the conical intersection is expected.

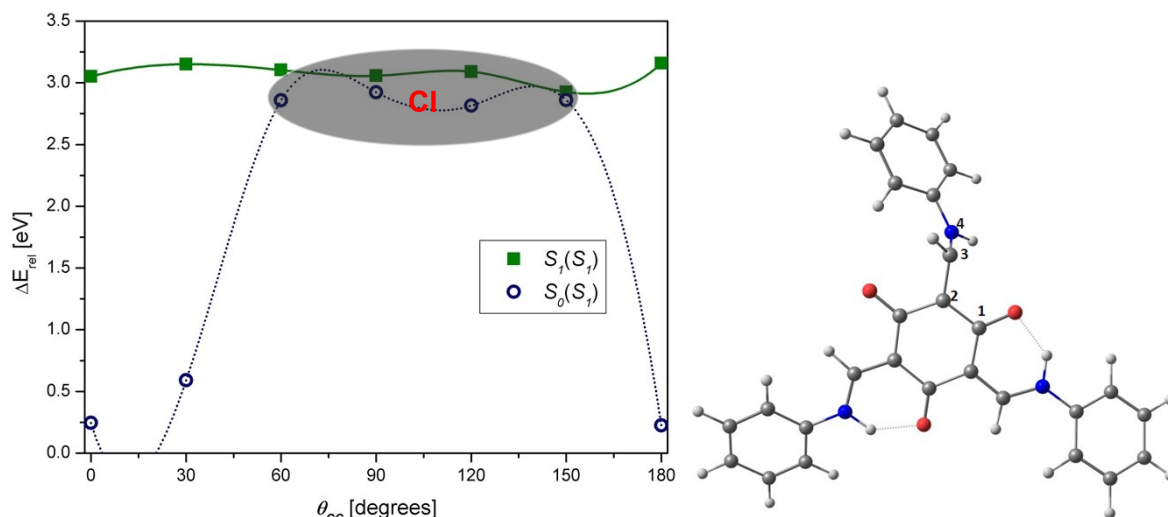


Figure S7. Minimum energy profiles for the C=C twist of the *kkk*, in the ground (S_0) and first excited singlet state (S_1) computed at MP2/ADC(2)/cc-pVDZ level of theory, respectively. Symbols connected by solid line denote energy profile optimized in the S_1 state, while dashed lines denotes vertical energy of the ground state computed along the minimum reaction path in the S_1 state. Molecular structure of *kkk* corresponding to $\theta_{CC}=90$ degrees.

Molecular Structures:

Ground State - MP2/cc-pVDZ

cis-kkk

H	3.447924170	-1.101654627	-0.022646828
N	3.764900728	-0.115456691	-0.066309656
C	-1.534386735	-5.602993722	-0.310530772
C	-2.392387339	-4.548288208	0.064825663
C	-3.722090918	-4.830936599	0.439889981
C	-4.186936174	-6.153774357	0.449470524
C	-3.329191538	-7.208407405	0.093086512
C	-2.005279402	-6.924395161	-0.285024423
N	-1.981414958	-3.203267117	0.072482408
C	-0.720454912	-2.745826845	0.041162978
C	-0.392121754	-1.394867550	0.026154242
C	1.042292148	-1.062850224	0.003033371
C	1.404227891	0.357264621	-0.020983889
C	0.399795460	1.433689300	0.005837571
C	-1.011144860	1.037388506	0.028900703
C	-1.440481026	-0.370916707	0.054134145
C	-2.016612257	1.997468121	0.049084857
N	-1.782231419	3.318538702	0.039875649
C	-2.742052187	4.346537313	0.035186223
C	-4.094703781	4.121719618	-0.295326912
C	-5.003196472	5.190588270	-0.269654676
C	-4.577291683	6.487936788	0.064806994
C	-3.225418181	6.712063837	0.376564446
C	-2.312075738	5.648216675	0.365965190
O	0.744203169	2.643028550	0.005537766
C	2.738207646	0.748166818	-0.049519560
C	5.134171969	0.201521084	-0.118202222
C	6.056292954	-0.812430934	0.213823011
C	7.433825785	-0.553170384	0.178149791
C	7.905577597	0.720884302	-0.181336787
C	6.985043467	1.729112638	-0.516704303

