

Electronic Supplementary Information (ESI)

Steric Effects in Light-Induced Solvent Proton Abstraction

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Experimental Methods

Materials. The alcohols methanol, ethanol, propan-1-ol (*n*-propanol), propan-2-ol (*i*-propanol), butan-1-ol (*n*-butanol), pentan-1-ol (*n*-pentanol), cyclopentanol, 2-methylbutan-2-ol (*t*-amyl alcohol, TAA), hexan-1-ol (*n*-hexanol), heptan-1-ol (*n*-heptanol), and octan-1-ol (*n*-octanol) were obtained from Millipore-Sigma in their highest purity grade available and were used as received. Acetonitrile (ACN) was purchased from Millipore-Sigma in its highest purity grade and used as received. The compound **FR0**-SB was synthesized from **FR0** and *n*-butylamine as described previously.^{1,2}

Steady-state absorbance and emission spectroscopy. UV-visible absorption spectra were recorded using a Shimadzu UV-2600 spectrometer. Spectral resolution was 1 nm for all measurements. The concentration of the samples was 2 μ M in all the solvents. The molar absorptivity of **FR0**-SB is $\epsilon_{\text{max}} = 81500 \text{ M}^{-1}\text{cm}^{-1}$ (*ca.* 370 nm). Fluorescence spectra of **FR0**-SB dissolved in each solvent were recorded using a Hitachi FL-4500 fluorescence spectrometer with excitation at the absorption maximum in each solvent. Excitation and emission spectral resolution

was 1 nm for all measurements. Temperature-dependent steady-state spectra of **FR0**-SB in *n*- and *i*-propanol were acquired using a Horiba Duetta spectrofluorometer with a Quantum Northwest temperature controller (QNW TC 1). Analysis of the spectra was performed using Microcal Origin 9.0 software.

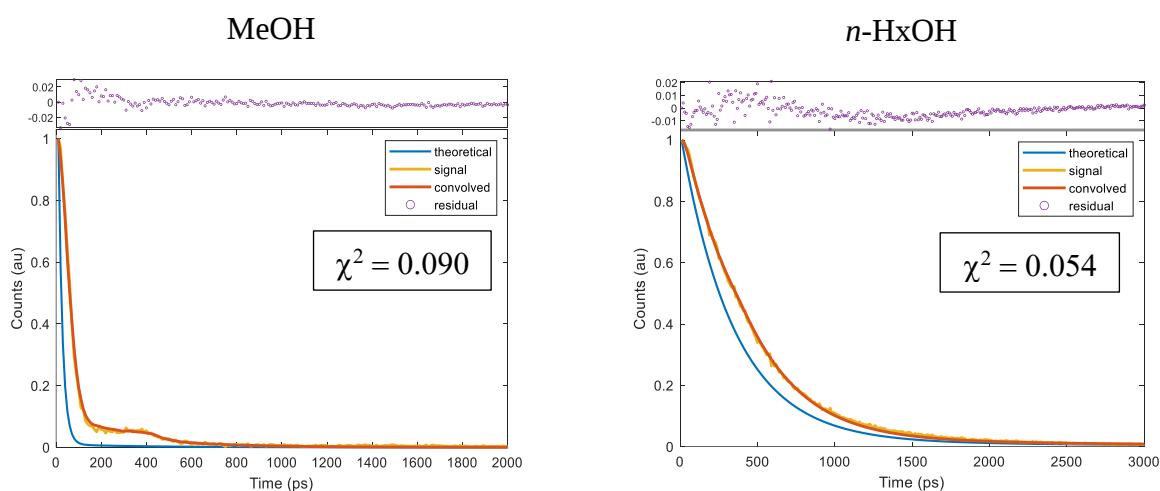
Time-resolved fluorescence measurements. The time-correlated single photon counting (TCSPC) instrument used in this work has been described elsewhere³ in detail and we provide only a brief synopsis here. The pump laser is a passively mode-locked Nd:YVO₄ laser (Spectra-Physics Vanguard) that operates at 1064 nm producing 13 ps pulses at 80 MHz repetition rate. The second harmonic (532 nm) and third harmonic (355 nm) outputs are 2.5 W average power with the same pulse width and repetition rate as the fundamental laser output. The 532 nm output of the Nd:YVO₄ laser excites synchronously a cavity-dumped dye laser (Coherent 701-3) operating at 700 nm (LDS 698 laser dye, Exciton). The output of the dye laser was frequency-doubled using a Type I LiIO₃ SHG crystal to produce 350 nm excitation pulses (*ca.* 5 ps pulses, 250 ns inter-pulse spacing) to excite the samples. Average power at the sample was less than 1 mW for all measurements. A portion of the dye laser fundamental output (700 nm) was sent to a reference photodiode (B&H). Sample fluorescence was collected using a 40× reflecting microscope objective (Ealing) and sent to a polarization-selective cube beamsplitter (Newport). Each polarized emission component was polarization-scrambled and sent through a subtractive double monochromator (CVI Digikrom CM112) equipped with a microchannel plate photomultiplier detector (MCP-PMT, Hamamatsu RG3809). The output of each MCP-PMT detector was input to one channel of a two-channel TCSPC system (B&H Simple Tau 152) with instrument control performed with a personal computer. Data were acquired and stored using a program written in-house using National Instruments LabVIEW[®] software. Temperature-dependent time-resolved data were recorded by

TCSPC as described above, the only differences being that the excitation wavelength was 430 nm and that the temperature was controlled using a Thermo Fisher Scientific bath circulator connected to the cuvette-holder. For the temperature-dependent measurements, data were collected at every 10 K between 273 K and 323 K while the sample was stirred.

Fluorescence Lifetime Fitting

Analysis of the fluorescence lifetime data was performed using a convolute-and-compare program written in-house using Matlab. The program generates and convolves a number of exponential functions with the experimental instrument response function. The resulting curves are then compared with the experimental signal to determine the one that best fits the experimental signal. The average chi-squared value across all fits presented in this manuscript was 0.186. Here we include a number of representative fits together with the residual (data – fit). Two of the data sets presented here (ethanol and heptanol) have the highest chi-squared values obtained.

Fig. S1. FR0-SB in methanol, *n*-hexanol, and *i*-propanol excited at 350 nm, detected at 460 nm.



i-PrOH

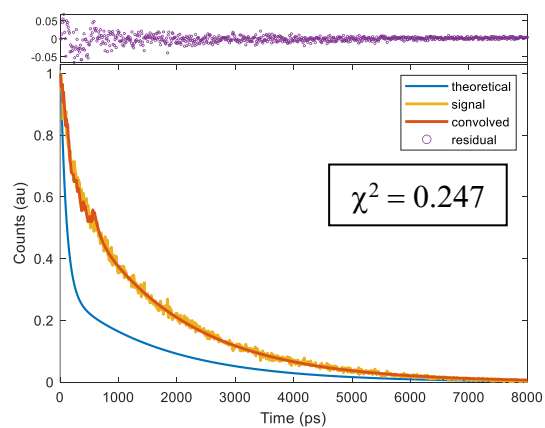
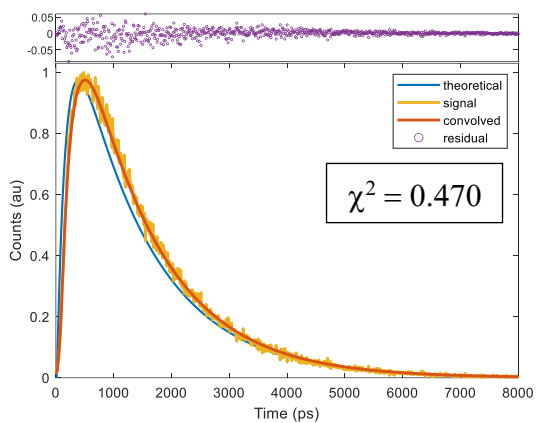
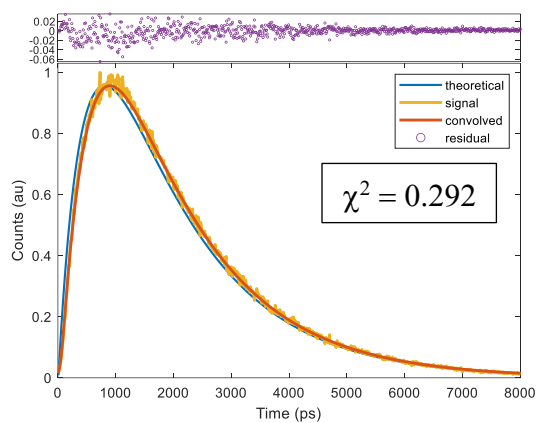


Fig. S2. FR0-SB in ethanol, *n*-butanol, and *n*-heptanol excited at 350 nm, detected at 630 nm.

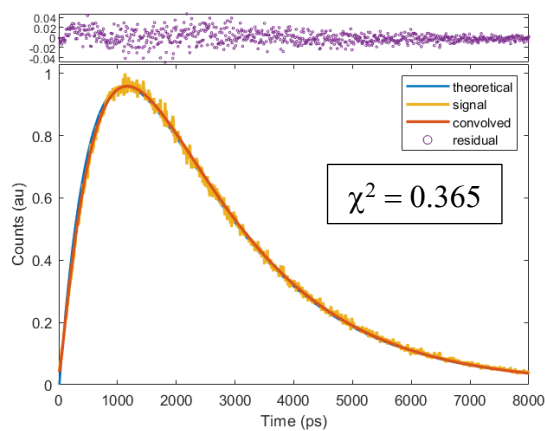
EtOH



n-BuOH



n-HpOH



Computational Details

All of the geometry optimizations relied on the Kohn–Sham formulation⁴ of density functional theory (DFT)⁵ using, in the case of the structures along the excited-state proton transfer reaction pathway, the time-dependent (TD)⁶ extension of DFT to excited states combined with the SMD continuum solvation model, described in ref. 27 of the main text, to account for the bulk solvation effects (the analogous protocol employing SMD was used in the DFT ground-state optimizations). All of the calculations reported in this work employed the 6-31+G* basis set⁷⁻⁹ using spherical components of d functions and the CAM-B3LYP functional.¹⁰ As explained in our previous work,² among the several benchmarked functionals, CAM-B3LYP provides the gas-phase vertical excitation energies of **FR0**-SB closest to those obtained in the high-level *ab initio* EOMCC calculations using the δ -CR-EOMCC(2,3) triples correction to EOMCCSD.¹¹ For example, the CAM-B3LYP/6-31+G* $S_0 \rightarrow S_1$ vertical excitation energy of 3.92 eV is close to the 3.70 eV value obtained with δ -CR-EOMCC(2,3), which is, in turn, within 0.2 eV from the experimental excitation energy of 3.52 eV. In addition, the CAM-B3LYP functional provides the ground-state geometry of **FR0**-SB that is essentially identical to that obtained using the second-order Møller–Plesset perturbation theory, when the 6-31+G* basis set is employed.²

All of the electronic structure calculations reported in this study, including the DFT and TD-DFT geometry optimizations using the CAM-B3LYP functional and the accompanying single-point DFT and TD-DFT calculations employing the same functional and the SMD continuum solvation model, were performed using the GAMESS package.¹² In the case of the optimized ground-state geometries, the $S_0 \rightarrow S_1$ vertical excitation energies, which, from the fundamental physics perspective, correspond to a very fast process resulting in an abrupt change in the solute electron density, were computed by taking advantage of the nonequilibrium solvation effects

associated with the solvent relaxation delay, incorporating a fast component of the solvent dielectric constant in addition to its bulk value,¹³ as implemented in GAMESS. All visualizations of optimized molecular structures presented in this work were performed using the VMD software.¹⁴

In what follows, we provide the SMD/CAM-B3LYP/6-31+G* optimized geometries, labeled A–L, obtained in this work, characterizing the interaction between **FR0**-SB and a cluster of three *n*-propanol molecules in a continuum solvation model of *n*-propanol. In particular, geometry A corresponds to the optimized structure of the [**FR0**-SB⋯HOR] complex in the ground electronic state (S_0), B corresponds to the optimized structure of the [**FR0**-SB*⋯HOR] reactant, *i.e.*, **FR0**-SB in its first-excited singlet state (S_1) hydrogen-bonded to a cluster of three *n*-propanol molecules, and L is the optimized geometry of the [**FR0**-HSB^{+*}⋯-OR] product of the excited-state proton transfer reaction. The partially optimized geometries C–K are the structures along the minimum-energy pathway defining the proton exchange process in the S_1 state, obtained using the procedure outlined in the main text. For each of the A–L structures, we also provide the total electronic energies of the S_0 and S_1 states, denoted as E_{S_0} and E_{S_1} , respectively.

FR0-SB in *n*-propanol, geometry A (in Å)

E_{S_0} = -1625.579223 hartree

E_{S_1} = -1625.445429 hartree

	X	Y	Z
C	-0.0690226790	-2.3122671680	1.6301606704
C	0.6207687767	-1.4368616386	0.7802318540
C	-0.1024028570	-0.6398032630	-0.1261478064
C	-1.4804810603	-0.7280931447	-0.1578790879
C	-2.1625217391	-1.6142086541	0.7006368383
C	-1.4564018842	-2.4113289000	1.5973571435
H	0.4933579322	-2.9235054805	2.3322011115
H	0.4285993863	0.0507263025	-0.7744873521
H	-1.9705232656	-3.0959028518	2.2666041286
C	-2.4668437005	0.0479484252	-1.0249684447
C	-3.7975544381	-0.5149203593	-0.5378037669
C	-5.0686621850	-0.1590383478	-0.9514807687
C	-6.2067263235	-0.7811623428	-0.3814361221
C	-5.9835196690	-1.7460339726	0.6346956440
C	-4.7028608164	-2.0958077477	1.0394716259
C	-3.5974616288	-1.4796511193	0.4582932744
H	-5.1832202943	0.6069647830	-1.7084719237
H	-6.8193928729	-2.2388316703	1.1142584913
H	-4.5836864916	-2.8441666008	1.8194933498
C	-2.3641645013	1.5595211395	-0.7642171505
H	-1.3844947901	1.9411849936	-1.0681850602
H	-3.1269674119	2.1024520883	-1.3340483636
H	-2.5109699489	1.7886315365	0.2969607593
C	-2.2508926097	-0.2434658776	-2.5187956809
H	-3.0038337643	0.2715911384	-3.1255630596
H	-1.2659403365	0.1075543363	-2.8437611790
H	-2.3193480827	-1.3153826791	-2.7318259057
C	2.0814966770	-1.3891450732	0.9031564699
H	2.4881685171	-1.9898303354	1.7283956337
N	2.8795484801	-0.7288818776	0.1584571675
C	4.3068255050	-0.8449833622	0.4557532920
H	4.4635708107	-1.1305768220	1.5058153365
H	4.7598931905	0.1425089006	0.3167950322
C	4.9963538147	-1.8566004899	-0.4594927866
H	4.7746569435	-1.6119265480	-1.5060999648
H	4.5685004929	-2.8514668610	-0.2748885172
C	6.5096042961	-1.8950701427	-0.2514987252
H	6.7287830200	-2.1009901515	0.8047840483
H	6.9297720029	-0.9037194968	-0.4670895861
C	7.1986194752	-2.9404836469	-1.1247347424
H	8.2836716078	-2.9345197380	-0.9712925426
H	6.8366974064	-3.9504459430	-0.8959265611
H	7.0131399930	-2.7546198173	-2.1896673467
N	-7.4841962789	-0.4724623840	-0.8049475892
C	-8.6547388717	-1.0207713477	-0.1278072211
C	-8.9908070240	-0.3653605969	1.2115712616
H	-8.5277217785	-2.1015464902	0.0034135044

	X	Y	Z
H	-9.5040887506	-0.9062219831	-0.8067463918
H	-9.8481460412	-0.8721764852	1.6698259944
H	-8.1532418766	-0.4198875669	1.9137460726
H	-9.2520408982	0.6896933407	1.0820625612
C	-7.7075807979	0.4813037992	-1.8848393871
C	-7.7150673874	1.9502804407	-1.4619286299
H	-8.6690804380	0.2354001308	-2.3460103359
H	-6.9586231083	0.3171297799	-2.6666011184
H	-7.8302233293	2.5926206157	-2.3429823735
H	-8.5461034646	2.1626965123	-0.7819323960
H	-6.7865935200	2.2337309189	-0.9560240011
C	3.5088093913	1.0918775293	-5.5506623056
C	3.4111513562	1.6776708934	-4.1442776126
C	3.0261441832	0.6254287913	-3.1215673576
O	2.8966753965	1.2312072883	-1.8271669811
H	3.7885707549	1.8626301057	-6.2762324142
H	2.5518716286	0.6653526787	-5.8738708791
H	4.2636219330	0.2982054451	-5.6034793426
H	2.6683152047	2.4845076565	-4.1271331270
H	4.3735195959	2.1195555929	-3.8581951660
H	2.0746499027	0.1519659430	-3.3966645368
H	3.7914224565	-0.1591849990	-3.0789163366
H	2.7668810508	0.5180888190	-1.1402748803
C	6.2789058042	6.2861464942	-1.3116299928
C	6.3187357504	4.7996415433	-0.9663157089
C	5.0114615056	4.1014550515	-1.2917130886
O	5.1077466529	2.7253782640	-0.9338612043
H	7.2296660283	6.7717123789	-1.0666090048
H	5.4898208332	6.8064221031	-0.7555638925
H	6.0931987752	6.4451948760	-2.3807272494
H	6.5327395888	4.6707690072	0.1019012209
H	7.1304732914	4.3083625071	-1.5168175000
H	4.1886546885	4.5769765608	-0.7392929171
H	4.7928329386	4.1987803605	-2.3647926649
H	4.3174578510	2.2424164940	-1.2599649836
C	0.1563320340	6.5609453306	-0.7736193492
C	-0.1519580598	5.1559206719	-1.2845976581
C	1.0836654910	4.2756734916	-1.3293433263
O	0.7207663571	2.9812346203	-1.7948675337
H	-0.7465913944	7.1807966855	-0.7599268811
H	0.8935483377	7.0663473896	-1.4092197733
H	0.5564017532	6.5377207174	0.2472168585
H	-0.5839913103	5.2117948504	-2.2916557871
H	-0.9019359059	4.6779473419	-0.6423553799
H	1.8349717775	4.7229626811	-1.9969071272
H	1.5272878121	4.2053111705	-0.3251904860
H	1.5116561077	2.3999075920	-1.7891902332

FR0-SB in *n*-propanol, geometry B (in Å)

