Supporting Information for:

Computational study on the luminescence quantum yields of terbium complexes with 2,2'-bipyridine derivative ligands

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1. Computational details

1.1. Comparison of the geometries and frequencies obtained from different calculation methods

  The geometries and frequencies calculated using different three methods are shown in Figure S1.

Calculation level (I): The ground state of Tb^{3+} was described as the septet state with the $(14s13p10d8f)/[10s8p5d4f]$ small-core RECP basis set.[S1] In this calculation, 28 electrons $(1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10})$ are included in the small-core RECP and 4s, 4p, 4d, 4f, 5s, 5p, 5d, and 6s valence orbitals are calculated explicitly. The lowest quintet state was also calculated with the same level of theory.

Calculation level (II): The ground state of Tb^{3+} was described as the singlet state with the $(7s6p5d)/[5s4p3d]$ large-core RECP basis set. In this calculation, 54 electrons $(1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 4f^8)$ are included in the large-core RECP and 5s, 5p, 5d, and 6s valence orbitals are calculated explicitly. (This is the same method used in the main text.)

In both calculation levels (I and II), the ωB97XD DFT functional was used with the cc-pVDZ basis set for other atoms.
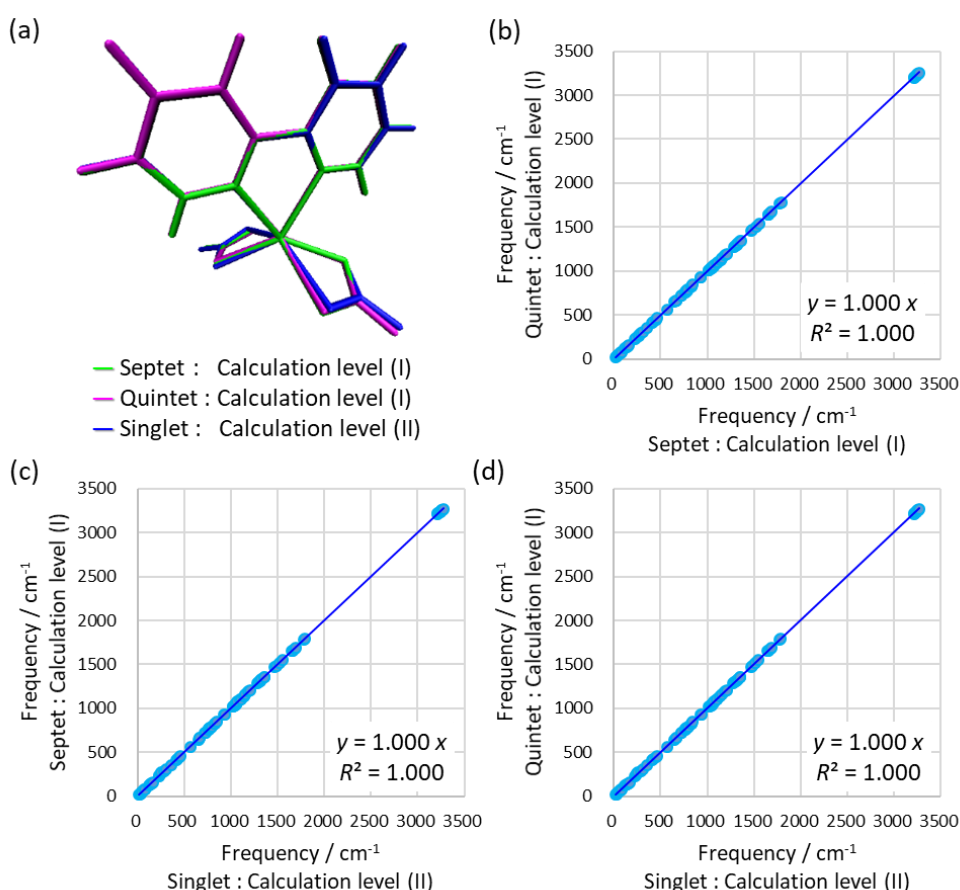

Figure S1. Comparison of (a) geometries and (b-d) frequencies (in cm^{-1}) of the LMs on the PESs of the lowest septet, quintet states calculated at the level (I), and the lowest singlet states calculated at the level (II).

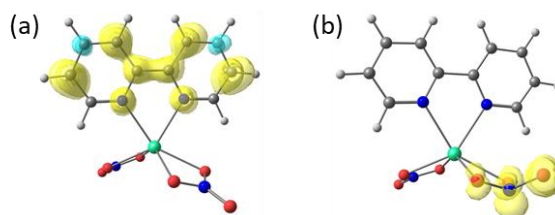## 1.2. Spin densities of Tb(bpy)(NO₃)₂ at the ligand-centered triplet states

Figure S2. Spin densities at the LMs on (a) bpy-centered T1 and (b) NO_3^--centered T1 of Tb(bpy)(NO₃)₂.

1.3. Geometries of Tb(bpy)(NO₃)₂ and TbL1(NO₃)₂ at the MEX between T1 and S0

$\Delta G = 79.0$
$(\Delta E = 83.9)$

$\Delta G = 84.4$
$(\Delta E = 86.6)$

$\Delta G = 82.8$
$(\Delta E = 86.8)$

$\Delta G = 91.5$
$(\Delta E = 96.5)$

$\Delta G = 100.0$
$(\Delta E = 105.7)$

$\Delta G = 110.3$
$(\Delta E = 117.4)$

Figure S3. Geometries of Tb(bpy)(NO₃)₂ at the MEX points between bpy-centered T1 and S0 PESs shown in Figure 2(a). Gibbs free energies (at 298.15 K and 1atm) and electronic energies are in kcal/mol. The moieties whose structures at the MEXs are quite different from those of the LMs on the S0 and T1 PESs are shown in yellow.

$\Delta G = 60.0$
$(\Delta E= 62.9)$

$\Delta G = 61.8$
$(\Delta E = 64.5)$

$\Delta G = 79.1$
$(\Delta E = 81.1)$

$\Delta G = 81.1$
$(\Delta E = 84.6)$

$\Delta G = 84.7$
$(\Delta E = 88.0)$

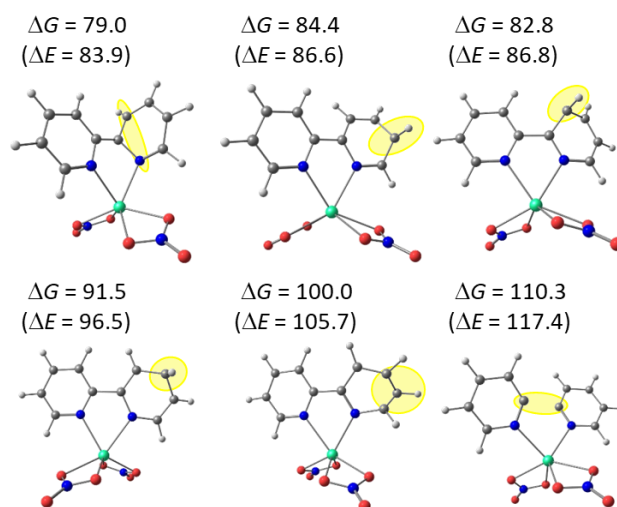$\Delta G = 94.6$
$(\Delta E = 97.8)$

Figure S4. Geometries of Tb**L1**(NO₃)₂ at the MEX points between **L1**-centered T1 and S0 PESs shown in Figure 3(a). Gibbs free energies (at 298.15 K and 1 atm) and electronic energies are in kcal/mol. The moieties whose structures at the MEX are quite different from those of the LM on the S0 and T1 PESs are shown in yellow.
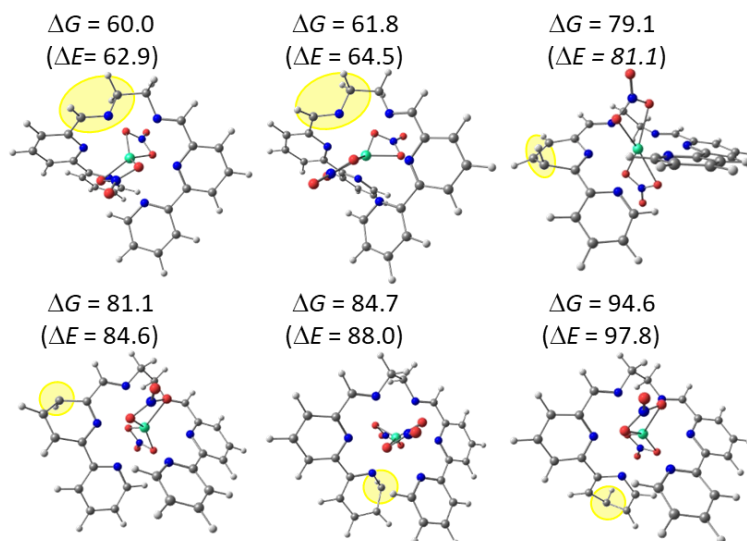
1.4. Potential energy profile of the TbL1(NO₃)₂ in the solid state

The structure and potential energy profile of the Tb**L1**(NO₃)₂ in the solid state are shown in Figure S4. The electronic energies were evaluated by the ONIOM method, in which the atoms shown in "ball and stick" and "wireframe" are described as high- and low-level regions, respectively. The ωB97XD method with the same basis set written in the main text and the MM method with the UFF force parameters and the QEq charges were used for the high- and low-level calculations. The initial structure was obtained from the crystal structure (CCDC: 919431) and the structure of one of the Tb**L1**(NO₃)₂ complexes (in high-level region) was optimized with fixing all the surrounding atoms.

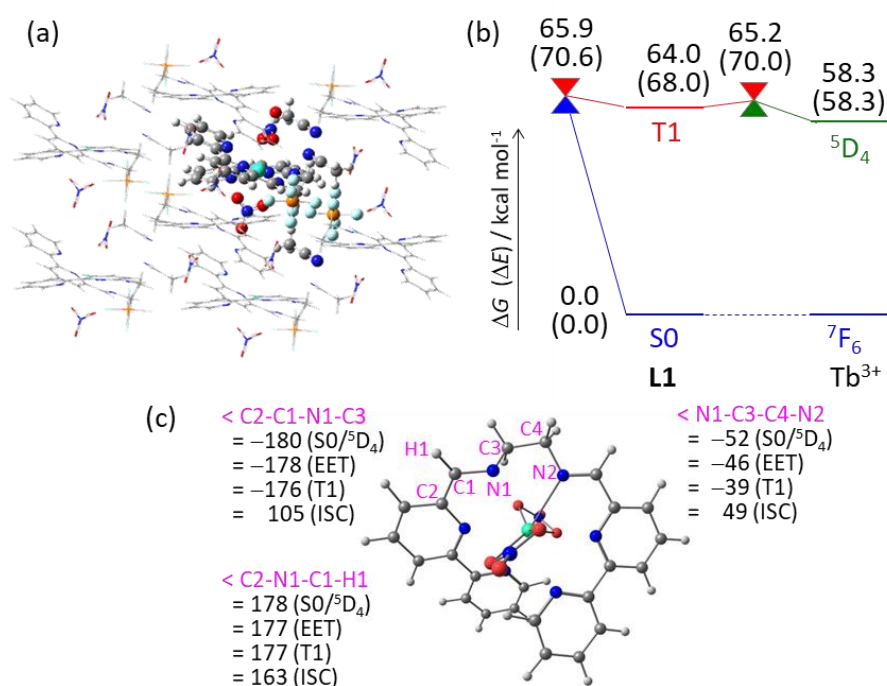**Figure S5.** (a) The optimized S0 structure of the Tb**L1**(NO₃)₂ complex in the solid state calculated by the ONIOM(ωB97XD:UFF) scheme. The high- and low-level regions are shown in ball/stick and in wireframe, respectively. (b) The Gibbs free energy (at 298.15 K and 1atm) and potential energy profile (in kcal/mol) calculated by the same level of theory. (c) The geometry parameters at the critical structures.

1.5. Comparison of the time scale of emission and quenching

According to the transition state theory, the rate constant for quenching from $^5D_4$ (k_{nr}) can be written as follows,

$$k_{nr} = \gamma \frac{k_B T}{h} \exp\left(-\frac{\Delta G^{\ddagger}}{RT}\right) \tag{1}$$

where k_B is Boltzmann's constant, h is Plank's constant, T is temperature, R is the gas constant, $\Delta G^{\ddagger}$ is the activation barrier of quenching (i.e. the Gibbs free energy difference between $^5D_4$ and the rate determining step of quenching), and γ is the transmission coefficient which is often taken as $\gamma = 1$. Though the hopping probability need to be considered for a pathway via a MEX between S0 and T1,[S2] the rate constant (1) is treated like a spin-allowed transition because Tb^{3+} has a large spin-orbit coupling constant. The rate constant for emission (k_e) can be evaluated by the inverse of the lifetime of $^5D_4$ at 77 K (1.5 ms).[25]

Table S1. Rate constants k and their inverses k^{-1} of each step for the Tb(**L1**)(NO$_3$)$_2$

Condition	T1→MEX(ISC)		T1→MEX(EET)		$^5D_4$→MEX(ISC)	
	k [s^{-1}]	k^{-1} [ms]	k [s^{-1}]	k^{-1} [ms]	k [s^{-1}]	k^{-1} [ms]
In solution / 298 K	3×10^{12}	3×10^{-10}	4×10^9	3×10^{-7}	4×10^{11}	3×10^{-9}
In solid / 298 K	3×10^{11}	4×10^{-9}	8×10^{11}	1×10^{-9}	2×10^7	6×10^{-5}
In solid / 77 K	6×10^6	2×10^{-4}	6×10^8	2×10^{-6}	4×10^{-10}	2×10^{12}

1.6. Gibbs free energy profile of the Tb complexes with modified ligands
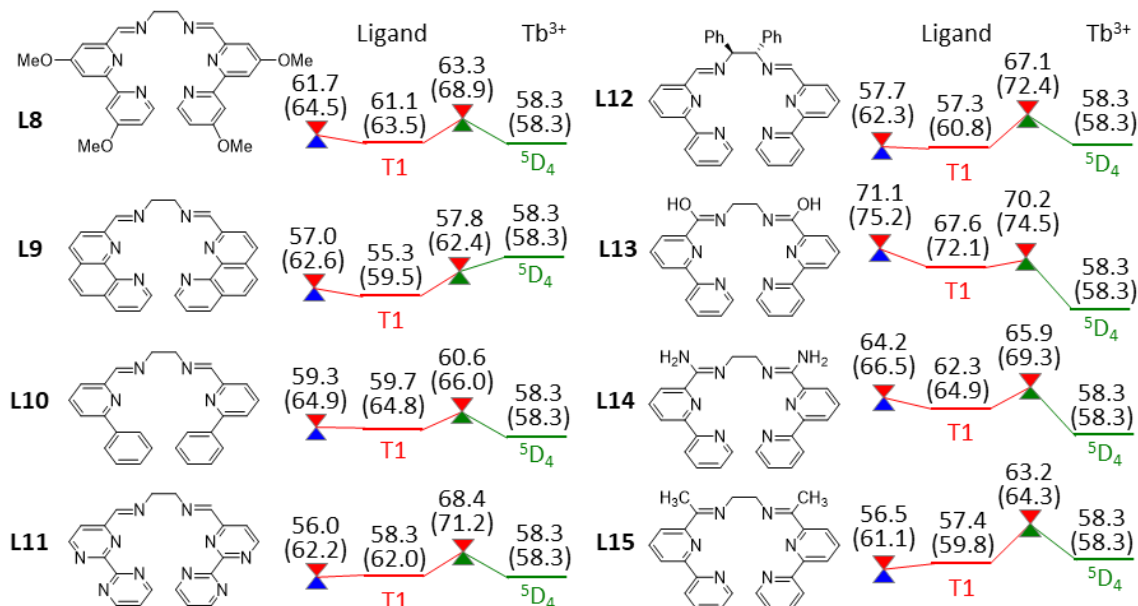
Figure S6. Gibbs free energy profiles (at 298.15 K and 1 atm, in kcal/mol) of Tb complexes with modified helical ligands calculated at the ωB97XD level of theory. The values in parentheses are electronic energies. The references (energy zero) are the energy levels of the LMs on the ground state.
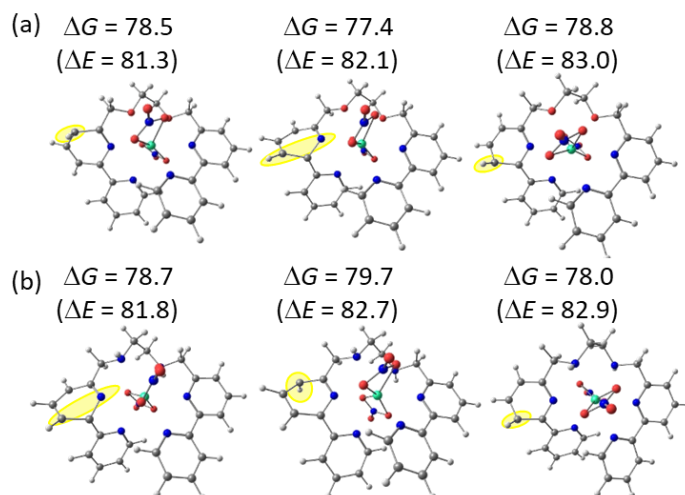
Figure S7. Structures of (a) TbL6(NO₃)₂ and (b) TbL7(NO₃)₂ at the MEX points between T1 and S0 shown in Figure 4. Gibbs free energies (at 298.15 K and 1 atm) and electronic energies are in kcal/mol.

2. Cartesian coordinates

✓ All the energies (electronic energy (E), electronic energy with zero-point correction (E+ZPE), and Gibbs free energy (G) at 298.15 K, 1 atm) are in atomic unit.

2.1. Tb(bpy)(NO$_3$)$_2$

S0
E = -1092.263592376880 / E+ZPE = -1092.068601346262 / G = -1092.121438621947

|			
Tb	0.185322540865	-0.141035845121	0.408072174591
N	0.061763289696	0.259979706297	2.846834878787
N	2.392023450282	-0.011659559874	1.519516008311
C	-1.132615578479	0.418964967502	3.446244305092
C	-1.264624788053	0.667795683363	4.805449416280
H	-2.254390295045	0.787622229256	5.244006779661
C	-0.108635309661	0.762612163077	5.570667840527
H	-0.165479834893	0.958807863627	6.641932865877
C	1.131403244439	0.609510275649	4.955152131229
H	2.038769888458	0.692498356841	5.549463868989
C	1.191445255172	0.357229732575	3.587551032614
C	2.480576987015	0.186497718553	2.856446035163
C	3.716910841601	0.218971247358	3.494876554951
H	3.789686833875	0.372896671388	4.569327750255
C	4.879926772149	0.046922853641	2.747798721321
H	5.852640784316	0.072296196915	3.240152012085
C	4.783647979748	-0.161242982670	1.377399845572
H	5.665837140558	-0.306932728786	0.755601488254
C	3.519197678596	-0.187157473208	0.805430283313
H	3.389227888404	-0.366890015111	-0.264317698591
N	-1.835809999526	1.697895722444	-0.169105271872
O	-2.071857734675	0.575030435922	0.423166849414
O	-0.591612515701	1.861087341047	-0.485569861655
O	-2.670125690238	2.500817268086	-0.395784620093
N	0.925428796121	-2.344611248629	-1.138889773270
O	0.061237405065	-2.391022032960	-0.177291777933
O	1.401330822690	-1.161559484965	-1.344720408488
O	1.250388323679	-3.292484811572	-1.761944357624
H	-2.010046215468	0.353493119378	2.798458774249

bpy-centered T1
E = -1092.154197353021 / E+ZEP = -1091.963422641008 / G = -1092.017036560560

Tb	0.165645154116	-0.145923528759	0.375576286285
N	0.046138507798	0.266082193148	2.793809688155
N	2.356227676235	-0.029720533135	1.479340810828
C	-1.105274745576	0.453671177189	3.417425819104
C	-1.231181904698	0.700324905642	4.802437063744
H	-2.221966052975	0.841487346346	5.231965267048
C	-0.063457844224	0.751787359881	5.592319440860
H	-0.130604247042	0.928700044683	6.665617120395
C	1.152364721601	0.578512703551	4.991856207515
H	2.061901063658	0.616835134133	5.587487171062
C	1.239672449674	0.343090521479	3.553505841839
C	2.429310722128	0.201366094412	2.875045618439
C	3.738356957721	0.263821042124	3.516900767176
H	3.806644667708	0.461734217370	4.584354965887
C	4.877941656586	0.071815255206	2.785935920119
H	5.855914858586	0.117147546258	3.264721348578
C	4.769421707302	-0.187053095411	1.403700981268
H	5.645969850284	-0.357212952478	0.780295076159
C	3.485401616597	-0.223131722898	0.817461142254
H	3.387102049016	-0.429280330244	-0.252922976541
N	-1.871228867116	1.693232641081	-0.168536479461
O	-2.095275546788	0.577380340025	0.441036694484
O	-0.637493794065	1.849708950409	-0.522430635463
O	-2.709799626838	2.497537028816	-0.378150127097
N	0.931771274409	-2.352052403403	-1.163764336858
O	0.042654956880	-2.396149287578	-0.226588005007
O	1.419833086246	-1.171944180679	-1.356544951433
O	1.269331731429	-3.301478180970	-1.779197204414
H	-2.003754117572	0.416045083781	2.793267332075

MEX for the EET from the bpy-centered T1 to $^5D_4$
E = -1092.153706777350 / E+ZPE = -1091.964586604675 / G = -1092.017254925800

Tb	0.170600510045	-0.143152716978	0.380591591889

N	0.051897948949	0.274164175025	2.800743283028
N	2.362534532979	-0.033035615574	1.488439848738
C	-1.105829881683	0.460650365901	3.420564517192
C	-1.233381577198	0.704137791194	4.802017157415
H	-2.223961029622	0.845483943491	5.231972671383
C	-0.067803373016	0.754101451241	5.589232094058
H	-0.133207198705	0.929992849090	6.662884592205
C	1.151109625026	0.580993949274	4.986350949029
H	2.059663370460	0.619643338057	5.583517333931
C	1.235192224770	0.347160067885	3.558348369192
C	2.437379224676	0.197510209699	2.874117823974
C	3.735221592509	0.257402837915	3.514729773293
H	3.804364734276	0.452349047439	4.582720127637
C	4.879070949653	0.067496008138	2.782763383793
H	5.855858524652	0.112711819990	3.264118841025
C	4.772778881911	-0.188375963008	1.403189374860
H	5.650348132895	-0.356619974950	0.780650335627
C	3.491966484990	-0.225616646225	0.819472064124
H	3.388942652402	-0.431324715364	-0.250246742331
N	-1.875901249472	1.683118489366	-0.167387793390
O	-2.094234465789	0.567779077824	0.444918426597
O	-0.642111752701	1.846081752243	-0.519085071373
O	-2.718808607272	2.481527626762	-0.381504711451
N	0.930909477948	-2.344572741753	-1.167212709501
O	0.044843906003	-2.391033642161	-0.227106712833
O	1.419581480225	-1.164228523848	-1.357170101641
O	1.265174044967	-3.291997768864	-1.787336657739
H	-2.000631202804	0.423986878192	2.791633788284