C	5.605164931	1.476064248	-0.496524848
O	1.917567368	-1.965627886	0.000794290
O	-2.659337592	-0.677313265	0.094641250
H	-2.675873323	-2.434631226	0.116101869
H	-0.768633489	3.536526825	0.048500275
H	0.098800054	-3.472647040	0.032281902
H	2.958045687	1.821109532	-0.053149076
H	-3.055297945	1.651443748	0.079563932
H	-4.382879931	-4.006532876	0.730499833
H	-5.221710248	-6.358675291	0.742387949
H	-3.689883386	-8.241516021	0.103396377
H	-0.511922414	-5.398138043	-0.640087059
H	5.683100473	-1.800138131	0.506901877
H	8.138436426	-1.349615026	0.438422912
H	8.980331965	0.925317205	-0.206414434
H	4.905405427	2.262419708	-0.793188435
H	-1.259677908	5.815427806	0.621377129
H	-2.877881716	7.717410655	0.635482867
H	-5.291655791	7.316839496	0.075891855
H	-4.437389601	3.125951914	-0.590328136
H	-6.051019724	5.006487029	-0.528320141
H	7.341208479	2.721421344	-0.812006952
H	-1.331889388	-7.736473287	-0.577957215

trans-kkk

H	2.960423127	-0.944990962	0.056500551
N	3.244445119	0.030559293	0.245193950
C	-2.115438505	-5.397184820	-0.854347831
C	-0.803128913	-4.907639698	-1.020275136
C	0.213718461	-5.776441101	-1.467151649
C	-0.078325784	-7.117531902	-1.754088783
C	-1.388395850	-7.603877000	-1.605991095
C	-2.400066013	-6.737393589	-1.156418631
N	-0.452221679	-3.573244481	-0.745650871
C	-1.290424556	-2.534243318	-0.600043386
C	-0.886773135	-1.237730139	-0.306625751
C	0.522617436	-0.906043114	-0.139697724
C	0.873606211	0.479407647	0.163610011
C	-0.146612187	1.536910831	0.315242757
C	-1.544386492	1.156091165	0.116880231
C	-1.967571723	-0.227163283	-0.193302305
C	-2.558389078	2.099191361	0.234606368
N	-2.344987584	3.392886540	0.521589911
C	-3.314947367	4.404881353	0.635744985
C	-4.632536121	4.253663335	0.155506185
C	-5.553350826	5.300679633	0.311398215
C	-5.173720190	6.506783181	0.925873852
C	-3.855739167	6.660669169	1.388525059
C	-2.931327136	5.615684959	1.248555264
O	0.187419743	2.715214846	0.598158784
C	2.196690073	0.864989565	0.340480045
C	4.603331437	0.364915688	0.388186956
C	5.520255981	-0.684806616	0.602394605
C	6.887134896	-0.409421210	0.750294957
C	7.352446087	0.915434121	0.694219489
C	6.437552218	1.960288281	0.476052134
C	5.069653584	1.693962230	0.313605916
O	1.425048370	-1.796491063	-0.253553215
O	-3.160307418	-0.530730993	-0.349487351
H	0.539624049	-3.302992994	-0.647403961
H	-1.342505541	3.601937059	0.675335566

H	-2.364252276	-2.710745860	-0.724241773
H	2.390939479	1.916142489	0.578529309
H	-3.589009455	1.758624637	0.087677008
H	1.230908547	-5.389411333	-1.595630149
H	0.721025063	-7.780577850	-2.100442336
H	-1.618599177	-8.649339300	-1.832892282
H	-2.908429525	-4.746889932	-0.474725466
H	5.151152225	-1.714971773	0.660810857
H	7.587728944	-1.234113678	0.916335739
H	8.418477158	1.132042758	0.813023607
H	4.377564774	2.515893764	0.110155785
H	-1.906228512	5.726295662	1.619746328
H	-3.543741717	7.595017773	1.866265846
H	-5.897121206	7.320288631	1.037348013
H	-4.937985807	3.334999830	-0.353025991
H	-6.573720055	5.173608872	-0.064677266
H	6.790197705	2.995049803	0.416226725
H	-3.421717677	-7.108138461	-1.024402068