E_{S_0} = -1625.568743 hartree

E_{S_1} = -1625.460711 hartree

	X	Y	Z
C	-0.0537141596	-2.3670337572	1.5390063941
C	0.6621682126	-1.4509293066	0.6970515529
C	-0.0902745887	-0.6085586614	-0.1943833723
C	-1.4542553088	-0.6888415655	-0.2085965848
C	-2.1572580806	-1.6052502815	0.6460022858
C	-1.4176573193	-2.4539910183	1.5323495280
H	0.5209080993	-3.0053570904	2.2068183513
H	0.4402013230	0.0903044600	-0.8332063504
H	-1.9307280193	-3.1556278174	2.1842241876
C	-2.4492168322	0.1033240429	-1.0538648733
C	-3.7749690070	-0.4701635449	-0.5672462024
C	-5.0355314007	-0.1372624764	-0.9581033464
C	-6.1734273198	-0.7941419154	-0.3720657515
C	-5.9285285587	-1.7832796063	0.6356212856
C	-4.6570680717	-2.1240477224	1.0260453605
C	-3.5388656586	-1.4726824223	0.4343217145
H	-5.1771077247	0.6355775109	-1.7028625905
H	-6.7597463358	-2.2957249262	1.1020584999
H	-4.5147615373	-2.8871771329	1.7854437823
C	-2.3480462121	1.6102541752	-0.7702995034
H	-1.3678781454	1.9931668778	-1.0713077477
H	-3.1114225204	2.1634483653	-1.3298166850
H	-2.4905638977	1.8233215268	0.2947075010
C	-2.2488662017	-0.1665305007	-2.5539920106
H	-2.9980675869	0.3675042831	-3.1492029172
H	-1.2601713564	0.1763208609	-2.8754979513
H	-2.3307657072	-1.2341332616	-2.7826977247
C	2.0837986955	-1.4160568634	0.7881149791
H	2.5196794653	-2.1003375144	1.5283461079
N	2.8893618545	-0.6445733742	0.1013323162
C	4.3095261234	-0.8171086192	0.3741338485
H	4.4813708438	-1.0033250095	1.4467799870
H	4.8219465666	0.1206474627	0.1289753394
C	4.9446569939	-1.9561754527	-0.4324587310
H	4.7516064702	-1.7914521490	-1.5005980902
H	4.4469723233	-2.8991860091	-0.1677202969
C	6.4484434618	-2.0798490469	-0.1924005324
H	6.6358238873	-2.2223208945	0.8805019666
H	6.9384059869	-1.1362781800	-0.4681224263
C	7.0832325971	-3.2276782252	-0.9734230650
H	8.1623610906	-3.2855005780	-0.7901184442
H	6.6461779243	-4.1924629272	-0.6881690150
H	6.9364890652	-3.1033678562	-2.0532770484
N	-7.4398730031	-0.4913443518	-0.7654545700
C	-8.6076770049	-1.0562946757	-0.0819751711
C	-8.9054051970	-0.4228882222	1.2761662148
H	-8.4770298339	-2.1385578735	0.0177864408

	X	Y	Z
H	-9.4645466166	-0.9186451420	-0.7444525159
H	-9.7610968756	-0.9320000787	1.7332489497
H	-8.0575099000	-0.5048384610	1.9623523375
H	-9.1566372503	0.6369720995	1.1743745951
C	-7.6980943448	0.4461796471	-1.8611918533
C	-7.7609846568	1.9112913542	-1.4325209700
H	-8.6481799279	0.1565580371	-2.3177921518
H	-6.9411380830	0.3027433740	-2.6361835432
H	-7.9019573066	2.5433795531	-2.3163813564
H	-8.5992672284	2.0942573117	-0.7538820457
H	-6.8421182747	2.2284307953	-0.9296304754
C	3.5779004811	1.1294560429	-5.4825628933
C	3.4255690357	1.7383849113	-4.0909070663
C	3.0420658222	0.6949203205	-3.0574147642
O	2.8612234230	1.3092630435	-1.7772085935
H	3.8542188364	1.8936177389	-6.2166074738
H	2.6429559077	0.6677275866	-5.8217010411
H	4.3566130318	0.3574190935	-5.4997777190
H	2.6609806422	2.5245024188	-4.1095229546
H	4.3671164064	2.2129444922	-3.7884869206
H	2.1122872168	0.1903210414	-3.3532985119
H	3.8268873447	-0.0688300598	-2.9850930796
H	2.7511482323	0.5828108851	-1.0772217457
C	6.2349753847	6.3421462002	-1.3701679874
C	6.2812262946	4.8608290844	-1.0036483948
C	4.9583220115	4.1645198367	-1.2654676463
O	5.0621719474	2.7925238931	-0.8974654766
H	7.1978446429	6.8256421370	-1.1731612271
H	5.4726441136	6.8758737100	-0.7899199062
H	6.0052666333	6.4850295191	-2.4329852810
H	6.5384360719	4.7469310580	0.0567259016
H	7.0672418069	4.3567795792	-1.5794368343
H	4.1613277015	4.6509730456	-0.6849418988
H	4.6952081176	4.2516112811	-2.3294391641
H	4.2687642519	2.3039737538	-1.2137143557
C	0.1518700042	6.6405098409	-0.8190317438
C	-0.1603044906	5.2397406088	-1.3390139478
C	1.0652355264	4.3441352583	-1.3549462514
O	0.6991690161	3.0552635909	-1.8300431511
H	-0.7435204163	7.2713935322	-0.8272437462
H	0.9108524650	7.1373792129	-1.4354225823
H	0.5264495048	6.6117866364	0.2112899358
H	-0.5665215644	5.3022674857	-2.3564292148
H	-0.9315906929	4.7702743832	-0.7160548359
H	1.8381113446	4.7842180334	-2.0023654777
H	1.4835299403	4.2680625112	-0.3402540898
H	1.4809610489	2.4598351991	-1.7928526986

FR0-SB in *n*-propanol, geometry C (in Å)

E_{S_0} = -1625.568266 hartree

E_{S_1} = -1625.460561 hartree

	X	Y	Z
C	-0.0566691703	-2.3760945122	1.5219276064
C	0.6599992182	-1.4556541352	0.6850150661
C	-0.0912351484	-0.6094162496	-0.2038607798
C	-1.4552312044	-0.6904296554	-0.2203147995
C	-2.1587734032	-1.6102606497	0.6299548626
C	-1.4204351475	-2.4629796064	1.5131385978
H	0.5172450149	-3.0171743954	2.1876408857
H	0.4393986118	0.0935705063	-0.8380602376
H	-1.9342969023	-3.1674933419	2.1612481160
C	-2.4495606749	0.1044938268	-1.0638146650
C	-3.7756721132	-0.4691381619	-0.5785482299
C	-5.0360312831	-0.1336718298	-0.9677603900
C	-6.1743041172	-0.7907394924	-0.3827975806
C	-5.9300143390	-1.7837018865	0.6214989656
C	-4.6587654302	-2.1275491743	1.0094486336
C	-3.5404220277	-1.4755589210	0.4190589260
H	-5.1771664017	0.6414512847	-1.7101834856
H	-6.7614830184	-2.2961737208	1.0874313860
H	-4.5166154156	-2.8932991385	1.7662346934
C	-2.3474847898	1.6108800211	-0.7780759999
H	-1.3670156858	1.9938333084	-1.0779231100
H	-3.1106085356	2.1650020513	-1.3370954142
H	-2.4905655933	1.8225910981	0.2871486974
C	-2.2497098255	-0.1633699977	-2.5644023686
H	-2.9991360862	0.3715191150	-3.1585422554
H	-1.2612117816	0.1800413754	-2.8858542658
H	-2.3315762459	-1.2306485340	-2.7945824235
C	2.0806570523	-1.4196439119	0.7815136160
H	2.5151063203	-2.1050409471	1.5210219414
N	2.8893618545	-0.6445733742	0.1013323162
C	4.3089994576	-0.8097295013	0.3834760028
H	4.4730241866	-1.0065391049	1.4551599734
H	4.8147640218	0.1352149697	0.1529292839
C	4.9619291618	-1.9325806364	-0.4313562171
H	4.7685100851	-1.7618368718	-1.4984207333
H	4.4787196281	-2.8855285367	-0.1754257864
C	6.4672787794	-2.0332968438	-0.1900630575
H	6.6559057327	-2.1818008392	0.8818408857
H	6.9410951837	-1.0789947300	-0.4569070262
C	7.1228715837	-3.1629292070	-0.9803558668
H	8.2028151266	-3.2028927082	-0.7972096030
H	6.7031877593	-4.1378406086	-0.7035842273
H	6.9740625975	-3.0320144152	-2.0591754885
N	-7.4404254216	-0.4843117257	-0.7735801074
C	-8.6084239650	-1.0511581986	-0.0918441459
C	-8.9058464795	-0.4216711953	1.2681282828
H	-8.4776418763	-2.1336327538	0.0046470470

	X	Y	Z
H	-9.4652769976	-0.9115866759	-0.7539208225
H	-9.7605781973	-0.9328882132	1.7246243728
H	-8.0572913356	-0.5045778320	1.9534364196
H	-9.1582348745	0.6381934255	1.1694400574
C	-7.6976690791	0.4602892739	-1.8635860561
C	-7.7499003514	1.9238012905	-1.4278522780
H	-8.6514039156	0.1787140919	-2.3174264861
H	-6.9447777264	0.3159540680	-2.6424556820
H	-7.8912313984	2.5606291697	-2.3082444971
H	-8.5840431814	2.1086990712	-0.7446736673
H	-6.8269858229	2.2336214691	-0.9278642678
C	3.5166431667	1.1292343076	-5.4533352700
C	3.4038375540	1.7236132669	-4.0516382578
C	3.0111493068	0.6773632887	-3.0236755122
O	2.8586398900	1.2772108992	-1.7345329954
H	3.8006184857	1.8951837237	-6.1826620496
H	2.5642056498	0.6966228035	-5.7821391036
H	4.2742863683	0.3373448177	-5.4933984464
H	2.6594107024	2.5292140475	-4.0468389526
H	4.3623166433	2.1704336278	-3.7602762754
H	2.0680202043	0.1947842598	-3.3156041687
H	3.7804397332	-0.1040104395	-2.9715877913
H	2.7563598722	0.5365297397	-1.0327818472
C	6.2262763134	6.3149465406	-1.4021004039
C	6.2773287430	4.8377520786	-1.0194803459
C	4.9536747306	4.1369785332	-1.2647883216
O	5.0619983333	2.7684681719	-0.8862408589
H	7.1894029920	6.8022696452	-1.2162948523
H	5.4664708781	6.8538455037	-0.8233132601
H	5.9897445613	6.4452211328	-2.4650365545
H	6.5420718242	4.7359743471	0.0402941923
H	7.0602178946	4.3286407910	-1.5950780611
H	4.1606286406	4.6276213292	-0.6825142170
H	4.6822825297	4.2149825848	-2.3273504570
H	4.2668201021	2.2753773087	-1.1930796257
C	0.1760885312	6.6397733738	-0.8372933166
C	-0.1422107684	5.2270441671	-1.3199659922
C	1.0832168706	4.3311672573	-1.3319121601
O	0.7121266373	3.0341884758	-1.7792034550
H	-0.7197857920	7.2699711878	-0.8474995452
H	0.9259830989	7.1223994946	-1.4757718470
H	0.5649995434	6.6357177208	0.1881477035
H	-0.5619340863	5.2653451095	-2.3331549207
H	-0.9051592001	4.7718440610	-0.6764481961
H	1.8493780295	4.7592933335	-1.9952977190
H	1.5120945903	4.2740961531	-0.3203534263
H	1.4933888545	2.4371127025	-1.7387674318

FR0-SB in *n*-propanol, geometry D (in Å)

E_{S_0} = -1625.567398 hartree

E_{S_1} = -1625.460093 hartree

	X	Y	Z
C	-0.0593027553	-2.3826298973	1.5085629250
C	0.6580360713	-1.4587671529	0.6755935307
C	-0.0921719436	-0.6089944896	-0.2107045287
C	-1.4562217959	-0.6898688825	-0.2283611397
C	-2.1601194076	-1.6125063748	0.6182843690
C	-1.4229358921	-2.4689135936	1.4983927200
H	0.5139508805	-3.0263334993	2.1722525964
H	0.4387318366	0.0970794879	-0.8412509793
H	-1.9376020008	-3.1756532157	2.1434058511
C	-2.4499722100	0.1075317754	-1.0701678112
C	-3.7764559549	-0.4656790937	-0.5855391259
C	-5.0367382645	-0.1271380002	-0.9723315137
C	-6.1751570641	-0.7848226869	-0.3885312956
C	-5.9313132003	-1.7820972565	0.6118110304
C	-4.6601984888	-2.1285709173	0.9973424410
C	-3.5418838707	-1.4758595928	0.4082169056
H	-5.1776725214	0.6511503149	-1.7114640563
H	-6.7630064376	-2.2954586024	1.0762997320
H	-4.5179847809	-2.8971779257	1.7512282115
C	-2.3461755847	1.6135730038	-0.7834310538
H	-1.3653445684	1.9956228545	-1.0831901148
H	-3.1091029945	2.1687548667	-1.3416465623
H	-2.4884152949	1.8247063897	0.2820490587
C	-2.2508322415	-0.1593858112	-2.5710974784
H	-2.9996204365	0.3771266573	-3.1646249599
H	-1.2618966592	0.1829317410	-2.8921721430
H	-2.3344234929	-1.2263357948	-2.8022038151
C	2.0776921907	-1.4227732345	0.7757645361
H	2.5115746067	-2.1102171460	1.5130606967
N	2.8893618545	-0.6445733742	0.1013323162
C	4.3090892246	-0.8066230690	0.3873609090
H	4.4695099778	-1.0127658322	1.4574967213
H	4.8101553881	0.1434080647	0.1677153471
C	4.9712334281	-1.9170779429	-0.4372169549
H	4.7729060860	-1.7409097690	-1.5023886064
H	4.4994950035	-2.8771686907	-0.1865127205
C	6.4786778795	-2.0016862478	-0.2019334031
H	6.6734968454	-2.1578155984	0.8677458890
H	6.9393952381	-1.0390435294	-0.4618291966
C	7.1452197443	-3.1152679982	-1.0059421367
H	8.2265182488	-3.1425637483	-0.8282172917
H	6.7397331765	-4.0982376601	-0.7365788116
H	6.9898019355	-2.9759914853	-2.0827780691
N	-7.4410702048	-0.4748088108	-0.7761181956
C	-8.6089673868	-1.0418944696	-0.0942393630
C	-8.9014179282	-0.4174803172	1.2691337731
H	-8.4805631654	-2.1251049810	-0.0028455027

	X	Y	Z
H	-9.4669295483	-0.8974289570	-0.7537870392
H	-9.7560404917	-0.9287582940	1.7257455531
H	-8.0512553698	-0.5050753069	1.9518663594
H	-9.1517168485	0.6433377068	1.1754807631
C	-7.6983482626	0.4743284467	-1.8622814695
C	-7.7469358735	1.9362855952	-1.4208481498
H	-8.6533531754	0.1962743503	-2.3155756807
H	-6.9470210060	0.3312449763	-2.6428789222
H	-7.8884854595	2.5766075927	-2.2986973779
H	-8.5795456398	2.1202315142	-0.7355875704
H	-6.8224806685	2.2424905671	-0.9214624481
C	3.5033921513	1.1306298083	-5.4175084880
C	3.3959108682	1.7140482209	-4.0107667881
C	3.0007993378	0.6617538411	-2.9891511648
O	2.8577717263	1.2469678514	-1.6940449971
H	3.7880308270	1.9012599328	-6.1416631267
H	2.5488554364	0.7034221761	-5.7474284536
H	4.2583839812	0.3365953931	-5.4656019404
H	2.6551484508	2.5229649671	-3.9984737703
H	4.3570249192	2.1543220038	-3.7181740753
H	2.0535957162	0.1878065063	-3.2836484347
H	3.7649842200	-0.1257643450	-2.9502189372
H	2.7615715121	0.4902485942	-0.9883419486
C	6.2101611605	6.2970708479	-1.4212496366
C	6.2658544516	4.8233295635	-1.0258909631
C	4.9405731906	4.1194087248	-1.2535004793
O	5.0529717002	2.7540639293	-0.8657831241
H	7.1745282067	6.7867340134	-1.2485768960
H	5.4550760643	6.8406310170	-0.8406255006
H	5.9637993700	6.4173086578	-2.4831367340
H	6.5401313683	4.7311804789	0.0323664781
H	7.0440425951	4.3097882168	-1.6039532428
H	4.1524918120	4.6142184505	-0.6680323848
H	4.6597801417	4.1895157185	-2.3141149117
H	4.2579761634	2.2555795599	-1.1669400784
C	0.1865205339	6.6295747572	-0.8723149121
C	-0.1315642293	5.2064552065	-1.3236182394
C	1.0945499786	4.3113358629	-1.3191390260
O	0.7232914354	3.0051663416	-1.7371345487
H	-0.7094554480	7.2593302437	-0.8961029800
H	0.9360302255	7.0980587353	-1.5217625793
H	0.5759864144	6.6486138675	0.1527444421
H	-0.5529491663	5.2225013477	-2.3366934037
H	-0.8929933211	4.7645221091	-0.6691326015
H	1.8585858859	4.7260833378	-1.9935756479
H	1.5263723944	4.2768239201	-0.3076912384
H	1.5061016743	2.4087591402	-1.6930774369

FR0-SB in *n*-propanol, geometry E (in Å)

E_{S_0} = -1625.564854 hartree

E_{S_1} = -1625.457925 hartree

	X	Y	Z
C	0.0142216029	-2.3472085071	1.6125329684
C	0.7326303543	-1.4003291199	0.8052593638
C	-0.0284358022	-0.5295629914	-0.0521457512
C	-1.3905839481	-0.6231901840	-0.0822742414
C	-2.0943813945	-1.5864346722	0.7165756321
C	-1.3499198835	-2.4501922084	1.5845299310
H	0.5855849960	-3.0028166537	2.2661695817
H	0.4885563730	0.2049899416	-0.6580748822
H	-1.8588414583	-3.1813931001	2.2065667408
C	-2.3793040245	0.2060596137	-0.8966426519
C	-3.6972957760	-0.4574904428	-0.5237004589
C	-4.9435381086	-0.1685395242	-0.9865335164
C	-6.0832809999	-0.8951271366	-0.4986056985
C	-5.8578175488	-1.8954027981	0.5031966795
C	-4.5984043199	-2.1939138553	0.9630394320
C	-3.4732954830	-1.4870862881	0.4534433529
H	-5.0753689389	0.6288234584	-1.7071048371
H	-6.6939507250	-2.4550303287	0.9022256383
H	-4.4711007525	-2.9720777559	1.7098469226
C	-2.3667250749	1.6769655103	-0.4446557386
H	-1.3989781926	2.1407847073	-0.6608580144
H	-3.1385546312	2.2485007455	-0.9734900424
H	-2.5615500409	1.7612811834	0.6298946624
C	-2.1038085914	0.1155659277	-2.4036667706
H	-2.8490707460	0.6826694915	-2.9726440719
H	-1.1207005361	0.5363439520	-2.6373780269
H	-2.1234279058	-0.9209027690	-2.7558470198
C	2.1565855520	-1.3623220798	0.8888602896
H	2.6074135447	-2.0607424950	1.6049315798
N	2.9503548995	-0.5679864300	0.2069429781
C	4.3789492638	-0.7049313548	0.4288714776
H	4.5822366182	-0.9773102238	1.4766316533
H	4.8466740057	0.2700191330	0.2511848076
C	5.0289416331	-1.7450192979	-0.4908163313
H	4.8092618874	-1.4867774877	-1.5351738843
H	4.5650128300	-2.7233575762	-0.3042562983
C	6.5405677571	-1.8409709770	-0.2909096629
H	6.7564911949	-2.0595859197	0.7637317480
H	6.9964011783	-0.8646159148	-0.5029501350
C	7.1893607761	-2.9061964621	-1.1710253180
H	8.2749467705	-2.9390750148	-1.0231287352
H	6.7933239411	-3.9036598989	-0.9440422974
H	7.0049411738	-2.7103571754	-2.2343560794
N	-7.3316125728	-0.6453290660	-0.9761471261
C	-8.5235120331	-1.2192788262	-0.3433026081
C	-8.8775533493	-0.5897423462	1.0025895371
H	-8.3948993145	-2.3020361708	-0.2412499281