MEX for ISC (1) from the bpy-centered T1 to S0
E = -1092.129892931693 / E+ZPE = -1091.941690234665 / G = -1091.995537727433

Tb	0.197832478589	0.226505579529	0.198350357351
N	0.241483145846	-0.087217235222	2.638696743390
N	2.435269726482	0.442175994136	1.176508479603
C	-0.807628748702	-0.551909605438	3.330429547906
C	-0.885704303405	-0.506901797852	4.718371823698
H	-1.765275069217	-0.900647081881	5.225213230680
C	0.169117357801	0.079685186690	5.425981003262
H	0.130522981075	0.150033854229	6.513730152677
C	1.258344875022	0.581644860580	4.735919551896
H	2.083887413194	1.062191716945	5.261212590056
C	1.301871664425	0.459885615255	3.328057407925
C	2.353147680449	0.989912367114	2.534848677823
C	3.658777557127	1.455567260786	3.097017217149
H	3.857838215519	2.491604250285	3.378052700251
C	4.606555579145	0.466477531256	3.086564905759
H	5.593094860097	0.577647059150	3.541556075417
C	4.348459093469	-0.628710998087	2.218952291513
H	5.047980921124	-1.462272517604	2.140848746615
C	3.338634285428	-0.489323585405	1.164391260083
H	3.387571258338	-1.151631981196	0.290851379614
N	-1.302984617980	2.524683169529	-0.306429569420
O	-1.737313110336	1.573466064813	0.443817602179
O	-0.123713463021	2.295338265828	-0.800045179322
O	-1.907235951708	3.514147061942	-0.525984217365
N	0.189058720100	-2.332181344237	-0.937279887389
O	-0.832130187605	-1.805519613390	-0.348948512767
O	1.211152786524	-1.541463047942	-0.992842583118
O	0.193598856571	-3.427970934887	-1.375668403415
H	-1.630646043649	-0.968882724876	2.743752454955

MEX for ISC (2) from the bpy-centered T1 to S0
E = -1092.125617996370 / E+ZPE = -1091.936096491101 / G = -1091.986870444158

Tb	0.140863013210	-0.251017776692	0.375141970375
N	-0.041747791983	0.228508203688	2.801823607508
N	2.319483706257	0.021022853859	1.505220673175
C	-1.147218444277	0.548311861807	3.402923793125
C	-1.062000795242	1.062143421170	4.786373178655
H	-0.904474211333	2.153831300746	4.816585858674
C	-0.128672769790	0.270003292928	5.633773192859
H	-0.368708369082	-0.037530485018	6.652379336795
C	1.042189142647	-0.002645285433	5.019931304811
H	1.865236519235	-0.501258414503	5.536094445294
C	1.139889810408	0.221798195154	3.590147482865
C	2.385947679331	0.175227422152	2.862276163973

C	3.625589902327	0.290136411937	3.511415264335
H	3.665713556984	0.448801968360	4.588060592298
C	4.797132009430	0.227944524248	2.768199415644
H	5.764634558054	0.321765297137	3.262686481688
C	4.720248419623	0.049840814104	1.388794709863
H	5.613125175286	-0.008281705933	0.767778138467
C	3.462459152301	-0.049942552929	0.803961258892
H	3.359439306973	-0.205887276786	-0.272802754575
N	-1.921780696165	1.546440548321	-0.196523063404
O	-2.124294970999	0.442684908424	0.443586907422
O	-0.692653288680	1.710350650798	-0.563751215026
O	-2.772841369865	2.333413405609	-0.418121555657
N	0.992056767131	-2.424631624015	-1.154309158621
O	0.114068855198	-2.501253429632	-0.205204158073
O	1.421903365119	-1.225134089649	-1.359610218152
O	1.364134542036	-3.362565410524	-1.765462334590
H	-2.088435336084	0.460323908710	2.848070351420

MEX for ISC (3) from the bpy-centered T1 to S0
E = -1092.125253845835 / E+ZPE = -1091.935510142186 / G = -1091.989504925566

Tb	0.003193800062	-2.342487975527	1.243065987050
N	-0.019320503050	-0.520725272045	2.919291609540
N	2.148395481904	-2.108600121576	2.478147251046
C	-1.142547337236	0.027863779802	3.411828924045
C	-1.200968884796	0.667595834705	4.711233517746
H	-2.173749521533	0.754472672137	5.197208447119
C	-0.044999060289	1.032752620234	5.309464756470
H	0.014711467114	1.396994111791	6.336808809219
C	1.115272398697	1.005654514850	4.380554732407
H	1.202591386299	1.924440552587	3.772154764059
C	1.143013695255	-0.230263437251	3.563210114683
C	2.284670990238	-1.089301615905	3.376659608407
C	3.479106332272	-0.886693977456	4.078757111389
H	3.562139157996	-0.046480320847	4.769117012067
C	4.537461055684	-1.767189802774	3.881589450038
H	5.472609693199	-1.632680106764	4.426295793817
C	4.390624467150	-2.812963320682	2.973873895341
H	5.194323738174	-3.523744127642	2.786154188932
C	3.182277669937	-2.941659198533	2.292423128511
H	3.025936816538	-3.750431285293	1.574116619900
N	-1.596874227794	-0.843790580659	-0.483647077962
O	-0.366525706864	-1.173479913751	-0.726837202114
O	-2.041593722557	-1.307695649907	0.633666853605
O	-2.240358355460	-0.179160456569	-1.215967050042
N	0.039526159297	-5.117342487177	1.532812858937
O	-0.808831139500	-4.337671596411	2.120690225169
O	0.858870539744	-4.491298200347	0.754328761534
O	0.065193335012	-6.285468432829	1.697172090115
H	-2.059914014120	-0.179649384833	2.854411267131

MEX for ISC (4) from the bpy-centered T1 to S0
E = -1092.109747785311 / E+ZPE = -1091.920819755359 / G = -1091.975657191982

Tb	0.994055315073	-1.114736996472	1.426555914923
N	0.824122519315	0.005240854528	3.602904651385
N	2.137646979737	1.075214001064	1.492876145549
C	0.145256880855	-0.591569977804	4.603051894547
C	0.041920678132	-0.044118181799	5.871415772236
H	-0.524254783625	-0.561387036119	6.644695435733
C	0.689638823540	1.162496026618	6.119794758138
H	0.643049135280	1.624896957528	7.106409705584
C	1.410591189298	1.772974085827	5.099466754678
H	1.938291193528	2.704357153195	5.295580994501
C	1.453561108705	1.179676221367	3.838644035565
C	2.200411821453	1.782984855098	2.701183241977
C	2.815304096330	3.000245804494	2.754967399239
H	2.740407077675	3.676620015959	3.606432655216
C	3.660268650972	3.297903813918	1.578930012388
H	4.594221159392	2.700702840718	1.693064891236
C	3.072147526168	2.918913926765	0.280203498866
H	3.121442821833	3.519019437798	-0.629852239967
C	2.458751526286	1.682664496742	0.316345582294
H	2.090256903006	1.191539190063	-0.589300442067
N	-0.740778966391	-0.570484961498	-0.695301310397
O	0.546243788099	-0.610022927949	-0.831101444711
O	-1.137992528768	-0.843760994286	0.501629137061

O	-1.475272327808	-0.304078522518	-1.579513228926
N	1.868902896660	-3.567552071911	2.436703013803
O	0.684189900998	-3.113092144757	2.662563257924
O	2.579299461390	-2.796229749928	1.674573491041
O	2.274320196144	-4.582565993606	2.881352876074
H	-0.320702872766	-1.551561895612	4.368979670404

MEX for ISC (5) from the bpy-centered T1 to S0
E = -1092.095098912158 / E+ZPE = -1091.907597442495 / G = -1091.962020499532

Tb	0.182902864813	-1.269341785660	0.352988430131
N	-0.262165406332	-0.516613319842	2.691767232744
N	1.827661796748	0.306078161411	1.184208721330
C	-1.344194704135	-0.908933652711	3.383382338176
C	-1.597190879503	-0.483120528081	4.683748532318
H	-2.488865114800	-0.831751909307	5.203201440170
C	-0.699386225424	0.390971390879	5.283952305701
H	-0.867883685464	0.751362990969	6.299344680052
C	0.420003747667	0.814307247279	4.567518833594
H	1.126674515097	1.515228916322	5.010135971045
C	0.611035453809	0.339081212412	3.276535066166
C	1.765622442923	0.730091062274	2.443146400395
C	2.870299066966	1.519191075137	2.818419405533
H	3.128853138853	1.813881626908	3.833711071695
C	3.703020267014	1.818314490240	1.687654888635
H	4.762359000725	2.039786841829	1.850220001993
C	3.158582815787	2.205815767785	0.364686566992
H	3.732238653095	2.724039849950	-0.403451649852
C	3.006264951959	0.795071727928	0.527556301326
H	3.543748995424	0.063519273307	-0.087294359071
N	-2.491331643755	-1.078878536348	-0.447592862099
O	-1.522252670160	-0.394219045156	-0.967628202958
O	-2.106421645844	-1.899507931471	0.468956777819
O	-3.617012525129	-0.955535458355	-0.780686574857
N	2.138985449430	-3.105671857821	-0.423774102551
O	1.261772629262	-3.332452493568	0.498470730000
O	2.003701667348	-1.953072650795	-0.990417255733
O	2.985764445486	-3.875537732117	-0.713894008010
H	-2.032109297513	-1.579023284058	2.862617796783

MEX for ISC (6) from the bpy-centered T1 to S0
E = -1092.076557677653 / E+ZPE = -1091.888407809546 / G = -1091.945666509218

Tb	-0.044055511539	-1.030035726318	0.823350687560
N	-0.748045517337	0.407898988898	2.723280816384
N	2.259348124881	-0.585095433057	1.635477088710
C	-1.941176586435	1.056959105883	2.830499284692
C	-2.223932025681	1.831973176576	3.940792414260
H	-3.184762710603	2.340844163215	4.009762178859
C	-1.272142200310	1.953545472412	4.959502716291
H	-1.486767889413	2.559668235741	5.842107008179
C	-0.042721345569	1.299646391983	4.850413330579
H	0.728113381711	1.364787404165	5.616618392890
C	0.114227664888	0.557612591567	3.697483992879
C	2.422355975965	0.482182410826	2.377104021659
C	3.593315555750	0.933427091338	2.951450957460
H	3.640995307378	1.839843389938	3.553034625589
C	4.712847461522	0.139274583098	2.692964960088
H	5.683761964161	0.421827343658	3.105001297264
C	4.588797167442	-1.015953253635	1.912599491637
H	5.452064541618	-1.648318590411	1.707763204578
C	3.353189393762	-1.361682346664	1.395787625647
H	3.196382175365	-2.259399571578	0.795412001548
N	-1.003513278948	0.304752941312	-1.434107921927
O	0.045710916284	-0.456397070762	-1.420193961477
O	-1.569078010594	0.407969988753	-0.280354733830
O	-1.393755765292	0.847829361609	-2.405454868446
N	-0.318430143357	-3.796080574387	1.083059708784
O	-1.282241565826	-2.941616710888	1.235547691815
O	0.811101033338	-3.241376296611	0.806239789505
O	-0.467115681203	-4.960892173770	1.192405398996
H	-2.642148617611	0.939492103711	2.002443191287

NO₃-centered T1
E = -1092.150419130330 / -1091.958965946032 / -1092.013805558857

Tb	-0.075729027641	-0.514415752082	0.504226903025
N	-0.103510230199	0.035923007101	2.910956979062

N	1.980849226658	0.595796053835	1.296770417716
C	-1.185481655878	-0.247061890662	3.658412141198
C	-1.276858375226	0.080169814661	5.004157357864
H	-2.175190882810	-0.172619097402	5.565763582243
C	-0.203438115921	0.735466371247	5.594534988686
H	-0.233111897438	1.013776380891	6.648656487905
C	0.916377091696	1.040779798699	4.824397911760
H	1.755684981768	1.560479160036	5.281549121904
C	0.943645971429	0.678773327942	3.480626677332
C	2.104450986964	0.973832812061	2.591195206698
C	3.263759253021	1.594866017289	3.047131852861
H	3.368269699152	1.893116185874	4.088030368755
C	4.309204377179	1.833308258470	2.157966994426
H	5.220434546430	2.320410999390	2.506805197627
C	4.179181135198	1.438267886469	0.832202625420
H	4.973526986861	1.597629058212	0.104245242109
C	2.999162660971	0.817794881197	0.446096637861
H	2.858507877529	0.467424416850	-0.579019120616
N	-2.625336433394	0.492905290353	0.177297950837
O	-1.555393082895	1.051837433669	-0.322056524700
O	-2.460889132476	-0.682214898023	0.737183490048
O	-3.328677380082	1.227418761613	1.032457691535
N	1.269289407331	-2.544514858312	-0.863264645089
O	0.500348260966	-2.750199190652	0.154805253269
O	1.331475485887	-1.302664499873	-1.217271886017
O	1.861369219655	-3.404743198450	-1.412586113409
H	-2.011111366944	-0.745679031720	3.145677413359

MEX for the EET from the NO₃-centered T1 to ⁵D₄
E = -1092.141363985128 / E+ZPE = -1091.950458662918 / G = -1092.002923942921

Tb	-0.157257419225	-0.490736099210	0.554040791738
N	-0.114773730410	0.071883956323	2.959371715547
N	1.928845029467	0.607007003787	1.286443766997
C	-1.183769834180	-0.187046877575	3.734117280042
C	-1.224260642681	0.121715451210	5.086879999051
H	-2.113300342228	-0.110753733672	5.671614061683
C	-0.112402242035	0.731836871211	5.654309863311
H	-0.101228716388	0.994166470599	6.712904448473
C	0.993722194235	1.012914653178	4.855625732860
H	1.861747406111	1.499626573309	5.295061539968
C	0.969652592342	0.670509058526	3.506657284039
C	2.111767250910	0.940873626036	2.586017199808
C	3.311429162198	1.497475384594	3.020230566382
H	3.463310225303	1.755617947233	4.065988003652
C	4.336209107777	1.719031589718	2.103224649196
H	5.278963909314	2.155557048196	2.434905015167
C	4.144398318195	1.372730444598	0.771395773502
H	4.920146813241	1.521699825145	0.021481239006
C	2.927011512859	0.813660119842	0.408251717968
H	2.736624519525	0.502288667967	-0.621488932940
N	-2.752387701522	0.478681425006	0.202031283652
O	-1.699392769018	1.030575537283	-0.306937292215
O	-2.496474771861	-0.598192015084	0.868810439212
O	-3.839463804878	0.919420810841	0.074581225533
N	1.284813916208	-2.409180215371	-0.796683348059
O	0.638233704480	-2.674269779669	0.300602370843
O	1.127654101990	-1.220944776588	-1.302089127316
O	2.401046186544	-2.990673402356	-0.988162683962
H	-2.040054388548	-0.649612066394	3.237765620436

MEX for ISC from the NO₃-centered T1 to S0
E = -1092.148025682282 / E+ZPE = -1091.958000310625 / G = -1092.009690979048

Tb	-0.059490092038	-0.495126574334	0.489864576668
N	-0.086924490927	0.013617633022	2.903995339081
N	1.989230860266	0.614785201070	1.293551940107
C	-1.165136221166	-0.287008528126	3.649541877855
C	-1.271781748961	0.053313524040	4.990819646689
H	-2.166717998651	-0.214849508081	5.550635039149
C	-0.218960510085	0.743599119276	5.578324432566
H	-0.262917438239	1.036874991277	6.627845840744
C	0.898428766223	1.064543944179	4.811092899423
H	1.721650579176	1.611747320332	5.265400465858
C	0.943110790814	0.684738912156	3.472848503274
C	2.106233706260	0.988347023032	2.589679164327
C	3.263293195018	1.607994821652	3.053185900399

H	3.364135078606	1.899686219111	4.096323424781
C	4.312346904046	1.850238763098	2.169266654126
H	5.222295951777	2.335390450189	2.524051000864
C	4.188498232352	1.460069784102	0.841382457793
H	4.986237288640	1.621801592935	0.117727124200
C	3.010724057805	0.840082778840	0.448064408867
H	2.875662829556	0.492105728560	-0.578553395919
N	-2.614739767484	0.540699779703	0.148633045559
O	-1.517280881658	1.044050563455	-0.356838611929
O	-2.483765800941	-0.651976430138	0.710847137016
O	-3.172512045067	1.199211730540	1.175769039402
N	1.205863277906	-2.584921428367	-0.857788714843
O	0.371044623835	-2.759235412383	0.112596938261
O	1.379942090071	-1.341112891517	-1.167181235177
O	1.759327369354	-3.471370889706	-1.405153655802
H	-1.976989018701	-0.811434719225	3.141018960313

2.2. Tb**L1**(NO$_3$)$_2$

S0

E = -1851.920561916115 / E+ZPE = -1851.482069450462 / G = -1851.549643278099

Tb	-0.017424541528	0.053897325630	0.059519117672
N	-1.462298539829	2.256629601258	0.031387486145
N	0.388731724641	1.833470887804	-1.868309268399
N	1.445111776782	-0.658847732863	-1.941835153977
N	0.087465266214	-2.478050545523	-0.413081566872
N	-0.507130915462	-1.598551271648	2.078895770495
N	-0.101190978451	1.017951825134	2.515641297248
C	1.347605725924	3.823723310388	-3.553444655964
H	1.730049062912	4.612560172229	-4.201566395763
C	1.837985149349	2.524112632854	-3.652474154344
H	2.601638496991	2.260819358504	-4.384575204986
C	1.335289951653	1.565513158662	-2.779977950170
C	1.806439314510	0.166830490215	-2.836918915766
H	2.450588183091	-0.122387672258	-3.681930720346
H	2.248138780745	-2.325104944424	-3.005062455806
C	-2.496140696442	2.358640624069	0.876643847154
H	-2.655344826267	1.506415421466	1.538856009879
C	-3.341303068979	3.460685690211	0.918470501398
H	-4.169889431914	3.486537464737	1.625062836101
C	-3.103404582193	4.504670504276	0.032889167347
H	-3.744769379346	5.386899834189	0.022930455669
C	-2.041201871281	4.401616957791	-0.858927683823
H	-1.863564282760	5.197129521738	-1.580092185491
C	-1.237230753066	3.261219537632	-0.835759853300
C	-0.118875208661	3.065562675460	-1.803608586578
C	0.355579857522	4.098352333267	-2.624312958101
H	-0.040135842012	5.108541713378	-2.537742709652
C	1.831418346851	-2.057721767547	-2.020600736346
H	2.594360450332	-2.235308896742	-1.245921483156
C	0.591588302785	-2.897456592322	-1.710194806208
H	-0.189214460625	-2.680611388183	-2.456428178737
C	-0.272873546442	-3.336609222253	0.451070253136
H	-0.255909484922	-4.419324905187	0.251320648279
C	-0.709952389539	-2.892607501609	1.790226628794
C	-1.271849610593	-3.789470628645	2.691653526907
H	-1.411992577892	-4.835758728979	2.419212173044
C	-1.661844498361	-3.309203612934	3.939255322599
H	-2.130341203349	-3.971392019450	4.667703840987
C	-1.435273413357	-1.976141957632	4.246548383218
H	-1.731927459723	-1.587551417357	5.218943547862
C	-0.832284968185	-1.146106526339	3.291278472523
C	-0.483009459892	0.276787624451	3.572234037147
C	-0.501958637696	0.800956188899	4.865361158480
H	-0.792884100684	0.185455643926	5.714674648839
C	-0.112550163477	2.120295197045	5.071120706885
H	-0.115546551711	2.543419346439	6.076310051483
C	0.294477555647	2.879051035268	3.980362177801
H	0.624816348098	3.910941557588	4.092972029880
C	0.284504507669	2.283167606001	2.725222825557
H	0.611281160423	2.832728710571	1.841134276483
H	0.829935726767	-3.972968515148	-1.741963734625
N	-2.627928254718	-0.672211193763	-0.976843946287
O	-1.635902406372	-0.405857104167	-1.732895111035
O	-2.378194595142	-0.613637809785	0.277079785304

O	-3.708747819560	-0.958980658059	-1.402452824524
N	2.730593934754	0.505417118800	0.866920009172
O	2.162831180264	-0.632238583048	0.966177081783
O	1.998090764216	1.429879964735	0.369453171759
O	3.861527152225	0.697309811276	1.206910963267

T1
E = -1851.821014984700 / E+ZPE = -1851.386521749733 / G = -1851.454655757654
Tb	5.902639673837	3.099662145685	2.678390379902
C	3.390354568158	5.305445948561	3.522130159089
H	3.303481008728	4.488523045650	4.239733786073
C	2.443111100694	6.321056073460	3.478831561561
H	1.602546231028	6.312354229903	4.171482854192
C	2.595018258562	7.322026486260	2.527278950755
H	1.867716523637	8.130713796977	2.446713086869
C	3.684606974926	7.271252041198	1.663836549539
H	3.801281744632	8.032639511449	0.894555731495
C	4.595483767807	6.221348598520	1.775957769241
C	5.764130528043	6.090822466978	0.859890344572
C	6.219657912254	7.152890234483	0.066283207960
H	5.756549154404	8.135908721885	0.129699228035
C	7.284467851246	6.944028557917	-0.796755494483
H	7.655591279987	7.756526971532	-1.421795986024
C	7.868583405232	5.680863810558	-0.855168593851
H	8.696776156800	5.471246578273	-1.532540540706
C	7.373853666237	4.689184301212	-0.015776599375
C	7.943653234478	3.327811490980	-0.042153365980
H	8.693194638508	3.112829902244	-0.819715016495
C	8.042774202406	1.075984780062	0.641079805078
H	9.142116706371	1.052764873339	0.585800726241
H	7.644243804541	0.662427148920	-0.298996314258
C	7.563681774025	0.213822764129	1.806742364194
H	7.712436430467	-0.858935596043	1.599228454019
H	8.137564883364	0.450453150212	2.726278041854
C	5.460139722036	-0.365193421049	2.884867588244
H	4.994176284299	-1.229857550520	2.402802606538
C	5.173150338396	0.004293960149	4.221055026377
C	4.529042331085	-0.879935232340	5.114501121354
H	4.243346006530	-1.877169503007	4.779960327323
C	4.277761130531	-0.451393766842	6.402531574371
H	3.771674028253	-1.104027184422	7.114507169440
C	4.672992769339	0.832592783821	6.783908678920
H	4.458443338270	1.195833773891	7.787366167149
C	5.299993166932	1.657706956509	5.843641079393
C	5.710400241317	3.047846338427	6.188878422372
C	5.979446770297	3.420487028169	7.506449198349
H	5.924507470786	2.687034766865	8.309352707981
C	6.353076330552	4.731211781903	7.780407123180
H	6.575241925297	5.036729157867	8.803596821177
C	6.447621553534	5.636436827640	6.729451704309
H	6.738398191576	6.673495642613	6.891774730314
C	6.178848473114	5.182176571575	5.444991121236
H	6.265350949007	5.851552952041	4.588201771492
N	4.444568944288	5.250426477464	2.697079653734
N	6.350992782050	4.893400292261	0.827381951629
N	7.545280777948	2.442443172334	0.780410637947
N	6.184769075420	0.512685668862	2.095641127568
N	5.531564041911	1.266702589092	4.587987101717
N	5.820522219188	3.919816281875	5.169128347062
N	3.314138307543	2.425138175533	1.590996099260
N	8.618718128703	3.654156564827	3.597395841847
O	4.294207784052	2.774118293821	0.855436793215
O	3.584766258659	2.348650913224	2.842417556420
O	2.224973364017	2.190704688787	1.156887614614
O	8.082220149866	2.498641788109	3.681538153601
O	7.875624521850	4.549218986266	3.074120319496
O	9.731732776959	3.878195249608	3.976472457873