Ground State - MP2/cc-pVTZ

cis-kkk

H	3.417634313	-1.098756821	-0.028449585
N	3.735538508	-0.118976583	-0.064103595
C	-1.518773493	-5.559905247	-0.288196634
C	-2.376889262	-4.514723072	0.066184998
C	-3.699897193	-4.795078432	0.419649613
C	-4.158621153	-6.107338799	0.429183493
C	-3.300945601	-7.152496813	0.092645400
C	-1.983633713	-6.870776699	-0.265151357
N	-1.970041415	-3.175846301	0.072713574
C	-0.718909931	-2.723477542	0.040715548
C	-0.391276759	-1.382767373	0.027931436
C	1.030480462	-1.053247154	0.001186505
C	1.393382160	0.352092226	-0.017887054
C	0.397280190	1.418830072	0.005432401
C	-1.001189951	1.030703479	0.031406453
C	-1.426473100	-0.365504022	0.051976758
C	-1.998258103	1.984948460	0.048910451
N	-1.764418582	3.295001422	0.041532212
C	-2.720883864	4.316424640	0.036926650
C	-4.064513234	4.087337252	-0.273761827
C	-4.966859866	5.145773604	-0.251502516
C	-4.542866628	6.435889506	0.062396438
C	-3.200012984	6.664130533	0.355439013
C	-2.292987352	5.610675465	0.346279997
O	0.739956660	2.624900361	0.002978321
C	2.718053359	0.738602066	-0.048123204
C	5.097480094	0.198288129	-0.115358127
C	6.013456193	-0.811736987	0.192401286
C	7.378842739	-0.552982610	0.156150194
C	7.843281931	0.716608285	-0.180976349
C	6.928806197	1.721082167	-0.493169579
C	5.561072999	1.468515857	-0.470253569
O	1.903682037	-1.952981772	-0.005176465
O	-2.641732130	-0.671767848	0.088980800
H	-2.658673475	-2.409882119	0.109551100
H	-0.756227770	3.509102785	0.044392986
H	0.090313395	-3.442365390	0.035603749
H	2.936086752	1.798850596	-0.047798427
H	-3.024971162	1.643669526	0.081401055
H	-4.357804660	-3.979906635	0.692289188

H	-5.183996717	-6.310947646	0.704794853
H	-3.655432540	-8.173306836	0.102051362
H	-0.504110160	-5.357200526	-0.598782605
H	5.646049234	-1.792522937	0.465796542
H	8.076986702	-1.342669501	0.396570405
H	8.904315187	0.919901870	-0.207131374
H	4.867792053	2.249820273	-0.745970029
H	-1.250820201	5.779403509	0.585224893
H	-2.856521180	7.660399427	0.596838979
H	-5.249531599	7.253413417	0.071441109
H	-4.404480777	3.099857437	-0.550165990
H	-6.004063165	4.960096488	-0.493993635
H	7.278946992	2.706000653	-0.769580425
H	-1.313620438	-7.673153869	-0.541445393

trans-kkk

H	2.952156648	-0.940186715	0.055211798
N	3.228795263	0.028876001	0.247059565
C	-2.113985993	-5.346870965	-0.864120761
C	-0.806900645	-4.875778248	-1.018125819
C	0.197039016	-5.748272366	-1.447732923
C	-0.102630064	-7.076138202	-1.729851100
C	-1.407622209	-7.544390555	-1.592947786
C	-2.406567919	-6.674272115	-1.159760512
N	-0.448055356	-3.550254968	-0.746108403
C	-1.275656267	-2.516765991	-0.598257444
C	-0.872425833	-1.230747386	-0.308186464
C	0.523058944	-0.900783553	-0.140092522
C	0.874211282	0.470637704	0.162569305
C	-0.138905329	1.518309108	0.309238140
C	-1.523947566	1.143049121	0.117331280
C	-1.942581825	-0.227584323	-0.193203312
C	-2.530585243	2.079695947	0.233193459
N	-2.318676632	3.362262253	0.518693237
C	-3.286523680	4.366726965	0.632546966
C	-4.595433699	4.206856469	0.168362843
C	-5.511195805	5.242922725	0.319795459
C	-5.134311651	6.444799825	0.916597359
C	-3.824980158	6.606892812	1.364307252
C	-2.905529571	5.573334120	1.226480111
O	0.192057088	2.694647145	0.587816634
C	2.186653676	0.854434563	0.337338950
C	4.578586193	0.369726904	0.391022876
C	5.495893406	-0.666299176	0.588849101
C	6.849241889	-0.384651677	0.735899643
C	7.299647972	0.933128041	0.693963722
C	6.384472624	1.964605870	0.491238167
C	5.029848088	1.691525882	0.331620126
O	1.422323689	-1.789415069	-0.253232534
O	-3.130881898	-0.529070906	-0.349315480
H	0.538014943	-3.288727544	-0.644223923
H	-1.320867128	3.569868521	0.663673611
H	-2.337631824	-2.685913371	-0.723121139
H	2.376001324	1.893449136	0.574168073
H	-3.549092985	1.740842069	0.092361872
H	1.206542522	-5.375707622	-1.566135253
H	0.683012748	-7.740606748	-2.061632625
H	-1.643027396	-8.575502887	-1.814650934
H	-2.894551355	-4.695006738	-0.499814309
H	5.138791544	-1.687189534	0.634887474
H	7.548308964	-1.195002383	0.889050254