	X	Y	Z
H	-9.3525442376	-1.0806228093	-1.0402778862
H	-9.7686759256	-1.0808335704	1.4086283152
H	-8.0704601230	-0.6972707690	1.7328928476
H	-9.0962411928	0.4769516987	0.8962940456
C	-7.5579763587	0.2465901351	-2.1161467822
C	-7.8311053610	1.6995143014	-1.7315718281
H	-8.4103869658	-0.1528156384	-2.6741043568
H	-6.7039169283	0.1805170311	-2.7927666428
H	-7.9377428246	2.3026584179	-2.6400681709
H	-8.7580181038	1.7952009845	-1.1580310644
H	-7.0163305918	2.1214389564	-1.1345438352
C	2.9110881251	0.9561460758	-5.2697771212
C	3.0688874647	1.5183848058	-3.8594421519
C	2.3578668083	0.6666967084	-2.8201016049
O	2.4382304121	1.2536301417	-1.5239678062
H	3.4357659700	1.5785011676	-6.0026408368
H	1.8563623490	0.9135882713	-5.5671247726
H	3.3196547982	-0.0588962876	-5.3451617084
H	2.6644426216	2.5373431798	-3.8186574023
H	4.1327188929	1.5847012416	-3.6011646097
H	1.3016455885	0.5454157780	-3.1037076031
H	2.8000652223	-0.3387436996	-2.7885232138
H	2.5266221948	0.4833791656	-0.7968182303
C	6.4366810695	5.9030639551	-1.6918020742
C	6.2961548789	4.4737392234	-1.1738437734
C	4.8932624092	3.9320272384	-1.3801615640
O	4.8025214761	2.6149523070	-0.8467563951
H	7.4522519897	6.2824212198	-1.5350936166
H	5.7475791171	6.5851035945	-1.1791310138
H	6.2245916394	5.9614239718	-2.7662495679
H	6.5358498142	4.4382917482	-0.1037751630
H	7.0115325897	3.8185281880	-1.6856078920
H	4.1698028759	4.5911102051	-0.8799809298
H	4.6513849252	3.9241001654	-2.4524538626
H	3.9581211896	2.1938037927	-1.1305475920
C	0.6270671606	7.0094347840	-0.7643793508
C	0.0768791433	5.6366387610	-1.1427292322
C	1.1555970487	4.5685769670	-1.1593111414
O	0.5755792903	3.3198392636	-1.5109574462
H	-0.1650889766	7.7658619674	-0.7684988433
H	1.4013497254	7.3385807209	-1.4680232209
H	1.0706052134	7.0012588717	0.2385080855
H	-0.3894026611	5.6836253846	-2.1349345194
H	-0.7061525863	5.3366810012	-0.4353790368
H	1.9360199874	4.8437066417	-1.8838163808
H	1.6278600117	4.5017363033	-0.1678883077
H	1.2585476372	2.6115988029	-1.4641127242

FR0-SB in *n*-propanol, geometry F (in Å)

E_{S_0} = -1625.563774 hartree

E_{S_1} = -1625.457257 hartree

	X	Y	Z
C	0.0055926344	-2.3454447443	1.5982634991
C	0.7244620956	-1.3977416360	0.7917008160
C	-0.0358248091	-0.5246656412	-0.0642238491
C	-1.3984486609	-0.6178953464	-0.0935328348
C	-2.1021807722	-1.5806004986	0.7056398431
C	-1.3585341526	-2.4462175069	1.5716530797
H	0.5765340978	-3.0023886422	2.2508470801
H	0.4818088712	0.2112574817	-0.6682333280
H	-1.8679616589	-3.1769620783	2.1938199110
C	-2.3875525770	0.2115524253	-0.9076395408
C	-3.7067070974	-0.4455074528	-0.5269087746
C	-4.9545735614	-0.1499829989	-0.9814650177
C	-6.0946901139	-0.8721526765	-0.4877672955
C	-5.8679257779	-1.8744466323	0.5119780997
C	-4.6070147439	-2.1796705710	0.9629351799
C	-3.4821315920	-1.4769206972	0.4477883394
H	-5.0871908129	0.6489011599	-1.7001985535
H	-6.7040358138	-2.4304559341	0.9160682663
H	-4.4785101470	-2.9591633368	1.7081480558
C	-2.3675372320	1.6850423521	-0.4654256211
H	-1.3996890991	2.1444486444	-0.6906135704
H	-3.1406690201	2.2555543706	-0.9934536739
H	-2.5560482929	1.7770363561	0.6096571911
C	-2.1187044830	0.1100905910	-2.4154101806
H	-2.8643362509	0.6764772014	-2.9846645889
H	-1.1347905764	0.5251217865	-2.6559678885
H	-2.1442255837	-0.9285782157	-2.7607485979
C	2.1476467196	-1.3632578144	0.8794093702
H	2.5947870684	-2.0664582269	1.5922641311
N	2.9503548995	-0.5679864300	0.2069429781
C	4.3774634719	-0.7049566671	0.4361164833
H	4.5678932162	-1.0591211861	1.4610610543
H	4.8356960447	0.2862251662	0.3445054724
C	5.0530947703	-1.6566218646	-0.5571904716
H	4.8783530888	-1.2914456098	-1.5777322324
H	4.5750836048	-2.6432503352	-0.4879367152
C	6.5546977364	-1.7903555838	-0.3058250278
H	6.7203514653	-2.1494950668	0.7189624720
H	7.0222044566	-0.7986187505	-0.3646431360
C	7.2407019137	-2.7347695119	-1.2892136264
H	8.3144038633	-2.8126976444	-1.0826386088
H	6.8175320151	-3.7450140079	-1.2308594136
H	7.1261899345	-2.3857511391	-2.3226234049
N	-7.3443970016	-0.6168961823	-0.9580183794
C	-8.5350653459	-1.1896739671	-0.3214238239
C	-8.8834118773	-0.5608902559	1.0263224001
H	-8.4075639976	-2.2726498918	-0.2209830880

	X	Y	Z
H	-9.3663297978	-1.0491631515	-1.0153464796
H	-9.7729237716	-1.0522393699	1.4355677546
H	-8.0733109819	-0.6689952765	1.7532104202
H	-9.1025489566	0.5058637276	0.9217116974
C	-7.5734124627	0.2780443015	-2.0952858572
C	-7.8372595440	1.7315593505	-1.7066073412
H	-8.4309240541	-0.1165088925	-2.6488201070
H	-6.7237391427	0.2091759266	-2.7770850624
H	-7.9470021667	2.3364985224	-2.6135237198
H	-8.7598799807	1.8307327667	-1.1268449431
H	-7.0165246369	2.1487813696	-1.1144856857
C	3.0040673694	0.8252075364	-5.2271806032
C	3.1555510352	1.4072778668	-3.8242142934
C	2.3536933343	0.6317805811	-2.7904319658
O	2.4406906551	1.2242817641	-1.4999456411
H	3.5886289221	1.3965819350	-5.9563160209
H	1.9580879217	0.8414228149	-5.5565329488
H	3.3498604452	-0.2149242276	-5.2689367162
H	2.8229014082	2.4527917033	-3.8176598983
H	4.2126082313	1.4062335638	-3.5323690565
H	1.2996648095	0.5876960673	-3.1046671347
H	2.7130188434	-0.4059983560	-2.7375998047
H	2.5446379040	0.4386785875	-0.7541416329
C	6.4271501182	5.8734859394	-1.6573573984
C	6.2771251730	4.4518114113	-1.1215729010
C	4.8801762344	3.9038069035	-1.3513537046
O	4.7749692508	2.6002623299	-0.7894287399
H	7.4391850731	6.2560876759	-1.4860896307
H	5.7274432828	6.5621833975	-1.1684920071
H	6.2365223171	5.9162721201	-2.7365989745
H	6.4923182765	4.4326769069	-0.0458301061
H	7.0054005328	3.7906113274	-1.6067401862
H	4.1439145975	4.5747362772	-0.8866508465
H	4.6663767301	3.8700504794	-2.4291485229
H	3.9424860991	2.1675563982	-1.0944740703
C	0.5729682339	6.9708035978	-0.7843187754
C	0.0461733499	5.5920326764	-1.1741239487
C	1.1380425405	4.5372374659	-1.1745634155
O	0.5817395090	3.2837684689	-1.5457391242
H	-0.2283268262	7.7174283620	-0.7997736550
H	1.3542036892	7.3109561170	-1.4748977470
H	1.0003575601	6.9661126132	0.2256095313
H	-0.4042336412	5.6353096469	-2.1738176112
H	-0.7447372769	5.2813288437	-0.4803203504
H	1.9301394163	4.8266232943	-1.8808655004
H	1.5907958916	4.4708278666	-0.1740426660
H	1.2695767716	2.5804651210	-1.4768143757

FR0-SB in *n*-propanol, geometry G (in Å)

E_{S_0} = -1625.562095 hartree

E_{S_1} = -1625.456433 hartree

	X	Y	Z
C	0.0015912096	-2.3457788962	1.5895240712
C	0.7217512696	-1.3963724004	0.7855287542
C	-0.0361751062	-0.5199345793	-0.0691924308
C	-1.3989703442	-0.6128907719	-0.1004884479
C	-2.1033066989	-1.5780544395	0.6946419336
C	-1.3622774780	-2.4456407431	1.5599061732
H	0.5712362221	-3.0041998507	2.2416621273
H	0.4832584800	0.2188686864	-0.6684554358
H	-1.8732854864	-3.1773982909	2.1795454531
C	-2.3875557814	0.2209007758	-0.9109833044
C	-3.7065374294	-0.4404797956	-0.5373149882
C	-4.9540206071	-0.1448694363	-0.9930745748
C	-6.0941276917	-0.8689429181	-0.5024754793
C	-5.8682718145	-1.8736073199	0.4954308387
C	-4.6078210886	-2.1789343844	0.9468813152
C	-3.4833176902	-1.4742708988	0.4347103174
H	-5.0864771849	0.6564504412	-1.7091006938
H	-6.7045272105	-2.4309177698	0.8972571673
H	-4.4793413964	-2.9601165298	1.6903211574
C	-2.3706378936	1.6906848040	-0.4559377735
H	-1.4030410754	2.1521949896	-0.6772119053
H	-3.1445697824	2.2639353624	-0.9798908394
H	-2.5602982151	1.7732226607	0.6197430034
C	-2.1146216201	0.1351638139	-2.4188337958
H	-2.8621756308	0.7028381495	-2.9842790875
H	-1.1329474612	0.5592222570	-2.6524683996
H	-2.1332340845	-0.9001608512	-2.7745128706
C	2.1434235030	-1.3638724768	0.8765505964
H	2.5907652209	-2.0666011906	1.5884973988
N	2.9503548995	-0.5679864300	0.2069429781
C	4.3780732674	-0.6951436685	0.4391660863
H	4.5662089771	-1.0400931214	1.4671491310
H	4.8286578337	0.2989162975	0.3422765255
C	5.0639349801	-1.6480562933	-0.5457308150
H	4.8919848106	-1.2892228307	-1.5689255151
H	4.5925616543	-2.6376030391	-0.4736582200
C	6.5651556563	-1.7694608224	-0.2854429929
H	6.7275784546	-2.1275019231	0.7402018889
H	7.0246894844	-0.7738854865	-0.3409659749
C	7.2652898699	-2.7073518624	-1.2651348312
H	8.3380888492	-2.7768149106	-1.0510700678
H	6.8497601951	-3.7209387647	-1.2111188530
H	7.1555092038	-2.3577071181	-2.2988170588
N	-7.3432085440	-0.6132581918	-0.9728151549
C	-8.5343322214	-1.1864045486	-0.3370058641
C	-8.8811731594	-0.5599017461	1.0121445246
H	-8.4078418183	-2.2696864765	-0.2390707108

	X	Y	Z
H	-9.3655876862	-1.0434751956	-1.0303873801
H	-9.7710912431	-1.0510281304	1.4207516841
H	-8.0709952566	-0.6705853091	1.7385592318
H	-9.0989699162	0.5073210892	0.9098354935
C	-7.5719815243	0.2833937508	-2.1089038399
C	-7.8393997928	1.7354908765	-1.7175509853
H	-8.4277356082	-0.1119278753	-2.6645675983
H	-6.7209497994	0.2174030270	-2.7892005394
H	-7.9488394256	2.3420584629	-2.6233931998
H	-8.7631649882	1.8316020596	-1.1391251894
H	-7.0205124812	2.1531553941	-1.1231947782
C	2.9643959229	0.8200650917	-5.2140878407
C	3.1291541124	1.4050636671	-3.8137769538
C	2.3487754192	0.6234629918	-2.7668487276
O	2.4476216583	1.2092735814	-1.4774791695
H	3.5317171333	1.3968987442	-5.9526334955
H	1.9135459094	0.8242986348	-5.5281212069
H	3.3207141376	-0.2163695776	-5.2599507415
H	2.7866900102	2.4473519148	-3.8041919642
H	4.1901978122	1.4149629055	-3.5366379879
H	1.2912034411	0.5695360405	-3.0700116962
H	2.7173526633	-0.4127865806	-2.7258948759
H	2.5626536132	0.3939780095	-0.7114650355
C	6.4118650499	5.8612177490	-1.7193150656
C	6.2734400215	4.4405167116	-1.1776960733
C	4.8731214943	3.8902923938	-1.3806247729
O	4.7780462697	2.5890523368	-0.8128202227
H	7.4261489401	6.2459279876	-1.5671502470
H	5.7200264950	6.5500551981	-1.2195497895
H	6.2016553886	5.9013213452	-2.7950218322
H	6.5080370953	4.4241473765	-0.1059468313
H	6.9937706095	3.7792299884	-1.6745222688
H	4.1451520627	4.5628876845	-0.9053770330
H	4.6402651084	3.8534779302	-2.4543668002
H	3.9411981839	2.1512260727	-1.1039817388
C	0.5943634319	6.9488498496	-0.7482663501
C	0.0593782301	5.5682884205	-1.1206472795
C	1.1499970738	4.5119695458	-1.1298821408
O	0.5880277308	3.2541188311	-1.4750357223
H	-0.2052616844	7.6973757037	-0.7592554342
H	1.3674650305	7.2818635374	-1.4514510645
H	1.0349072515	6.9510202210	0.2559829944
H	-0.4053942665	5.6065005270	-2.1138857413
H	-0.7221363595	5.2648375291	-0.4131887939
H	1.9280490746	4.7938969866	-1.8544602799
H	1.6226723305	4.4580681891	-0.1376375859
H	1.2831380469	2.5532986565	-1.4299233499

FR0-SB in *n*-propanol, geometry H (in Å)

E_{S_0} = -1625.560340 hartree

E_{S_1} = -1625.455794 hartree

	X	Y	Z
C	-0.0037027804	-2.3377508333	1.5871010703
C	0.7182976279	-1.3884908917	0.7840541605
C	-0.0360219802	-0.5069287127	-0.0685650470
C	-1.3993181589	-0.5963277181	-0.0996489220
C	-2.1046753013	-1.5626157482	0.6925282958
C	-1.3675083339	-2.4333407984	1.5565220620
H	0.5642819414	-2.9987015309	2.2379808737
H	0.4864363462	0.2321405763	-0.6653138012
H	-1.8811423606	-3.1647400612	2.1743669230
C	-2.3871264252	0.2420987503	-0.9066435530
C	-3.7059283449	-0.4245552014	-0.5414203312
C	-4.9527269526	-0.1314634355	-1.0009153953
C	-6.0923924569	-0.8590951248	-0.5148118092
C	-5.8676435538	-1.8652031599	0.4822544918
C	-4.6080724405	-2.1677170629	0.9369630960
C	-3.4845686932	-1.4594407170	0.4292393705
H	-5.0850731428	0.6706983366	-1.7159695465
H	-6.7037203296	-2.4257411361	0.8797537744
H	-4.4793727666	-2.9499697891	1.6792263865
C	-2.3755336527	1.7080026845	-0.4379146063
H	-1.4096263441	2.1738874182	-0.6571366980
H	-3.1526321611	2.2821843213	-0.9562162068
H	-2.5647567461	1.7800385957	0.6386536693
C	-2.1079781380	0.1737506903	-2.4140965012
H	-2.8573490641	0.7422706714	-2.9762785973
H	-1.1287386303	0.6080704639	-2.6386856140
H	-2.1182724058	-0.8578095371	-2.7809198014
C	2.1381956731	-1.3623555378	0.8753472489
H	2.5864301307	-2.0659230779	1.5842954516
N	2.9503548995	-0.5679864300	0.2069429781
C	4.3795199549	-0.6864798225	0.4373810751
H	4.5671399494	-1.0263548008	1.4664986559
H	4.8215321947	0.3109894413	0.3381865711
C	5.0733461045	-1.6363100160	-0.5446614625
H	4.9025756579	-1.2789029171	-1.5684869504
H	4.6084637343	-2.6289255815	-0.4735040496
C	6.5745171116	-1.7469792790	-0.2785550291
H	6.7354748316	-2.1077392196	0.7463677559
H	7.0266548620	-0.7477697446	-0.3282115055
C	7.2863750312	-2.6751974292	-1.2589653450
H	8.3586399445	-2.7371210241	-1.0399868345
H	6.8787232827	-3.6922893070	-1.2112440073
H	7.1786425297	-2.3219737210	-2.2916178304
N	-7.3404043207	-0.6056752519	-0.9875036235
C	-8.5318651462	-1.1813433436	-0.3541103254
C	-8.8800454265	-0.5577914328	0.9960374704
H	-8.4045026400	-2.2646635209	-0.2584706065