MEX for EET
E = -1851.811408643713 / E+ZPE = -1851.379057182120 / G = -1851.447640314457
Tb	-0.023323675036	0.060568511711	0.051005569287
N	-1.465498628847	2.271749095064	0.016595117712
N	0.376867040061	1.836152230963	-1.890512226007
N	1.463966584172	-0.645071293237	-1.930859778560
N	0.119289940463	-2.440438497901	-0.393981495583

N	-0.548069711741	-1.573931814932	2.049841641998
N	-0.111670951444	1.021799306140	2.521160073551
C	1.321266084077	3.815832050639	-3.596743516669
H	1.697698112500	4.600531429893	-4.253360330422
C	1.816272561347	2.517442282228	-3.686442982057
H	2.578508868117	2.250967860213	-4.418870638773
C	1.321996445297	1.564822633416	-2.802364860196
C	1.809553377087	0.171244234067	-2.840701319198
H	2.458373101997	-0.121243675891	-3.680991920152
H	2.308285188978	-2.313804526244	-2.958155158315
C	-2.496165446939	2.378448824051	0.865019743919
H	-2.650955422991	1.531160472762	1.534453393507
C	-3.344042487459	3.478557311045	0.901391959929
H	-4.169741069799	3.508383219217	1.611233866019
C	-3.112994606330	4.515237395869	0.005341940065
H	-3.756893393456	5.395548908499	-0.009588328187
C	-2.055058054843	4.406641195309	-0.890737748334
H	-1.883605911093	5.195867230518	-1.620262285685
C	-1.247629335928	3.268577236472	-0.861119529158
C	-0.133902167685	3.067272943343	-1.833351202805
C	0.333323763593	4.094917470710	-2.664541111583
H	-0.064175010065	5.104843608501	-2.583225818297
C	1.885102450212	-2.034421307927	-1.979747429800
H	2.652538703164	-2.173280624906	-1.201680472241
C	0.671859644215	-2.905010681892	-1.642252273217
H	-0.099408745509	-2.768842690251	-2.423692814231
C	-0.405807793661	-3.330097146198	0.459146367544
H	-0.514805214600	-4.386391562097	0.185972966572
C	-0.792577693101	-2.902466144436	1.725624048070
C	-1.380380888477	-3.808705152675	2.689808543081
H	-1.572781738660	-4.841692050412	2.398991932722
C	-1.678752996019	-3.346926447474	3.942879964839
H	-2.131710278671	-4.000852049993	4.687862203059
C	-1.387041646145	-2.008547810108	4.262686542520
H	-1.631750666876	-1.620881717613	5.248862349652
C	-0.805152907531	-1.161681021841	3.268178487431
C	-0.447679546895	0.253362064882	3.575058490977
C	-0.414934333997	0.743197425193	4.880651784067
H	-0.670355225167	0.107870901027	5.726427635966
C	-0.018161364435	2.059363588403	5.103736307340
H	0.022431425466	2.456532415717	6.118583414083
C	0.335788376600	2.845920144473	4.016324625371
H	0.664781789991	3.877056132835	4.139884225183
C	0.273239432806	2.281802444833	2.745080820989
H	0.558185476424	2.856214615994	1.862284456334
H	0.953165289448	-3.970576546918	-1.615056456154
N	-2.623888011304	-0.679608218705	-1.008948832526
O	-1.620006570790	-0.428766752463	-1.754991760763
O	-2.397017866691	-0.582607546928	0.246199081378
O	-3.694890180762	-0.986800905811	-1.445670864158
N	2.696401066173	0.590596847600	0.913524646716
O	2.155606020319	-0.559438866887	1.015229382583
O	1.957990431617	1.486128052598	0.373331345636
O	3.808296568868	0.820564619648	1.291999195049

MEX for ISC (1)
E = -1851.820280020198 / E+ZPE = -1851.387375678096 / G = -1851.454050354017

Tb	5.908395719251	3.145654658053	2.699812854554
C	3.446078275237	5.387299140065	3.563726728897
H	3.382418005930	4.595528760262	4.311052870256
C	2.498803551551	6.402588216887	3.518866528711
H	1.683014885260	6.419069457466	4.240292763627
C	2.619215426950	7.370213462121	2.529372209867
H	1.891694205239	8.178508323019	2.447137094214
C	3.676073598492	7.285158299810	1.628932785083
H	3.765591048490	8.020660083298	0.831710196255
C	4.588967685214	6.237134067476	1.743047886986
C	5.719090162962	6.069661913758	0.784872145430
C	6.109024829424	7.085120393834	-0.099662622281
H	5.622182352339	8.058254582083	-0.082892137582
C	7.137574425929	6.844280637164	-0.997384299548
H	7.455187212548	7.620331683955	-1.694012400755
C	7.755722885147	5.596313626662	-0.996047538827
H	8.559230880670	5.362048104120	-1.694679243733
C	7.327611303081	4.652595822617	-0.069190759067

C	7.949742609472	3.315245184195	-0.020997221864
H	8.689704191790	3.079031498343	-0.801487770091
C	8.221727550523	1.144886639938	0.851047244252
H	9.304927110179	1.214081409489	1.032597948231
H	8.070218162979	0.696999466086	-0.143697601239
C	7.586098813856	0.254134864728	1.919371836984
H	7.768392718833	-0.814849999321	1.719255762729
H	8.028186165749	0.468999177176	2.915045130957
C	5.411392311839	-0.343278564575	2.799246569800
H	4.878367097573	-1.135372509950	2.267422311841
C	5.137701499797	-0.000068963821	4.143973064744
C	4.454168843615	-0.881275315183	5.012069787608
H	4.131841269295	-1.857272882866	4.649490309146
C	4.212268054127	-0.477462455149	6.308822833975
H	3.677981930832	-1.129080070217	7.000889590428
C	4.650428947461	0.782263918509	6.725627835371
H	4.441351103573	1.129342432107	7.735962440727
C	5.308742110431	1.607829872451	5.809446365000
C	5.742750926265	2.980764058622	6.192016748739
C	6.047901998906	3.301839291420	7.515228190334
H	6.012747735715	2.536938475560	8.289397166691
C	6.430330228026	4.600702743367	7.830028492087
H	6.680420752310	4.866009088483	8.858044166498
C	6.495633681264	5.546710564589	6.813331255262
H	6.789899128616	6.577230694596	7.007973912558
C	6.192721899629	5.143306841277	5.519735123644
H	6.257465136806	5.846444914995	4.688514645721
N	4.471552566209	5.301677250857	2.705434184105
N	6.336228160818	4.886838355366	0.803439614679
N	7.620394622457	2.476441356520	0.877239347934
N	6.182687069882	0.537863559968	2.040656552819
N	5.539794911071	1.239797090371	4.545010931641
N	5.827929904171	3.891590416474	5.203828087039
N	3.301816921598	2.506730121745	1.630618653103
N	8.610182637711	3.743478020380	3.629929148258
O	4.282071928950	2.837928959437	0.886872856966
O	3.581930279071	2.423277706207	2.879158616544
O	2.204276401852	2.295574669263	1.205574359406
O	8.091681432788	2.581426726019	3.729999085049
O	7.850405050272	4.623266376033	3.104022378881
O	9.723265313946	3.987360843555	3.997054666342

MEX for ISC (2)
E = -1851.817784682803 / E+ZPE = -1851.384395066060 / G = -1851.451136142740

Tb	-0.038311486427	0.144142542988	0.234263770158
N	-1.433036145180	2.353010790768	-0.052417588814
N	0.538404541112	1.703496023201	-1.854777777150
N	1.500707356151	-0.765003129024	-1.709627149732
N	-0.198709366397	-2.331988123821	-0.469628458724
N	-0.433125238779	-1.607112914849	2.133506956430
N	-0.218017819648	1.036633256638	2.656210077366
C	1.719660260189	3.735880024027	-3.362178646391
H	2.179423807547	4.543205674367	-3.933207641482
C	2.336151929110	2.503558394668	-3.270755411132
H	3.283447832052	2.302148911921	-3.770521206895
C	1.712680580868	1.491086978543	-2.511007337438
C	2.296925103447	0.208231949471	-2.336308033928
H	3.377597491418	0.044536244484	-2.356474958462
H	0.767382907350	-1.483837211051	-3.543828906148
C	-2.532421334295	2.525891945310	0.696057263504
H	-2.610187127500	1.893468885480	1.581659080732
C	-3.539580213358	3.427442908735	0.377462798074
H	-4.413444680079	3.518096240033	1.021367883640
C	-3.406880899568	4.179119678131	-0.784579233600
H	-4.183788684779	4.882054513256	-1.087471093478
C	-2.267352324917	4.014531404547	-1.564320938394
H	-2.149504626184	4.572740769819	-2.492122758616
C	-1.294068921802	3.098425052596	-1.165803256590
C	-0.046511242404	2.901022476941	-1.955576074834
C	0.506224447382	3.945082304412	-2.702898301717
H	0.026119505601	4.921767956208	-2.732270293577
C	1.035089698757	-1.842654958946	-2.534242856474
H	1.928393838849	-2.486846788812	-2.675783492840
C	-0.110376619864	-2.640059985546	-1.885097201579
H	-1.059494752165	-2.313050552293	-2.333888402153

C	-0.441124503269	-3.244584123621	0.381201172655
H	-0.549324800937	-4.303282885665	0.098588202686
C	-0.605617850560	-2.897498640805	1.807165592574
C	-0.932126899787	-3.875204398381	2.739765678027
H	-1.059903933635	-4.913488411371	2.432752379147
C	-1.103539850639	-3.487753874419	4.066321945910
H	-1.378775138885	-4.217981719816	4.827418803219
C	-0.921296283933	-2.156053222346	4.405074237489
H	-1.064654561585	-1.837240410928	5.435636593359
C	-0.567783591263	-1.235157343581	3.408416180691
C	-0.312541899814	0.203286540087	3.710951837067
C	-0.143799037803	0.660986745217	5.017612348258
H	-0.192305151182	-0.025031251283	5.860908402283
C	0.121827603968	2.008057035801	5.240944020746
H	0.262834144286	2.378515514701	6.256942686078
C	0.218505846130	2.864506857971	4.151560877894
H	0.434867455400	3.924896662086	4.274155407770
C	0.047719676417	2.330578620523	2.880513646252
H	0.136528071622	2.958747148111	1.993279395912
H	0.014033319235	-3.718530638504	-2.072522044470
N	-2.714409636659	-0.443080749147	-0.751564974299
O	-1.747767941184	-0.161782479163	-1.536174064212
O	-2.418262919315	-0.436167027782	0.490848211232
O	-3.815246021596	-0.696360674159	-1.149494699231
N	2.628929047942	0.678119431463	1.232480248229
O	2.081602041408	-0.468132568498	1.334806232638
O	1.930784389163	1.551118296247	0.606154916080
O	3.707408210060	0.926585955109	1.687036926299

MEX for ISC (3)
E = -1851.791365548811 / E+ZPE = -1851.357828831116 / G = -1851.423589116569

Tb	-0.029948293011	0.058260692082	0.030304188368
N	-1.400680735051	2.321644011507	0.048508261195
N	0.371180545288	1.828819145118	-1.911344798024
N	1.356725851878	-0.695236538087	-2.005135750665
N	0.033004734530	-2.492946077072	-0.412547555746
N	-0.503140414672	-1.569788500341	2.040079201252
N	-0.044414299921	1.030653391399	2.522405550022
C	1.336600066130	3.780211663694	-3.639691248443
H	1.720441678578	4.553318813011	-4.305702124426
C	1.778899725235	2.464589619530	-3.749965480602
H	2.507067290092	2.172720687137	-4.506961145983
C	1.275805888698	1.527062518136	-2.855099547070
C	1.706371071736	0.116210156923	-2.917965888256
H	2.316674804016	-0.193984659164	-3.780571131535
H	2.095514149610	-2.379281980714	-3.084830991621
C	-2.398477644241	2.468538287514	0.929772536337
H	-2.579718571264	1.618803787823	1.589279500339
C	-3.186240107163	3.610061163592	1.009638337572
H	-3.986988465521	3.670486631507	1.745622046827
C	-2.928781394827	4.648309002522	0.122851815420
H	-3.524355309076	5.561898028665	0.141469107969
C	-1.906757922246	4.499700537492	-0.808100545490
H	-1.716903969760	5.290383372878	-1.530134340695
C	-1.158971688406	3.320115094655	-0.821000775778
C	-0.088028540587	3.078902129321	-1.831460735188
C	0.391214857978	4.091605525387	-2.674453035756
H	0.035544347804	5.115577975920	-2.578484349251
C	1.720608724118	-2.100219689277	-2.086722769875
H	2.511562171093	-2.281242242930	-1.341547690925
C	0.486456091778	-2.927120245823	-1.720276902686
H	-0.318215819499	-2.714678099946	-2.443091735560
C	-0.189730381528	-3.368153257272	0.509928597282
H	-0.092919677172	-4.447164661173	0.319705567031
C	-0.547012017438	-2.942094348899	1.833451333468
C	-0.623424731461	-3.873376868765	2.941340386419
H	-0.258062910349	-4.892159535748	2.795072201039
C	-0.990645039040	-3.402141452932	4.153827638736
H	-0.893628342867	-3.971385022117	5.079070144513
C	-1.600874818853	-2.045682681968	4.097822151174
H	-2.674259291553	-2.065488833947	3.836922256495
C	-0.865338525039	-1.111844073894	3.198606679776
C	-0.568684857264	0.288859061932	3.520904566652
C	-0.778417596983	0.794108250170	4.802732565206
H	-1.228054160976	0.161869041516	5.569539592647

C	-0.389102795565	2.103874134619	5.077170539498
H	-0.529150383982	2.525020806166	6.073440123903
C	0.185337249684	2.856893918199	4.060851639676
H	0.518382762399	3.880324122081	4.230583532541
C	0.330311475618	2.280138178968	2.797827181436
H	0.774238989649	2.834965034834	1.969011546342
H	0.720983166417	-4.003767424079	-1.753763885759
N	-2.713964078182	-0.547832933070	-0.877404705231
O	-1.744283132178	-0.350279161057	-1.681183967817
O	-2.400654270743	-0.502287199101	0.363873884627
O	-3.831487540507	-0.759060962636	-1.247618520823
N	2.709050087259	0.516838171429	0.851417062090
O	2.161269300686	-0.633450944739	0.903571489339
O	1.978568180638	1.437689618768	0.342564817632
O	3.818892166012	0.725031360214	1.246386690357

MEX for ISC (4)
E = -1851.785763981318 / E+ZPE = -1851.352205247586 / G = -1851.420472478562

Tb	0.024503841603	0.032604870107	0.032387633307
N	-1.397145564752	2.266388216280	0.057923701321
N	0.383158315649	1.816096241142	-1.904758475439
N	1.370209573687	-0.704143313310	-2.046271258382
N	0.104918613063	-2.515336969146	-0.433140885915
N	-0.333709328960	-1.617347861501	2.057539077500
N	-0.031875829988	0.981566625458	2.520023137072
C	1.354638143495	3.803734438334	-3.586892450473
H	1.742364278748	4.591129407917	-4.233616388946
C	1.792962088830	2.489572715257	-3.727636270090
H	2.520973636235	2.213261312937	-4.490593220437
C	1.287311267732	1.533370797327	-2.854287041753
C	1.710242227718	0.121785850246	-2.949770765714
H	2.303719867687	-0.175480610540	-3.828587195987
H	2.054747192285	-2.375257336325	-3.180572074647
C	-2.404986440179	2.390009603565	0.931584431196
H	-2.585625940749	1.527159256256	1.574169897515
C	-3.201209015161	3.524917807432	1.023837466210
H	-4.010067755506	3.566138268741	1.752229879875
C	-2.941786255735	4.581317860429	0.159417941665
H	-3.543463113676	5.490615219546	0.189155143105
C	-1.909789285277	4.455522018396	-0.764151241300
H	-1.718316968188	5.260970432963	-1.470410861242
C	-1.154863343061	3.281921790808	-0.791611070233
C	-0.076540969518	3.064373261082	-1.799444081570
C	0.406643322131	4.095049925870	-2.617850377849
H	0.052241996873	5.117168783021	-2.499429592750
C	1.719548696730	-2.110704178582	-2.164650367695
H	2.536082784623	-2.311965845210	-1.453082463016
C	0.492443059667	-2.934019824232	-1.765827914984
H	-0.340061277169	-2.696264318190	-2.447927294687
C	-0.115385445011	-3.387209522269	0.486975963152
H	-0.079435337061	-4.469341529240	0.298147792050
C	-0.358722051362	-2.927816311299	1.834723494546
C	-0.501113755165	-3.792589220068	3.036745770936
H	0.450786223460	-3.914083570058	3.582597913750
C	-1.627700050375	-3.347522201606	3.899266165990
H	-2.323766833989	-4.036826562974	4.379965949287
C	-1.666085126325	-2.013648595364	4.075713757878
H	-2.393738545478	-1.537440237548	4.734643487962
C	-0.812144727158	-1.170027541748	3.232998056751
C	-0.562620781350	0.244277911121	3.523437224048
C	-0.794022671303	0.785582948234	4.792498625867
H	-1.206424921560	0.167814545386	5.589275281044
C	-0.450893523851	2.112155508425	5.035713542338
H	-0.614806088106	2.551289658111	6.020532107834
C	0.122970066406	2.855922072247	4.011539030715
H	0.428954585871	3.890761330941	4.160917459424
C	0.310079691890	2.245915867010	2.771556985556
H	0.761811938162	2.787806929152	1.938258125166
H	0.711041263744	-4.012448150075	-1.827826652804
N	-2.658835806975	-0.638912616220	-0.823373083851
O	-1.711788919185	-0.413377903491	-1.647032121786
O	-2.320476055803	-0.590269503094	0.411121212610
O	-3.777895085499	-0.878197828145	-1.170938182247
N	2.775023265395	0.515697380047	0.799048967317
O	2.244297112433	-0.642732348171	0.845234136817

| O | 2.015993616491 | 1.436381049377 | 0.332353635430 |
| O | 3.894438392932 | 0.731269125186 | 1.160702468578 |

MEX for ISC (5)

E = -1851.780285168444 / E+ZPE = -1851.347454975826 / G = -1851.414609192992

Tb	-0.040635613731	0.015704284838	0.009384740271
N	-1.402669808275	2.268392323032	0.038771351477
N	0.426473525813	1.819600887232	-1.864699005671
N	1.333567940389	-0.731863427476	-2.042834565958
N	-0.007195371731	-2.531426000955	-0.465658600058
N	-0.442357854549	-1.661331926284	2.057700295451
N	-0.135925402548	0.943739919058	2.407327482465
C	1.471224351795	3.797714128406	-3.512227985166
H	1.885060518013	4.580921196645	-4.147724709099
C	1.866174755962	2.472103020268	-3.671273968882
H	2.587134140676	2.183083072039	-4.436210562522
C	1.324518071152	1.520156201604	-2.815210216194
C	1.705186957932	0.097718019533	-2.930128601238
H	2.298205528702	-0.202575772481	-3.808312387453
H	1.983752092656	-2.408847750050	-3.189173262923
C	-2.415771365181	2.404029922626	0.903730828002
H	-2.681267085417	1.507327381953	1.466199318182
C	-3.113991944531	3.593446774606	1.077735486707
H	-3.934335914538	3.645056625302	1.792722188692
C	-2.741087483302	4.691633868808	0.312301755229
H	-3.259033788984	5.646234656536	0.412732578421
C	-1.704514430682	4.552231496535	-0.604804087492
H	-1.423938275774	5.397148366503	-1.230482509235
C	-1.056925442930	3.321729903368	-0.723368948494
C	0.013446930323	3.082552388585	-1.736039931924
C	0.533123232876	4.107180206067	-2.539306890897
H	0.212079124191	5.138792225496	-2.411011309767
C	1.643737714524	-2.145748292603	-2.174398859072
H	2.445524924551	-2.379066821794	-1.455845936818
C	0.389727961868	-2.939323395195	-1.802601933051
H	-0.428293098529	-2.668106467967	-2.488273366010
C	-0.259988359655	-3.399252748826	0.426705688268
H	-0.232161251345	-4.481131458554	0.223347626898
C	-0.568088736486	-2.968715408720	1.806980333789
C	-0.921753741400	-3.893106383099	2.787925525642
H	-1.008270808845	-4.952670747947	2.545648150794
C	-1.156989940789	-3.428116359919	4.077376559506
H	-1.440665908133	-4.117406788717	4.872866181377
C	-1.015923261360	-2.070833572848	4.340708608335
H	-1.186915701133	-1.694461543276	5.347413922817
C	-0.650267095156	-1.213812469154	3.297958087264
C	-0.433414064484	0.253892485548	3.476593265484
C	-0.677240738103	0.917918575725	4.737147304199
H	-0.907696647842	0.331753454874	5.625505526547
C	-0.900396170175	2.325346671768	4.755588433609
H	-1.425745513278	2.772909945928	5.601412680309
C	-0.543256843543	3.044199229113	3.650690565752
H	-0.789827580364	4.097145124743	3.507738084348
C	0.307504757616	2.271174831961	2.702728413190
H	1.367920255449	2.252616931265	3.015811778008
H	0.579568698122	-4.022540711236	-1.876006347284
N	-2.696675681344	-0.650402903651	-0.933465753864
O	-1.726193468124	-0.411430283239	-1.726400244202
O	-2.400241118256	-0.597945132392	0.310902852261
O	-3.799528767821	-0.907491610903	-1.318987907455
N	2.711212241785	0.349853103547	0.873221888530
O	2.111254847983	-0.776887836159	0.904374750788
O	2.036555682249	1.303179992393	0.356416399855
O	3.818777823746	0.503422757564	1.302215538288