H	8.350982113	1.153986945	0.810853224
H	4.339239826	2.500483932	0.142727783
H	-1.890061301	5.689039440	1.583130913
H	-3.517691438	7.534885336	1.826097816
H	-5.850928509	7.246369036	1.025059211
H	-4.897478505	3.293420780	-0.322927405
H	-6.521183597	5.111201549	-0.043021507
H	6.725107564	2.989620699	0.442900783
H	-3.420075968	-7.030459866	-1.037584841

First singlet excited state – ADC(2)/cc-pVDZ

cis-kkk

H	3.532212300	-1.050187642	-0.042812360
N	3.837921029	-0.059446629	-0.069412566
C	-1.567609769	-5.650450438	0.028321312
C	-2.387997502	-4.482508359	0.046679508
C	-3.807579339	-4.625443801	0.073913885
C	-4.386324192	-5.894901804	0.082467173
C	-3.571599280	-7.047527610	0.064217474
C	-2.168002533	-6.912381652	0.037253158
N	-1.874211659	-3.218773805	0.039090191
C	-0.545218839	-2.840953108	0.015057749
C	-0.275475928	-1.433880222	0.011591723
C	1.140165285	-1.052276469	-0.010558541
C	1.469794852	0.365462577	-0.026606625
C	0.429725317	1.404581149	-0.000566363
C	-0.969892366	0.965918070	0.028388571
C	-1.347331447	-0.441080948	0.036890523
C	-2.020611884	1.894286733	0.049137103
N	-1.821716482	3.231216429	0.045210602
C	-2.789799607	4.236598268	0.064401935
C	-4.178322703	3.969061671	0.096535049
C	-5.090263296	5.033712648	0.114003237
C	-4.644833157	6.367857940	0.100338446
C	-3.263838026	6.632776723	0.068737669
C	-2.342411332	5.578273873	0.050817584
O	0.738289037	2.623741648	-0.006473653
C	2.795280439	0.794037336	-0.052297413
C	5.201166677	0.261190629	-0.113758604
C	6.126560787	-0.796416708	0.026153638
C	7.504151187	-0.541568188	-0.009022102
C	7.978197210	0.770684972	-0.180241338
C	7.056524692	1.823146144	-0.322096697
C	5.675678805	1.579039743	-0.294541856
O	2.023927169	-1.958880103	-0.016531910
O	-2.580353326	-0.785541544	0.062278648
H	-2.488048102	-2.336111149	0.054073009
H	-0.816773013	3.478586943	0.024947670
H	0.262684793	-3.573338733	-0.000343034
H	2.992103667	1.870470418	-0.056086391
H	-3.044062046	1.509607756	0.069173346
H	-4.428303971	-3.721975071	0.087969569
H	-5.476683346	-5.992002924	0.103384983
H	-4.026675347	-8.043013919	0.070895247
H	-0.478376741	-5.559854647	0.007165160
H	5.753613458	-1.817437026	0.166491540
H	8.207933538	-1.373039174	0.100895951
H	9.053582987	0.971650975	-0.206193566
H	4.978475735	2.411181276	-0.424048330
H	-1.265557422	5.781624837	0.025904544
H	-2.899801687	7.665338037	0.057857579