	X	Y	Z
H	-9.3624658835	-1.0375181699	-1.0480294274
H	-9.7697839783	-1.0504802057	1.4030698453
H	-8.0702110642	-0.6688986004	1.7227519725
H	-9.0988440211	0.5094224829	0.8957036828
C	-7.5684950998	0.2924997959	-2.1226316519
C	-7.8392059261	1.7432550040	-1.7287380069
H	-8.4223842561	-0.1035252130	-2.6805745034
H	-6.7159107242	0.2290308351	-2.8011789047
H	-7.9481076954	2.3513917819	-2.6335598556
H	-8.7642860606	1.8364844588	-1.1519575761
H	-7.0222240202	2.1611899636	-1.1319776698
C	2.9570339776	0.7913440156	-5.2090926074
C	3.1292254640	1.3871299222	-3.8142103945
C	2.3540687722	0.6150940692	-2.7548245803
O	2.4597619598	1.2016143962	-1.4702189872
H	3.5201834526	1.3618129421	-5.9558699779
H	1.9043902683	0.7931162373	-5.5173511738
H	3.3125254547	-0.2457068760	-5.2487846597
H	2.7879643035	2.4299154905	-3.8112254763
H	4.1918463460	1.3988875354	-3.5431399899
H	1.2949968886	0.5598458461	-3.0557060059
H	2.7206118740	-0.4233474653	-2.7164282686
H	2.5806693224	0.3492774314	-0.6687884381
C	6.4015599278	5.8499025518	-1.7731207385
C	6.2693597819	4.4312679978	-1.2244692151
C	4.8672603088	3.8790077395	-1.4102779521
O	4.7773755868	2.5815586483	-0.8347402105
H	7.4171116184	6.2359082761	-1.6330460645
H	5.7144625046	6.5404056766	-1.2691062570
H	6.1802424371	5.8856735646	-2.8467922226
H	6.5149714873	4.4194253768	-0.1550752184
H	6.9851516623	3.7685128789	-1.7259784678
H	4.1440514478	4.5549834194	-0.9322991208
H	4.6237699548	3.8368781368	-2.4815263934
H	3.9384132668	2.1379365722	-1.1189309368
C	0.5804574857	6.9016408509	-0.6980555484
C	0.0504051080	5.5185672313	-1.0683627402
C	1.1469754130	4.4683861113	-1.0883176173
O	0.5903691618	3.2060928674	-1.4223463794
H	-0.2227789106	7.6463830735	-0.7035633083
H	1.3477196981	7.2389558975	-1.4056373918
H	1.0272886325	6.9052564644	0.3034235339
H	-0.4225817643	5.5564259277	-2.0577114417
H	-0.7238766082	5.2096264283	-0.3553026791
H	1.9143406384	4.7538932981	-1.8229728959
H	1.6332286192	4.4215608418	-0.1019944766
H	1.2971852081	2.5117523026	-1.4011145833

FR0-SB in *n*-propanol, geometry I (in Å)

E_{S_0} = -1625.558757 hartree

E_{S_1} = -1625.455729 hartree

	X	Y	Z
C	-0.0074368799	-2.3401865365	1.5756182122
C	0.7147211743	-1.3899153515	0.7733197192
C	-0.0362186736	-0.5083927588	-0.0818884484
C	-1.3997873223	-0.5992798456	-0.1152454124
C	-2.1045287669	-1.5657861626	0.6760751206
C	-1.3706633850	-2.4361026213	1.5413291268
H	0.5598648680	-3.0005357335	2.2276256832
H	0.4889544510	0.2310316712	-0.6767793371
H	-1.8860202053	-3.1671583350	2.1581025252
C	-2.3876969419	0.2377385429	-0.9237037068
C	-3.7066783842	-0.4285239010	-0.5575047017
C	-4.9545757058	-0.1350531938	-1.0143059244
C	-6.0933316310	-0.8615821934	-0.5245284371
C	-5.8668701043	-1.8692984508	0.4710264403
C	-4.6063895828	-2.1725773972	0.9214231472
C	-3.4851087889	-1.4634589641	0.4120601034
H	-5.0883613653	0.6669912221	-1.7291767265
H	-6.7021089308	-2.4292028722	0.8709127113
H	-4.4753953926	-2.9559787906	1.6620544797
C	-2.3752167205	1.7046072886	-0.4582124745
H	-1.4089547105	2.1696181427	-0.6780589433
H	-3.1520058871	2.2779804336	-0.9779179704
H	-2.5646346641	1.7791980629	0.6181595186
C	-2.1082192350	0.1659313306	-2.4310148250
H	-2.8576210236	0.7331282840	-2.9943916315
H	-1.1288650106	0.5997476377	-2.6560401196
H	-2.1184697902	-0.8664864077	-2.7955049208
C	2.1316077767	-1.3633913509	0.8704893146
H	2.5818110667	-2.0641400493	1.5789712389
N	2.9503548995	-0.5679864300	0.2069429781
C	4.3802939103	-0.6720437927	0.4420530254
H	4.5634596636	-0.9712380616	1.4838755756
H	4.8139623286	0.3245548930	0.3080146309
C	5.0831227029	-1.6538490897	-0.5008889322
H	4.9192033974	-1.3330448594	-1.5377876558
H	4.6208867736	-2.6449867772	-0.3986488362
C	6.5822492748	-1.7490718403	-0.2178333580
H	6.7347451629	-2.0815298990	0.8178932947
H	7.0295897163	-0.7490050976	-0.2896287360
C	7.3086186596	-2.6987795508	-1.1664788251
H	8.3779234410	-2.7529867618	-0.9316458441
H	6.9022216430	-3.7153470852	-1.1003521775
H	7.2139786620	-2.3699338444	-2.2084174863
N	-7.3424450058	-0.6058197771	-0.9907739936
C	-8.5318551599	-1.1825979239	-0.3538334621
C	-8.8738584031	-0.5621982067	0.9992829385
H	-8.4043620354	-2.2661237980	-0.2617464347

	X	Y	Z
H	-9.3651517801	-1.0365612040	-1.0439768913
H	-9.7608826641	-1.0568438600	1.4097650132
H	-8.0603247774	-0.6738857752	1.7217723508
H	-9.0941533705	0.5050018156	0.9024773466
C	-7.5744155170	0.2960228026	-2.1224359594
C	-7.8386635047	1.7462443893	-1.7225926333
H	-8.4325713324	-0.0962146786	-2.6763669791
H	-6.7258860136	0.2316825107	-2.8059030653
H	-7.9511881411	2.3573626801	-2.6248864359
H	-8.7598009263	1.8404414057	-1.1397627800
H	-7.0168830140	2.1600375578	-1.1295582805
C	2.8847756896	0.8717238974	-5.2313027851
C	3.0691519547	1.4599136724	-3.8347613313
C	2.3671168250	0.6389722126	-2.7592421446
O	2.4711773283	1.2176313893	-1.4755672105
H	3.4034566718	1.4720282114	-5.9870728197
H	1.8248610658	0.8331736077	-5.5112942039
H	3.2809849078	-0.1494855629	-5.2918257125
H	2.6765024823	2.4841858470	-3.8073575006
H	4.1379270263	1.5224615211	-3.5956866878
H	1.3056285059	0.5236474145	-3.0385829041
H	2.7933088382	-0.3787485225	-2.7458677667
H	2.5986850317	0.3045768533	-0.6261118407
C	6.4080664394	5.8316402508	-1.8172459839
C	6.2783347416	4.4110438224	-1.2729104304
C	4.8715775304	3.8643507957	-1.4412573315
O	4.7850330088	2.5628006854	-0.8767762938
H	7.4262427664	6.2145392293	-1.6878144838
H	5.7288870202	6.5219391314	-1.3022748939
H	6.1740038180	5.8723414096	-2.8880397880
H	6.5393231441	4.3936478030	-0.2072246821
H	6.9846496967	3.7481163197	-1.7876239777
H	4.1586607442	4.5391647889	-0.9460822971
H	4.6109401725	3.8342082071	-2.5089322125
H	3.9349891974	2.1240948660	-1.1484985805
C	0.6009823560	6.8847156660	-0.6627889225
C	0.0662566770	5.5028509524	-1.0310008934
C	1.1622454386	4.4522262157	-1.0679782761
O	0.6028194477	3.1894486307	-1.3904076959
H	-0.2015930077	7.6302179431	-0.6575619843
H	1.3609120285	7.2233034854	-1.3777019655
H	1.0589502914	6.8853181639	0.3336588830
H	-0.4188461791	5.5445282938	-2.0143118290
H	-0.6995092314	5.1917465256	-0.3096441249
H	1.9176172223	4.7376205496	-1.8153174195
H	1.6655366751	4.4084283235	-0.0897551800
H	1.3163157534	2.4962750232	-1.3921156208

FR0-SB in *n*-propanol, geometry J (in Å)

E_{S_0} = -1625.557649 hartree

E_{S_1} = -1625.456702 hartree

	X	Y	Z
C	-0.0089488020	-2.3308518207	1.5806857964
C	0.7133610637	-1.3834275523	0.7749280520
C	-0.0322335222	-0.5034146790	-0.0855396542
C	-1.3962795505	-0.5936569598	-0.1196147490
C	-2.1006436635	-1.5567348997	0.6744990310
C	-1.3718001550	-2.4245994460	1.5437602700
H	0.5574120993	-2.9891884693	2.2352008342
H	0.4966122883	0.2315457423	-0.6840936994
H	-1.8899114458	-3.1528501888	2.1614069763
C	-2.3834931311	0.2395886743	-0.9327032687
C	-3.7024895673	-0.4279384582	-0.5673555326
C	-4.9505557997	-0.1408717142	-1.0283422666
C	-6.0872161488	-0.8709471765	-0.5388874064
C	-5.8596866699	-1.8759019609	0.4597508542
C	-4.5996214018	-2.1706465122	0.9150888677
C	-3.4816631738	-1.4578966133	0.4064161288
H	-5.0860824847	0.6582256970	-1.7460936352
H	-6.6933412025	-2.4394555551	0.8574594571
H	-4.4662762997	-2.9512423259	1.6582252356
C	-2.3734527106	1.7075979828	-0.4701720026
H	-1.4062942026	2.1724826348	-0.6867821340
H	-3.1488450547	2.2790663606	-0.9939209745
H	-2.5670962261	1.7843614748	0.6053508634
C	-2.0991579438	0.1647740378	-2.4388805330
H	-2.8475496334	0.7297202410	-3.0058661786
H	-1.1197461631	0.5997960226	-2.6614597298
H	-2.1064114519	-0.8684049396	-2.8012062510
C	2.1268146245	-1.3609650400	0.8726771633
H	2.5825516589	-2.0578811746	1.5789846556
N	2.9503548995	-0.5679864300	0.2069429781
C	4.3844242876	-0.6604001303	0.4295666685
H	4.5791922061	-0.8609419734	1.4922774458
H	4.8144842311	0.3186131623	0.1970853312
C	5.0690271414	-1.7314680876	-0.4256063322
H	4.8596373930	-1.5317219873	-1.4843776833
H	4.6300030216	-2.7117211209	-0.1947704116
C	6.5790860912	-1.7723255151	-0.1947977213
H	6.7808734787	-1.9505785152	0.8701390577
H	7.0083273915	-0.7892154538	-0.4290363363
C	7.2790803712	-2.8420042632	-1.0288163462
H	8.3611208141	-2.8376998770	-0.8544636791
H	6.9071986718	-3.8442496388	-0.7832200294
H	7.1153124982	-2.6804000637	-2.1011851567
N	-7.3357752091	-0.6229703071	-1.0079321152
C	-8.5235099719	-1.2051264828	-0.3717798146
C	-8.8683512663	-0.5866802624	0.9814921121
H	-8.3913638489	-2.2880981860	-0.2806169780

	X	Y	Z
H	-9.3568808045	-1.0621927372	-1.0623435014
H	-9.7524394770	-1.0863813232	1.3920492950
H	-8.0541801361	-0.6940745198	1.7038978981
H	-9.0944975717	0.4792820057	0.8848931477
C	-7.5706698367	0.2774950146	-2.1402976291
C	-7.8410610555	1.7263607606	-1.7399993081
H	-8.4265753891	-0.1189926311	-2.6944915268
H	-6.7211880334	0.2162755665	-2.8228488996
H	-7.9553497402	2.3372587501	-2.6421436333
H	-8.7629937257	1.8163062878	-1.1577819477
H	-7.0213685967	2.1430952230	-1.1461221501
C	2.8483463770	0.9735143607	-5.2688484602
C	3.0331562454	1.5605358232	-3.8718262424
C	2.3894926657	0.7028921625	-2.7855774599
O	2.4890221281	1.2689742663	-1.5010797192
H	3.3314429729	1.5962513993	-6.0302994806
H	1.7861735522	0.8960730092	-5.5321746219
H	3.2816731378	-0.0318203764	-5.3416837283
H	2.5966146991	2.5665226700	-3.8297099412
H	4.1026255677	1.6701048581	-3.6533006556
H	1.3296855505	0.5396920870	-3.0526329485
H	2.8616594984	-0.2964373953	-2.7971573375
H	2.6167007409	0.2598762752	-0.5834352432
C	6.3954845367	5.8391242150	-1.8888933463
C	6.2918896141	4.3907504300	-1.4159876527
C	4.8594377147	3.8855808090	-1.4364808379
O	4.8023721142	2.5551730112	-0.9433188105
H	7.4330732427	6.1897095692	-1.8685464667
H	5.8076604916	6.5112986831	-1.2520958239
H	6.0291486810	5.9511897722	-2.9165866653
H	6.6853385554	4.3023680963	-0.3954074830
H	6.9075044584	3.7447749323	-2.0541794645
H	4.2327936829	4.5458106146	-0.8187606205
H	4.4683453591	3.9287544971	-2.4630024260
H	3.9341358221	2.1268581188	-1.1933678384
C	6.6206699180	6.8858412912	-0.5878263336
C	0.0822833008	5.5064158527	-0.9598830864
C	1.1766680423	4.4543097542	-1.0111771494
O	0.6150470882	3.1933357333	-1.3320286091
H	-0.1808033804	7.6324846985	-0.5738597386
H	1.3766838067	7.2270091028	-1.3057118185
H	1.0850488978	6.8807684215	0.4056321701
H	-0.4102653717	5.5540221434	-1.9392622363
H	-0.6787346300	5.1920813904	-0.2347339410
H	1.9261472294	4.7429902444	-1.7633229814
H	1.6899035156	4.4081248550	-0.0378057240
H	1.3378196832	2.5038270884	-1.3753843838

FR0-SB in *n*-propanol, geometry K (in Å)

E_{S_0} = -1625.557564 hartree

E_{S_1} = -1625.458238 hartree

	X	Y	Z
C	-0.0131438950	-2.3447518908	1.5539921476
C	0.7052228855	-1.4004994431	0.7403563881
C	-0.0394040557	-0.5433667104	-0.1429600242
C	-1.4035811968	-0.6485561990	-0.1835519358
C	-2.1040948148	-1.5937393846	0.6334328658
C	-1.3749391332	-2.4464079240	1.5148282251
H	0.5552231004	-2.9905533251	2.2189768626
H	0.4894943086	0.1814546736	-0.7561704885
H	-1.8914840969	-3.1675764398	2.1419480613
C	-2.3928414966	0.1468947540	-1.0315836531
C	-3.7169945044	-0.4673696464	-0.5963990177
C	-4.9733201901	-0.1522712399	-1.0162208119
C	-6.1115027592	-0.8399035696	-0.4710292174
C	-5.8734696980	-1.8440855253	0.5267413247
C	-4.6057013934	-2.1668451235	0.9391560917
C	-3.4900457469	-1.4832275569	0.3888568729
H	-5.1113174474	0.6335160871	-1.7477850788
H	-6.7057912726	-2.3807980525	0.9624059504
H	-4.4658288073	-2.9422864344	1.6863962360
C	-2.3374865129	1.6455973619	-0.6979685797
H	-1.3651959926	2.0694554231	-0.9695441517
H	-3.1082826955	2.1930010860	-1.2531083794
H	-2.5060779880	1.8199791405	0.3704792863
C	-2.1487989146	-0.0736904651	-2.5329202807
H	-2.8916672125	0.4654051785	-3.1313428343
H	-1.1589295106	0.2965029486	-2.8173873136
H	-2.2046140287	-1.1350777326	-2.7957808094
C	2.1148129408	-1.3676043223	0.8552334193
H	2.5706426427	-2.0636782601	1.5602400174
N	2.9503548995	-0.5679864300	0.2069429781
C	4.3862001179	-0.6774399060	0.4139686071
H	4.5847566243	-0.8742507144	1.4760159521
H	4.8225249529	0.2959816331	0.1733278137
C	5.0410140651	-1.7661749190	-0.4423413772
H	4.8191204649	-1.5710849279	-1.4991624276
H	4.5885946304	-2.7369236057	-0.1975616632
C	6.5531842620	-1.8323312388	-0.2347965546
H	6.7693471670	-2.0047943687	0.8281884808
H	6.9963252179	-0.8596196286	-0.4861761306
C	7.2174816036	-2.9233651826	-1.0704882753
H	8.3020937820	-2.9396087694	-0.9137864405
H	6.8292803385	-3.9155966258	-0.8101199499
H	7.0395221646	-2.7675988712	-2.1414341393
N	-7.3697392937	-0.5528344729	-0.8869267185
C	-8.5462074019	-1.1347796668	-0.2290835973
C	-8.8658221257	-0.5178042327	1.1311259210
H	-8.4104731400	-2.2170228399	-0.1417059299

	X	Y	Z
H	-9.3925745906	-0.9926335360	-0.9036109472
H	-9.7295275266	-1.0322164994	1.5662932912
H	-8.0303014674	-0.6087982863	1.8310876744
H	-9.1149928897	0.5432874129	1.0384543800
C	-7.6204039187	0.3903007967	-1.9816740458
C	-7.7361073644	1.8471585665	-1.5373689671
H	-8.5481008149	0.0789784039	-2.4687997293
H	-6.8370079749	0.2748513038	-2.7340767069
H	-7.8695105238	2.4848198739	-2.4182469270
H	-8.5989816731	1.9993455969	-0.8824280369
H	-6.8411759733	2.1840345886	-1.0050779364
C	3.1648384583	1.0594294183	-5.2936826536
C	3.1133394018	1.7028592376	-3.9099132679
C	2.6208928761	0.7382392802	-2.8315473611
O	2.5194284156	1.3252843190	-1.5602978330
H	3.5116948108	1.7695660939	-6.0532634074
H	2.1760114754	0.7003970198	-5.6050418558
H	3.8485481096	0.2015668754	-5.3089434880
H	2.4531300239	2.5790578198	-3.9273731019
H	4.1116152498	2.0646576765	-3.6333822551
H	1.6422021242	0.3319507521	-3.1493458359
H	3.3100280666	-0.1266304778	-2.8022542391
H	2.6347164501	0.2151756972	-0.5407586458
C	6.3484489908	5.8929499619	-1.5910215085
C	6.2389192466	4.4290208344	-1.1709300313
C	4.8052577266	3.9282739022	-1.2187856044
O	4.7352874684	2.5814005114	-0.7769795998
H	7.3864351499	6.2410743359	-1.5538453819
H	5.7587593460	6.5430900140	-0.9333190248
H	5.9863889316	6.0424429792	-2.6155526343
H	6.6270369111	4.3037951203	-0.1520343621
H	6.8568514622	3.8041686932	-1.8278337648
H	4.1758479471	4.5690409969	-0.5823741500
H	4.4206406513	4.0123706061	-2.2451220074
H	3.8873225117	2.1499984573	-1.1078644925
C	0.4508415222	6.8345990390	-0.7889297454
C	-0.0234013367	5.4532468325	-1.2341685891
C	1.1010142987	4.4314352320	-1.2474961162
O	0.5999858683	3.1693588652	-1.6466512797
H	-0.3724590655	7.5573353106	-0.7966471738
H	1.2351767742	7.2211815531	-1.4512039558
H	0.8583875492	6.8094585866	0.2289873902
H	-0.4581285189	5.5166306697	-2.2398199867
H	-0.8172251779	5.0964318581	-0.5659600039
H	1.8934769110	4.7672079363	-1.9339585168
H	1.5471935201	4.3660015951	-0.2427832988
H	1.3386426587	2.4878594177	-1.6106245947