MEX for ISC (6)

E = -1851.764780888032 / E+ZPE = -1851.332456724791 / G = -1851.398822748171

Tb	-0.077346808632	0.072360281991	0.062069898603
N	-1.565900381981	2.219151761955	-0.068895828527
N	0.400497667840	1.829546698719	-1.846625572704
N	1.461616978671	-0.661118845647	-1.867984274372
N	0.024521672871	-2.463352053111	-0.404213622764
N	-0.567370563278	-1.584661934132	2.068910115502
N	-0.188249260143	1.077846038831	2.520464028136
C	1.440454407237	3.825072456098	-3.472360534684

H	1.854201953181	4.616835757307	-4.097265390532
C	1.933255891014	2.525195998565	-3.555934838326
H	2.729117319248	2.264638050311	-4.253995988951
C	1.388814933034	1.563202782062	-2.712731495701
C	1.851033030141	0.160676118226	-2.755371001194
H	2.509283869637	-0.136442474438	-3.586602483063
H	2.260852951572	-2.331401597996	-2.927442781174
C	-2.650273410869	2.302521662851	0.713061866814
H	-2.852753580393	1.432175827230	1.339010360326
C	-3.488957867089	3.410394726166	0.734140058964
H	-4.361031123807	3.422709897784	1.386932090568
C	-3.186764938433	4.479297596286	-0.100806814540
H	-3.818512624017	5.368270092874	-0.121806729218
C	-2.071874795935	4.394259571139	-0.928561044611
H	-1.842299201439	5.211186124443	-1.609999102985
C	-1.280497009496	3.245686378978	-0.892616780928
C	-0.110552818335	3.061077573404	-1.800159226696
C	0.404045251520	4.096995159419	-2.591728868866
H	0.004290673337	5.106885297441	-2.522449266720
C	1.818598791772	-2.068327090632	-1.953039142631
H	2.553496322108	-2.276929165499	-1.159202157815
C	0.549009534221	-2.881622215340	-1.693256255672
H	-0.202990089992	-2.634288644797	-2.459129002774
C	-0.438349365053	-3.309950784494	0.423251463536
H	-0.503301009974	-4.385563206597	0.197219264683
C	-0.853285710418	-2.862791747457	1.768218810543
C	-1.429291801150	-3.739759135285	2.676558859464
H	-1.643785243030	-4.770720383422	2.394192020897
C	-1.727737254187	-3.261988002562	3.953789276157
H	-2.207072568355	-3.909261356417	4.688743398673
C	-1.386789171557	-1.960281818495	4.282306645804
H	-1.592398514650	-1.569208327908	5.278179619353
C	-0.780517836434	-1.149494317462	3.310097622868
C	-0.257099737472	0.207589438909	3.608791114012
C	0.148888064189	0.585101447899	4.853748189091
H	0.019236589076	-0.036199861863	5.740181559133
C	0.942788229857	1.836013837226	4.852791815507
H	1.955362860671	1.572908754738	4.469698528650
C	0.412560264327	2.893032045137	3.968152455070
H	0.368916675522	3.954231523001	4.215508726319
C	0.031915106851	2.399272699451	2.737873955785
H	-0.194690846636	3.058902691920	1.898754438372
H	0.760956759518	-3.962224364449	-1.732355280488
N	-2.615204557845	-0.735890542050	-1.092233757259
O	-1.600964214602	-0.433958825522	-1.804132443465
O	-2.427952462401	-0.655197310307	0.170754913519
O	-3.660738696160	-1.075531302292	-1.565096591033
N	2.464405656077	0.749412703714	1.267951013420
O	2.040237344189	-0.450702993143	1.227301230675
O	1.850872612295	1.564420460535	0.500650958931
O	3.350343223776	1.098308906744	1.999812678333

2.3. TbL2(NO₃)₂

S0

E = -2248.774707777709 / E+ZPE = -2248.369117360163 / G = -2248.441151449570

Tb	-0.015211534874	0.049605836412	0.056170265190
N	-1.462734715790	2.251075924900	0.028789632527
N	0.381678072456	1.827547002275	-1.873136074662
N	1.439651084214	-0.662067932056	-1.954073612193
N	0.098180879114	-2.485723171014	-0.409881149366
N	-0.496713262579	-1.600020076275	2.078133182656
N	-0.094528716537	1.013784603717	2.512318142603
C	1.332224498765	3.804162340191	-3.543825067008
C	1.833782218467	2.513965315866	-3.661556462798
H	2.596863574110	2.277193963992	-4.402168718894
C	1.325614111944	1.561595634094	-2.788050696323
C	1.798262111441	0.162047862177	-2.850915817235
H	2.440216695672	-0.124935876823	-3.698031719820
H	2.243588183242	-2.329534512274	-3.015288302170
C	-2.495294331002	2.360145388066	0.876894686297
H	-2.669415303233	1.503392948421	1.529045360855
C	-3.328080652065	3.467078437316	0.941077451331
H	-4.161232581529	3.518409873578	1.639782660342
F	1.795711820636	4.760723677479	-4.329473228567

F	-3.815079483307	5.590117093610	0.068041162267
C	-3.059994988432	4.504798230908	0.061612991633
C	-2.010331787264	4.415809591580	-0.841916034813
H	-1.847386406981	5.231070109455	-1.543444857530
C	-1.230545569058	3.262240326124	-0.828520032273
H	0.841474293780	-3.979149968696	-1.740395859097
C	-0.119581305849	3.062900836718	-1.804922606351
C	0.343913864899	4.098958965350	-2.620665754766
H	-0.033846586571	5.117025604929	-2.556983787449
C	1.831160650341	-2.060092370279	-2.029807158502
H	2.599618136895	-2.229811322520	-1.258815035717
C	0.597652221082	-2.905045081836	-1.709308058827
H	-0.189645189269	-2.694221275856	-2.450440770432
C	-0.257026761074	-3.344814572594	0.455069276473
H	-0.237101286072	-4.427894420653	0.259062040091
C	-0.696486937721	-2.895331766496	1.793323720184
C	-1.258056582591	-3.797059292860	2.687541816728
H	-1.407491271345	-4.847593654877	2.440559541675
C	-1.642890967577	-3.296520789947	3.925021425855
C	-1.429229685742	-1.967982072547	4.249584987243
H	-1.734785596077	-1.606938417698	5.229224813420
C	-0.830810848698	-1.147787568998	3.289052800390
C	-0.492642966532	0.278996406470	3.567138277756
C	-0.543631999179	0.801779482438	4.856752801603
H	-0.844973843849	0.215226971745	5.722055579132
C	-0.159818462836	2.122876184277	5.040870836433
C	0.272747869283	2.891451019512	3.971071209295
H	0.595944608953	3.921644122670	4.109562187896
C	0.286677123071	2.281134025259	2.725998856719
H	0.635094261475	2.827657495375	1.848610314135
F	-2.209804221432	-4.099836410977	4.808306622297
F	-0.199016205287	2.642288849414	6.256148424170
N	-2.632876181519	-0.671888479179	-0.958730251578
O	-1.642116559709	-0.421598735491	-1.722330143444
O	-2.372913798363	-0.609580898820	0.294133009094
O	-3.719613158671	-0.946575543661	-1.374626736283
N	2.728827879660	0.517085220208	0.861051764121
O	2.171202300364	-0.626761542546	0.948981383344
O	1.988465785894	1.437902639228	0.365481687863
O	3.854815507865	0.718524194199	1.208765159445

T1
E = -2248.673832236374 / E+ZPE = -2248.272274007274 / G = -2248.345260556037

Tb	-0.035590703921	0.135717191732	0.201781928987
N	-1.435137248063	2.350422210382	-0.030425064740
N	0.511878238016	1.746285943525	-1.850703871803
N	1.482769428815	-0.721889558903	-1.745326360832
N	-0.163556249251	-2.355508136015	-0.467194616500
N	-0.455606274322	-1.605819287791	2.117775053526
N	-0.199173971345	1.034469947715	2.634168053636
C	1.648994918559	3.762707888436	-3.373493923931
C	2.280760936665	2.538600562272	-3.314148696916
H	3.212389147570	2.362345322747	-3.849739987040
C	1.669705990481	1.533508787021	-2.538197408257
C	2.249802561531	0.248483343327	-2.388052806586
H	3.313828888258	0.058731737582	-2.557806648353
H	1.107870435824	-1.790540131299	-3.535212369955
C	-2.527239142265	2.507858810968	0.733474136171
H	-2.606433661740	1.845705384372	1.596430721454
C	-3.529948518675	3.427456126322	0.468239609346
H	-4.406201698214	3.520140978011	1.107279797215
F	2.181658140794	4.744979881071	-4.084119664949
F	-4.309113608915	5.094887120831	-0.986573381801
C	-3.379158961118	4.211899935866	-0.665453781726
C	-2.260262360992	4.078999660460	-1.476071478744
H	-2.172774042750	4.685042687255	-2.376010337429
C	-1.303046631317	3.134624247004	-1.117790963772
H	0.050729714022	-3.751774153538	-2.068167518502
C	-0.069877865974	2.943691222912	-1.933572721760
C	0.457838202929	3.992841469056	-2.690193439516
H	0.001740286267	4.980170836593	-2.723004433560
C	1.207124976628	-1.945778650001	-2.447591624264
H	2.120470119880	-2.561447858475	-2.299872043445
C	-0.018794121236	-2.669117950851	-1.876435712330
H	-0.918501400578	-2.277303674301	-2.373987762234

C	-0.457835672412	-3.257578075210	0.377449893286
H	-0.582517629643	-4.315266570966	0.098893369916
C	-0.659543416846	-2.892419692965	1.795888300883
C	-1.044529193461	-3.858013097204	2.716260952683
H	-1.204776957822	-4.898877266324	2.437249066766
C	-1.233885405895	-3.437136917394	4.026822682977
C	-1.021143691203	-2.117341856331	4.384254905970
H	-1.187118406937	-1.815756904365	5.416169701976
C	-0.614263300745	-1.225089168805	3.387788991991
C	-0.321051847167	0.206535696250	3.689898809605
C	-0.151249688636	0.648770189352	4.998337600725
H	-0.217432025480	-0.013855230076	5.858541911210
C	0.150453852208	1.988399956875	5.202464524539
C	0.282738148527	2.857018899727	4.130308941582
H	0.530581770534	3.906355961239	4.279387628235
C	0.101937834278	2.321090000149	2.864477770565
H	0.212441691478	2.950620343022	1.980938708502
F	-1.620772008400	-4.306905987486	4.943350812940
F	0.320440372922	2.429081264776	6.436641607888
N	-2.710624607654	-0.451077750441	-0.783529886143
O	-1.739132197371	-0.180374838608	-1.566781809281
O	-2.413978065074	-0.448311575991	0.459849283650
O	-3.813932203395	-0.688670683427	-1.181256521684
N	2.637565656391	0.648138477247	1.191106509873
O	2.085952235929	-0.497348655909	1.281748198194
O	1.940474811994	1.530416502862	0.574739177544
O	3.716512423360	0.888655508749	1.646922319211

MEX for EET

E = -2248.663731884216 / E+ZPE = -2248.264370247030 / G = -2248.337244983008

Tb	-0.018409104058	0.063155401437	0.084235432957
N	-1.444783584242	2.276451663330	0.031062679446
N	0.431121673665	1.824323846098	-1.842998111320
N	1.380790056244	-0.667956020752	-1.927230024278
N	0.014455888631	-2.465681734561	-0.420108728362
N	-0.484835141129	-1.603473495761	2.099258003630
N	-0.095074584973	1.014083041332	2.540590666713
C	1.449208497964	3.834137450825	-3.479851804730
C	2.007540530179	2.579207981135	-3.553941512814
H	2.831597501200	2.370122841592	-4.234988606650
C	1.467924810051	1.568590178285	-2.708791042431
C	1.955256916161	0.256492150719	-2.745342676121
H	2.770122585834	-0.017308270943	-3.423944553154
H	1.902741848692	-2.272584188538	-3.220686970484
C	-2.492992367138	2.394534084559	0.857668786868
H	-2.624770133418	1.589158731844	1.581076354166
C	-3.390956789467	3.451295365616	0.819978265166
H	-4.235498795447	3.510254299987	1.504273168588
F	1.921093647899	4.817612142395	-4.230110258696
F	-3.994502597970	5.456877844454	-0.237361646308
C	-3.173498660222	4.425352898638	-0.141593166496
C	-2.101293537690	4.329334068238	-1.018750923768
H	-1.973665185343	5.093179445478	-1.783043574070
C	-1.253885553620	3.231661058404	-0.897948876708
H	0.595795850176	-3.949141917948	-1.841680541912
C	-0.100316617262	3.034505088396	-1.824970379899
C	0.380384379522	4.092670289210	-2.624247412397
H	-0.029640169811	5.098946657746	-2.575686827478
C	1.633133583526	-2.062232798877	-2.172849353298
H	2.490183453578	-2.353304235288	-1.532566751763
C	0.398432402469	-2.868224250975	-1.761379724990
H	-0.435612537344	-2.603713469910	-2.430400779362
C	-0.318975688602	-3.331806745877	0.446735823162
H	-0.344008949857	-4.410628853744	0.228871814507
C	-0.687979080099	-2.897558888458	1.810786317595
C	-1.206747641199	-3.811376275973	2.718627210285
H	-1.360206067948	-4.860408176100	2.467756258080
C	-1.543912748560	-3.325049969176	3.975443377437
C	-1.330666348733	-1.997035646557	4.301592870172
H	-1.602688667449	-1.646483966043	5.294772054543
C	-0.777304549591	-1.163503452069	3.325309861736
C	-0.449344083479	0.266117059898	3.602001175375
C	-0.468596880828	0.780322090795	4.895948679849
H	-0.735559148596	0.184225557981	5.765998254142
C	-0.099757369142	2.106028652497	5.077456894891

C	0.288953562689	2.887799833980	4.000427510036
H	0.600380515983	3.921923842341	4.136463416251
C	0.274028770843	2.285602134441	2.751535969959
H	0.585662454752	2.843943400457	1.867905673421
F	-2.067667189651	-4.140699150680	4.873999041496
F	-0.111178832452	2.616899465797	6.296843738735
N	-2.664401272112	-0.618021423953	-0.896653611262
O	-1.687240700082	-0.356872447959	-1.674852112759
O	-2.383784845777	-0.569058617035	0.351426261430
O	-3.757738599966	-0.890043871148	-1.297829021091
N	2.733328763494	0.482187295022	0.897424702314
O	2.162766087225	-0.657317084701	0.959296143715
O	2.003713859612	1.421441248439	0.422426868777
O	3.861355387917	0.662498264672	1.250541852182

MEX for ISC
E = -2248.672258145999 / E+ZPE = -2248.271558383343 / G = -2248.342746136112

Tb	-0.028956940693	0.148092726246	0.234918872752
N	-1.413287599792	2.365263639296	-0.035505760772
N	0.535515950882	1.710697677175	-1.856123825916
N	1.513863842336	-0.752136804549	-1.707613803334
N	-0.193576560983	-2.327566592478	-0.472799741403
N	-0.442524793964	-1.607009237454	2.125919864678
N	-0.202232825854	1.030916917439	2.660654825739
C	1.674066799849	3.716823828517	-3.388781780724
C	2.315908796587	2.499442012196	-3.302920936136
H	3.255888008353	2.323406745899	-3.823578999007
C	1.704604703535	1.501450452005	-2.521625226040
C	2.304354718400	0.223238971177	-2.334082897600
H	3.388526097370	0.080705537944	-2.327907454984
H	0.872432778301	-1.551990277521	-3.550645725885
C	-2.506466322480	2.541341784272	0.723170173546
H	-2.577078269896	1.914037301672	1.612661751156
C	-3.520948973735	3.436419307615	0.422106417106
H	-4.397534729905	3.544523621495	1.058178155624
F	2.208104923402	4.693117374220	-4.106668721982
F	-4.323305078002	5.031305263404	-1.099714620620
C	-3.381606420054	4.174387543082	-0.743970543057
C	-2.262285001792	4.021932155014	-1.550293168875
H	-2.181890691513	4.590452959221	-2.475097832547
C	-1.292433368643	3.105758680348	-1.154725081513
H	0.000564426881	-3.706426367537	-2.087140723089
C	-0.054854899596	2.905195965782	-1.960971343651
C	0.472651486529	3.947192649059	-2.723718209125
H	0.009495930736	4.930490027634	-2.774345805445
C	1.085858949199	-1.860658800107	-2.512453982069
H	1.984159622497	-2.511877703082	-2.571700892685
C	-0.092847351306	-2.626837750291	-1.889474084539
H	-1.024687069242	-2.263924349340	-2.347245806001
C	-0.460299902875	-3.241105749319	0.368834209415
H	-0.583059997036	-4.296594051766	0.081340071824
C	-0.637544633318	-2.892632270829	1.794592610706
C	-0.998714670689	-3.870853724538	2.711172916163
H	-1.151556297881	-4.910755238869	2.424546502758
C	-1.174900890896	-3.463790169412	4.027886600784
C	-0.974535234249	-2.144452630492	4.394191929465
H	-1.131984281286	-1.854866953752	5.430800354831
C	-0.591006315738	-1.238430895239	3.401010913308
C	-0.313848473563	0.194710766638	3.711438909641
C	-0.148523592838	0.631515355373	5.022089374832
H	-0.207571298820	-0.036264419791	5.878767875641
C	0.138321792012	1.973297602744	5.233920087526
C	0.261300157760	2.849632885015	4.166981935579
H	0.498069291575	3.900649646078	4.322076982040
C	0.085846111831	2.319292973589	2.898047259457
H	0.189493345017	2.955030708188	2.017958920125
F	-1.538838314402	-4.346258345770	4.941484151530
F	0.303088606942	2.408487856583	6.470594961368
N	-2.716164151718	-0.404358659503	-0.739978722135
O	-1.746084839382	-0.144494116362	-1.528445950247
O	-2.411590532816	-0.411301388829	0.501263834897
O	-3.825649218639	-0.622858117554	-1.131838504017
N	2.642236701689	0.668173811520	1.222611386394
O	2.089018239999	-0.475065231841	1.328378429836
O	1.942148515323	1.546020006181	0.602630782155

| O | 3.725327751698 | 0.910955516677 | 1.667065217537 |

2.4. TbL3(NO₃)₂

S0
E = -2007.949968293529 / E+ZPE = -2007.416792411233 / G = -2007.487769004992

Tb	-0.012675077803	0.047528746943	0.049088958313
N	-1.487886313410	2.238139244355	0.054946452969
N	0.380613699648	1.840565764954	-1.826935307434
N	1.451638602624	-0.666122446228	-1.936773721531
N	0.066829497328	-2.471805151517	-0.438611379633
N	-0.516357231422	-1.560580374055	2.069781621127
N	-0.066616680916	1.042845070081	2.499901958395
C	1.351475646255	3.853147438120	-3.476352680383
H	1.739329468473	4.650766868514	-4.110401219536
C	1.862179131011	2.561327246586	-3.569272006190
H	2.647198189084	2.313188699684	-4.283910135001
C	1.351029107126	1.588755715325	-2.716375691052
C	1.839100464340	0.196345346360	-2.787417692531
H	2.519245168866	-0.038956147858	-3.616219719136
C	-2.526637463936	2.322917858639	0.895379337225
H	-2.665357288019	1.475831299870	1.568719086768
C	-3.400671304297	3.402895807693	0.919842388806
H	-4.232761273667	3.416064382982	1.622673874697
C	-3.187280497302	4.441567349794	0.021516671094
H	-3.853797529197	5.304586301182	-0.003286392272
C	-2.116226923281	4.358238660393	-0.861729290797
H	-1.954146914143	5.149300772708	-1.591687026386
C	-1.282349967331	3.240214578532	-0.818807441767
C	-0.145413654938	3.065628512169	-1.767553175236
C	0.332279342075	4.109252100699	-2.571211165399
H	-0.080564370138	5.112937884859	-2.487925561294
C	1.839920024303	-2.076140912436	-2.031795999794
H	2.529673914038	-2.250056154487	-1.186563133234
C	0.559939350751	-2.902140945496	-1.749904073135
H	-0.203316643143	-2.567553280660	-2.475177027122
C	-0.337614246369	-3.305516496730	0.432710278107
H	-0.385409483358	-4.387552700985	0.254638536781
C	-0.750075580786	-2.846779247668	1.775110856015
C	-1.319742217536	-3.735281392781	2.680961543232
H	-1.487420991956	-4.776639037635	2.405192971665
C	-1.678123884263	-3.255109879267	3.937594556325
H	-2.148783038910	-3.911812755092	4.669638596550
C	-1.418036315892	-1.928943506721	4.249767617885
H	-1.689254269246	-1.539682608159	5.229340619588
C	-0.814579051931	-1.106865938180	3.288892441742
C	-0.439003058912	0.309841813766	3.564847251641
C	-0.429394546570	0.837122634502	4.856771408669
H	-0.712678402600	0.227293608253	5.712828424876
C	-0.021440982842	2.152587537493	5.051025655633
H	-0.000508185073	2.578625113303	6.054779914471
C	0.372759774423	2.904326241906	3.950567164535
H	0.715355864878	3.933167389052	4.054322693935
C	0.334277865024	2.304764302578	2.697617170921
H	0.650303883612	2.848069867346	1.805745945342
N	-2.620004542637	-0.683562303206	-1.009070435520
O	-1.632825760503	-0.381964278327	-1.757013717097
O	-2.377189146098	-0.637539237201	0.246029887268
O	-3.691971741119	-0.992616479474	-1.443643216967
N	2.747957906283	0.462341671777	0.855569897306
O	2.158949519309	-0.661670676174	0.973623670895
O	2.030362158607	1.395772554506	0.354428654058
O	3.886934265085	0.634967488130	1.181452846592
C	0.794961838978	-4.403800862186	-1.903368055093
H	-0.160302520500	-4.940888655301	-1.798300773518
H	1.459604637901	-4.749190160485	-1.091065996655
C	1.434450636720	-4.746506322854	-3.247482880238
H	1.599060274722	-5.831601549048	-3.310183059106
H	0.741964722731	-4.483684581238	-4.065643891238
C	2.513030725971	-2.483360510537	-3.341691538216
C	2.747001615816	-3.990791074681	-3.423152561046
H	3.472255187863	-1.953485717450	-3.447467855517
H	1.870656312884	-2.175032033725	-4.186307319059
H	3.211861519526	-4.236750289907	-4.388473416062
H	3.460968593802	-4.299975565243	-2.640478639215