H	-5.366086513	7.190773769	0.114345911
H	-4.549043100	2.940769463	0.108293118
H	-6.162924863	4.814690789	0.138855353
H	7.412943249	2.848829260	-0.463188708
H	-1.535203377	-7.806118405	0.023041891

trans-kkk

H	2.715198934	-0.910282427	-0.008090575
N	3.134833005	0.043944096	0.193958406
C	-1.966781720	-5.365143540	-1.126214199
C	-0.671553261	-4.810281985	-0.948872694
C	0.466196827	-5.654286587	-1.048910393
C	0.313041750	-7.017672361	-1.318862028
C	-0.972200214	-7.566087706	-1.496351475
C	-2.102653937	-6.731680845	-1.397211901
N	-0.456791686	-3.473464386	-0.680007757
C	-1.384676993	-2.484485353	-0.545250130
C	-0.957396792	-1.163643752	-0.265881124
C	0.441530955	-0.825856806	-0.110425126
C	0.790186646	0.551510249	0.162318808
C	-0.230517119	1.607619643	0.310832017
C	-1.628511942	1.231389087	0.143210202
C	-2.034818679	-0.155764112	-0.136396378
C	-2.643950832	2.173775656	0.265595866
N	-2.425227603	3.472205626	0.530064499
C	-3.391752687	4.487587810	0.641537079
C	-4.718726934	4.327624232	0.190660975
C	-5.634693085	5.379699031	0.340670538
C	-5.241786322	6.598070649	0.921697913
C	-3.914741372	6.760074470	1.354984921
C	-2.994678268	5.710665623	1.220785804
O	0.121043575	2.787994800	0.571535422
C	2.138327633	0.969450773	0.317462481
C	4.493687937	0.238763309	0.309656682
C	5.339877771	-0.891863768	0.148731013
C	6.727152294	-0.756756021	0.253627861
C	7.299803804	0.502339670	0.522302014
C	6.464329317	1.625472512	0.681412706
C	5.073626048	1.508337789	0.578319384
O	1.372300135	-1.744628369	-0.227739531
O	-3.228482731	-0.484167549	-0.267293117
H	0.516011758	-3.076666932	-0.544143080
H	-1.422641577	3.686985681	0.666741960
H	-2.450592339	-2.698989436	-0.649322795
H	2.367033854	2.015638068	0.530168255
H	-3.677287587	1.831996962	0.143700061
H	1.462886845	-5.218863586	-0.911933931
H	1.199562870	-7.656321651	-1.390814455
H	-1.092525807	-8.632689199	-1.710317612
H	-2.856264613	-4.733732977	-1.052539184
H	4.885623840	-1.868040103	-0.057435946
H	7.366243902	-1.636510155	0.124721622
H	8.385853481	0.607880194	0.607708195
H	4.441596877	2.391525251	0.703962616
H	-1.962834301	5.827486713	1.570920847
H	-3.592003323	7.704658579	1.804568403
H	-5.962226115	7.414517186	1.030591833
H	-5.035955428	3.398216953	-0.290404590
H	-6.661917630	5.246757001	-0.014055308
H	6.903272992	2.607357495	0.887893097
H	-3.105032145	-7.151665517	-1.531868158