FR0-SB in *n*-propanol, geometry L (in Å)

E_{S_0} = -1625.557211 hartree

E_{S_1} = -1625.459402 hartree

	X	Y	Z
C	-0.0190951116	-2.3388424798	1.5481834009
C	0.6991206909	-1.3968254842	0.7317594603
C	-0.0428911418	-0.5428050479	-0.1560795929
C	-1.4078353323	-0.6485915610	-0.1972461476
C	-2.1073373153	-1.5883880718	0.6252839063
C	-1.3809142386	-2.4386916277	1.5089245885
H	0.5488187430	-2.9826644041	2.2152572154
H	0.4865801413	0.1793707169	-0.7726176986
H	-1.8987521100	-3.1570858881	2.1381294947
C	-2.3978920525	0.1404395975	-1.0508435481
C	-3.7229711577	-0.4625267496	-0.6016841673
C	-4.9810787428	-0.1440390785	-1.0142745715
C	-6.1181521310	-0.8255190036	-0.4588642625
C	-5.8775191954	-1.8285181137	0.5397917275
C	-4.6083480033	-2.1533243406	0.9453717458
C	-3.4951427851	-1.4747944573	0.3858876882
H	-5.1210531399	0.6383865134	-1.7489686364
H	-6.7086839241	-2.3614287176	0.9820902090
H	-4.4656185614	-2.9272380462	1.6935558551
C	-2.3311573536	1.6438264398	-0.7420115982
H	-1.3575810796	2.0563539956	-1.0257245166
H	-3.1015028140	2.1873242977	-1.3015468315
H	-2.4926045421	1.8363714634	0.3243787648
C	-2.1635611090	-0.1068264911	-2.5499041257
H	-2.9073617511	0.4262314803	-3.1524208814
H	-1.1735889784	0.2530821607	-2.8463399851
H	-2.2266704917	-1.1721645882	-2.7944450226
C	2.1065182342	-1.3667622948	0.8506907098
H	2.5623935955	-2.0629362118	1.5539859099
N	2.9503548995	-0.5679864300	0.2069429781
C	4.3876292172	-0.6785458483	0.4112129061
H	4.5853618307	-0.8569280519	1.4761662816
H	4.8223477660	0.2910833555	0.1544813237
C	5.0358965383	-1.7841540793	-0.4276392934
H	4.8165465075	-1.6044761380	-1.4875332697
H	4.5776851567	-2.7483843467	-0.1682287260
C	6.5471315415	-1.8562106913	-0.2162045072
H	6.7601220757	-2.0127589861	0.8499018315
H	6.9968285213	-0.8905309992	-0.4827703959
C	7.2051814491	-2.9655204947	-1.0326110657
H	8.2890744263	-2.9877917347	-0.8719363879
H	6.8083858292	-3.9505050975	-0.7579615690
H	7.0317088273	-2.8250979630	-2.1063994493
N	-7.3779594955	-0.5351136728	-0.8657426802
C	-8.5514870264	-1.1164855560	-0.2016825647
C	-8.8643981102	-0.4991368898	1.1598913451
H	-8.4153117246	-2.1986374412	-0.1151943311

	X	Y	Z
H	-9.4009984102	-0.9743502840	-0.8722062729
H	-9.7247050318	-1.0149116774	1.5999950441
H	-8.0247652618	-0.5884376756	1.8551689961
H	-9.1160925368	0.5613576506	1.0680252733
C	-7.6338574919	0.4114206929	-1.9565880006
C	-7.7363985888	1.8679491594	-1.5081844895
H	-8.5679391784	0.1061006796	-2.4349586771
H	-6.8585614204	0.2928144695	-2.7168348925
H	-7.8743064168	2.5081155844	-2.3865199296
H	-8.5917455398	2.0243672377	-0.8445243911
H	-6.8342185283	2.1982983847	-0.9840763026
C	3.2400095042	1.0845623248	-5.3412453396
C	3.1659482102	1.7450101208	-3.9667430796
C	2.7148549437	0.7774398096	-2.8711153684
O	2.5742693254	1.3760559546	-1.6134945303
H	3.5612606038	1.7945809751	-6.1123104313
H	2.2641969174	0.6861133827	-5.6457737382
H	3.9527802113	0.2502731890	-5.3446950629
H	2.4705661201	2.5934837361	-3.9927159559
H	4.1491484392	2.1519141477	-3.6979891929
H	1.7597768048	0.3171059980	-3.1907356160
H	3.4459308380	-0.0531670119	-2.8275846314
H	2.6527321593	0.1704751191	-0.4980820484
C	6.3621277579	5.8983009866	-1.5801058969
C	6.2423021252	4.4409505866	-1.1401577353
C	4.8062482186	3.9451496528	-1.1888937564
O	4.7233046107	2.6055294915	-0.7310259317
H	7.4016024445	6.2418403946	-1.5410464012
H	5.7712943161	6.5607924531	-0.9358474943
H	6.0075834652	6.0345065040	-2.6089963599
H	6.6242985176	4.3280290012	-0.1174712491
H	6.8609185600	3.8044246536	-1.7850746117
H	4.1763475064	4.5992174120	-0.5659709998
H	4.4270388230	4.0182612322	-2.2179426222
H	3.8935528070	2.1615833367	-1.1088043015
C	0.3512555132	6.7816320112	-0.7639067240
C	-0.0828305618	5.3861967999	-1.2059059389
C	1.0819890989	4.4128861831	-1.2853062880
O	0.6147453172	3.1357011149	-1.6717772251
H	-0.5023417214	7.4670975021	-0.7219565924
H	1.0850089861	7.2106982514	-1.4574432247
H	0.8091216733	6.7620620110	0.2326041368
H	-0.5659697579	5.4424150494	-2.1898896481
H	-0.8291701391	4.9856510418	-0.5081785083
H	1.8257242425	4.7888481244	-2.0057714687
H	1.5806198817	4.3594205039	-0.3046817277
H	1.3805429206	2.4754082821	-1.6562041497

In what follows, we provide the SMD/CAM-B3LYP/6-31+G* optimized geometries, labeled A'–L', obtained in this work, characterizing the interaction between **FR0**-SB and a cluster of three *i*-propanol molecules in a continuum solvation model of *i*-propanol. In particular, geometry A' corresponds to the optimized structure of the [**FR0**-SB...HOR] complex in the ground electronic state (S_0), B' corresponds to the optimized structure of the [**FR0**-SB*...HOR] reactant, *i.e.*, **FR0**-SB in its first-excited singlet state (S_1) hydrogen-bonded to a cluster of three *i*-propanol molecules, and L' is the optimized geometry of the [**FR0**-HSB⁺*...⁻OR] product of the excited-state proton transfer reaction. The partially optimized geometries C'–K' are the structures along the minimum-energy pathway defining the proton exchange process in the S_1 state, obtained using the procedure outlined in the main text. For each of the A'–L' structures, we also provide the total electronic energies of the S_0 and S_1 states, denoted as E_{S_0} and E_{S_1} , respectively.

FR0-SB in *i*-propanol, geometry A' (in Å)

E_{S_0} = -1625.593769 hartree

E_{S_1} = -1625.459494 hartree

	X	Y	Z
C	0.0248039283	-3.1267966368	0.7995283445
C	0.8011198076	-1.9832107930	0.5662729545
C	0.1689575049	-0.7836284490	0.1899005940
C	-1.2050100037	-0.7573303846	0.0451838606
C	-1.9724268631	-1.9189591701	0.2679146159
C	-1.3580274433	-3.1077405071	0.6508483160
H	0.5163985698	-4.0498813462	1.0980159048
H	0.7662631227	0.1080762947	0.0244425856
H	-1.9377205231	-4.0087224044	0.8330637791
C	-2.1032048598	0.4131890761	-0.3447149100
C	-3.4774836372	-0.2485626705	-0.3315139866
C	-4.6997615059	0.3332362492	-0.6161108863
C	-5.8880577299	-0.4368385459	-0.5593777045
C	-5.7669248580	-1.7982469595	-0.1788579533
C	-4.5350943439	-2.3696779446	0.1052293537
C	-3.3778280143	-1.5984138472	0.0291985458
H	-4.7381937397	1.3842226776	-0.8743816530
H	-6.6464796055	-2.4244937579	-0.1050139767
H	-4.4920617987	-3.4193786702	0.3858074052
C	-2.0182706599	1.5486347870	0.6886011339
H	-1.0130357307	1.9817970381	0.7159913526
H	-2.7233836873	2.3495525062	0.4383493320
H	-2.2619088888	1.1872202623	1.6936117314
C	-1.7553533953	0.9477514262	-1.7428648448
H	-2.4443961736	1.7476183318	-2.0355693768
H	-0.7421930175	1.3620813335	-1.7573102615
H	-1.8098032130	0.1584002966	-2.4999663040
C	2.2532578822	-2.1181863495	0.7261132752
H	2.5753627058	-3.0981028442	1.1065187108
N	3.1309948817	-1.2320018794	0.4593945257
C	4.5284816135	-1.6205254775	0.6495339655
H	4.6091474974	-2.4390185453	1.3798240281
H	5.0661462353	-0.7597142584	1.0603828350
C	5.1742244406	-2.0491325689	-0.6687725704
H	5.0915793958	-1.2334175922	-1.3982927791
H	4.6076034020	-2.8946817782	-1.0818207256
C	6.6406386657	-2.4473954366	-0.5048058410
H	6.7152749993	-3.2651167125	0.2243790200
H	7.2049283623	-1.6053687963	-0.0835909048
C	7.2828883119	-2.8817133229	-1.8196545596
H	8.3310858582	-3.1666286754	-1.6750127704
H	6.7607605198	-3.7447082240	-2.2506134444
H	7.2580482117	-2.0740076882	-2.5612193773
N	-7.1149025861	0.1085680392	-0.8812389775
C	-8.3460006876	-0.6571331383	-0.7166406737
C	-8.8435115610	-0.7791173402	0.7235060844
H	-8.2180703868	-1.6526325807	-1.1573597291

	X	Y	Z
H	-9.1149966649	-0.1676619283	-1.3203197781
H	-9.7492531259	-1.3960695842	0.7543012599
H	-8.0981135409	-1.2430327923	1.3768691490
H	-9.0904966080	0.2025675933	1.1400704946
C	-7.2315496311	1.5032212876	-1.2917595486
C	-7.2608115767	2.5162366379	-0.1478744456
H	-8.1507728705	1.5940755265	-1.8779617110
H	-6.4178537527	1.7406213132	-1.9856752090
H	-7.2810526271	3.5356329992	-0.5508589944
H	-8.1503038635	2.3855090922	0.4768626935
H	-6.3818266311	2.4267414025	0.4984169029
C	3.7195774688	1.6439472117	-1.6127762983
C	2.6145175337	1.1127929853	-2.5123493793
C	4.0150159588	3.1105659032	-1.8660580033
O	3.3635918353	1.5003698100	-0.2220194622
H	4.6356189517	1.0630840819	-1.7859793967
H	2.3944216294	0.0613796758	-2.3003425493
H	1.6949716134	1.6933167716	-2.3797089723
H	2.9127249728	1.1853855834	-3.5642622750
H	4.8067604017	3.4734572516	-1.2034505938
H	4.3499860795	3.2540619923	-2.8988134237
H	3.1194584313	3.7218423353	-1.7110306147
H	3.1669235029	0.5436307813	-0.0274133765
C	5.6506343685	2.5582551768	2.4979478476
C	4.9146983386	1.6277094097	3.4538835349
C	7.0539298603	2.8843045323	2.9769044553
O	5.7765778541	1.9693029801	1.2026155152
H	5.0846959588	3.4974917795	2.4068116740
H	3.9225193327	1.3653034521	3.0689082956
H	5.4784439868	0.6990864232	3.5995679239
H	4.7761868475	2.1031778995	4.4321161564
H	7.5554810237	3.5575739613	2.2736990153
H	7.0262850900	3.3726948653	3.9570196504
H	7.6517295249	1.9696241731	3.0644965200
H	4.8918134153	1.8433653095	0.7984904917
C	1.7636094341	4.0069304328	1.9095077260
C	2.5913477399	5.1044538565	1.2524210248
C	0.5371763768	4.5622616835	2.6111592265
O	1.3042206751	3.0557529261	0.9474463372
H	2.3869869028	3.4871228888	2.6529557716
H	3.4631091406	4.6905946082	0.7353296361
H	1.9895468371	5.6512059097	0.5171651112
H	2.9558001775	5.8192194604	1.9996192303
H	-0.0365774377	3.7606114899	3.0868759926
H	0.8260416700	5.2814182276	3.3855135493
H	-0.1165210449	5.0726237260	1.8941664736
H	2.0656413879	2.5902801947	0.5407261691

FR0-SB in *i*-propanol, geometry B' (in Å)

E_{S_0} = -1625.583577 hartree

E_{S_1} = -1625.474434 hartree

	X	Y	Z
C	-0.0128720322	-3.1516474760	0.7207268604
C	0.7967782840	-1.9881570263	0.4977245634
C	0.1438654385	-0.7584476288	0.1344880245
C	-1.2154931782	-0.7300837207	0.0005988451
C	-2.0123716555	-1.9077504060	0.2127609394
C	-1.3730119628	-3.1346456339	0.5872995072
H	0.4857491003	-4.0766674445	1.0029009493
H	0.7451798390	0.1313915918	-0.0210122912
H	-1.9566638455	-4.0345324654	0.7614181847
C	-2.1154504128	0.4473113875	-0.3692633536
C	-3.4890154617	-0.2145364679	-0.3627446754
C	-4.6992617925	0.3448171283	-0.6353175823
C	-5.8961533570	-0.4523911318	-0.5759821743
C	-5.7625320074	-1.8313846816	-0.2096507721
C	-4.5425208613	-2.3968164547	0.0670151118
C	-3.3640954305	-1.6012090831	-0.0059167548
H	-4.7572431160	1.3957137564	-0.8883700025
H	-6.6408338277	-2.4607788189	-0.1508125762
H	-4.4832364101	-3.4474542776	0.3351311656
C	-2.0309422689	1.5655860171	0.6824285685
H	-1.0213116189	1.9877081815	0.7204886501
H	-2.7280151166	2.3767416979	0.4418587254
H	-2.2814317391	1.1897020986	1.6803018331
C	-1.7734486890	1.0037278082	-1.7598939144
H	-2.4563260805	1.8148436605	-2.0364915883
H	-0.7561911862	1.4072465225	-1.7692443633
H	-1.8367327893	0.2275919816	-2.5296058795
C	2.2096518540	-2.1129749876	0.6495007021
H	2.5538823214	-3.1105299303	0.9560172312
N	3.1028759983	-1.1756501995	0.4675917936
C	4.4876222221	-1.5871881269	0.6490022328
H	4.5663146345	-2.3786905861	1.4121375452
H	5.0575459657	-0.7272587551	1.0198780430
C	5.1295221433	-2.0886951329	-0.6504773065
H	5.0554735989	-1.3027790610	-1.4134202566
H	4.5493153911	-2.9427636564	-1.0263027215
C	6.5907839027	-2.4995354565	-0.4728633849
H	6.6551998142	-3.2982199862	0.2785368448
H	7.1624677135	-1.6523386949	-0.0713476930
C	7.2355166845	-2.9748780762	-1.7725313444
H	8.2792463531	-3.2707248070	-1.6153006402
H	6.7049018061	-3.8411151555	-2.1865930848
H	7.2263434371	-2.1852685522	-2.5337968991
N	-7.1122225734	0.0832653330	-0.8693671952
C	-8.3457088201	-0.6946668083	-0.7219803210
C	-8.8289453623	-0.8387515442	0.7204978354
H	-8.2062575402	-1.6783561006	-1.1816624778

	X	Y	Z
H	-9.1150308906	-0.1968252205	-1.3150656408
H	-9.7356558960	-1.4535401077	0.7393679587
H	-8.0815978259	-1.3179454387	1.3599705163
H	-9.0724655058	0.1346725412	1.1562182877
C	-7.2501713395	1.4817438058	-1.2852876598
C	-7.2871937049	2.4835589125	-0.1325373236
H	-8.1737148573	1.5552600674	-1.8644217255
H	-6.4424777861	1.7256195601	-1.9810179130
H	-7.3303446607	3.5008203560	-0.5371782282
H	-8.1678136311	2.3365186732	0.4997705996
H	-6.3997238024	2.4089244949	0.5032162181
C	3.7099283798	1.6374188673	-1.5512387180
C	2.6009465861	1.1285832962	-2.4595648624
C	4.0356920922	3.0974297083	-1.8102290227
O	3.3463988380	1.5001779061	-0.1649722190
H	4.6147637265	1.0380189511	-1.7225905931
H	2.3575686560	0.0836889892	-2.2440492461
H	1.6928067128	1.7286489099	-2.3345633075
H	2.9089943960	1.1934438116	-3.5094493724
H	4.8307072685	3.4481723311	-1.1451326045
H	4.3775799823	3.2302217245	-2.8423442619
H	3.1511022881	3.7263195456	-1.6618783697
H	3.1461288324	0.5329930141	0.0352422996
C	5.7005455573	2.6022178037	2.4803867988
C	5.0182024434	1.6840937685	3.4863730116
C	7.1151640360	2.9619686569	2.8980271428
O	5.7880292370	1.9852513651	1.1960380434
H	5.1155945838	3.5297284490	2.3897758452
H	4.0160889146	1.3985538955	3.1472194782
H	5.6014445330	0.7670882041	3.6290588822
H	4.9126771115	2.1805394893	4.4582693989
H	7.5780491056	3.6295213100	2.1634109464
H	7.1172885580	3.4689696963	3.8690037099
H	7.7320169573	2.0593336730	2.9795593743
H	4.8908295067	1.8383257227	0.8246122244
C	1.7856602390	4.0259553190	1.9340098220
C	2.6235620055	5.1123204285	1.2707839665
C	0.5728261437	4.6009937983	2.6438843335
O	1.3069918022	3.0806872017	0.9769699955
H	2.4074360484	3.4991782987	2.6739899567
H	3.4864105925	4.6863003284	0.7493509817
H	2.0239236364	5.6651062167	0.5381738694
H	3.0007004106	5.8239746413	2.0148113998
H	-0.0069574199	3.8105398725	3.1310020390
H	0.8780088405	5.3222717918	3.4099557841
H	-0.0809600811	5.1142297527	1.9289697673
H	2.0588679629	2.5920711074	0.5758653536

FR0-SB in *i*-propanol, geometry C' (in Å)