T1
E = -2007.850910800596 / E+ZPE = -2007.321750458228 / G = -2007.393244484158

Tb	-0.264776585642	0.182532280308	-0.086124147344
N	-1.489695902478	2.469641641277	0.053235085570
N	0.162367854655	1.911851274084	-2.009079320073
N	1.270607159075	-0.563430500451	-2.011440058123
N	-0.373274742970	-2.303283512920	-0.850868654024
N	-0.695791263479	-1.722649319904	1.720970654371
N	-0.106061035031	0.843254948286	2.465665453380
C	0.916223609991	3.795850097135	-3.906547466049
H	1.217582364791	4.543760396251	-4.640150646330
C	1.447998487480	2.509576069901	-3.944586033515
H	2.168421274547	2.217103033878	-4.708755715018
C	1.046980051395	1.603287186034	-2.969231896112
C	1.603879009776	0.234526669216	-2.942960937714
H	2.309209686034	-0.033146973597	-3.741636387671
C	-2.419357075692	2.638321366085	1.003184835744
H	-2.473764599267	1.855007088111	1.760116543899
C	-3.282546778325	3.726376015369	1.039815268386
H	-4.023876033523	3.808660709029	1.833574678985
C	-3.179240691754	4.679901462660	0.034880943050
H	-3.843636944501	5.544602521161	0.014620073396
C	-2.222603750472	4.508908320124	-0.960206838078
H	-2.151252485968	5.234731818728	-1.767912843478
C	-1.389516167649	3.390807751011	-0.924610611351
C	-0.372744785410	3.134156469716	-1.985562085768
C	-0.002904490314	4.113212195540	-2.918372422426
H	-0.418871742214	5.117587537155	-2.868822994180
C	1.818264824496	-1.907482702189	-1.883554281837
H	2.362488083162	-1.883731422406	-0.923496863730
C	0.645701116439	-2.891638164660	-1.685701658065
H	0.124004493448	-2.978200161454	-2.668947578506
C	-1.218862878816	-3.118485951289	-0.101503311751
H	-1.950094313106	-3.745296816370	-0.620599665753
C	-1.284533626886	-2.875003375658	1.291612081947
C	-1.962109444641	-3.740435360185	2.178683460772
H	-2.434490231698	-4.645952480581	1.798174599554
C	-2.002668009948	-3.413417177055	3.519646617809
H	-2.522433086309	-4.056756374868	4.230295470842
C	-1.384923251763	-2.239114974272	3.956906002785
H	-1.444637274648	-1.945227553533	5.003646060964
C	-0.748018129050	-1.418535646536	3.018950253211
C	-0.148809056666	-0.112798371940	3.413555263581
C	0.344377795018	0.101936674963	4.700239397777
H	0.333986302522	-0.701162153100	5.435842948780
C	0.884626600562	1.342064255291	5.022810096778
H	1.290521930639	1.523270069928	6.018803897126
C	0.907839732333	2.336683049650	4.052222755306
H	1.322583278376	3.323600391269	4.253871922295
C	0.406136690442	2.038658457341	2.791611822933
H	0.429558070690	2.781985084893	1.993843631036
N	-3.003503280295	-0.178583109127	-0.977008138138
O	-2.053933141380	0.078346491411	-1.786226888388
O	-2.646973312441	-0.302868462756	0.246831090650
O	-4.142593610548	-0.294393206677	-1.326583289256
N	2.512621632516	0.562118137154	0.715809556499
O	1.911229912400	-0.555900615762	0.848061095052
O	1.799471668384	1.501024677497	0.226232638133
O	3.658886292630	0.718690135246	1.026504204875
C	1.165160038967	-4.272040614829	-1.281464900288
H	0.325066027937	-4.972168738124	-1.161973162907
H	1.658817382911	-4.186234708656	-0.298428275790
C	2.148327012363	-4.793678949705	-2.332462380437
H	2.553914850090	-5.763258877985	-2.009842345922
H	1.603243241809	-4.979067380824	-3.274623701923
C	2.762604525842	-2.414855471378	-2.967799215521
C	3.286235528988	-3.804916092499	-2.589612559250
H	3.610175646350	-1.721582998993	-3.082034755579
H	2.236578664087	-2.458742827011	-3.938489836895
H	3.945164086099	-4.181541318727	-3.384819713703
H	3.907169565593	-3.716869389679	-1.681812024561

MEX for EET
E = -2007.840300707277 / E+ZPE = -2007.313192271588 / G = -2007.384115330297

Tb	-0.058741170194	0.063312481060	0.014058859580
N	-1.496295437037	2.281779303133	0.048683949430
N	0.333695536028	1.859701318925	-1.870623212379
N	1.427178894702	-0.637191339543	-1.954265417765
N	0.022534840511	-2.429327222525	-0.486965218554
N	-0.591722090872	-1.556660421597	1.993272363630
N	-0.082676055168	1.017935729322	2.493438776153
C	1.266286501472	3.855072164982	-3.563430498219
H	1.638473502390	4.645645460868	-4.215429824280
C	1.780284247515	2.564129589170	-3.649049941319
H	2.554187240491	2.310084190020	-4.373682140201
C	1.288891788463	1.600539247939	-2.774224946493
C	1.793304922361	0.213146706867	-2.826264850376
H	2.473763635952	-0.028238128609	-3.653182300922
C	-2.515647244727	2.380692385551	0.911098403478
H	-2.643027579589	1.541775297235	1.596543445752
C	-3.383994993915	3.464869691087	0.944331900623
H	-4.199024201671	3.489995075115	1.666556530239
C	-3.187880310264	4.491881376288	0.028729866703
H	-3.851259910023	5.357475544018	0.009017827421
C	-2.138865273490	4.392755871405	-0.878767671236
H	-1.991911372487	5.174268422546	-1.622081810918
C	-1.307663173709	3.272246878516	-0.841924793837
C	-0.193010063816	3.084474217868	-1.814543587826
C	0.265570519588	4.119344518277	-2.640342797519
H	-0.146983364303	5.123340982645	-2.560121458498
C	1.855056408889	-2.035687485521	-2.006893067056
H	2.518171587196	-2.169644769608	-1.133722897523
C	0.590082399442	-2.896206048730	-1.739280580354
H	-0.146418532938	-2.622886091117	-2.522922300908
C	-0.549664589327	-3.293923137281	0.370715329314
H	-0.736094188136	-4.337430055800	0.103647330425
C	-0.899214009750	-2.864403995099	1.645744825448
C	-1.520701201993	-3.757884849097	2.598556190207
H	-1.768230712037	-4.773969528659	2.290129081744
C	-1.780095075715	-3.308555411696	3.865480720158
H	-2.255968713590	-3.955050995830	4.602628838700
C	-1.419959107636	-1.993216858485	4.208185807065
H	-1.633554662622	-1.613309974182	5.204709398647
C	-0.816200482440	-1.155620524521	3.223018486112
C	-0.406578034983	0.241797442486	3.544503616388
C	-0.322049898042	0.708193429207	4.856299525843
H	-0.566221500698	0.063812650616	5.698725352610
C	0.112330187382	2.010955399075	5.086919203323
H	0.193859100950	2.390867818162	6.105959379432
C	0.450382714106	2.807474418350	4.001228586256
H	0.806451273155	3.828851846256	4.130795493389
C	0.337346458048	2.265372678829	2.724118682729
H	0.609300668117	2.846374230222	1.841518788805
N	-2.676744873756	-0.621226261395	-1.052698661312
O	-1.680061351631	-0.343901514198	-1.797775648316
O	-2.440686992717	-0.565987078634	0.202828317907
O	-3.751340663878	-0.916320749925	-1.490864610295
N	2.684292256170	0.522726772593	0.863131177067
O	2.112464872518	-0.610810661841	0.973592725306
O	1.966046985100	1.438929580897	0.332559718877
O	3.808481949229	0.719601216184	1.226071222042
C	0.890079050923	-4.395263294222	-1.821173924255
H	-0.047302284947	-4.967161912255	-1.753089425979
H	1.514095717521	-4.680575942942	-0.955621640793
C	1.611737247478	-4.766316246276	-3.115553703081
H	1.828582166273	-5.844172533469	-3.116951439960
H	0.946053258178	-4.576881768256	-3.975563238524
C	2.587524301680	-2.461128046662	-3.277039654156
C	2.894361780505	-3.957861908473	-3.276127560309
H	3.524125513055	-1.890179628341	-3.373403632170
H	1.962276306566	-2.221218028308	-4.156109610118
H	3.409105373185	-4.227904727296	-4.209188026571
H	3.588936682938	-4.193624275346	-2.451554828858

MEX for ISC
E = -2007.848586778168 / E+ZPE = -2007.320774657569 / G = -2007.392114853033

Tb	-0.304884178060	0.210040382769	-0.107539898728
N	-1.499099749909	2.500751098028	0.030460627053
N	0.145564534248	1.921219521296	-2.034232316553

N	1.253412836794	-0.549124600527	-2.005115390774
N	-0.460920574299	-2.270631006889	-0.939945092635
N	-0.691025796910	-1.761589511583	1.651861906757
N	-0.133982107419	0.809543354336	2.455695336585
C	0.908350925193	3.790185176420	-3.941831894128
H	1.212276623162	4.532093658995	-4.680452914220
C	1.437670669123	2.502494664347	-3.970147857111
H	2.159523714826	2.203581594377	-4.730489833334
C	1.032682744863	1.603895313131	-2.989565829943
C	1.591394565003	0.235696582253	-2.945852022633
H	2.302393285870	-0.041859087386	-3.736341953176
C	-2.423823007460	2.681298197014	0.983223619243
H	-2.481872125390	1.901209167560	1.743504544039
C	-3.277110122456	3.777203702831	1.018105238950
H	-4.014737806482	3.869617673280	1.814194752995
C	-3.168724715111	4.725227032144	0.008581036390
H	-3.824636275009	5.596379613359	-0.012560362839
C	-2.217789517232	4.541196754264	-0.989786351935
H	-2.143325992781	5.263163425550	-1.800632005795
C	-1.394600054967	3.416058132194	-0.952968661188
C	-0.383512602927	3.146333928335	-2.016450912469
C	-0.009533469201	4.117627943328	-2.955808668664
H	-0.420741739437	5.124249830110	-2.913007215674
C	1.799630070836	-1.889543505477	-1.846521104521
H	2.320891623304	-1.848433044510	-0.874975270810
C	0.627810930898	-2.877067504242	-1.662944906475
H	0.155284283063	-3.007379052770	-2.667702188549
C	-1.325181102235	-3.091111584514	-0.195202092073
H	-2.218859041648	-3.466978632897	-0.702049742741
C	-1.298466220810	-2.898662904927	1.221351888184
C	-1.922147218569	-3.793463627220	2.112354116877
H	-2.405796556531	-4.691329377852	1.728267270384
C	-1.899788646220	-3.505240564875	3.463568043614
H	-2.377388121776	-4.174866951879	4.179709658042
C	-1.273920893828	-2.337364775637	3.903716809573
H	-1.288078637746	-2.071530988323	4.959562708788
C	-0.687525863518	-1.488962676615	2.961918303983
C	-0.097493706135	-0.182429191932	3.366922557626
C	0.457112349740	0.000743791238	4.633344379640
H	0.509201970045	-0.829651362051	5.336285292477
C	0.975299972897	1.244646551831	4.976172005686
H	1.427822755453	1.401495056002	5.956085818009
C	0.915769923912	2.275479688068	4.045628364000
H	1.309506844147	3.267294717531	4.263987632822
C	0.358200527217	2.007974047551	2.802130935032
H	0.319444127615	2.780230881049	2.033000146569
N	-3.055521083480	-0.130970623932	-0.963643729103
O	-2.121001296994	0.146620182908	-1.783004313191
O	-2.679724587280	-0.267832239996	0.253541780015
O	-4.198288862486	-0.255962872910	-1.297897730994
N	2.464139726394	0.612797335457	0.729109783271
O	1.876370753035	-0.513783057251	0.846974022140
O	1.747305259017	1.542087132900	0.227072459844
O	3.600783113208	0.785638081258	1.065701016629
C	1.137903612748	-4.237476550236	-1.189126699202
H	0.297204472648	-4.937376637633	-1.074537977463
H	1.596851985016	-4.114111236148	-0.193384667093
C	2.159949300841	-4.783530764573	-2.191049970165
H	2.567906445940	-5.734878707290	-1.820558665665
H	1.643450824340	-5.011715922037	-3.139870914661
C	2.773000197903	-2.418618510819	-2.893923600206
C	3.295234724682	-3.792386628686	-2.455475282007
H	3.618797121239	-1.723176415127	-3.008263025229
H	2.271542151140	-2.496732791993	-3.875417123511
H	3.976244491893	-4.191451172927	-3.220662408760
H	3.893098986046	-3.667167908042	-1.536726661037

2.5. TbL4(NO₃)₂

S0

E = -2050.369223290269 / E+ZPE = -2049.945579450534 / G = -2050.014733316770

Tb	-0.012047695578	0.051888405464	0.061455246536
N	-1.459261837441	2.253999567010	0.036306863808
N	0.396270924324	1.836895693045	-1.863775861684
N	1.450098115895	-0.672354933141	-1.941315346063

N	0.095530757839	-2.482472385610	-0.415113744174
N	-0.517455785745	-1.593362988558	2.085615601279
N	-0.090187988115	1.021784307486	2.515685630543
C	1.363155412106	3.837694392937	-3.528674967652
H	1.748646301235	4.631718525536	-4.168500678987
C	1.878116496661	2.546401209825	-3.618683201901
H	2.660379189652	2.289683965863	-4.330608522551
C	1.362366403464	1.588528468196	-2.755890764656
C	1.830829199590	0.184919107032	-2.781539603996
H	2.232576039099	-2.337887203059	-3.023425134209
C	-2.496608675938	2.349921605387	0.878182899220
H	-2.629760415037	1.515757419646	1.568217888772
C	-3.375741727395	3.425946235778	0.886409414281
H	-4.205795917798	3.446687416856	1.591419329235
C	-3.170252467972	4.449791802840	-0.030092018102
H	-3.840932768207	5.309020179453	-0.068131793869
C	-2.100983548356	4.355751682157	-0.914667106294
H	-1.945236713405	5.134793414379	-1.658802992928
C	-1.261677457158	3.242959128888	-0.855388650677
C	-0.129026929585	3.061950415238	-1.807717627377
C	0.347939815175	4.099154626562	-2.620987415209
H	-0.062412714319	5.104208287860	-2.541563622263
C	1.835850940393	-2.074882736535	-2.033330961905
H	2.617118158996	-2.253897156542	-1.278265186544
C	0.605042698994	-2.917116345225	-1.709636665500
H	-0.180951382052	-2.727576448515	-2.457261731559
C	-0.326259541885	-3.298641726919	0.446417630411
C	-0.754845293342	-2.879037439138	1.799453733173
C	-1.331790339494	-3.772299750832	2.692143570100
H	-1.498168384624	-4.810821585241	2.411980822282
C	-1.695444038724	-3.285286197868	3.945609811910
H	-2.173274346680	-3.939691025363	4.674919244719
C	-1.435290306400	-1.959436585101	4.257504775241
H	-1.715175218376	-1.568482982225	5.234019306302
C	-0.823528614074	-1.136993201457	3.301475295430
C	-0.447927603797	0.278829193497	3.579656546265
C	-0.422411145365	0.794038865268	4.875835969442
H	-0.691898960676	0.174983054606	5.729738381003
C	-0.014223345151	2.108464666239	5.077634904022
H	0.020152397522	2.524641585403	6.085125069536
C	0.363571238949	2.870984281721	3.979168220628
H	0.705743803175	3.899447064015	4.087656814033
C	0.310065448950	2.283329986709	2.721129600986
H	0.613406581399	2.836803533452	1.831234335483
H	0.855959152393	-3.986732413532	-1.724336326957
N	-2.627486270785	-0.645590193369	-0.977631590705
O	-1.633870727947	-0.379606195473	-1.731645806679
O	-2.368545877746	-0.623144070199	0.276790869906
O	-3.716081233147	-0.898300812726	-1.402762020689
N	2.721846028388	0.508515515551	0.902961964568
O	2.152506220428	-0.628380262903	1.000137598834
O	2.004803896879	1.422367895938	0.361723820002
O	3.836883552274	0.711161254916	1.283827235608
F	-0.400279023266	-4.608167811527	0.227545377223
F	2.662120841764	-0.098898714223	-3.780041337580

T1

E = -2050.254572250541 / E+ZPE = -2049.835153729620 / G = -2049.905793510943

Tb	-0.027625906880	0.114751910528	0.164191580574
N	-1.460896144679	2.303241923594	-0.023070611342
N	0.489025435628	1.783904869478	-1.842531549750
N	1.448134442907	-0.708152488742	-1.787951169679
N	-0.085588630701	-2.403043490998	-0.451542190253
N	-0.474941258157	-1.594807446878	2.126753011069
N	-0.171391015636	1.046763722923	2.595296282161
C	1.625142520915	3.841413644074	-3.364086723912
H	2.063532440551	4.662193551617	-3.932352632369
C	2.226780932442	2.601959436481	-3.353289112776
H	3.137546027177	2.396712373831	-3.913898074637
C	1.621684097780	1.575085711678	-2.582862319575
C	2.140848993176	0.284762651779	-2.498955525362
H	1.287827408680	-1.940889500175	-3.501756234771
C	-2.546895267484	2.426617087152	0.753157089384
H	-2.631553389922	1.711952859952	1.572797622232
C	-3.531123639978	3.383577641540	0.542283113354

H	-4.395421200390	3.431529559485	1.203565607519
C	-3.386514750931	4.249662605232	-0.535096642039
H	-4.143859207055	5.003991887962	-0.751600666803
C	-2.261547698104	4.133655080882	-1.344857805241
H	-2.140413516938	4.785133587097	-2.208935448042
C	-1.312315548539	3.152708755590	-1.058010688599
C	-0.088191146216	2.981996192832	-1.891498960222
C	0.445290918847	4.043381547846	-2.637561392141
H	-0.021805356843	5.026236879630	-2.617727921804
C	1.319138977412	-1.996567647260	-2.400446639725
H	2.262251208874	-2.527341716205	-2.143369349227
C	0.114201723636	-2.762549258361	-1.846771979068
H	-0.787690414765	-2.440435152574	-2.388656985573
C	-0.443040068102	-3.245360754703	0.414985870944
C	-0.691575906233	-2.882036449491	1.828429526889
C	-1.115930545478	-3.825043162827	2.755040297531
H	-1.276529674257	-4.860922613319	2.462405917394
C	-1.336446811654	-3.391904311542	4.060611621995
H	-1.688623131366	-4.088803111348	4.821325877670
C	-1.101758182809	-2.063712590310	4.380574551591
H	-1.279697300932	-1.712502784010	5.395276152190
C	-0.652342804401	-1.185306286180	3.384463955247
C	-0.334006390473	0.244343678401	3.664910728210
C	-0.175829559772	0.720288947600	4.966263506622
H	-0.280300194473	0.055279465837	5.821477445511
C	0.153376773481	2.056808633866	5.168207868452
H	0.288734463457	2.442338213897	6.179370100862
C	0.320659852071	2.882634201173	4.063698210268
H	0.588441762510	3.933019860911	4.169867327426
C	0.152804404045	2.330563972235	2.799889463353
H	0.294059041108	2.934657310172	1.902896490321
H	0.249278509488	-3.842115214845	-1.996961080003
N	-2.648021966280	-0.570776287602	-0.893492751211
O	-1.660064736178	-0.269709251204	-1.645097781720
O	-2.396232432942	-0.545127541790	0.359348444649
O	-3.725154853978	-0.858447741096	-1.327735041931
N	2.651281166390	0.581385604395	1.157022486836
O	2.087186655267	-0.560314568517	1.226157510459
O	1.980687847151	1.470589048819	0.522203049532
O	3.715770134408	0.811414162425	1.649889958271
F	-0.633250538592	-4.531108224992	0.135784687128
F	3.359038773750	-0.023617395884	-2.920834987756

MEX for EET

E = -2050.253506774012 / E+ZPE = -2049.836816880319 / G = -2049.906941820503

Tb	0.006439349796	0.048547843363	0.076878347119
N	-1.461970498432	2.267629390295	0.044810091843
N	0.436278500094	1.845077997816	-1.775746843205
N	1.402281948200	-0.664323562145	-1.940889782352
N	0.072290691854	-2.478980774043	-0.423871846162
N	-0.495052451576	-1.609633592737	2.098045862989
N	-0.083143338911	1.007220584999	2.534117639595
C	1.406794365821	3.841957307513	-3.572306323483
H	1.771184105331	4.647085993809	-4.209893452044
C	2.013610907847	2.630037439238	-3.563457126043
H	2.878174063972	2.401250677752	-4.184313626858
C	1.466906937903	1.577522658901	-2.686071595894
C	1.887669885033	0.250328520776	-2.744803775471
H	2.102861456991	-2.294509969104	-3.117623845316
C	-2.497753735568	2.381823559938	0.877909687821
H	-2.615292260841	1.579045208061	1.607126767285
C	-3.403622290220	3.440931820136	0.830336446493
H	-4.235652673092	3.476495996495	1.532657997495
C	-3.218973675958	4.423904655455	-0.129969335156
H	-3.907259924496	5.265973281727	-0.209236125055
C	-2.139776650278	4.313925429257	-1.005143844723
H	-1.995240673296	5.067436113653	-1.776542566040
C	-1.281727545058	3.220159550138	-0.892863506860
C	-0.144096425092	3.008164550068	-1.826530424998
C	0.283148438127	4.063591652136	-2.727853029581
H	-0.199510105419	5.037113733378	-2.709084917338
C	1.759161954046	-2.058101091973	-2.100565066071
H	2.581848331800	-2.281906327063	-1.398438017985
C	0.538104815189	-2.901772205976	-1.738539083406
H	-0.272276769925	-2.699768362977	-2.456144916754