cis-kke

H	3.394663808	-1.136850312	0.037982057
N	3.720893210	-0.147949307	-0.015394063
C	-1.461797333	-5.586801475	-0.371918317
C	-2.344991410	-4.548246260	0.041218299
C	-3.683443950	-4.887264712	0.379281660
C	-4.119899984	-6.215354443	0.339877730
C	-3.232344365	-7.234464331	-0.055869798
C	-1.908253488	-6.911914161	-0.415391684
N	-2.012794338	-3.207183114	0.122891293
C	-0.721064233	-2.809562356	0.087262360
C	-0.385377623	-1.457569461	0.063147758
C	1.042360587	-1.115774034	0.044467214
C	1.364653572	0.300244482	0.003553452
C	0.345125195	1.365439765	0.008631341
C	-1.072006895	0.972956249	0.034868727
C	-1.414993373	-0.368146421	0.077330238
C	-2.139140666	1.962045324	0.030883112
N	-1.855405996	3.299985261	0.031300136
C	-2.748509277	4.352720066	0.035516287
C	-4.156547630	4.170240917	0.055293667
C	-5.003420341	5.286821873	0.058302532
C	-4.484600408	6.594661393	0.042581062
C	-3.087699442	6.777097879	0.023759979
C	-2.227903561	5.674539740	0.020259308
O	0.699584383	2.571057116	-0.014986469
C	2.699366078	0.713285322	-0.019282780
C	5.093360640	0.168397679	-0.062183941
C	6.008474291	-0.828320471	0.331838311
C	7.386060913	-0.567256579	0.305111880
C	7.859453201	0.689724276	-0.108106372
C	6.943908762	1.679832092	-0.506391311
C	5.564509513	1.424544974	-0.495224570
O	1.926771787	-2.020737156	0.060570639
O	-2.712836608	-0.714450306	0.124183597
H	-2.729623480	-1.722951338	0.142949757
H	-0.840835751	3.492229355	0.016906589
H	0.116334057	-3.523210979	0.091867483
H	2.911982427	1.787685247	-0.036232221
H	-3.179246847	1.632462319	0.040953022
H	-4.355209517	-4.078124292	0.685077724
H	-5.151804520	-6.458981743	0.612724986
H	-3.571667803	-8.274676194	-0.094359945
H	-0.440536170	-5.351488608	-0.685872485
H	5.631124218	-1.801002606	0.666550578
H	8.088770119	-1.347764028	0.613670224
H	8.934118910	0.895216973	-0.126709915
H	4.866299128	2.191863754	-0.841643661
H	-1.140653641	5.817402246	0.005456452
H	-2.664448693	7.787377207	0.011629988
H	-5.157380826	7.457950362	0.045297271
H	-4.586185898	3.165120740	0.069427161
H	-6.087652003	5.129888316	0.073721021
H	7.304044631	2.656783227	-0.844347392
H	-1.223583352	-7.701529453	-0.742429960

trans-kke

H	2.563162262	2.103926645	-0.079078481
N	3.330452721	1.409398091	-0.045099099
C	-1.216765687	-6.155762100	-0.328327215
C	-2.120359001	-5.115050128	0.036314286

C	-3.469213156	-5.457970654	0.331678489
C	-3.897562194	-6.788208025	0.293815359
C	-2.990610604	-7.807797469	-0.054851503
C	-1.655165150	-7.483182004	-0.368784429
N	-1.800659445	-3.773781486	0.112013594
C	-0.509023380	-3.357829087	0.073496402
C	-0.194822499	-2.006360807	0.043125189
C	1.238492593	-1.640371588	0.020501586
C	1.527541245	-0.198400081	0.005618979
C	0.485269037	0.824370977	-0.008321656
C	-0.920619064	0.412013077	0.023013511
C	-1.242447135	-0.934313441	0.054894800
C	-2.015037118	1.377177790	0.016518236
N	-1.767372423	2.722412483	0.027577437
C	-2.689054911	3.750004029	0.037752992
C	-4.091487764	3.528221425	0.063051818
C	-4.969327911	4.620612731	0.072268139
C	-4.487826485	5.942635767	0.057759522
C	-3.096618174	6.164288003	0.033916970
C	-2.206374768	5.086283577	0.023879690
O	0.803297705	2.056891001	-0.043087808
C	2.877521023	0.150807039	-0.018626875
C	4.677464555	1.821989691	-0.047524811
C	4.957271560	3.145193481	-0.444599299
C	6.280363043	3.609114745	-0.465209081
C	7.334827829	2.755889839	-0.097539803
C	7.052217311	1.438283998	0.303051815
C	5.730755975	0.968368785	0.339476476
O	2.126422367	-2.514414200	0.019142400
O	-2.528388708	-1.303737026	0.097107190
H	-2.526188886	-2.317436664	0.120642972
H	-0.760308055	2.943956771	0.009288071
H	0.338803628	-4.058792410	0.079140818
H	3.607691629	-0.666108297	-0.020413319
H	-3.045813253	1.020070683	0.024373830
H	-4.155671662	-4.648482173	0.602095307
H	-4.937529725	-7.033859623	0.531994652
H	-3.322881253	-8.850370245	-0.090736382
H	-0.184302260	-5.921332758	-0.603381436
H	4.132404495	3.801304249	-0.744295151
H	6.485588315	4.638589432	-0.775613115
H	8.367999163	3.115975584	-0.116255675
H	5.525094402	-0.048026492	0.687065827
H	-1.123662093	5.260379050	0.004898461
H	-2.701993348	7.186123212	0.022896235
H	-5.184586956	6.786635881	0.065420527
H	-4.492735201	2.511446394	0.077301472
H	-6.048630499	4.433108081	0.091908616
H	7.864909341	0.770057685	0.605509660
H	-0.954511416	-8.273943447	-0.656766175
<i>cis-kee</i>			
H	2.762897971	-1.671219896	0.033288027
N	3.695160771	-0.281214834	0.021652240
C	-1.603648570	-5.512761127	-0.735820451
C	-2.374337114	-4.563620304	-0.026004670
C	-3.555118674	-4.974088803	0.628536760
C	-3.935829954	-6.323273253	0.617970741
C	-3.157263940	-7.269324824	-0.073239015
C	-1.997784717	-6.859043961	-0.755583243
N	-2.046667408	-3.192098996	0.033045796