E_{S_0} = -1625.582875 hartree

E_{S_1} = -1625.474136 hartree

	X	Y	Z
C	-2.4425044400	-0.1025858651	-2.4585977332
C	-2.1964371804	-0.0923839502	-1.0452424980
C	-0.8479303183	-0.2810928014	-0.5812286491
C	0.1532347278	-0.4903066055	-1.4873296391
C	-0.1109735323	-0.5169492480	-2.8995453448
C	-1.4484794097	-0.3145221059	-3.3726712162
H	-3.4620080617	0.0568181099	-2.8035114768
H	-0.6458214823	-0.2492944607	0.4844886679
H	-1.6693728036	-0.3229056132	-4.4366992183
C	1.6413636498	-0.7168673489	-1.2305719474
C	2.1684711572	-0.8681824349	-2.6528597221
C	3.4474166666	-1.0865246306	-3.0634523490
C	3.7475778680	-1.2122869688	-4.4651250702
C	2.6639525425	-1.0865214903	-5.3943308100
C	1.3744558298	-0.8571480145	-4.9823665182
C	1.0882475744	-0.7442949357	-3.5928147848
H	4.2381237426	-1.1690662391	-2.3287386221
H	2.8532243425	-1.1568475704	-6.4573787143
H	0.5836829986	-0.7628947843	-5.7205373265
C	2.2747031146	0.4862946604	-0.5150949735
H	1.8260179166	0.6211012393	0.4739403771
H	3.3520890410	0.3354294271	-0.3795364942
H	2.1323997675	1.4086154494	-1.0888386025
C	1.8786365812	-1.9955473222	-0.4109111531
H	2.9503350676	-2.1799706453	-0.2765269435
H	1.4297627466	-1.8971437949	0.5826457684
H	1.4401654731	-2.8727748095	-0.8982492564
C	-3.3018989126	0.1101238605	-0.1670677750
H	-4.2653850937	0.2869655227	-0.6637983102
N	-3.2640636000	0.1023857900	1.1398785100
C	-4.5435561148	0.2925553176	1.8090717183
H	-5.1733169678	1.0078207288	1.2555871628
H	-4.3541413221	0.7334553824	2.7940114925
C	-5.3182332678	-1.0191877065	1.9875170981
H	-4.6718876946	-1.7501688633	2.4907711640
H	-5.5440960509	-1.4355865596	0.9961721875
C	-6.6118772096	-0.8429864879	2.7815790837
H	-7.2456197616	-0.0944878726	2.2870132709
H	-6.3756965903	-0.4386855380	3.7751197758
C	-7.3938196452	-2.1449705631	2.9371054558
H	-8.3126948516	-1.9922227126	3.5148871377
H	-7.6803766456	-2.5553819698	1.9611767261
H	-6.7989744327	-2.9067972337	3.4557583803
N	5.0165809882	-1.4527172519	-4.8914828780
C	5.3272195436	-1.6242672687	-6.3132448722
C	5.5225584914	-0.3153582941	-7.0765173002
H	4.5434921618	-2.2290113081	-6.7776580476

	X	Y	Z
H	6.2394895983	-2.2222202415	-6.3717497360
H	5.6853101441	-0.5337111738	-8.1378694666
H	4.6494337526	0.3393808504	-6.9952990977
H	6.3945619291	0.2347051606	-6.7105149396
C	6.1437730332	-1.4851712198	-3.9549661384
C	6.6221226854	-0.1052347751	-3.5043708217
H	6.9609535405	-2.0085434194	-4.4551529388
H	5.8777963038	-2.1034162390	-3.0915013807
H	7.4442668841	-0.2201794955	-2.7894572366
H	6.9915343700	0.4814936341	-4.3506967337
H	5.8273159063	0.4675533777	-3.0176333700
C	-2.4802939104	3.3049037060	4.5337690022
C	-2.9279306349	3.6487868026	3.1190270793
C	-3.0969868166	4.2230403411	5.5734058045
O	-2.8385296469	1.9644863622	4.8792714398
H	-1.3865819028	3.4010069354	4.5928555009
H	-2.5039872563	2.9509167435	2.3886768906
H	-4.0198587409	3.6046915458	3.0361557126
H	-2.6016665858	4.6592734541	2.8453070922
H	-2.7547453264	3.9571282825	6.5791206902
H	-2.8154068654	5.2646138813	5.3831880494
H	-4.1911944288	4.1568515427	5.5520313793
H	-2.3736527547	1.3352809013	4.2835699815
C	1.2710969367	2.2697492160	3.3256337146
C	1.3194772622	2.2389625049	4.8487825911
C	2.5512424707	2.8264611664	2.7270394746
O	1.0819685114	0.9594113638	2.7928715603
H	0.4320157602	2.9065303689	3.0066697251
H	0.4063458066	1.8004675553	5.2648331839
H	2.1693068974	1.6373068608	5.1921039903
H	1.4253681468	3.2499678688	5.2601196678
H	2.4862090743	2.8616853731	1.6348246727
H	2.7416333391	3.8417217525	3.0922907419
H	3.4079991979	2.1987390653	2.9993793196
H	0.1683149251	0.6532795848	2.9857337168
C	-1.6316593549	-1.2567503743	3.8210751004
C	-0.8427026335	-2.2716910591	3.0061719388
C	-1.1328575819	-1.1589514551	5.2524620548
O	-1.5511967648	0.0483257968	3.2215895419
H	-2.6888372989	-1.5543772207	3.8352208381
H	-1.2066998636	-2.3181375586	1.9750668642
H	0.2206661409	-2.0074330767	2.9884492179
H	-0.9391664323	-3.2731393577	3.4414857142
H	-1.7094228842	-0.4242853782	5.8228463571
H	-1.2285964036	-2.1287786369	5.7526543442
H	-0.0773568829	-0.8667704632	5.2797936736
H	-2.0909187800	0.0461430800	2.3596341600

FR0-SB in *i*-propanol, geometry D' (in Å)

E_{S_0} = -1625.582096 hartree

E_{S_1} = -1625.473415 hartree

	X	Y	Z
C	-2.3840933479	-0.2463064329	-2.4392303391
C	-2.1548606238	-0.1393600450	-1.0262993334
C	-0.8205880524	-0.3454218736	-0.5317811536
C	0.1823056543	-0.6579667923	-1.4067948862
C	-0.0665380195	-0.7849513915	-2.8161579468
C	-1.3877900670	-0.5589340957	-3.3217668311
H	-3.3924467347	-0.0747182528	-2.8101246306
H	-0.6280318864	-0.2432568818	0.5310899591
H	-1.5981014704	-0.6380029864	-4.3849242811
C	1.6548950194	-0.9306412490	-1.1105135098
C	2.1857320667	-1.2438000875	-2.5046259333
C	3.4541142987	-1.5714862333	-2.8727099084
C	3.7604037073	-1.8471699921	-4.2510155692
C	2.6971465317	-1.7434841876	-5.2058242564
C	1.4187635605	-1.4029207675	-4.8372407175
C	1.1251896675	-1.1420801231	-3.4690099827
H	4.2299639405	-1.6364415733	-2.1205677949
H	2.8953396020	-1.9204889639	-6.2551261581
H	0.6432731820	-1.3270897074	-5.5934695702
C	2.3427420536	0.3087905366	-0.5172952767
H	1.8907067731	0.5791758646	0.4422347609
H	3.4093893946	0.1187622461	-0.3494195516
H	2.2554138422	1.1689419919	-1.1899876732
C	1.8245043936	-2.1300798867	-0.1651750549
H	2.8847907792	-2.3505154392	0.0013666886
H	1.3730974408	-1.9143931954	0.8087115369
H	1.3490699150	-3.0301807816	-0.5685138291
C	-3.2652782776	0.1694328134	-0.1866452960
H	-4.2156217270	0.3197939591	-0.7159815572
N	-3.2604181800	0.2765648700	1.1181285400
C	-4.5554073289	0.5348451923	1.7315494858
H	-5.2060257629	1.1025612538	1.0470171687
H	-4.3997099388	1.1624068368	2.6163321583
C	-5.2800335973	-0.7512701509	2.1481687263
H	-4.6328670521	-1.3264071889	2.8231089206
H	-5.4359551430	-1.3761798104	1.2579894457
C	-6.6203375919	-0.4764456390	2.8287670955
H	-7.2700127951	0.0803332204	2.1398873432
H	-6.4593512063	0.1766991345	3.6970030141
C	-7.3332752881	-1.7493627723	3.2786223637
H	-8.2943294421	-1.5204966283	3.7534202087
H	-7.5333296724	-2.4161591588	2.4311247466
H	-6.7293943971	-2.3077568805	4.0042858003
N	5.0183898217	-2.1998540357	-4.6294750243
C	5.3229594769	-2.6024099043	-6.0047777309
C	5.6686158668	-1.4431557897	-6.9370647131
H	4.4820210479	-3.1784354171	-6.3985752128

	X	Y	Z
H	6.1648956855	-3.2980712011	-5.9572730087
H	5.8223516088	-1.8267697350	-7.9518166922
H	4.8703587520	-0.6951206131	-6.9731654284
H	6.5900138791	-0.9412705063	-6.6264407595
C	6.1421594517	-2.1428710987	-3.6896984587
C	6.6288847122	-0.7258545903	-3.3880419446
H	6.9556061421	-2.7217473096	-4.1308395883
H	5.8702694715	-2.6638251687	-2.7655265228
H	7.4537194314	-0.7701516739	-2.6682537102
H	6.9956945999	-0.2317031693	-4.2925263610
H	5.8391153895	-0.1023486004	-2.9590759343
C	-2.6317501182	3.9059392316	3.9810106161
C	-3.0711951637	4.1242437923	2.5381156781
C	-3.2468183697	4.9207002529	4.9277988544
O	-3.0033941231	2.6067379987	4.4455811321
H	-1.5374451332	3.9988135440	4.0354876279
H	-2.6543201790	3.3576845563	1.8760949671
H	-4.1634372537	4.0856315093	2.4552800516
H	-2.7321423368	5.1017865623	2.1749490795
H	-2.9174465237	4.7395567192	5.9565461335
H	-2.9515589046	5.9382434362	4.6493599251
H	-4.3415061898	4.8644631269	4.9006123938
H	-2.4897108929	1.9217181864	3.9607555054
C	1.2305798187	2.7851984766	2.9500434455
C	1.2283556367	2.9379234974	4.4666020624
C	2.5494530122	3.2246784574	2.3385146879
O	1.0137047531	1.4285744519	2.5668367659
H	0.4258897666	3.4066827039	2.5277949105
H	0.2842162217	2.5914160620	4.8986986063
H	2.0386614595	2.3478811694	4.9108761842
H	1.3652765049	3.9870474651	4.7545535999
H	2.5293472096	3.1181380923	1.2492136704
H	2.7568030949	4.2735893057	2.5773580101
H	3.3742573639	2.6156963487	2.7268065455
H	0.0995251891	1.1521013015	2.8033570395
C	-1.6097758156	-0.6504059674	3.9396888123
C	-0.8388953869	-1.7794235677	3.2693640287
C	-1.0490556858	-0.3145525045	5.3112067598
O	-1.5789903620	0.5384902911	3.1338089916
H	-2.6592602256	-0.9547697388	4.0541512597
H	-1.2548632798	-2.0122762894	2.2842369262
H	0.2145410631	-1.5040319181	3.1472675396
H	-0.8856747849	-2.6910542695	3.8765670324
H	-1.6179642435	0.4929687321	5.7816787750
H	-1.0992885843	-1.1912758030	5.9661157192
H	-0.0011146098	-0.0040179020	5.2377901354
H	-2.1307399300	0.3879562300	2.2788746400

FR0-SB in *i*-propanol, geometry E' (in Å)

E_{S_0} = -1625.580082 hartree

E_{S_1} = -1625.471689 hartree

	X	Y	Z
C	-0.6005542082	-0.8259490557	-3.0151954609
C	-1.0778399119	-0.9147256949	-1.6637818763
C	-0.1267884496	-0.7665626268	-0.5941539004
C	1.1964512657	-0.5779403632	-0.8854415445
C	1.6596073237	-0.5106393743	-2.2440028851
C	0.7175034581	-0.6256496417	-3.3163813520
H	-1.3227421593	-0.9299078731	-3.8220164430
H	-0.4789707958	-0.8210247313	0.4305691255
H	1.0439633209	-0.5654556397	-4.3510675520
C	2.3787088366	-0.4308744108	0.0731184575
C	3.5411823770	-0.2897958933	-0.9042656006
C	4.8652319885	-0.1323671222	-0.6280306447
C	5.8215308398	-0.0251555932	-1.6981511184
C	5.3256151758	-0.0715283698	-3.0421326335
C	3.9896792408	-0.2223098962	-3.3210147972
C	3.0545786878	-0.3407285957	-2.2547892492
H	5.1928955612	-0.0724299477	0.4020740664
H	6.0135521375	0.0095376550	-3.8736238433
H	3.6589190674	-0.2566739691	-4.3549316539
C	2.2423612430	0.8224993823	0.9503835608
H	1.3467994982	0.7589467815	1.5763207022
H	3.1094672030	0.9329702693	1.6114233813
H	2.1628542734	1.7285267051	0.3411830011
C	2.5438516187	-1.6777259325	0.9566313893
H	3.4242674362	-1.5854773187	1.6023811516
H	1.6698502322	-1.8093184299	1.6032184750
H	2.6573281913	-2.5838586618	0.3529654704
C	-2.4597703581	-1.2171815319	-1.4637853019
H	-3.0159231488	-1.4342907964	-2.3858702003
N	-3.1065454500	-1.2935699200	-0.3269517400
C	-4.4532501497	-1.8370817319	-0.3981622314
H	-4.8948675707	-1.6776595806	-1.3951584137
H	-5.0855729645	-1.3056782762	0.3225884354
C	-4.4740639264	-3.3363184477	-0.0747664303
H	-4.0176400180	-3.4944954896	0.9111196107
H	-3.8378705943	-3.8613007751	-0.8004916159
C	-5.8799510721	-3.9339234286	-0.0925330293
H	-6.3295231546	-3.7798460163	-1.0826166315
H	-6.5150700017	-3.3938098200	0.6224557147
C	-5.8894579503	-5.4230350773	0.2445303294
H	-6.9048373418	-5.8346489469	0.2155644644
H	-5.2795387117	-5.9945657833	-0.4658413267
H	-5.4851418464	-5.6046622388	1.2478091958
N	7.1523277292	0.1016172853	-1.4466534786
C	8.1177441907	0.3266995418	-2.5275736210
C	8.1173907581	1.7475949358	-3.0902445247
H	7.9411510974	-0.4044210678	-3.3235033393

	X	Y	Z
H	9.1064879465	0.0987384717	-2.1249038131
H	8.8539168719	1.8156871991	-3.8985770725
H	7.1426959781	2.0321063520	-3.4969737551
H	8.3895149176	2.4788365985	-2.3235404696
C	7.6850938345	0.0646256582	-0.0816943877
C	7.7073968628	1.4232575916	0.6169037782
H	8.6993854314	-0.3375624650	-0.1428727832
H	7.1136124787	-0.6598685977	0.5027195252
H	8.0511702725	1.2969037153	1.6496694923
H	8.3922252542	2.1170991060	0.1199559177
H	6.7148375022	1.8840502261	0.6416840118
C	-5.9270640305	2.0829579836	1.1848590897
C	-5.5016857343	1.8700964543	-0.2622771756
C	-7.3970724839	2.4420503994	1.3044572526
O	-5.7151733453	0.9078668497	1.9669805082
H	-5.3328000342	2.9043468731	1.6125075047
H	-4.4495628445	1.5720741979	-0.3292878023
H	-6.1060543809	1.0849531024	-0.7304717828
H	-5.6247545110	2.7928011615	-0.8419709559
H	-7.6743272219	2.5909421555	2.3533163115
H	-7.6157900424	3.3659553465	0.7579754918
H	-8.0232742303	1.6417835693	0.8926525602
H	-4.7692979070	0.6361432871	1.9298924210
C	-2.2761457688	3.4712164880	2.0911976767
C	-2.9966483870	3.6167207501	3.4258499194
C	-1.3372750418	4.6352746890	1.8242028142
O	-1.4953405437	2.2768989061	2.0487512181
H	-3.0235193660	3.4343945266	1.2843269942
H	-3.6638339391	2.7692695241	3.6124382049
H	-2.2726820882	3.6667115406	4.2475198598
H	-3.6012903448	4.5311063160	3.4448387677
H	-0.8480064631	4.5289703647	0.8505292025
H	-1.8846229567	5.5840923830	1.8278492339
H	-0.5602052894	4.6871116499	2.5959748383
H	-2.0742875070	1.4813456837	2.0525423909
C	-2.9619556104	-1.0067258158	3.0415087710
C	-1.6175872216	-1.7226023234	3.0166480604
C	-3.1756884192	-0.2567285994	4.3454587796
O	-3.0738199893	-0.0745864517	1.9574200509
H	-3.7608332565	-1.7550577121	2.9318642456
H	-1.4653838865	-2.2463103793	2.0679606300
H	-0.7975222924	-1.0102440963	3.1609481625
H	-1.5658649858	-2.4671562211	3.8200826627
H	-4.1480421276	0.2450420588	4.3563208706
H	-3.1448316181	-0.9505666756	5.1931664821
H	-2.3930849716	0.4960524252	4.4927405114
H	-2.9975767100	-0.5813201700	1.0497047900

FR0-SB in *i*-propanol, geometry F' (in Å)

E_{S_0} = -1625.578850 hartree

E_{S_1} = -1625.470952 hartree

	X	Y	Z
C	-1.3965092132	-0.6706653255	-3.0133537210
C	-1.6411993820	-0.5215775765	-1.6059671441
C	-0.5096093301	-0.4394423287	-0.7217793319
C	0.7547779580	-0.5260099338	-1.2344777784
C	0.9836474718	-0.6990953234	-2.6422169224
C	-0.1356340865	-0.7618748314	-3.5335011728
H	-2.2539137152	-0.7219590127	-3.6809632298
H	-0.6771733562	-0.3049839732	0.3417209072
H	0.0108137838	-0.8836842384	-4.6033366536
C	2.0882402518	-0.4577880085	-0.4939894993
C	3.0740106536	-0.6684666514	-1.6365853180
C	4.4313180967	-0.7454546210	-1.5763908661
C	5.1984521443	-0.9617582538	-2.7737629851
C	4.4865821998	-1.0512152185	-4.0145430553
C	3.1173872154	-0.9683131167	-4.0771695987
C	2.3663257556	-0.7871742016	-2.8816830826
H	4.9302725856	-0.6497293344	-0.6207439622
H	5.0309131110	-1.1801910502	-4.9407711390
H	2.6196165683	-1.0406235823	-5.0395615362
C	2.2813493491	0.9220935538	0.1580806030
H	1.4955153159	1.1122588621	0.8958688197
H	3.2517936753	0.9793665945	0.6653576453
H	2.2454454455	1.7207810138	-0.5909807082
C	2.2100516270	-1.5639885040	0.5640885983
H	3.1939698484	-1.5395095455	1.0456193027
H	1.4553537818	-1.4288863145	1.3446033139
H	2.0695707538	-2.5573206855	0.1252638823
C	-2.9955731986	-0.4839310753	-1.1629359418
H	-3.7447915698	-0.5559225358	-1.9612255887
N	-3.4254517600	-0.3785486500	0.0713145700
C	-4.8678999307	-0.4511411464	0.2537989302
H	-5.3938455440	-0.0184871590	-0.6117345015
H	-5.1334478925	0.1535291248	1.1274324716
C	-5.3590017528	-1.8882510801	0.4694403913
H	-4.8145519315	-2.3297163464	1.3143913988
H	-5.1029700416	-2.4878694785	-0.4148529354
C	-6.8623515857	-1.9681574590	0.7310209327
H	-7.4041763146	-1.5213817098	-0.1135371250
H	-7.1098877674	-1.3619795291	1.6127358325
C	-7.3494255425	-3.3990629199	0.9465462416
H	-8.4284742016	-3.4294423294	1.1370625083
H	-7.1497943848	-4.0236457429	0.0672289031
H	-6.8476990195	-3.8637748947	1.8041360731
N	6.5519138199	-1.0866919360	-2.7263040218
C	7.3408099940	-1.3383089596	-3.9356733664
C	7.6748419829	-0.0841388868	-4.7420398214
H	6.8131203227	-2.0669057041	-4.5573437716