C	-0.320021939891	-3.303276027521	0.443887695119
C	-0.723445988411	-2.895835503306	1.808476025851
C	-1.279798059274	-3.799415439924	2.704343351350
H	-1.438883805201	-4.838294245428	2.421291546531
C	-1.634302869739	-3.321567867597	3.963727411022
H	-2.095243113463	-3.984554883041	4.696180695702
C	-1.388956077514	-1.993086800646	4.276723145284
H	-1.664600160799	-1.609400174333	5.257243787594
C	-0.796844243303	-1.160238787046	3.317455489724
C	-0.440646450256	0.261018674417	3.595990046791
C	-0.432979132724	0.779589505971	4.891368233467
H	-0.703676688861	0.159823780715	5.744287324817
C	-0.042848182011	2.099198822830	5.094316342281
H	-0.024646900536	2.518157189564	6.101083161049
C	0.339067461855	2.863483263251	3.998320802866
H	0.670063591619	3.895462178394	4.108287667373
C	0.304475914545	2.272431900924	2.741355592638
H	0.613648927507	2.826041649603	1.853508687839
H	0.783517211956	-3.972108567666	-1.773798120447
N	-2.665405182609	-0.544679709439	-0.891481365481
O	-1.688038335510	-0.310548670896	-1.675346051446
O	-2.359799474144	-0.576232028858	0.352236783211
O	-3.783889938687	-0.716595345852	-1.279815780993
N	2.747993380667	0.453379591743	0.933528007614
O	2.165742236170	-0.680246473971	0.991318423646
O	2.039803532122	1.393132768103	0.428350296623
O	3.866439123410	0.628741280228	1.318299315765
F	-0.391811265728	-4.612060279953	0.218064647427
F	2.805825014996	-0.064586289086	-3.664003862923

MEX for ISC

E = -2050.250129620387 / E+ZPE = -2049.831885057125 / G = -2049.901028020311

Tb	-0.026359608287	0.104656203688	0.161767966062
N	-1.461551944954	2.292736306765	-0.042283646884
N	0.489416939404	1.766589474361	-1.880964116564
N	1.402145518687	-0.722363135937	-1.818100792093
N	-0.112322470649	-2.409820973724	-0.459821987113
N	-0.461625763198	-1.596252847186	2.125293579245
N	-0.158528080803	1.046304239814	2.583656094122
C	1.666647426358	3.854427331911	-3.298915330726
H	2.131540506056	4.683981010252	-3.832502341038
C	2.255398904263	2.600311322087	-3.299882195500
H	3.182585619832	2.400048338504	-3.835448728429
C	1.626564844186	1.578030617381	-2.579826145928
C	2.182784777508	0.238011459147	-2.527722172375
H	1.062364147777	-1.837635017166	-3.568884629375
C	-2.550172187785	2.415105427008	0.731019778709
H	-2.629836842313	1.708769877235	1.558413712590
C	-3.542510321191	3.360627010458	0.508155272278
H	-4.408339413342	3.408132970960	1.167424371749
C	-3.404221766133	4.216127514786	-0.578806558668
H	-4.168115501606	4.961107202762	-0.804602339179
C	-2.276978728354	4.101964538788	-1.385493917848
H	-2.157838507760	4.744731390140	-2.256638115239
C	-1.319452175727	3.132888705830	-1.085620419957
C	-0.085545358549	2.975340311952	-1.904663976036
C	0.474491133636	4.047419159770	-2.603206276251
H	0.011539235282	5.032539161392	-2.572887560848
C	1.185923246748	-1.967614885136	-2.479591369097
H	2.155023076444	-2.500894794648	-2.352241981701
C	0.039078049942	-2.772975545393	-1.860928919096
H	-0.898775345881	-2.495281668155	-2.364093937388
C	-0.454834245787	-3.250019105973	0.414806629854
C	-0.676945295801	-2.885100683457	1.832218175252
C	-1.084048181296	-3.828090096937	2.766492478526
H	-1.244268559316	-4.865226805632	2.478186209036
C	-1.288984856847	-3.393366824082	4.073984028289
H	-1.627847196079	-4.090113089925	4.840824405624
C	-1.057686789035	-2.063122868246	4.387802688341
H	-1.225251037429	-1.710448626299	5.403732991965
C	-0.625493034587	-1.184406050709	3.384456848487
C	-0.313131450411	0.248075706110	3.657675286834
C	-0.153421096528	0.731766030935	4.955945769269
H	-0.252895599528	0.071495995015	5.815371972982
C	0.169822301956	2.071047035336	5.149601927264

H	0.305416171692	2.462689131776	6.158396687479
C	0.330494312420	2.891851086561	4.040392221231
H	0.594512453898	3.943781467953	4.140424280353
C	0.160801863275	2.332515634820	2.780061326588
H	0.296152097520	2.931972781476	1.879064691017
H	0.207233008258	-3.848560295754	-2.006099721576
N	-2.650374197045	-0.571404463049	-0.892450846193
O	-1.662719641009	-0.271481773521	-1.645019132943
O	-2.397709040836	-0.547359659003	0.359951041685
O	-3.728280838961	-0.856763694278	-1.326565162988
N	2.659314345333	0.582587412028	1.117712933958
O	2.097316379715	-0.559045557041	1.203681676637
O	1.978116662438	1.465699533004	0.483523964274
O	3.728360556317	0.819174583841	1.595272698088
F	-0.658552272996	-4.534371979572	0.139330309727
F	3.487719091064	0.113176057128	-2.244186606403

2.6. Tb**L5**(NO₃)₂

S0

E = -1883.925341306762 / E+ZPE = -1883.511610225082 / G = -1883.578698643242

Tb	-0.072390947777	0.126824581951	0.096787808296
N	-1.468790806095	2.332130107255	0.005599192458
N	0.302013841893	1.760117051627	-1.931751975055
N	1.341246489245	-0.612926459855	-1.962417092898
N	0.087866462391	-2.440635430714	-0.346508856037
N	-0.426262814212	-1.601290879592	2.048722478858
N	-0.131208113795	1.018847725197	2.553165656897
C	1.285297337358	3.641713760010	-3.724713391013
H	1.676125625574	4.388585983404	-4.416092603799
C	1.731803040787	2.323756672234	-3.778791122795
H	2.464455810085	1.978120537192	-4.506557880023
C	1.214201420255	1.434324699655	-2.848865485879
H	2.151288462780	-2.253820310061	-3.028481225731
C	-2.476038824562	2.500922971555	0.872737329434
H	-2.632388699329	1.690987110389	1.586643298899
C	-3.297446579477	3.621322673668	0.877860373811
H	-4.104196239185	3.703008436113	1.605182735100
C	-3.065047811368	4.610717531741	-0.069586113377
H	-3.688398518604	5.504874734907	-0.109040511062
C	-2.031981767187	4.437347753209	-0.984914499679
H	-1.860097690169	5.189057363677	-1.753018288082
C	-1.250149280399	3.283676551916	-0.922735469935
C	-0.165642968598	3.011117576975	-1.909504852493
C	0.323753114202	3.989198432645	-2.786195969307
H	-0.036620822127	5.014975777418	-2.735778597824
C	1.763736787423	-2.009733833804	-2.030300657680
H	2.559215014304	-2.129201140654	-1.276822546020
C	0.562730235451	-2.877376698588	-1.656858102913
H	-0.263064721311	-2.695399351420	-2.363714773996
C	-0.584811730968	-2.888425380610	1.736067937484
C	-1.105767355092	-3.839206867322	2.601053864638
H	-1.190876687346	-4.875306163086	2.276728841938
C	-1.512146201336	-3.407103158219	3.860961631059
H	-1.951719035778	-4.106768898572	4.572185127673
C	-1.335456521315	-2.074246517514	4.205163477220
H	-1.643868275198	-1.724270991102	5.188573919215
C	-0.766166027275	-1.194205358489	3.274895496953
C	-0.470038738492	0.232335628656	3.592830946516
C	-0.488758459458	0.717729690961	4.900567955124
H	-0.745321663912	0.067165090898	5.734642521704
C	-0.143509100149	2.043868815756	5.139967748158
H	-0.147594074061	2.436991569139	6.157289529298
C	0.223601397053	2.847930601716	4.067534241186
H	0.520034971180	3.886766204934	4.206853403468
C	0.216848632299	2.289698171030	2.795333310339
H	0.515031968388	2.875086933886	1.923942794946
H	0.816427327064	-3.946047555979	-1.645710880379
N	-2.701133353979	-0.645619669394	-0.833184657830
O	-1.714504476123	-0.462839610626	-1.624473940295
O	-2.418278906488	-0.526490846449	0.410233931614
O	-3.800747393386	-0.906690144788	-1.219546506481
N	2.680591260215	0.638876486481	0.821367512373
O	2.159448131850	-0.526230475445	0.877730002543
O	1.907877188912	1.548379837195	0.355291395054

O	3.798871497912	0.865698671868	1.174287464352
N	-0.168156112224	-3.350824904207	0.449356566534
N	1.681703930175	0.085744571257	-2.923496302549

T1

E = -1883.856468019216 / E+ZPE = -1883.444159182629 / G = -1883.511748522476

Tb	-0.055309024232	0.207273457629	0.234204193520
N	-1.446727382389	2.410815359452	-0.048625723058
N	0.445292124831	1.709159875836	-1.871380493303
N	1.536283115228	-0.717737026104	-1.750961922249
N	-0.109168802448	-2.313839208712	-0.405913800274
N	-0.395942477578	-1.596860301111	2.069485639512
N	-0.232172890600	1.034364384307	2.668909071026
C	1.580350006503	3.605979017378	-3.570205003919
H	2.019825091949	4.359449422098	-4.224277362591
C	2.176696596324	2.364228297139	-3.435650577500
H	3.089957545467	2.090388174088	-3.961469795400
C	1.558524321786	1.438207970111	-2.582816710225
H	1.281340449170	-1.956084583957	-3.454508096125
C	-2.513591852941	2.613755974561	0.737678612337
H	-2.598327778269	1.957481353289	1.605031375868
C	-3.481596696896	3.575861718037	0.478479532205
H	-4.330023705979	3.689930929314	1.151972343125
C	-3.343074938710	4.358362282852	-0.661664237763
H	-4.089438849485	5.111153172932	-0.917468105541
C	-2.239591672537	4.157659894924	-1.484521113269
H	-2.126519177692	4.738894167721	-2.398332809749
C	-1.304876279864	3.179789901434	-1.146374484467
C	-0.107801200270	2.920031165443	-1.994316906619
C	0.424694547700	3.894900677766	-2.844202685163
H	-0.028318749005	4.882406361635	-2.910977029764
C	1.328676688125	-2.031636495450	-2.358382876098
H	2.207226891416	-2.641034807854	-2.085466280575
C	0.049421559688	-2.665612673964	-1.812478118119
H	-0.824359517031	-2.223504399329	-2.316082735023
C	-0.558489962026	-2.873154919722	1.713168069138
C	-0.920415576093	-3.883378354298	2.591281528931
H	-1.030017409392	-4.902410798377	2.223239542778
C	-1.143839207522	-3.531545164217	3.920245878727
H	-1.450163189823	-4.281682371835	4.649344061951
C	-0.972733063849	-2.209250531367	4.303293881124
H	-1.156353684942	-1.919036270890	5.335949749598
C	-0.580421038954	-1.259772603086	3.348747972978
C	-0.337273658237	0.169338164852	3.697450573736
C	-0.187074874616	0.587372956779	5.019195864915
H	-0.243794207904	-0.125429106502	5.839631362845
C	0.072959128462	1.927684818257	5.286205572623
H	0.201234827589	2.267089548350	6.314633420592
C	0.182129013753	2.816778191411	4.224340300179
H	0.395990806165	3.873122001297	4.381460387212
C	0.028162710758	2.321637824777	2.935416801488
H	0.129082063394	2.976881326325	2.068972045582
H	0.052020677101	-3.755572648566	-1.948958684537
N	-2.746454816241	-0.392391969572	-0.685716640190
O	-1.778546973337	-0.200216596577	-1.496939385248
O	-2.416784543692	-0.385072619334	0.550388579728
O	-3.872881958683	-0.558108091075	-1.050321398129
N	2.597330099225	0.816344612399	1.190032314186
O	2.087799256705	-0.347481420104	1.293059886626
O	1.865895395122	1.665866645282	0.563538837875
O	3.662735640232	1.104184718148	1.646502651264
N	-0.359755540196	-3.258691308680	0.351508187449
N	2.133801374659	0.206349564814	-2.394859074224

MEX for EET

E = -1883.832289121963 / E+ZPE = -1883.421709787166 / G = -1883.487931648466

Tb	-0.072359731366	0.122345032155	0.093363847824
N	-1.470439862648	2.329504060946	0.002861379578
N	0.300331922698	1.759760462518	-1.934527558766
N	1.335402384523	-0.614597124935	-1.969765367634
N	0.091872270905	-2.441650768027	-0.343031215255
N	-0.417733288998	-1.603851433383	2.048663953319
N	-0.130997273645	1.015922285932	2.550055098503
C	1.290758625306	3.643780647214	-3.721013053225
H	1.684063975234	4.391585272389	-4.409994897762

C	1.729763114366	2.323598479058	-3.781861105298
H	2.459209775556	1.977330937995	-4.512537457046
C	1.209792053146	1.433276362791	-2.854079807628
H	2.139273888782	-2.258143787993	-3.037207506983
C	-2.477447223348	2.499167710433	0.870065048218
H	-2.643058236159	1.683118868538	1.574926026760
C	-3.288213353822	3.627241054557	0.885246924532
H	-4.094989656856	3.709448420086	1.612485680993
C	-3.045005318228	4.623686512420	-0.052051819900
H	-3.659296305724	5.524441571798	-0.083050308218
C	-2.013091507681	4.448989223224	-0.968411324676
H	-1.833603819131	5.206320177524	-1.729179724611
C	-1.242331385676	3.287330949018	-0.916633426915
C	-0.160306186533	3.013291560097	-1.905857166232
C	0.333528552256	3.992680762581	-2.778611145377
H	-0.020133292243	5.020477541535	-2.722309056156
C	1.756853912012	-2.011819321519	-2.037631644036
H	2.556779804086	-2.129541653971	-1.288517760477
C	0.557919632367	-2.879122109383	-1.655659760938
H	-0.272819151058	-2.693261945675	-2.355804429651
C	-0.563301136464	-2.892322530563	1.737886077884
C	-1.076074985148	-3.846203800903	2.602960876022
H	-1.147860797367	-4.883983884227	2.280650710274
C	-1.492174825224	-3.415480484912	3.861013299141
H	-1.926825728112	-4.117992200239	4.572467734197
C	-1.330148706708	-2.080676944215	4.202295280637
H	-1.645915457639	-1.731804648505	5.183769528518
C	-0.764868447480	-1.196829818458	3.272227844941
C	-0.481124663239	0.232716664167	3.588458101596
C	-0.521766618017	0.724422556120	4.893284383473
H	-0.788805381456	0.077322296602	5.726746966272
C	-0.186071440889	2.053343722408	5.131141225082
H	-0.208393405978	2.451651149187	6.146199616825
C	0.195169374255	2.853304579688	4.060631233689
H	0.485283620664	3.893986646468	4.199413949423
C	0.209931037435	2.288745642063	2.791197556195
H	0.519645605661	2.870588318336	1.921417240166
H	0.809332138441	-3.948428696951	-1.647448808304
N	-2.705641408274	-0.651361874954	-0.822101735938
O	-1.722843946975	-0.471264377963	-1.618642835549
O	-2.416456592050	-0.530507789632	0.419836060736
O	-3.807484639348	-0.911729694023	-1.202505581080
N	2.683159008018	0.634599022175	0.809646891914
O	2.163195241963	-0.531171837237	0.864442971663
O	1.907414867908	1.545245470282	0.351049807918
O	3.803272342665	0.860668065490	1.157139352171
N	-0.142444243458	-3.358369265353	0.449424035866
N	1.673664098654	0.083463627182	-2.932038016814

MEX for ISC
E = -1883.856114871669 / E+ZPE = -1883.445392165932 / G = -1883.510623452171
Tb	-0.053163276372	0.212602788700	0.253477978943
N	-1.439720623345	2.417658529704	-0.056591721784
N	0.464690712508	1.691537764582	-1.862896939415
N	1.554093538811	-0.733432996300	-1.717182636198
N	-0.120049662829	-2.301458639023	-0.407320905950
N	-0.386463760896	-1.600744074358	2.075652472706
N	-0.242241124765	1.029325506586	2.686564220199
C	1.607856143303	3.574337026532	-3.570959829581
H	2.049694837326	4.322218685465	-4.229878741160
C	2.212465072313	2.339093679200	-3.411153745187
H	3.135782984317	2.066237009610	-3.919612085993
C	1.590083769416	1.419535899880	-2.554799920655
H	1.122832330350	-1.815581809507	-3.492043880173
C	-2.510222620412	2.632338713267	0.721572561985
H	-2.596203542890	1.992258555456	1.600913016072
C	-3.481155702945	3.585245863196	0.439687132925
H	-4.332171177540	3.709953832865	1.107981836865
C	-3.342099852261	4.344559237788	-0.715891978850
H	-4.090828565404	5.088447411692	-0.990074996548
C	-2.234944061454	4.131503564512	-1.530702338559
H	-2.120692665055	4.694174929109	-2.455953672301
C	-1.297401020622	3.164990646957	-1.169199831074
C	-0.094260077486	2.897169279736	-2.005942280500
C	0.442205656243	3.864576516993	-2.862385805528

H	-0.015242004820	4.848833320292	-2.945574783483
C	1.251298281354	-1.984342557156	-2.412407807951
H	2.132028781377	-2.632686557106	-2.265669523926
C	0.001088773780	-2.639537821764	-1.820877275248
H	-0.895884950635	-2.205573736494	-2.289228141685
C	-0.537504196510	-2.877065365414	1.714132401888
C	-0.875267499198	-3.896353532393	2.591435120528
H	-0.977743937861	-4.914550529855	2.219067524372
C	-1.085389848383	-3.554233133736	3.925065068700
H	-1.372287868259	-4.312124642561	4.654040362764
C	-0.927491950551	-2.231695169340	4.312957239958
H	-1.102088323963	-1.949989451036	5.349460082418
C	-0.560387275269	-1.271931397078	3.358711695964
C	-0.334769955478	0.159137086437	3.712035392846
C	-0.188309574415	0.575063846433	5.034880557993
H	-0.235509266998	-0.140572221364	5.853362245059
C	0.055748228883	1.917610887110	5.305893102164
H	0.181000247822	2.254904569669	6.335387940939
C	0.152767330218	2.811644224050	4.247063401509
H	0.354524979904	3.869850185819	4.407505188274
C	0.002905946848	2.318753334020	2.956830671928
H	0.096136636513	2.977596378357	2.092129126543
H	0.009733862154	-3.728290574470	-1.965706230062
N	-2.751743413348	-0.363485154435	-0.660654356210
O	-1.785877266160	-0.178075468474	-1.475761882803
O	-2.416388141778	-0.363779920620	0.573822185106
O	-3.881671658042	-0.515799639186	-1.020533123319
N	2.586563605826	0.845894396836	1.227285437007
O	2.085555770591	-0.321042451826	1.332062886940
O	1.853503799475	1.686208159004	0.589697410266
O	3.645279634542	1.144994944245	1.691909157953
N	-0.357357500864	-3.252386329094	0.346821443909
N	2.180280672925	0.199716058484	-2.327904240608

2.7. TbL6(NO₃)₂

S0
E = -1894.058473838527 / E+ZPE = -1893.596706831381 / G = -1893.664505407348

Tb	-0.021510388498	0.054193265264	0.052913178096
N	-1.443007190656	2.237572982694	0.041367564455
N	0.325091734737	1.776320557441	-1.910466155197
O	1.544382574238	-0.631078419768	-1.844089918831
O	-0.037136362093	-2.445857534683	-0.470162104212
N	-0.415781955424	-1.605558075117	2.069288614893
N	-0.138886999898	1.025254697305	2.478945633085
C	1.377767151700	3.753388359906	-3.545761033004
H	1.806669194560	4.535662469407	-4.172638705133
C	1.712651826474	2.420976093614	-3.750783045144
H	2.400240550198	2.127897831634	-4.544085166337
C	1.159257524224	1.463390824899	-2.905622205777
C	1.428189523543	-0.001456504426	-3.112406436604
H	2.360526046565	-0.143648184055	-3.680600226812
H	2.318770774628	-2.281024173322	-2.862247861651
C	-2.464149709139	2.364390115659	0.899377737931
H	-2.732990780708	1.463038692510	1.452789607699
C	-3.158639609535	3.552341564813	1.084041176095
H	-3.984273618049	3.597992208967	1.793082890056
C	-2.770948586632	4.661400084849	0.340442587291
H	-3.282064221395	5.618045541999	0.455389908084
C	-1.731967725968	4.530347033509	-0.574150887498
H	-1.444121190499	5.381366275584	-1.188214372425
C	-1.091597271076	3.297129315200	-0.710001909875
C	-0.041952257534	3.056143023604	-1.741785511855
C	0.480853039642	4.077786360225	-2.535199993981
H	0.202833066912	5.117127949154	-2.373381371066
C	1.830550910670	-2.033817823312	-1.907341653549
H	2.529149491504	-2.237233979904	-1.084076655462
C	0.538257140762	-2.799738564222	-1.733902186188
H	-0.200765226958	-2.513153525874	-2.494659342615
C	0.194761589307	-3.391251050666	0.563983586571
H	1.279261876621	-3.487888079070	0.754923189196
C	-0.481077983680	-2.916607529199	1.820803511530
C	-1.085925504538	-3.817250938587	2.692993153618
H	-1.131320044917	-4.878834264763	2.449781593730
C	-1.640516093718	-3.326218235389	3.868109399610

H	-2.143995819523	-3.995975368965	4.565811369302
C	-1.540466806291	-1.968873206464	4.147011721932
H	-1.962156649930	-1.573249754628	5.068782306967
C	-0.903023919810	-1.134895532401	3.227881350783
C	-0.654840427865	0.310758754951	3.495494931815
C	-0.873976869989	0.882341860447	4.750370590780
H	-1.284691415462	0.294646755041	5.568907363573
C	-0.532946126806	2.213417358097	4.961837223951
H	-0.693531794278	2.672267158048	5.938249231164
C	0.035747093406	2.936952088523	3.919553897339
H	0.344324970424	3.974078029095	4.044682437590
C	0.211445633104	2.299651621964	2.698584766623
H	0.661134557221	2.820045365467	1.851410032289
H	0.706114249817	-3.886068952861	-1.788175627655
N	-2.577869638511	-0.779688562708	-1.002128895931
O	-1.586762799241	-0.479785666796	-1.750614700760
O	-2.373870976694	-0.616935437450	0.249417826736
O	-3.614152321853	-1.187048766240	-1.437197993703
N	2.737011686435	0.487420558398	0.787777399052
O	2.162619224299	-0.647652950813	0.905658797019
O	1.979494937183	1.432446779492	0.377417532749
O	3.894379859379	0.653394141301	1.036249334757
H	0.589062011483	-0.443239258502	-3.680301343988
H	-0.203545296879	-4.372742709976	0.263055899883