C	-0.785539861	-2.832609808	0.029870913
C	-0.401128489	-1.441921811	0.028390788
C	0.960855717	-1.138515273	0.029004803
C	1.363819932	0.245640957	0.023852998
C	0.369305097	1.332648112	0.032909771
C	-1.047215396	0.997732709	0.038223415
C	-1.405335343	-0.348256204	0.036022275
C	-2.078948828	2.004943305	0.046144468
N	-1.780163331	3.346138725	0.047867077
C	-2.669679605	4.404104235	0.062728470
C	-4.077567444	4.231122014	0.068633321
C	-4.919861978	5.352197319	0.082893394
C	-4.396864948	6.657521316	0.091509156
C	-2.999525177	6.830977760	0.085535459
C	-2.145248118	5.723411349	0.071257765
O	0.796818475	2.526959855	0.032167796
C	2.746201487	0.629497682	0.027434210
C	5.045399406	0.121953628	-0.036984785
C	5.995481381	-0.732373888	0.562051666
C	7.355603217	-0.392855162	0.552677582
C	7.779879141	0.787206986	-0.084289501
C	6.840160784	1.625536246	-0.712007316
C	5.476539309	1.298988919	-0.691500735
O	1.871929302	-2.130897333	0.031795017
O	-2.714463521	-0.669771220	0.040263038
H	-2.760273638	-1.668497184	0.043333632
H	-0.771889972	3.543215451	0.044888180
H	0.030204136	-3.572853901	0.041793932
H	2.959808588	1.709709815	0.047148910
H	-3.125360336	1.697014884	0.055318020
H	-4.150455028	-4.221162067	1.155109981
H	-4.845651838	-6.635610531	1.140570852
H	-3.461128894	-8.320819143	-0.093271390
H	-0.723728841	-5.188916319	-1.301346298
H	5.643231630	-1.648421607	1.047336467
H	8.085268908	-1.052794025	1.032400947
H	8.843007701	1.047191689	-0.104345842
H	4.752397366	1.933091465	-1.213066600
H	-1.057330212	5.862753789	0.067081673
H	-2.569717101	7.838650725	0.092265583
H	-5.065294888	7.524012103	0.102546507
H	-4.513811749	3.228939453	0.061474304
H	-6.004744454	5.198649587	0.087083461
H	7.172023707	2.531243434	-1.229615793
H	-1.404414654	-7.588132034	-1.317003743

trans-kee

H	3.214504524	-1.178453455	0.047302996
N	4.099387365	0.235974217	0.029585247
C	-1.006488777	-5.186783756	-0.724318509
C	-1.813352915	-4.265125986	-0.018213545
C	-2.980134530	-4.719246692	0.633090632
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O	-2.308917778	-0.414254625	0.029193063
H	-2.301161103	-1.420743751	0.039170129
H	-3.290980093	1.252653456	0.031027440
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H	-2.762026601	-8.061148580	-0.085871582
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