	X	Y	Z
H	8.2655630218	-1.8283754278	-3.6214263656
H	8.2039164132	-0.3725668027	-5.6572001754
H	6.7760481178	0.4703835232	-5.0292131784
H	8.3255991905	0.5925203792	-4.1802095407
C	7.2919748585	-0.9084525794	-1.4734316854
C	7.5030733189	0.5509263671	-1.0729547467
H	8.2597352032	-1.3979006181	-1.6000173393
H	6.7834004461	-1.4565611465	-0.6745044467
H	8.0344872441	0.5901100920	-0.1155949238
H	8.1042829197	1.0858820737	-1.8136631981
H	6.5559901720	1.0862281733	-0.9557805631
C	-4.6231023152	3.0519526306	2.9875068182
C	-4.7186967590	3.2574606640	1.4803312933
C	-5.7682553072	3.7204823586	3.7276781281
O	-4.6502274843	1.6669678939	3.3285852919
H	-3.6769193598	3.4859449651	3.3431880412
H	-3.9199280357	2.7231629314	0.9544583695
H	-5.6796271483	2.8928093557	1.0995209032
H	-4.6306314673	4.3214551808	1.2303821569
H	-5.6713400311	3.5738906358	4.8084912928
H	-5.7839230014	4.7976351625	3.5291936320
H	-6.7290317535	3.2994878459	3.4086888882
H	-3.8569491588	1.2069426574	2.9670589803
C	-0.5197252567	3.0886239926	2.8411109252
C	-0.8716516956	3.2409168076	4.3167989411
C	0.6868301990	3.9289457498	2.4574144732
O	-0.2183952710	1.7340484933	2.5170268531
H	-1.3784442750	3.4161800578	2.2351233399
H	-1.7103966985	2.5937926675	4.5938486192
H	-0.0155061016	2.9720886489	4.9468213833
H	-1.1526868620	4.2757749690	4.5470908657
H	0.9205581407	3.8117557184	1.3943156854
H	0.4983835711	4.9907050190	2.6523311878
H	1.5676213587	3.6284906039	3.0371009437
H	-1.0400798872	1.1896579812	2.5220227757
C	-2.4855520151	-1.0495268430	3.2065612752
C	-1.5399022114	-2.1103767603	2.6576255452
C	-2.1088859302	-0.6472437379	4.6237294163
O	-2.4888164919	0.1210339168	2.3828324696
H	-3.5055013703	-1.4629062845	3.2210601082
H	-1.7911046097	-2.3742248122	1.6259934710
H	-0.5048271699	-1.7516256251	2.6784474842
H	-1.5940697845	-3.0232276917	3.2626979838
H	-2.7985705576	0.1066926279	5.0138962486
H	-2.1434882649	-1.5161340417	5.2906214658
H	-1.0941260243	-0.2341373377	4.6515738036
H	-2.7892313000	-0.1234504300	1.3876129400

FR0-SB in *i*-propanol, geometry G' (in Å)

E_{S_0} = -1625.576563 hartree

E_{S_1} = -1625.469586 hartree

	X	Y	Z
C	0.1436929135	3.0998271679	1.3878755886
C	-0.7125225753	2.1102356191	0.7954160125
C	-0.1069772187	0.9748838406	0.1536090840
C	1.2557644847	0.8721150248	0.1148866957
C	2.0997584422	1.8808346739	0.6912165946
C	1.5066392893	3.0082792825	1.3442182901
H	-0.3203339248	3.9509552578	1.8814290202
H	-0.7417752606	0.2106011189	-0.2824890156
H	2.1262797231	3.7769719540	1.7978402129
C	2.1088805402	-0.2441315245	-0.4817277093
C	3.5141275482	0.2816070751	-0.2162192540
C	4.7057033537	-0.2869631735	-0.5470267257
C	5.9404787450	0.3627573649	-0.1984203951
C	5.8633570138	1.6110067748	0.5026724223
C	4.6614354521	2.1820051899	0.8409063345
C	3.4468332484	1.5325234313	0.4863939540
H	4.7178875298	-1.2365257624	-1.0661389918
H	6.7705228825	2.1261931223	0.7894348900
H	4.6489231025	3.1281314055	1.3742239641
C	1.8665374714	-1.5720230562	0.2556240123
H	0.8291642054	-1.8963203567	0.1272339052
H	2.5213185999	-2.3578713163	-0.1392707896
H	2.0683610559	-1.4725279476	1.3277448648
C	1.8456395190	-0.4231966482	-1.9840332009
H	2.5029778761	-1.1907990702	-2.4074325317
H	0.8123296966	-0.7421660892	-2.1520596280
H	2.0103108345	0.5080969633	-2.5355899767
C	-2.1200844668	2.3104898160	0.8761550081
H	-2.4294361187	3.2207966468	1.4034772863
N	-3.0637869144	1.5311267187	0.4003642508
C	-4.4296724521	2.0152808571	0.5595650886
H	-4.5587647229	2.4844447931	1.5476339197
H	-5.1004947345	1.1509195086	0.5251361342
C	-4.8380477713	3.0178246441	-0.5274836983
H	-4.6817366720	2.5609060310	-1.5133046640
H	-4.1711987728	3.8896209262	-0.4788999162
C	-6.2909282530	3.4713360237	-0.3945823108
H	-6.4469302402	3.9104559977	0.6001428196
H	-6.9505748374	2.5950914015	-0.4515760811
C	-6.6974267017	4.4829986085	-1.4632156632
H	-7.7470127654	4.7790570136	-1.3527627815
H	-6.0879396911	5.3929008794	-1.4023944729
H	-6.5742157680	4.0683796381	-2.4712042435
N	7.1399416038	-0.1846596760	-0.5296766798
C	8.4037206319	0.4502132799	-0.1426030561
C	8.8120598264	0.2077098030	1.3097838395
H	8.3409645561	1.5221297922	-0.3526387617

	X	Y	Z
H	9.1766086659	0.0600366493	-0.8080064289
H	9.7369535083	0.7552353674	1.5222648494
H	8.0475137381	0.5486700754	2.0142059794
H	8.9977874338	-0.8530380469	1.5012793277
C	7.2249244341	-1.4727602842	-1.2246253814
C	7.0631430076	-2.6890025053	-0.3139072804
H	8.2005781663	-1.5110326268	-1.7140230201
H	6.4871314295	-1.4917520831	-2.0318694993
H	7.0998495909	-3.6023881260	-0.9179532611
H	7.8676078273	-2.7436499821	0.4256652411
H	6.1107743311	-2.6758621675	0.2246072223
C	-5.6304261658	-2.1473122084	1.5193829768
C	-4.9224700195	-1.3255602990	2.5897610150
C	-7.0417528916	-2.5257695266	1.9324051522
O	-5.7249929839	-1.4293270503	0.2890111433
H	-5.0574768506	-3.0706634909	1.3466960098
H	-3.9278337180	-1.0118211975	2.2553347540
H	-5.4988503043	-0.4255277367	2.8324771865
H	-4.7983600587	-1.9124679049	3.5076305592
H	-7.5242643564	-3.1339963314	1.1601125870
H	-7.0332661103	-3.1022529533	2.8638453095
H	-7.6475487583	-1.6258164757	2.0904561076
H	-4.8219153213	-1.2108027622	-0.0455982884
C	-1.9788113427	-3.6509480189	0.6167740005
C	-2.8610067389	-4.6494605691	-0.1247932482
C	-0.8106862227	-4.3306668129	1.3116582896
O	-1.4450148136	-2.6773261181	-0.2764389436
H	-2.5850374346	-3.1391564498	1.3788529225
H	-3.6828216845	-4.1417025649	-0.6396569339
H	-2.2746979002	-5.1919304422	-0.8757976682
H	-3.2949590782	-5.3808825091	0.5674713145
H	-0.2018876397	-3.5980427476	1.8509225470
H	-1.1666774877	-5.0783518248	2.0290785918
H	-0.1684207217	-4.8361312073	0.5808372781
H	-2.1284775883	-1.9979975997	-0.4898274955
C	-3.5924123496	-0.4011021136	-2.1915067742
C	-2.4777090321	0.3543517008	-2.9065782853
C	-3.8948041974	-1.7264399457	-2.8737384326
O	-3.2624662323	-0.6456904061	-0.8231611141
H	-4.5034985259	0.2169857855	-2.2222569696
H	-2.2597861104	1.3044889299	-2.4093666301
H	-1.5580606472	-0.2411915551	-2.9270033895
H	-2.7642059965	0.5726977685	-3.9424186049
H	-4.7001137394	-2.2568797434	-2.3570154569
H	-4.2072881747	-1.5625714389	-3.9115150583
H	-3.0078830916	-2.3693623136	-2.8814874568
H	-3.0748478223	0.3030226369	-0.3010597694

FR0-SB in *i*-propanol, geometry H' (in Å)

E_{S_0} = -1625.574450 hartree

E_{S_1} = -1625.468452 hartree

	X	Y	Z
C	-1.9133545548	-0.5978031194	-2.7093789654
C	-1.9079800112	-0.4352811844	-1.2809712758
C	-0.6417038108	-0.4168363971	-0.5994960254
C	0.5114592260	-0.5762074209	-1.3171865325
C	0.4882825580	-0.7671277932	-2.7400417492
C	-0.7650073766	-0.7679148852	-3.4305267229
H	-2.8721689613	-0.5952848785	-3.2230496783
H	-0.6187921802	-0.2667549234	0.4747100326
H	-0.8055309742	-0.8960159458	-4.5089473748
C	1.9530877977	-0.5748878405	-0.8142295383
C	2.7195871575	-0.8243388669	-2.1072638164
C	4.0635015239	-0.9490076676	-2.2823621638
C	4.6016811001	-1.2049784847	-3.5908481735
C	3.6822411747	-1.2894646246	-4.6875949464
C	2.3277750468	-1.1527621813	-4.5133262841
C	1.8049014389	-0.9242815448	-3.2103237626
H	4.7257040360	-0.8727541897	-1.4294358741
H	4.0573784923	-1.4440718053	-5.6907537474
H	1.6671418720	-1.2178601284	-5.3729110445
C	2.3238496838	0.7872231373	-0.2036333977
H	1.7101716421	0.9992607447	0.6777108842
H	3.3774842738	0.7991560278	0.1001403050
H	2.1720525201	1.5977813485	-0.9246343021
C	2.1996296462	-1.6960923405	0.2058995912
H	3.2495328522	-1.7173723900	0.5183769291
H	1.5904921999	-1.5373641478	1.1009182092
H	1.9468565059	-2.6781806570	-0.2071181035
C	-3.1635712507	-0.2989359888	-0.6249474850
H	-4.0366869422	-0.3248970168	-1.2863149989
N	-3.3896019500	-0.1566823400	0.6619356900
C	-4.7854989406	-0.1231601413	1.0792533596
H	-5.4017686531	0.3754341692	0.3157858122
H	-4.8499860416	0.4799506995	1.9906528345
C	-5.3579524133	-1.5195614241	1.3537592912
H	-4.7253853861	-2.0268453551	2.0936866116
H	-5.3035920225	-2.1173156034	0.4334587263
C	-6.8000061495	-1.4746621269	1.8567447178
H	-7.4303097850	-0.9682208847	1.1131996500
H	-6.8467378980	-0.8640307867	2.7683275618
C	-7.3709886402	-2.8612709901	2.1447041399
H	-8.4066551602	-2.8004692057	2.4985078408
H	-7.3634702592	-3.4888859909	1.2452411659
H	-6.7871196119	-3.3793302578	2.9152890406
N	5.9373489637	-1.3714198164	-3.7761768233
C	6.4899510323	-1.7932714117	-5.0663106640
C	6.8508537723	-0.6399276458	-5.9996942531
H	5.7818943554	-2.4721118937	-5.5459298296

	X	Y	Z
H	7.3792920012	-2.3937385503	-4.8553422524
H	7.1867807151	-1.0428136644	-6.9615876254
H	5.9946463525	0.0165208171	-6.1847137388
H	7.6638388455	-0.0316397749	-5.5916790799
C	6.8988682281	-1.0896933437	-2.7053640406
C	7.0878157115	0.3978328944	-2.4115319484
H	7.8526440038	-1.5215159551	-3.0135100050
H	6.6047557467	-1.6287879100	-1.7980626056
H	7.8173245659	0.5164580605	-1.6029328671
H	7.4659138535	0.9301230693	-3.2894247455
H	6.1572403484	0.8804746517	-2.0993912897
C	-3.8286031694	3.2288453885	3.6793548057
C	-4.0083525046	3.4818978255	2.1867481526
C	-4.8954919727	3.9224915469	4.5083927588
O	-3.8961276539	1.8387875109	3.9844093080
H	-2.8439884030	3.6133467031	3.9862280108
H	-3.2727128087	2.9228488374	1.5981749883
H	-5.0083484228	3.1753855304	1.8590933618
H	-3.8825135005	4.5468362032	1.9572395489
H	-4.7414052712	3.7319352481	5.5759219079
H	-4.8715284806	5.0060133717	4.3482846838
H	-5.8916992129	3.5557151093	4.2338052546
H	-3.1851226167	1.3412220615	3.5083562187
C	0.1281401940	3.0651896418	2.9884976639
C	0.1120665703	3.0097593377	4.5117071305
C	1.2986907006	3.8806255708	2.4643515559
O	0.2289910603	1.7625532337	2.4222309934
H	-0.8049962656	3.5343914666	2.6401454251
H	-0.7332989402	2.4188423491	4.8780354495
H	1.0347059828	2.5484989714	4.8836593456
H	0.0314358593	4.0163734816	4.9394226677
H	1.2840104915	3.9248268653	1.3704584828
H	1.2636681238	4.9054574121	2.8503920499
H	2.2489390383	3.4301764029	2.7743966949
H	-0.5925361978	1.2380126833	2.5943017680
C	-1.9839557957	-0.9526044686	3.5104017132
C	-1.1909281474	-2.0655643364	2.8329649252
C	-1.3925742140	-0.6126906599	4.8714163210
O	-2.0316374804	0.2208105571	2.7039374081
H	-3.0149813184	-1.3101716810	3.6654459156
H	-1.5990923139	-2.3053115898	1.8463506464
H	-0.1441910950	-1.7671140278	2.7062597423
H	-1.2117828085	-2.9800826020	3.4380429432
H	-1.9719039288	0.1728181093	5.3652661747
H	-1.3929233337	-1.4946382297	5.5225404354
H	-0.3583617030	-0.2651305986	4.7667817667
H	-2.5748961000	0.0129716400	1.7180792100

FR0-SB in *i*-propanol, geometry I' (in Å)

E_{S_0} = -1625.571553 hartree

E_{S_1} = -1625.467245 hartree

	X	Y	Z
C	-1.2516504441	-0.8631443964	-3.0233813281
C	-1.5189156507	-0.7709420933	-1.6134820216
C	-0.4408902093	-0.4110078337	-0.7323130631
C	0.8032300825	-0.1802325021	-1.2532319899
C	1.0584209798	-0.2987681427	-2.6606176800
C	-0.0103211978	-0.6382603835	-3.5472101395
H	-2.0729951102	-1.1265919884	-3.6860157252
H	-0.6286365754	-0.3189422299	0.3323042587
H	0.1586635163	-0.7207879154	-4.6175454285
C	2.0860520455	0.2101972360	-0.5217233372
C	3.0859827465	0.2377540794	-1.6707385358
C	4.4211988321	0.4978560672	-1.6223267363
C	5.2051340587	0.4812246560	-2.8271694391
C	4.5313321845	0.1972798150	-4.0605756929
C	3.1851652993	-0.0640362973	-4.1095217954
C	2.4226945473	-0.0552362731	-2.9095408876
H	4.8861762882	0.7366547149	-0.6743548873
H	5.0930545176	0.1699444309	-4.9848270866
H	2.7157918471	-0.2872678355	-5.0629268262
C	1.9528637113	1.5944471278	0.1346571900
H	1.2002724798	1.5640072190	0.9282095645
H	2.9062911618	1.9035561442	0.5790847481
H	1.6598203003	2.3559779516	-0.5963688410
C	2.4751034659	-0.8297667884	0.5395130862
H	3.4266412956	-0.5656672129	1.0146636020
H	1.7123135112	-0.8701704577	1.3230434067
H	2.5765866679	-1.8305657725	0.1071948159
C	-2.8441123685	-1.0423893823	-1.1796449587
H	-3.5589665198	-1.2636254095	-1.9780291439
N	-3.3105642800	-1.0465518200	0.0522481200
C	-4.7153548113	-1.3959715199	0.2242202304
H	-5.3261148650	-0.8735939411	-0.5274812414
H	-5.0290919952	-1.0287170465	1.2053674855
C	-4.9834276528	-2.9035377975	0.1343905305
H	-4.3793146211	-3.4207308836	0.8910160709
H	-4.6452860265	-3.2738681549	-0.8428333718
C	-6.4599036968	-3.2454244794	0.3291346491
H	-7.0576084086	-2.7165948135	-0.4256118787
H	-6.7946385820	-2.8706009574	1.3055042097
C	-6.7391899485	-4.7434796150	0.2370849579
H	-7.8047623927	-4.9595771072	0.3762295212
H	-6.4449615874	-5.1434097272	-0.7409470240
H	-6.1855390517	-5.2995925278	1.0034168662
N	6.5415425090	0.7202004054	-2.7999169572
C	7.3163690535	0.8836195958	-4.0346772384
C	7.0665466954	2.2056135467	-4.7591095199
H	7.1236270329	0.0358135548	-4.7007106155