T1

E = -1893.950795875887 / E+ZPE = -1893.493814991995 / G = -1893.561915203300

Tb	0.076153140901	0.102959931959	0.120508034024
N	-1.441392212707	2.184789771799	-0.001202777037
N	0.469032710231	1.776354894086	-1.805178762254
O	1.683045614321	-0.540942173144	-1.735393876231
O	0.361637185215	-2.386518561382	-0.253510393784
N	-0.579448091406	-1.586976589760	2.047817226123
N	-0.186465286957	1.040227249783	2.560691881422
C	1.027321621989	3.722298922895	-3.806290674652
H	1.344075824106	4.454969222306	-4.548667852756
C	1.304456959211	2.348973856080	-4.002029003094
H	1.793995307611	1.989113284625	-4.906597196012
C	1.070758375129	1.440627899882	-2.900302635292
C	1.571648273456	0.031040627775	-3.021781238155
H	2.555717207669	0.026250659016	-3.520547601512
H	2.637731069742	-2.156150347569	-2.655276102009
C	-2.508852427170	2.291697400379	0.771923393740
H	-2.767806929294	1.401773721840	1.351134854756
C	-3.286655739388	3.455365485787	0.885888706102
H	-4.154133845403	3.465147644495	1.544207680830
C	-2.901725065371	4.588794393177	0.155327693678
H	-3.463754677156	5.519608429385	0.238287894327
C	-1.808863768635	4.511191663864	-0.677688805709
H	-1.507802456436	5.376912921408	-1.264463035149
C	-1.086907937313	3.272474745104	-0.793906447914
C	-0.066058212642	3.078718136528	-1.711903155795
C	0.397094282278	4.113553572994	-2.663537588331
H	0.221425676651	5.167386775876	-2.454575794116
C	2.124066651243	-1.903856840430	-1.716121563819
H	2.829828097326	-1.981300746062	-0.878120258679
C	0.940297972795	-2.813569890104	-1.483535396408
H	0.192474959930	-2.739071147833	-2.291185430039
C	-0.583446385256	-3.278425942367	0.305377431105
H	-0.169769672405	-4.300410865717	0.310194712618
C	-0.877693820827	-2.846125661808	1.718128518732
C	-1.452732596806	-3.744510938262	2.614285838498
H	-1.672395370195	-4.767151734172	2.306069101834
C	-1.741199194286	-3.303426087788	3.897355008216
H	-2.205839985118	-3.971673603441	4.623017126752
C	-1.422815588633	-1.995986509715	4.248720111626
H	-1.651606584619	-1.631429354270	5.248220039730
C	-0.827263479734	-1.166108157460	3.299744552660
C	-0.442053843740	0.238952137838	3.611116268416
C	-0.340392297111	0.699833490023	4.925034438290
H	-0.513026534825	0.029094957878	5.764653041796
C	0.014301582566	2.023464398401	5.157599547186
H	0.105896863531	2.396892937446	6.178260216173
C	0.260510407857	2.854418016353	4.070702151050
H	0.545077159779	3.897695737042	4.200680913059

C	0.153394777670	2.315698264520	2.795677143584
H	0.365634019705	2.922734162490	1.914830602161
H	1.285086686326	-3.857021957724	-1.393712257997
N	-2.321130235817	-0.843129640901	-1.269344905510
O	-1.247015516992	-0.538422466551	-1.885117700988
O	-2.264409571022	-0.717611125493	-0.000007888766
O	-3.301599961762	-1.235081864156	-1.834837022518
N	2.714183518060	0.728905830339	1.121765266947
O	2.206610742448	-0.444554609587	1.169541804520
O	1.966250194324	1.612164710536	0.582478675329
O	3.802641947424	0.978170978218	1.549385549087
H	0.854518059899	-0.533678791701	-3.647160753556
H	-1.514524945449	-3.282708555741	-0.290237265392

MEX for EET

E = -1893.950012099202 / E+ZPE = -1893.494575266965 / G = -1893.561860012460

Tb	0.053899066162	0.096628065676	0.099516835005
N	-1.453701869032	2.180607701224	-0.003189103297
N	0.411826241517	1.762183319123	-1.849906174116
O	1.683152606626	-0.543808887276	-1.730528822794
O	0.361436121757	-2.393194423381	-0.251457523536
N	-0.588626016270	-1.587930213358	2.039421018628
N	-0.193870417077	1.041591292729	2.546728820962
C	1.050995205920	3.714688452954	-3.802089058710
H	1.357004982229	4.456688452067	-4.539422689676
C	1.419301130937	2.364324728331	-3.960049806240
H	1.995848642399	2.028726549858	-4.821671980084
C	1.101734482408	1.443922421163	-2.906505465357
C	1.584348957997	0.025637404796	-3.020833183946
H	2.569811051548	0.001885101903	-3.514749433045
H	2.646737406908	-2.157704629805	-2.642609830100
C	-2.502583811656	2.293725786637	0.794546135204
H	-2.766107904300	1.398733992013	1.363774712329
C	-3.252825048950	3.470870856650	0.946124695066
H	-4.104587613741	3.487947656458	1.624429868237
C	-2.858845735623	4.607522992079	0.226224347764
H	-3.395416064739	5.550039670408	0.339245728213
C	-1.790764643400	4.517593450381	-0.637845096008
H	-1.486844457633	5.387423118554	-1.216591079220
C	-1.098884389413	3.268162095829	-0.790015392878
C	-0.108278570021	3.058873638303	-1.751841262820
C	0.320302156027	4.081609025258	-2.706366400416
H	0.042712334136	5.122512650823	-2.554214134121
C	2.127852944867	-1.905669672355	-1.706299380967
H	2.830295133556	-1.980254847961	-0.865317543407
C	0.946285640805	-2.819420377655	-1.478869470723
H	0.201438216506	-2.747159999546	-2.289334554441
C	-0.586269565714	-3.284645027262	0.303532773835
H	-0.173159446375	-4.306810860907	0.311501669398
C	-0.885211011886	-2.848824642828	1.714220646331
C	-1.460200425842	-3.744517321998	2.612936245721
H	-1.678193144643	-4.768668840512	2.308552543743
C	-1.750517005516	-3.298881760727	3.894116295671
H	-2.215474813865	-3.964692785030	4.621810095031
C	-1.432859422643	-1.990186357045	4.241146898684
H	-1.662255798435	-1.622409185811	5.239323718666
C	-0.836702901237	-1.163254751850	3.289833193811
C	-0.449565350839	0.241893991415	3.598153698838
C	-0.345959062754	0.703503657899	4.911743995125
H	-0.518396807728	0.033329710721	5.751779025092
C	0.010458558479	2.026700783899	5.143304009887
H	0.102889397166	2.400796333747	6.163655803890
C	0.257323624105	2.856361437477	4.055534921434
H	0.543604428995	3.899313186147	4.184384198500
C	0.148416701103	2.316683238995	2.781068552900
H	0.361004906933	2.922940699694	1.899764551862
H	1.294011329308	-3.861705081599	-1.386965178971
N	-2.335448069156	-0.880926045097	-1.276475519686
O	-1.261634721959	-0.585506956841	-1.896714067033
O	-2.282724449501	-0.724693952621	-0.009832404034
O	-3.312374363680	-1.292421622304	-1.834090701355
N	2.688246382372	0.766855985920	1.078708502192
O	2.192720057896	-0.409242302158	1.157146293878
O	1.926473364783	1.631959722723	0.527680748578
O	3.778501104791	1.036482390881	1.489122309721

H	0.860420646453	-0.534214153453	-3.642507696379
H	-1.514685266056	-3.289562194540	-0.296347859810

MEX for ISC(1)

E = -1893.927562345686 / E+ZPE = -1893.472462037743 / G = -1893.541221013437

Tb	-0.259496026640	0.101753662651	-0.088601488770
N	-1.334059397193	2.447959076373	0.090569006601
N	0.190524440487	1.793738938063	-2.022122857323
O	1.407845283136	-0.617970910160	-1.896255262605
O	0.053976756862	-2.492119326395	-0.402175342228
N	-1.106116193616	-1.601345741693	1.673491337712
N	-0.258310797303	0.805098580646	2.508845157034
C	1.273215536815	3.664071166654	-3.762440244354
H	1.710355658635	4.402930716945	-4.434828095907
C	1.520620126478	2.309332393396	-3.944566656215
H	2.150214717393	1.956806414127	-4.761478657890
C	0.962396584777	1.406468372712	-3.044774232246
C	1.184215635184	-0.074196355360	-3.193352656802
H	2.063152371915	-0.262171415928	-3.828663324360
H	2.356026169181	-2.224372071901	-2.831300775234
C	-2.266697007995	2.669755363346	1.025314884661
H	-2.518457604079	1.822550958988	1.664898509980
C	-2.903455607375	3.892041098397	1.191009640412
H	-3.657969399278	4.014404851903	1.967023264751
C	-2.557938269243	4.932836971933	0.337030636631
H	-3.032326363384	5.910738398755	0.427324652197
C	-1.612998586517	4.702925900487	-0.656394349095
H	-1.363715870935	5.496246793810	-1.358157111608
C	-1.021713471141	3.442586262486	-0.759469798315
C	-0.075853603409	3.100382339743	-1.859757002132
C	0.464559139502	4.067591666288	-2.707725572974
H	0.270916115176	5.126313890606	-2.548582999058
C	1.864336840482	-1.975464079306	-1.878523755943
H	2.603514779167	-2.034211574717	-1.068616221390
C	0.691195945948	-2.894556631759	-1.615124950342
H	-0.075038530203	-2.796556153943	-2.395832917938
C	0.441920028879	-3.182671428794	0.760661937466
H	1.521448514476	-3.069823118661	0.968853987380
C	-0.329069634603	-2.596128354751	1.905153714589
C	-0.246457758333	-3.261744246293	3.233486025804
H	0.510717604631	-4.035590556013	3.375332166425
C	-1.331779907790	-3.130291750540	4.124227293083
H	-1.527098428167	-3.906660475000	4.867730121908
C	-2.223179006855	-2.122126245425	3.823931515464
H	-3.281268314899	-2.146562780872	4.092504867063
C	-1.615664807388	-1.086894917532	2.929203870797
C	-0.963044376508	0.067243440957	3.424739127967
C	-1.117818543223	0.508710716426	4.763182538383
H	-1.729772041432	-0.070860598854	5.454799837791
C	-0.481997474380	1.665551241498	5.171262035055
H	-0.572420972295	2.009013608563	6.202774438783
C	0.268222973293	2.392613306775	4.241506832371
H	0.780211273459	3.313982636202	4.515546531167
C	0.333738081518	1.925873802833	2.930161898342
H	0.888279717684	2.479475757529	2.169525426280
H	1.014140299931	-3.945891076215	-1.555813408229
N	-2.710512865686	-0.605941495074	-1.453126723704
O	-1.547409099569	-0.726750298335	-1.983027901824
O	-2.714175747845	-0.074393792565	-0.297049603022
O	-3.704480069043	-0.967787118482	-2.008225258315
N	2.462581602171	0.448579986974	0.856303938033
O	1.854437120224	-0.675002800629	0.916799274927
O	1.783109110817	1.397811223124	0.344859931215
O	3.582360771690	0.591783231033	1.251146552408
H	0.293739328645	-0.537554575865	-3.652889102373
H	0.204407902745	-4.259120210022	0.676067358369

MEX for ISC (2)

E = -1893.928889193886 / E+ZPE = -1893.473243993565 / G = -1893.539770344516

Tb	0.083026133940	0.060459358588	-0.132621315315
N	-1.249594294258	2.246559570884	-0.447460741788
N	0.771750680377	1.656798207478	-2.080203243939
O	1.900480997816	-0.754984376001	-1.688295241923
O	0.224579557701	-2.456677882820	-0.402992376971
N	-0.890608447222	-1.491455244032	1.718240211284

N	-0.389551304779	1.082070131154	2.275711338192
C	2.015556822618	3.488003519064	-3.745021265441
H	2.515234787129	4.213863280006	-4.387138788611
C	2.357324545459	2.142936818743	-3.802176317156
H	3.121493053209	1.785239067524	-4.492388212097
C	1.704825398159	1.257976125261	-2.947782261929
C	1.979480383644	-0.220616347624	-3.003919908245
H	2.983202981270	-0.406290479656	-3.416903104595
H	2.843081246016	-2.461758719565	-2.434294425935
C	-2.369056140167	2.437718075098	0.262094312268
H	-2.756832177640	1.560448319423	0.783375857181
C	-3.015079807280	3.663884620110	0.344089162206
H	-3.927513420247	3.764728706260	0.930342861322
C	-2.462612210252	4.741510785054	-0.339783513719
H	-2.926130478355	5.727677038505	-0.293723096482
C	-1.319319774401	4.542447288368	-1.106161427137
H	-0.897197027653	5.372132108255	-1.669545227067
C	-0.742345823587	3.272570485973	-1.156562569591
C	0.407972799348	2.947818644844	-2.049471522108
C	1.021184451561	3.898717017315	-2.864663250594
H	0.734245108614	4.947484366583	-2.825270863115
C	2.214613484777	-2.148472982027	-1.587674296647
H	2.776344786471	-2.263152943540	-0.651009944178
C	0.941760602984	-2.963715930735	-1.527313382193
H	0.329104135300	-2.852883127231	-2.437259785290
C	-0.805278785039	-3.276867537462	0.104789717231
H	-0.428927098952	-4.295834419833	0.309477392114
C	-1.288211806462	-2.674495169208	1.381829145498
C	-2.253380638849	-3.367102370244	2.273859289477
H	-3.297861710236	-3.077852971976	2.067312640574
C	-1.841899783281	-3.274655379804	3.700544683757
H	-1.892766052675	-4.116950491933	4.391540933889
C	-1.435633863709	-2.038943352518	4.058240092194
H	-1.179506035910	-1.800721023303	5.091987393993
C	-1.173102805336	-1.058803347110	3.014371576362
C	-0.898899194445	0.334791926181	3.290449688799
C	-1.145579123158	0.896867969280	4.556431244392
H	-1.597161685147	0.297000238436	5.344778185264
C	-0.820282221556	2.224465107233	4.790936906459
H	-1.002000647501	2.670912049324	5.769303915118
C	-0.256001642508	2.970859155713	3.759946200768
H	0.030834782182	4.012462599694	3.898253381218
C	-0.067582996031	2.354672886773	2.526024880995
H	0.374618833431	2.904965270790	1.693869763269
H	1.185486294428	-4.027063397045	-1.369821913872
N	-2.166389652300	-0.838967279425	-1.779842704604
O	-1.013937764161	-0.600125138578	-2.266175990202
O	-2.278637034219	-0.608937251682	-0.528018918803
O	-3.070805473565	-1.269897427255	-2.437144904034
N	2.587484041551	0.639789142013	1.170362641120
O	2.039090831285	-0.512906670333	1.209748440536
O	1.956887896017	1.509972074585	0.474861002960
O	3.607737570001	0.890568187407	1.740203740750
H	1.225383273426	-0.700335605141	-3.653163338364
H	-1.643558391479	-3.361738888663	-0.612750085593

MEX for ISC (3)
E = -1893.926161789979 / E+ZPE = -1893.470405706733 / G = -1893.539001159333

Tb	-0.272433323996	-0.026934091649	-0.126235135442
N	-1.468184034779	2.272627478455	0.020015219625
N	-0.049970278206	1.634633140271	-2.152546856656
O	1.047862306669	-0.837549841889	-2.164064940640
O	-0.297036480751	-2.595926674297	-0.489389108638
N	-0.581859216232	-1.612156422560	1.886792819135
N	0.031924996633	0.959065405051	2.320760143510
C	0.907183372919	3.488135231669	-3.978528070607
H	1.299111263755	4.221101770401	-4.684449089121
C	1.110713687379	2.129430419973	-4.185565986391
H	1.654483350915	1.767388237871	-5.058053318772
C	0.612394245339	1.235543249401	-3.242232092229
C	0.750633693865	-0.250706826641	-3.425569302574
H	1.560886998066	-0.474131849244	-4.136608209569
H	1.655266627631	-2.530430000185	-3.222389583718
C	-2.341846942976	2.493995746299	1.010822179986
H	-2.593282288212	1.629683159210	1.627923990599

C	-2.916096953597	3.734291817877	1.254555986109
H	-3.628029336649	3.856820204541	2.069778228687
C	-2.561644229894	4.794954398846	0.428312967459
H	-2.984614870946	5.788494931637	0.582174242262
C	-1.675997988190	4.567472421558	-0.619054231037
H	-1.419395846720	5.380564537299	-1.295059244398
C	-1.152876523131	3.286855187884	-0.806345287168
C	-0.287938739806	2.942619811740	-1.971473006975
C	0.191942118939	3.903384193476	-2.862046377358
H	0.019257068475	4.964409346660	-2.694060554691
C	1.321016121482	-2.242712581768	-2.213963680258
H	2.140549255591	-2.415939917914	-1.502909713694
C	0.077118636279	-3.003954572629	-1.810523417446
H	-0.773735142772	-2.747783398991	-2.455782371813
C	0.161932240148	-3.448611380736	0.537596976779
H	1.261914235717	-3.570159989903	0.497230016386
C	-0.188350300070	-2.855013887613	1.864591508655
C	0.076597332402	-3.639067077419	3.088676880347
H	0.693315114614	-4.536473894693	3.011775920046
C	-0.436182800666	-3.215190805905	4.257100600468
H	-0.269954075625	-3.743534480376	5.198422442335
C	-1.352273623654	-2.057925369605	4.129331371455
H	-2.423157873611	-2.310236356298	4.067581852568
C	-0.847162148453	-1.085321956454	3.137262233452
C	-0.447994637578	0.259142918519	3.387756130530
C	-0.524054090848	0.829547671775	4.674929261097
H	-0.959393550360	0.255420328445	5.493646001299
C	-0.026578334241	2.107560113728	4.872862248103
H	-0.056515058115	2.562990082728	5.863565436081
C	0.510751535156	2.801794992560	3.787579745909
H	0.924232380349	3.803273676055	3.899842332902
C	0.502289041881	2.188435339096	2.535350247868
H	0.898639105220	2.701599898914	1.656546722272
H	0.243332071351	-4.091614462191	-1.846804450950
N	-2.940153791583	-0.770112308522	-0.956563934891
O	-1.962889318678	-0.643272322927	-1.775566696588
O	-2.663707208398	-0.478913652088	0.253765263941
O	-4.022264774200	-1.139474727478	-1.303719255773
N	2.564156591054	0.255996803939	0.357890542076
O	1.935991944380	-0.843990926118	0.540340193557
O	1.840204456562	1.226607638079	-0.044562412892
O	3.739619167841	0.361974716394	0.548044996925
H	-0.198574897896	-0.657212275066	-3.819144165578
H	-0.300960247426	-4.447042935784	0.439200450856

MEX for ISC (4)
E = -1893.907188329470 / E+ZPE = -1893.452002573462 / G = -1893.519943791051

Tb	-0.160364748450	0.359630224712	-0.071744756281
N	-1.181649939642	2.693399292011	-0.026267947143
N	-0.227864282586	1.616520720025	-2.282092667362
O	0.838684582102	-0.834217841068	-2.045419855540
O	1.072850466197	-3.907572315055	-0.260694928754
N	-0.384730498178	-1.731183193202	1.389593141799
N	-0.013007622213	0.695598710222	2.480153503166
C	0.045836286195	3.013325154308	-4.655154975301
H	0.160655641010	3.567820197033	-5.587004706204
C	0.251444306611	1.640200286706	-4.623981003427
H	0.527745575227	1.091175662809	-5.524219232822
C	0.102585724602	0.976325012000	-3.409422023290
C	0.271073403832	-0.517085706990	-3.312427229092
H	0.939380796286	-0.868473026328	-4.113031510487
H	1.723266404909	-2.462335997416	-2.964741074691
C	-1.755512374743	3.154200837196	1.091363549475
H	-1.984768704411	2.407404682731	1.853023868597
C	-2.056581806001	4.495548531956	1.291100786974
H	-2.524223370380	4.818778984670	2.220139569266
C	-1.741565641909	5.394900831577	0.279562612256
H	-1.941575850904	6.460354097510	0.398368753825
C	-1.184129671599	4.916744436405	-0.902290877659
H	-0.954497051754	5.610734161136	-1.708251521831
C	-0.931855818314	3.552047733208	-1.034065796855
C	-0.450261483309	2.943699877576	-2.308264186532
C	-0.313469024569	3.675675122391	-3.486284396604
H	-0.495302098785	4.747949438788	-3.508386732613
C	1.419476621748	-2.149381890032	-1.955896426956

H	2.332927518371	-2.026317154908	-1.361144902262
C	0.469223866655	-3.170414125528	-1.307382468708
H	-0.447091445059	-2.653837128555	-0.971706673273
C	1.515632177671	-3.175344797074	0.857972995911
H	2.114957366528	-2.290899183459	0.590262600481
C	0.377383358949	-2.711399098919	1.749641771288
C	0.091187660679	-3.477874503566	2.988920536989
H	0.824804780996	-4.222416949897	3.303206433953
C	-1.228426297612	-3.475725690878	3.538189573026
H	-1.595425780277	-4.348309802824	4.082867265808
C	-2.011191253966	-2.431973209820	3.153067523564
H	-3.101518950625	-2.413722030205	3.203199085983
C	-1.201097479398	-1.337903218336	2.539608063296
C	-0.752443213148	-0.187037193181	3.228280136796
C	-1.105628546097	0.115706749100	4.567008291917
H	-1.745720624112	-0.566695352672	5.126290210076
C	-0.598337854784	1.258633422968	5.153119559192
H	-0.834618125746	1.491389956900	6.192574795811
C	0.226088534384	2.111408653134	4.405897165677
H	0.650508335813	3.016840202768	4.837305268869
C	0.471209289050	1.791768045257	3.075608053264
H	1.064181682323	2.450525856875	2.435634999422
H	0.157717431415	-3.933786297134	-2.031179757712
N	-2.869774899463	-0.606795326181	-0.404253193780
O	-1.956451061846	-0.764388202490	-1.288031402840
O	-2.516814726153	0.088406617253	0.606402896322
O	-3.959197839316	-1.083679918343	-0.512857059770
N	2.604538342797	1.060099741852	0.374837225841
O	2.185797104594	-0.148947431254	0.397878229439
O	1.699279750116	1.930032506028	0.128064511131
O	3.744071607464	1.350736517209	0.574325339513
H	-0.712720485032	-1.006657984211	-3.419752802012
H	2.163519986137	-3.858787811425	1.421296448337

2.8. TbL7(NO₃)₂

S0

E = -1854.366891417728 / E+ZPE = -1853.877248482170 / G = -1853.943741269091

Tb	-0.008155052283	0.005017723487	0.015473896100
N	-1.431527552062	2.218283540422	0.015121763729
N	0.358921385672	1.758615039936	-1.908161425440
N	1.677863363222	-0.688837476828	-1.862330422759
N	-0.147443644089	-2.540192966891	-0.563385727501
N	-0.423151469002	-1.626367835259	2.044749749996
N	-0.123985108528	0.993348492561	2.463611291294
C	1.294273909569	3.701396948675	-3.648564214046
H	1.673786011061	4.470379578170	-4.322186462323
C	1.611151849628	2.364014022059	-3.853606966867
H	2.233569891270	2.054421773558	-4.693266968394
C	1.116751353362	1.419796817727	-2.957781645659
C	1.360874032657	-0.055916106236	-3.145524701549
H	2.151956819675	-0.222357401961	-3.896481746812
H	2.356067109996	-2.445222144703	-2.882666123624
C	-2.433626466697	2.365394189227	0.891698237910
H	-2.778736274942	1.447396398330	1.371581702596
C	-3.014335521412	3.592468756511	1.183945531031
H	-3.831888333525	3.653702895173	1.901097399728
C	-2.517197719480	4.721345952412	0.542701890100
H	-2.929000565629	5.709598290477	0.751252446189
C	-1.499333152099	4.573081953072	-0.393439981170
H	-1.122040204586	5.446976402939	-0.920540547127
C	-0.989654120843	3.299668023043	-0.653855393745
C	0.003712607013	3.040757747887	-1.737401742603
C	0.469239805678	4.046777930900	-2.585284737245
H	0.190763183103	5.087650168593	-2.435298974729
C	1.850608617731	-2.148499906521	-1.947304064770
H	2.502084826952	-2.447716837848	-1.114073208401
C	0.507567149718	-2.855550355903	-1.843055664393
H	-0.163893972596	-2.513263260043	-2.643127832791
C	0.292250452783	-3.383936520417	0.551402120843
H	1.379804992430	-3.259755293595	0.677420440643
C	-0.368168594263	-2.946879266081	1.834330408520
C	-0.844557076107	-3.868279432837	2.763190527910
H	-0.790916476883	-4.937264064016	2.556898568955
C	-1.384370098406	-3.392457275357	3.951997046422

H	-1.776687697141	-4.084016175174	4.698376747643
C	-1.399860962187	-2.023610331368	4.188365229638
H	-1.790465923205	-1.642845701815	5.129707240966
C	-0.894838639179	-1.163672723551	3.211896553320
C	-0.753418539036	0.305198026990	3.434205805919
C	-1.175214765297	0.928120674367	4.610376518238
H	-1.706858124563	0.372027560772	5.379924823200
C	-0.896022770624	2.276370497340	4.805467517053
H	-1.216082652119	2.774555676080	5.721463859592
C	-0.187242072289	2.966785476652	3.828699954928
H	0.082409541099	4.015054980379	3.950536067794
C	0.168941957573	2.283475325781	2.673438439123
H	0.716045280365	2.778692329288	1.868683123677
H	0.648735442223	-3.942708523053	-1.973304959379
N	-2.664321240727	-0.481849168794	-1.051504690658
O	-1.644873824102	-0.373106682264	-1.809767757758
O	-2.394625319509	-0.592669123116	0.196600054549
O	-3.785847967039	-0.481899998339	-1.468057843698
N	2.657431661509	0.479910514035	1.062033133407
O	2.156348235555	-0.691482900288	1.003226474833
O	2.000795247390	1.375853515152	0.423357322970
O	3.661724112303	0.726506221432	1.663553643601
H	0.431461494508	-0.501349054298	-3.535551135097
H	0.097194178471	-4.453400806814	0.363221971962
H	-1.152319269990	-2.679824393883	-0.676625957417
H	2.553683917889	-0.285459186194	-1.527404698384

T1

E = -1854.255856090037 / E+ZPE = -1853.771700060257 / G = -1853.839957630116

Tb	0.071927392523	0.014707688592	0.085128612143
N	-1.338908922584	2.235027531904	0.058334234817
N	0.541380720551	1.764740114310	-1.766686523199
N	1.670821802280	-0.676430573571	-1.870736320773
N	-0.127638823605	-2.522769842920	-0.533080734997
N	-0.412256719882	-1.641688706860	2.075396597334
N	-0.094475458106	0.966715167557	2.531600428219
C	1.135199351612	3.744746226167	-3.720127433478
H	1.487590604043	4.475880755685	-4.448187525158
C	1.216072048876	2.359790549730	-4.008417078164
H	1.575530634864	1.999875316484	-4.972206052108
C	0.996626741460	1.418459982968	-2.930337188448
C	1.330835858100	-0.034888560737	-3.139497868919
H	2.132706395505	-0.139373436167	-3.891731428411
H	2.321062187650	-2.433261262384	-2.912593016943
C	-2.390101030901	2.399020132851	0.846480325204
H	-2.734388430588	1.501934799489	1.367557448639
C	-3.047702809295	3.622927598314	1.040609272206
H	-3.908102601846	3.675625997518	1.706097984162
C	-2.557244742864	4.755559982271	0.377707830018
H	-3.026506762685	5.729629802259	0.520673885437
C	-1.479544863617	4.621780057029	-0.469690546772
H	-1.095046667375	5.486913134839	-1.006569623220
C	-0.883213493526	3.330464381577	-0.663088908708
C	0.123741092078	3.101312705393	-1.593014042878
C	0.655405622222	4.138136877078	-2.507850062001
H	0.639047137804	5.188664823856	-2.220944757845
C	1.838780497609	-2.136383427804	-1.965089697338
H	2.507936452494	-2.437223842918	-1.146930885822
C	0.495542919620	-2.837988972712	-1.828018997078
H	-0.193325140669	-2.490729528018	-2.611022645083
C	0.314663885293	-3.384281163039	0.567164829066
H	1.403581172950	-3.267337557234	0.688430094296
C	-0.337891556382	-2.960098338113	1.858964559996
C	-0.792345974692	-3.891533914978	2.789466607288
H	-0.723802383261	-4.958941117386	2.579394106450
C	-1.327204052413	-3.428372558440	3.985344560582
H	-1.697826232373	-4.128921155742	4.734420886551
C	-1.366581653464	-2.060170721136	4.225291644578
H	-1.749744040695	-1.687815462227	5.173208603251
C	-0.887999968584	-1.190088903542	3.245254004526
C	-0.778548777611	0.281546696151	3.466173466439
C	-1.285654505617	0.911442049498	4.604159227967
H	-1.869588396413	0.358171933899	5.337202335598
C	-1.031012527383	2.264328564684	4.801912798630
H	-1.418747956928	2.769834095359	5.687252558657

C	-0.262488793700	2.951539440500	3.868345183410
H	-0.010914463500	4.003367504441	3.998015988823
C	0.175374339039	2.260643820618	2.745825007826
H	0.770490686110	2.752066352783	1.973273612574
H	0.629423560445	-3.925334960445	-1.964553114016
N	-2.566305846133	-0.399793842384	-1.066438000695
O	-1.523272456279	-0.287716072574	-1.792739662539
O	-2.335036385756	-0.556191469402	0.182546851150
O	-3.674884393962	-0.360985342456	-1.515774190412
N	2.765816910957	0.293034036957	1.141032765671
O	2.200965907874	-0.845591725631	1.007840981288
O	2.146274385715	1.264086829999	0.586170008044
O	3.795433371513	0.437362727883	1.732594673586
H	0.426983611467	-0.510900039486	-3.556250746532
H	0.110480753158	-4.450007025420	0.366944305663
H	-1.137437492709	-2.639202621756	-0.626571018626
H	2.551405541543	-0.273063003178	-1.547616299932

MEX for EET
E = -1854.254784971839 / E+ZPE = -1853.771373836677 / G = -1853.837746552408
Tb	0.037222141585	0.008994526049	0.055935718596
N	-1.360616325486	2.220887831268	0.056217749667
N	0.459242159959	1.750160521740	-1.823629417616
N	1.665819930570	-0.688368770528	-1.868733111027
N	-0.144672545662	-2.532606597720	-0.544256331361
N	-0.415941147702	-1.639916369497	2.062414125849
N	-0.088597120928	0.969698062262	2.510687668354
C	1.201802380645	3.737771022788	-3.697605762965
H	1.556674947753	4.487094089857	-4.405268861538
C	1.403128773794	2.366298859922	-3.955094897753
H	1.889975478102	2.025633531223	-4.868320869720
C	1.047694068360	1.418873173999	-2.940819681938
C	1.353399870066	-0.043255139402	-3.143603654144
H	2.161567853477	-0.168919896372	-3.884849397551
H	2.314616298771	-2.444381708340	-2.911361881829
C	-2.392061228454	2.385698265258	0.868654702679
H	-2.740836680538	1.484265761334	1.379098019575
C	-3.023736060510	3.617337537291	1.102121032985
H	-3.869195114042	3.671529571389	1.786313811745
C	-2.523150778362	4.754561198638	0.454626430658
H	-2.967212775383	5.735067838048	0.629675516976
C	-1.470209732502	4.616458300590	-0.422362620302
H	-1.084182964151	5.487453050372	-0.947805399287
C	-0.903706457679	3.318873515027	-0.658440061632
C	0.063146780751	3.079844903393	-1.640253492392
C	0.566183267077	4.111242348483	-2.546525673763
H	0.409663485225	5.164274864547	-2.320960447079
C	1.828206098910	-2.149002735059	-1.965599183163
H	2.492781298930	-2.455812009786	-1.145893335785
C	0.481882110920	-2.846316939173	-1.837882592326
H	-0.202461449599	-2.493376136054	-2.622386890170
C	0.303422094103	-3.388053643737	0.558153749839
H	1.392722143651	-3.268892772489	0.673875960285
C	-0.342265898874	-2.959123974998	1.851691115699
C	-0.789225289502	-3.887016254843	2.789297664503
H	-0.721399627610	-4.955250500602	2.583188560080
C	-1.315081933358	-3.419035831112	3.987332829938
H	-1.679416630864	-4.116659346905	4.742158779778
C	-1.353017623148	-2.049853217339	4.221474989946
H	-1.728044390463	-1.673589034175	5.171129408270
C	-0.883163227860	-1.183649737077	3.233734744399
C	-0.773429534999	0.288877882590	3.447859133432
C	-1.282316522696	0.923684219896	4.582428643577
H	-1.868912531281	0.373852972381	5.315958011203
C	-1.026703508596	2.277053845865	4.775480799860
H	-1.416187339982	2.786530441703	5.657784039573
C	-0.254708056431	2.959286477950	3.841112337138
H	-0.001223159117	4.011081886892	3.967489465204
C	0.183343341101	2.263937807286	2.721350996203
H	0.779522615442	2.751337763461	1.946959713742
H	0.612334509867	-3.933738128300	-1.977400356355
N	-2.614568161320	-0.432094033685	-1.050431665960
O	-1.584554876334	-0.325312072060	-1.794909964314
O	-2.362020998772	-0.571894589921	0.197288336785
O	-3.731032001672	-0.403686739199	-1.480597836781

N	2.723277271391	0.359189878304	1.107547241963
O	2.184392972529	-0.793188181483	0.997710724057
O	2.093493802991	1.302234315385	0.514475721676
O	3.738629270880	0.543464872207	1.712729667298
H	0.444684710560	-0.504737391963	-3.565419020678
H	0.101179411256	-4.455122215915	0.363358963669
H	-1.153696077479	-2.655667184812	-0.638455045523
H	2.542895942660	-0.291777454857	-1.528397012242

MEX for ISC(1)
E = -1854.234811218057 / E+ZPE = -1853.751962432005 / G = -1853.819519338806

Tb	-0.166371409459	0.037936878300	-0.060119347837
N	-1.472900132894	2.299393307148	-0.054182515642
N	0.331438519228	1.787771091940	-1.947763389523
N	1.596641808350	-0.674174821267	-1.854655870118
N	-0.194554320697	-2.546295242159	-0.541080677442
N	-0.775534612437	-1.587360057543	1.872109134234
N	-0.264698257034	0.991361243210	2.438314878709
C	1.258626041707	3.686173967678	-3.739597625918
H	1.630763619667	4.436791803578	-4.437673276119
C	1.565439057606	2.342898878208	-3.918425045498
H	2.175351661918	2.011313718336	-4.758885927859
C	1.074989687497	1.419839385113	-2.997719446494
C	1.313932584342	-0.060904980544	-3.156333888303
H	2.124742764190	-0.240753115489	-3.882824380151
H	2.325498283045	-2.430679875622	-2.838717602687
C	-2.451585426070	2.481082926358	0.841003654439
H	-2.855829737736	1.572152409534	1.291067486631
C	-2.936499906781	3.734583759556	1.191034485526
H	-3.737618905082	3.827144428898	1.923231061801
C	-2.362553648414	4.849421196090	0.589819544625
H	-2.693508343563	5.855884172450	0.849353893378
C	-1.369956525974	4.667143242126	-0.367678501356
H	-0.928366905003	5.531925922309	-0.859168905401
C	-0.961492195003	3.371277692411	-0.687655074527
C	-0.001583796574	3.078013646430	-1.792127629334
C	0.455579271095	4.061724573876	-2.669160633079
H	0.183484911059	5.106979070132	-2.538172504940
C	1.803713927128	-2.130923622874	-1.913363703601
H	2.455140141536	-2.399890771075	-1.069708208926
C	0.479047174685	-2.873434131163	-1.808206283874
H	-0.193576593207	-2.561209394571	-2.619033996282
C	0.253069820310	-3.344135179742	0.598584374198
H	1.353367098229	-3.295400431278	0.670452208976
C	-0.286296582829	-2.795118346251	1.886688272574
C	-0.106023797972	-3.570588750358	3.134571954279
H	0.573007988446	-4.425001581613	3.121377221438
C	-0.779994836225	-3.204131934782	4.239365047026
H	-0.696022061582	-3.746478930703	5.183839730837
C	-1.745143188136	-2.104144194447	4.023526983717
H	-2.793404394246	-2.406999618494	3.875024863843
C	-1.193157195103	-1.092002879069	3.098879004377
C	-0.856659005082	0.252420955751	3.421201975377
C	-1.109699195329	0.791156728997	4.700916864089
H	-1.625103069023	0.183766720864	5.445893346893
C	-0.687297134992	2.078754199569	4.986158902458
H	-0.855435112372	2.508175476177	5.974708062927
C	-0.045841600740	2.816689353763	3.989594298339
H	0.311648485027	3.829604007750	4.169750391779
C	0.128173447319	2.230694283695	2.736787770793
H	0.618000129357	2.778701477955	1.928624840584
H	0.650327683130	-3.958608595323	-1.917267266780
N	-2.707887042487	-0.489400079068	-1.373484591822
O	-1.604051016278	-0.417573621805	-2.015627697537
O	-2.585276578687	-0.484952570714	-0.102052615018
O	-3.768216428372	-0.563736166649	-1.921687106676
N	2.455594953918	0.403399261405	1.140073550399
O	1.900273289722	-0.744146000064	1.065730497227
O	1.894677391799	1.314884987022	0.440418383676
O	3.422911244863	0.610436394668	1.813346474600
H	0.393040529872	-0.508831371430	-3.562693970207
H	-0.013818018980	-4.412941984465	0.501475408898
H	-1.196999214788	-2.700731203261	-0.656491941561
H	2.450045680966	-0.245515874603	-1.493658371264

MEX for ISC(2)

E = -1854.236506835120 / E+ZPE = -1853.753685977578 / G = -1853.818211720841

Tb	0.151098859352	0.026861814868	0.200502998853
N	-1.235081225870	2.311821152989	-0.131232919141
N	1.041572271274	1.802705897027	-1.505841512581
N	1.570223976762	-0.711706564618	-1.946798258009
N	-0.130154411760	-2.496881615284	-0.461467393892
N	-0.286299266212	-1.669587933467	2.163993008653
N	-0.392575387872	0.981057616967	2.580982184743
C	1.020022348342	3.809274409150	-3.589699794998
H	1.279195878283	4.452488689328	-4.433960983095
C	0.643643337917	2.465700604019	-3.811959398440
H	0.433285718066	2.096056161022	-4.817376701528
C	0.897944498233	1.465938363969	-2.738795224912
C	1.126850460639	0.030946690369	-3.117862651660
H	1.841497529335	-0.011370504893	-3.962706097632
H	1.993708721935	-2.444697649065	-3.136170279565
C	-2.439728513905	2.486301266422	0.420272956609
H	-2.851397453487	1.616831342217	0.937342114175
C	-3.155334299491	3.680126852396	0.365532450101
H	-4.135529970344	3.747689788693	0.835192932775
C	-2.573581594433	4.775290239657	-0.281134493634
H	-3.094343902339	5.732530037094	-0.331120049834
C	-1.322796647813	4.631807389510	-0.849409079035
H	-0.831027154527	5.471939617543	-1.340425593175
C	-0.674659258193	3.371181514173	-0.797662924682
C	0.622767645868	3.176258733111	-1.327227980158
C	1.256788475803	4.147057579379	-2.276983785460
H	1.922980359284	4.954223362627	-1.966008411295
C	1.658694067292	-2.166728852249	-2.121575213941
H	2.419634876540	-2.528072227013	-1.415942515303
C	0.319284138780	-2.822693806185	-1.824361917959
H	-0.446304272257	-2.444290262375	-2.515827641048
C	0.445657554860	-3.351566221638	0.582535419941
H	1.531968115065	-3.177138899544	0.627559564643
C	-0.152231913128	-2.981118527563	1.915671871864
C	-0.539194911824	-3.955372855617	2.831682618088
H	-0.414809550295	-5.012143134909	2.595639862740
C	-1.093517743155	-3.549743871495	4.039002237588
H	-1.422349232519	-4.285138404795	4.773926082975
C	-1.224227282075	-2.192173820320	4.300072040506
H	-1.657300240425	-1.863727434717	5.242144875524
C	-0.793388068350	-1.271997306663	3.343029718764
C	-0.803754505866	0.198650870352	3.594473913824
C	-1.143038240024	0.735269034785	4.838294526448
H	-1.477003157053	0.096553643382	5.653009157176
C	-1.024939677016	2.104528297788	5.045652413329
H	-1.282158937607	2.537061971581	6.013167393647
C	-0.550012112411	2.902755683246	4.011828001432
H	-0.408800740245	3.975671095269	4.134827530482
C	-0.247589254617	2.293500299932	2.801653379628
H	0.137512451295	2.880192466975	1.966919854368
H	0.398468205878	-3.913313729768	-1.977672894405
N	-2.470912894299	-0.339543501184	-1.023567251938
O	-1.417517768663	-0.180665471809	-1.724578911652
O	-2.261726440435	-0.517050490991	0.225335738207
O	-3.570242273285	-0.320083571567	-1.496527061161
N	2.872510121198	0.147850551828	1.241853092436
O	2.342305754018	-0.926121505105	0.776238232454
O	2.118020795919	1.168634257772	1.209267208972
O	3.991705190325	0.173739385010	1.662360428662
H	0.168716898713	-0.374764325999	-3.479834539199
H	0.278769083861	-4.422978504620	0.378497009203
H	-1.143718937369	-2.616568959100	-0.424665572668
H	2.490004204272	-0.366071315954	-1.671882846681

MEX for ISC(3)

E = -1854.235061087857 / E+ZPE = -1853.751502560814 / G = -1853.816709038322

Tb	0.035623976995	0.007865127575	0.061985840414
N	-1.385478945071	2.256500758049	0.033770643321
N	0.416483994289	1.710748064313	-1.845590314084
N	1.683500066118	-0.678542065285	-1.880889523033
N	-0.116773572277	-2.530475482122	-0.547837698658
N	-0.406453544419	-1.643135276503	2.061914764220
N	-0.107589433065	0.970553237675	2.504637926726

C	1.295536878094	3.703097156141	-3.645337527586
H	1.967645915530	4.333608181519	-4.228693515504
C	0.869685247190	2.346210226308	-4.091676523555
H	-0.059184106141	2.308592834947	-4.683711685570
C	0.904095979652	1.353271515341	-2.981385259460
C	1.398208542464	-0.046648306643	-3.168533009353
H	2.265445303750	-0.049363980011	-3.853599054803
H	2.367238437421	-2.441368657027	-2.892253222496
C	-2.395944873282	2.438114517332	0.886882884850
H	-2.723005366794	1.547648264076	1.428373445944
C	-3.017043358743	3.667197001650	1.094624629595
H	-3.841027978358	3.747916339214	1.802400682886
C	-2.559445936826	4.769414082509	0.374543506218
H	-3.015027082375	5.751261944457	0.509845964274
C	-1.531891527669	4.596317441765	-0.540359323453
H	-1.189074453189	5.431369148081	-1.149843446386
C	-0.963064713715	3.318596128126	-0.705626724641
C	0.032523144324	3.054891333036	-1.709926714268
C	0.732344610627	4.075996195653	-2.480646658417
H	0.866566406614	5.073867135312	-2.057279797408
C	1.865900083120	-2.137861183656	-1.957125766999
H	2.522842608593	-2.426750513508	-1.124823069834
C	0.523525837840	-2.844290786768	-1.835767433370
H	-0.157012453121	-2.498440014592	-2.627067262866
C	0.327323978744	-3.384726656737	0.558122705745
H	1.414837470924	-3.259077707387	0.682826580749
C	-0.332021367963	-2.961606266824	1.846603874913
C	-0.790841042456	-3.892227784756	2.775463126032
H	-0.721754273731	-4.959859572630	2.566692518701
C	-1.331438398030	-3.427569383376	3.968332495766
H	-1.706763961932	-4.127173145114	4.715945785098
C	-1.370415767526	-2.059260749549	4.207358601417
H	-1.759656616920	-1.686504827915	5.152580358169
C	-0.886029412691	-1.189834136306	3.229415344897
C	-0.774778531139	0.281790194062	3.449650764214
C	-1.262103000171	0.908367565122	4.597806611832
H	-1.831587121398	0.352490315407	5.340110169455
C	-1.004454526964	2.260767129966	4.796045068696
H	-1.377463162305	2.762992119205	5.689539786010
C	-0.251039104741	2.950474234443	3.852598337977
H	0.003194528611	4.001763961428	3.981298426134
C	0.166465009229	2.263695449548	2.719805015775
H	0.747830300999	2.758223478545	1.938979291091
H	0.660424879971	-3.931519418846	-1.969770639919
N	-2.624965344409	-0.426697677889	-1.019560620705
O	-1.600190448536	-0.327307922417	-1.774015399712
O	-2.361498675231	-0.559059348052	0.226166599592
O	-3.744257989167	-0.397890084544	-1.441135103851
N	2.718867535152	0.383443788044	1.103228025687
O	2.190824159679	-0.774601659737	0.991578847576
O	2.077865586302	1.321212493687	0.513986252491
O	3.733402203475	0.575690727715	1.706483754576
H	0.592150433971	-0.601994510737	-3.679204272895
H	0.132445303974	-4.452465612887	0.360148166278
H	-1.123722883060	-2.662277922686	-0.653124880011
H	2.544302853723	-0.264720152737	-1.520961334516

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