	X	Y	Z
H	8.3711122130	0.8157650061	-3.7621615270
H	7.6670480379	2.2341424831	-5.6749249963
H	6.0170916054	2.3321060992	-5.0396413755
H	7.3540883718	3.0596713835	-4.1387349621
C	7.2652840170	0.8962984663	-1.5375134598
C	7.2941428784	2.3373364180	-1.0311261896
H	8.2866421415	0.5421095508	-1.6995941561
H	6.8358076614	0.2291716183	-0.7867731513
H	7.8015018237	2.3718842083	-0.0606057120
H	7.8413310647	2.9923593224	-1.7159746387
H	6.2860195857	2.7440359948	-0.9031949847
C	-4.8703913331	1.5647833438	3.4687565783
C	-5.01111110686	2.0439926293	2.0286665794
C	-6.0874663944	1.9172867740	4.3060530055
O	-4.6949578446	0.1511514155	3.5285543489
H	-3.9918122557	2.0501669371	3.9178982137
H	-4.1437959367	1.7487295042	1.4287644942
H	-5.9075603262	1.6146894299	1.5663761806
H	-5.0922579683	3.1367935814	1.9891256828
H	-5.9577057203	1.5848378562	5.3414253568
H	-6.2503324620	3.0007245635	4.3155120338
H	-6.9876441153	1.4404201741	3.9008875369
H	-3.8387906893	-0.1032142034	3.0959586460
C	-1.0023427624	2.3761035422	3.2732111459
C	-1.1507356089	2.1156571378	4.7681070426
C	-0.0584504111	3.5340398445	2.9932606756
O	-0.4942718094	1.2314617183	2.5973431636
H	-1.9897147524	2.6276446188	2.8569979726
H	-1.8199107164	1.2704262125	4.9586383346
H	-0.1752486736	1.8815618455	5.2113271966
H	-1.5599836967	2.9934517778	5.2826709822
H	0.0284880208	3.7121775418	1.9163526633
H	-0.4201443913	4.4547817539	3.4646441162
H	0.9418555681	3.3182066499	3.3867074592
H	-1.1761338251	0.5096031086	2.5754866599
C	-2.1248031876	-2.0204103896	2.9130428837
C	-1.0087283470	-2.7789923271	2.1992293945
C	-1.8143247252	-1.8584136277	4.3959523077
O	-2.3539490146	-0.7504051155	2.3204340999
H	-3.0468407462	-2.6207874677	2.8267211020
H	-1.2306347997	-2.9011283160	1.1342768711
H	-0.0579006945	-2.2411436536	2.2882956561
H	-0.8770698542	-3.7779982664	2.6333446744
H	-2.6311192778	-1.3448491027	4.9118477727
H	-1.6737502028	-2.8358445724	4.8735003833
H	-0.8975319053	-1.2749997004	4.5378638791
H	-2.7178480600	-0.8830266600	1.1690373400

FR0-SB in *i*-propanol, geometry J' (in Å)

E_{S_0} = -1625.570205 hartree

E_{S_1} = -1625.467186 hartree

	X	Y	Z
C	-1.8366451036	-0.4847900245	-2.8282424822
C	-1.8793618058	-0.3880667468	-1.3943428299
C	-0.6417604547	-0.2886437992	-0.6713045682
C	0.5382833097	-0.3063367861	-1.3633674571
C	0.5661866220	-0.4256363360	-2.7917370221
C	-0.6593495145	-0.5098470483	-3.5199485870
H	-2.7782629387	-0.5462571829	-3.3690367608
H	-0.6590029763	-0.1971441993	0.4105755465
H	-0.6587020832	-0.5879071980	-4.6038657216
C	1.9596605707	-0.2116280899	-0.8169419722
C	2.7768067127	-0.2985174910	-2.0998033303
C	4.1298590314	-0.2707899309	-2.2441318657
C	4.7198845422	-0.3943479798	-3.5488794643
C	3.8394444398	-0.5165221291	-4.6747781105
C	2.4753717846	-0.5326739644	-4.5293773608
C	1.9051325944	-0.4290939167	-3.2322053812
H	4.7608058721	-0.1748610004	-1.3700212621
H	4.2511415353	-0.5775535729	-5.6733767259
H	1.8431429091	-0.6201200074	-5.4082301230
C	2.1884017513	1.1223192602	-0.0886887503
H	1.5443478232	1.1869521487	0.7940294539
H	3.2296549420	1.2089386263	0.2436771843
H	1.9719027333	1.9739887536	-0.7430144314
C	2.2739628046	-1.3849992263	0.1244440979
H	3.3089474804	-1.3347810223	0.4803502834
H	1.6161932851	-1.3523766806	0.9980844608
H	2.1309064319	-2.3492842824	-0.3744029266
C	-3.1553717724	-0.3984404312	-0.7773320435
H	-4.0106578959	-0.4393528940	-1.4557576262
N	-3.4346067900	-0.3495582300	0.5113609400
C	-4.8381368584	-0.3998415581	0.9039241747
H	-5.4311651578	0.2381207425	0.2328637615
H	-4.9145614582	0.0264727835	1.9078110002
C	-5.4154659059	-1.8206301149	0.8991572504
H	-4.8187714515	-2.4498102094	1.5718403333
H	-5.3100573601	-2.2506586575	-0.1061487036
C	-6.8832254601	-1.8587448238	1.3230870939
H	-7.4738604428	-1.2229713269	0.6495971608
H	-6.9848873189	-1.4237547449	2.3261908291
C	-7.4607239563	-3.2720100330	1.3202763216
H	-8.5161305994	-3.2730493507	1.6165557879
H	-7.3948987583	-3.7248989635	0.3235185219
H	-6.9200871705	-3.9238530503	2.0172539369
N	6.0677739716	-0.4006201650	-3.7068080326
C	6.6923768781	-0.6858873704	-5.0021662671
C	6.9298635975	0.5487782551	-5.8685735480
H	6.0821278620	-1.4207857318	-5.5316530348

	X	Y	Z
H	7.6438751533	-1.1832763584	-4.7956353379
H	7.3456952986	0.2404346682	-6.8340071942
H	6.0023509208	1.0990622689	-6.0559805092
H	7.6438726612	1.2346532770	-5.4025654479
C	6.9678508863	-0.0759727079	-2.5947089223
C	6.9859090618	1.4055539873	-2.2220154266
H	7.9706165381	-0.3869684424	-2.8938400454
H	6.7111051814	-0.6917814862	-1.7260456598
H	7.6689087212	1.5582599861	-1.3793819210
H	7.3356768129	2.0201346441	-3.0569212855
H	5.9979874778	1.7702896911	-1.9259133282
C	-3.8587899233	2.4222979864	3.9889009232
C	-3.8587975729	2.9479658642	2.5577341855
C	-4.9981405927	3.0055803196	4.8072105893
O	-3.9855992556	1.0054025346	4.0239220633
H	-2.9090680070	2.7072026291	4.4669053639
H	-3.0673156308	2.4768133719	1.9652354639
H	-4.8184956560	2.7409406798	2.0698598128
H	-3.6914973759	4.0317908998	2.5423149011
H	-4.9841588325	2.6122306414	5.8293107569
H	-4.9193940974	4.0972076185	4.8618053928
H	-5.9655753660	2.7557475496	4.3551999352
H	-3.2347496049	0.5747626016	3.5259422065
C	0.0817189382	2.2585016470	3.5918650214
C	-0.0703633253	1.9373133749	5.0749914431
C	1.3006940633	3.1286701267	3.3287651574
O	0.2168373927	1.0777725399	2.8108553174
H	-0.8120717456	2.8081694591	3.2579877332
H	-0.9434205231	1.3022040222	5.2529110032
H	0.8158300381	1.4065975881	5.4433495602
H	-0.1922080152	2.8546505178	5.6635866197
H	1.3891652886	3.3658540931	2.2634939646
H	1.2345695048	4.0706050153	3.8849666192
H	2.2165439047	2.6117432666	3.6392768307
H	-0.6373115676	0.5613050448	2.7979795887
C	-2.0818959451	-1.6374658630	3.1954016443
C	-1.2754997296	-2.6191248159	2.3461898083
C	-1.5608340422	-1.6132980086	4.6297226620
O	-2.0731375730	-0.3396321911	2.6339619583
H	-3.1241841429	-2.0039216062	3.2291998098
H	-1.6338608596	-2.6335433247	1.3116841785
H	-0.2165030177	-2.3351143732	2.3334387742
H	-1.3505610010	-3.6392897369	2.7435915493
H	-2.1499505444	-0.9278272151	5.2471749653
H	-1.6166093794	-2.6119864302	5.0807791087
H	-0.5154837260	-1.2845766117	4.6551041580
H	-2.6852674500	-0.3483488300	1.4551923300

FR0-SB in *i*-propanol, geometry K' (in Å)

E_{S_0} = -1625.569170 hartree

E_{S_1} = -1625.468443 hartree

	X	Y	Z
C	-1.9547438715	-0.5182569333	-2.7539832285
C	-1.9534482490	-0.3680960111	-1.3228335707
C	-0.6915124879	-0.3352696443	-0.6349684003
C	0.4653632927	-0.4802959177	-1.3537077717
C	0.4455090480	-0.6549945132	-2.7758689261
C	-0.8007572546	-0.6650507436	-3.4704870849
H	-2.9114092113	-0.5250997929	-3.2708784510
H	-0.6708302471	-0.1982954680	0.4422397010
H	-0.8351995652	-0.7828371476	-4.5502308774
C	1.9049949303	-0.4923168959	-0.8448073937
C	2.6775307906	-0.6910371743	-2.1426094171
C	4.0241921672	-0.7874069330	-2.3176993291
C	4.5672699305	-1.0154569361	-3.6285813700
C	3.6498779491	-1.1013164581	-4.7286457265
C	2.2941277739	-0.9894294103	-4.5521783487
C	1.7691659597	-0.7878810343	-3.2480253692
H	4.6836706732	-0.7146103848	-1.4624846113
H	4.0281565642	-1.2363041850	-5.7332005908
H	1.6345738117	-1.0531879807	-5.4126049275
C	2.2740130748	0.8354173954	-0.1650048292
H	1.6684576330	0.9924719276	0.7334726738
H	3.3297996146	0.8350379919	0.1315527356
H	2.1142745608	1.6838318827	-0.8393489119
C	2.1450853436	-1.6653791261	0.1187806617
H	3.1923569575	-1.7000155633	0.4386424488
H	1.5260594012	-1.5539786286	1.0137139265
H	1.8986803019	-2.6251476906	-0.3471517976
C	-3.2117559387	-0.2718439423	-0.6800441310
H	-4.0877615042	-0.3193147652	-1.3285108992
N	-3.4660339400	-0.1401675800	0.6119014000
C	-4.8455385798	-0.1484224555	1.0784641413
H	-5.4799057563	0.3642524816	0.3427631189
H	-4.8777416879	0.4316034003	2.0046195330
C	-5.3820270229	-1.5631539208	1.3248111714
H	-4.7369328427	-2.0660780123	2.0563371076
H	-5.3138641785	-2.1427282242	0.3937262870
C	-6.8250363501	-1.5605879860	1.8266217215
H	-7.4674058333	-1.0611812631	1.0887051043
H	-6.8887971242	-0.9634882111	2.7461119826
C	-7.3591283722	-2.9653786057	2.0953844787
H	-8.3972685975	-2.9365611139	2.4458924830
H	-7.3323537825	-3.5817621413	1.1884245335
H	-6.7643168314	-3.4769959914	2.8617840815
N	5.9029494737	-1.1573113900	-3.8151013652
C	6.4633603801	-1.5669152703	-5.1069536197
C	6.8206397599	-0.4036620468	-6.0288238686
H	5.7606537080	-2.2458854478	-5.5934422009

	X	Y	Z
H	7.3544400865	-2.1646267076	-4.8959266885
H	7.1656019794	-0.7973455471	-6.9912301209
H	5.9601102428	0.2469771018	-6.2143580449
H	7.6266124645	0.2080003284	-5.6117753287
C	6.8602983082	-0.8739840320	-2.7396319008
C	7.0192513040	0.6125996545	-2.4249793203
H	7.8216403162	-1.2826954170	-3.0552167659
H	6.5766435109	-1.4331882477	-1.8412255788
H	7.7419011719	0.7332337941	-1.6106357159
H	7.3925602366	1.1636201283	-3.2933056262
H	6.0783460580	1.0737148541	-2.1111738964
C	-3.7182725306	2.9710226727	3.8403932606
C	-3.7328357053	3.4402429617	2.3888369255
C	-4.8165450767	3.6293749341	4.6587948265
O	-3.8970013243	1.5647005206	3.9296259105
H	-2.7469076785	3.2376511728	4.2853609243
H	-2.9820922004	2.9054206614	1.7974628986
H	-4.7147013740	3.2589932396	1.9353883461
H	-3.5146797952	4.5131525403	2.3218717147
H	-4.7913155490	3.2777989832	5.6958694301
H	-4.7001271576	4.7191189213	4.6655632817
H	-5.8022941832	3.3947041186	4.2390690348
H	-3.1315378874	1.0855337447	3.4879342094
C	0.2247648554	2.8135765157	3.1662571131
C	0.2548949013	2.7523342004	4.6904840527
C	1.3782236991	3.6398889629	2.6171764479
O	0.3078437336	1.5174046174	2.5938833652
H	-0.7187371894	3.2859464773	2.8520805482
H	-0.5738142337	2.1507276072	5.0758291945
H	1.1913626505	2.2950540852	5.0321443967
H	0.1799682151	3.7558695656	5.1271411295
H	1.3308571453	3.6983027343	1.5246937758
H	1.3552376970	4.6599904019	3.0173083611
H	2.3383012175	3.1865279198	2.8913693405
H	-0.5542079449	1.0148400515	2.7070586930
C	-1.9301816918	-1.0714576074	3.4760587938
C	-1.1619091115	-2.1704891401	2.7406386512
C	-1.3289050361	-0.8443752193	4.8634945090
O	-1.9670663720	0.1252017705	2.7349354749
H	-2.9637807322	-1.4393286712	3.6247589030
H	-1.5844588794	-2.3539652081	1.7470446932
H	-0.1121732406	-1.8818558709	2.6139540893
H	-1.1886648060	-3.1158754591	3.2980275045
H	-1.8971722999	-0.0863889516	5.4113342170
H	-1.3361334457	-1.7685847974	5.4560019774
H	-0.2919567327	-0.4990178598	4.7797525548
H	-2.6994438200	-0.0400226300	1.4434158800

FR0-SB in *i*-propanol, geometry L' (in Å)

$E_{S_0} = -1625.568112$ hartree

$E_{S_1} = -1625.469529$ hartree

	X	Y	Z
C	0.0150964635	-2.7780116363	0.7184206846
C	0.7760880544	-1.5970601956	0.4060566360
C	0.0761070536	-0.4213777557	-0.0338353627
C	-1.2894375564	-0.4574666726	-0.1373889339
C	-2.0306302500	-1.6415592240	0.1757777791
C	-1.3459090163	-2.8136802692	0.6105256341
H	0.5501303550	-3.6634552125	1.0528801729
H	0.6332362425	0.4814299624	-0.2688773174
H	-1.8926809273	-3.7203173451	0.8548867064
C	-2.2393486393	0.6581029066	-0.5671533919
C	-3.5892381801	-0.0379496373	-0.4442540880
C	-4.8291218335	0.4723126448	-0.6813635367
C	-5.9945510825	-0.3525789010	-0.5134650504
C	-5.7992950341	-1.7089774705	-0.0855863616
C	-4.5496701672	-2.2179746804	0.1595132388
C	-3.4084082542	-1.3922163486	-0.0115536431
H	-4.9314420987	1.5033928258	-0.9936200256
H	-6.6518922726	-2.3598333791	0.0546745247
H	-4.4444218939	-3.2487304640	0.4845008051
C	-2.1410478084	1.8692344587	0.3731903937
H	-1.1363035639	2.3027562576	0.3439644248
H	-2.8569698034	2.6462620039	0.0806420668
H	-2.3593355459	1.5824707044	1.4078304692
C	-1.9731211660	1.0871731255	-2.0189858151
H	-2.6854788452	1.8572677251	-2.3351873065
H	-0.9657472937	1.5031736617	-2.1147320120
H	-2.0567209612	0.2414276199	-2.7095662856
C	2.1784846356	-1.6770457952	0.5607201485
H	2.5763099706	-2.6334679604	0.8991425526
N	3.0869402852	-0.7292879080	0.3658770813
C	4.5032711730	-1.0341315909	0.5233433441
H	4.6339617517	-1.6691196243	1.4096496046
H	5.0132391983	-0.0874576711	0.7179191785
C	5.1022142758	-1.7289705034	-0.7044809912
H	4.9747257640	-1.0797439741	-1.5799699100
H	4.5345856771	-2.6473641782	-0.9073211019
C	6.5800753795	-2.0712848156	-0.5212012580
H	6.7013551378	-2.6935282188	0.3758608040
H	7.1496581670	-1.1511081645	-0.3382727724
C	7.1691108816	-2.8016955280	-1.7256204318
H	8.2283483466	-3.0356065336	-1.5691449118
H	6.6444900928	-3.7464078592	-1.9126871353
H	7.0949502162	-2.1941614269	-2.6356758764
N	-7.2369522693	0.1302388713	-0.7587781071
C	-8.4362579530	-0.6901714120	-0.5486068682
C	-8.8709287520	-0.8012122483	0.9123592403
H	-8.2688341546	-1.6814360673	-0.9799669073

	X	Y	Z
H	-9.2382885707	-0.2397347903	-1.1350005464
H	-9.7417564077	-1.4624927725	0.9802636653
H	-8.0815922667	-1.2138686618	1.5476016448
H	-9.1569051129	0.1735941741	1.3177509272
C	-7.4469595923	1.5189489606	-1.1851706404
C	-7.4372222282	2.5322599516	-0.0419814191
H	-8.4106120456	1.5540648290	-1.6974629513
H	-6.6983543007	1.7769491570	-1.9390126712
H	-7.5328250756	3.5423809787	-0.4549995953
H	-8.2749153201	2.3700456503	0.6425571800
H	-6.5104584486	2.4900342498	0.5382787471
C	3.4138536785	1.9836232803	-1.7420326363
C	2.3704293205	1.3708277549	-2.6791868555
C	3.6706608074	3.4454972498	-2.1176925538
O	3.0426752177	1.8551814303	-0.3951076115
H	4.3616990750	1.4353830741	-1.9169890086
H	2.1980636163	0.3158605177	-2.4381845502
H	1.4140860207	1.8989738163	-2.5859656809
H	2.6896264100	1.4284597743	-3.7282130441
H	4.4198582606	3.8849002197	-1.4503911439
H	4.0358450878	3.5357012900	-3.1493822192
H	2.7501775531	4.0340246075	-2.0271087660
H	2.8887759861	0.2656211357	0.0395398604
C	5.0915236025	3.1017644464	2.0846808761
C	4.4441502309	2.2545680741	3.1768332035
C	6.4234131111	3.6800886910	2.5361306519
O	5.3083793322	2.3386513973	0.9069732735
H	4.4177132802	3.9386167725	1.8469587472
H	3.5122699181	1.8046160928	2.8187161703
H	5.1149724502	1.4426072151	3.4816452667
H	4.2114803557	2.8604351964	4.0613892803
H	6.8712090266	4.2897965594	1.7440623156
H	6.2928614729	4.3155302533	3.4199208190
H	7.1278181133	2.8809619270	2.7964928999
H	4.4224269879	2.1781562307	0.4460863488
C	1.3276017584	4.2627401091	1.4579963787
C	2.0351792964	5.4894270871	0.8896417346
C	0.0420835634	4.6420132307	2.1776084611
O	0.9968905097	3.3311921405	0.4406512053
H	1.9996230107	3.7797741717	2.1842941138
H	2.9400933567	5.2023777042	0.3453179257
H	1.3774076146	6.0234681359	0.1930681878
H	2.3247772149	6.1826963522	1.6890407392
H	-0.4424691389	3.7542399384	2.5968454682
H	0.2418947445	5.3448204434	2.9946474326
H	-0.6606518619	5.1168003373	1.4819899452
H	1.8116983264	2.8312829209	0.1172351561

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