

SUPPLEMENTARY INFORMATION

The effect of molecular structure on the properties of fluorene derivatives for OLED applications

Anna Pidluzhna^{*,a}, Aivars Vembris^a, Raitis Grzibovskis^a, Margarita Anna Zommere^a, Oleksandr Bezvikonnyi^{*,b-d}, Jurate Simokaitiene^b, Melita Baronaite^b, Dmytro Volyniuk^b, Juozas V. Grazulevicius^b, Amjad Ali^c, Glib Baryshnikov^{e,f}, Khrystyna Ivaniuk^g, Hryhorii Starykov^b, Pavlo Stakhira^g

^a Institute of Solid State Physics, University of Latvia, Kengaraga str. 8, Riga LV-1063 Latvia. *Corresponding author: anna.pidluzhna@cfi.lu.lv

^b Department of Polymer Chemistry and Technology, Faculty of Chemical Technology, Kaunas University of Technology, K. Baršausko st. 59, LT-51423 Kaunas, Lithuania *Corresponding author: o.bezvikonnyi@ktu.lt

^c Department of Physics, Faculty of Mathematics and Natural Sciences, Kaunas University of Technology, Studentų st. 50, LT-51369 Kaunas, Lithuania

^d KTU "M-Lab" laboratory center, Kaunas University of Technology, Studentų st. 63A, LT-51369 Kaunas, Lithuania

^e Laboratory of Organic Electronics, Department of Science and Technology, Linköping University, Norrköping, SE-60174, Sweden

^f Department of Chemistry and Nanomaterials Science, Bohdan Khmelnytsky National University, Cherkasy, 18031, Ukraine

^g Department of Electronic Engineering, Institute of Telecommunications, Radioelectronics and Electronic Engineering, Lviv Polytechnic National University, Stepan Bandera 12, 79013, Lviv, Ukraine

Table S1. Emission decay characteristics of the solid samples compounds 1-4

| Sample | $\lambda_{\text{max}}^{\text{em}}$, nm | τ_1 , ns | B, % | τ_2 , ns | B, % | $\lambda_{\text{max}2}^{\text{em}}$, nm | τ_1 , ns | B, % | τ_2 , ns | B, % |
|--------|---|---------------|------|---------------|------|--|---------------|------|---------------|------|
| 1 | 396 | 0.7005 | 94 | 1.536 | 6 | 416 | 0.7821 | 85 | 1.6060 | 15 |
| 2 | 386 | 0.7850 | 100 | - | - | 406 | 0.8139 | 94 | 1.6530 | 6 |
| 3 | 400 | 1.0000 | 100 | - | - | 419 | 1.0370 | 100 | - | - |
| 4 | 399 | 0.7625 | 100 | - | - | 419 | 0.8301 | 98 | 2.5940 | 2 |

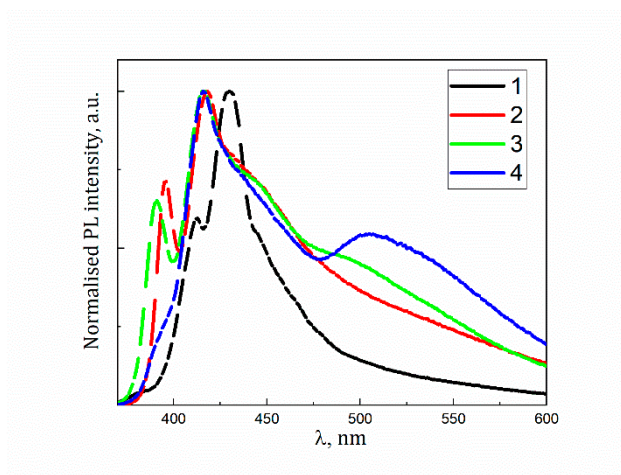


Figure S1. Photoluminescence intensity of 1-4 compounds in thin film state without encapsulation

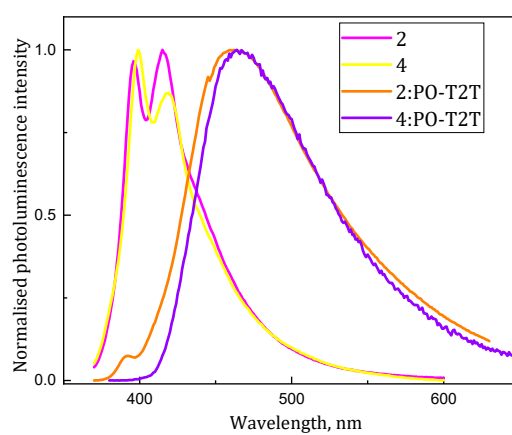


Figure S2. Photoluminescence intensity of 2 and 4 compounds in thin film state encapsulated (magenta and yellow plots) and in mixture with PO-T2T (orange and violet plots)

Table S2. EL characteristics of the fabricated devices

| Device, Emitting layers | V _{on} , V | V ^{Bright} , V* | Brightn ess (Cd*m ⁻²) | EQE (%) | U _c , V | Max Current efficien cy (Cd*A ⁻¹) | U _p , V | Max Power efficiency (lm*W ⁻¹) | x | y |
|-------------------------------|------------------------|-----------------------------|---|------------|-----------------------|---|-----------------------|---|--------|--------|
| A 4/PO-T2T | 3.8 | 7.8 | 520.3 | 0.18 | 5.4 | 0.80 | 4.6 | 0.51 | 0.2406 | 0.3510 |
| B 4/1 | 3.7 | 10.2 | 37.1 | 0.10 | 3.6 | 0.93 | 3.7 | 0.81 | 0.2341 | 0.2890 |
| C 2/1 | 4.7 | 9.0 | 14.9 | 0.14 | 4.7 | 0.52 | 4.8 | 0.33 | 0.1896 | 0.1544 |
| D 2/PO-T2T | 4.1 | 5.8 | 27.3 | 0.24 | 4.8 | 0.65 | 4.6 | 0.43 | 0.2218 | 0.3183 |
| E 4:PO-T2T thick | 3.9 | 8.8 | 1182.1 | 0.42 | 8.4 | 1.40 | 5.0 | 0.73 | 0.1992 | 0.2603 |
| F 4:PO-T2T thin | 3.4 | 6.6 | 1479.2 | 0.45 | 4.6 | 1.19 | 4.4 | 0.83 | 0.1623 | 0.1942 |

V_{on}, V is turn on voltage of OLED; V^{Bright}, V – Voltage for maximal brightness; **Brightness**, (cd*m⁻²) - Maximal value for Brightness; **EQE (%)** is the External Quantum Efficiency at maximal brightness; U_c, V is the voltage at maximal current efficiency; **Max Current efficiency** (cd*A⁻¹) is the maximal current efficiency; U_p, V is the voltage at maximal power efficiency; **Max Power efficiency** (lm*W⁻¹) is the maximal power efficiency; x and y are CIE 1931 coordinates.

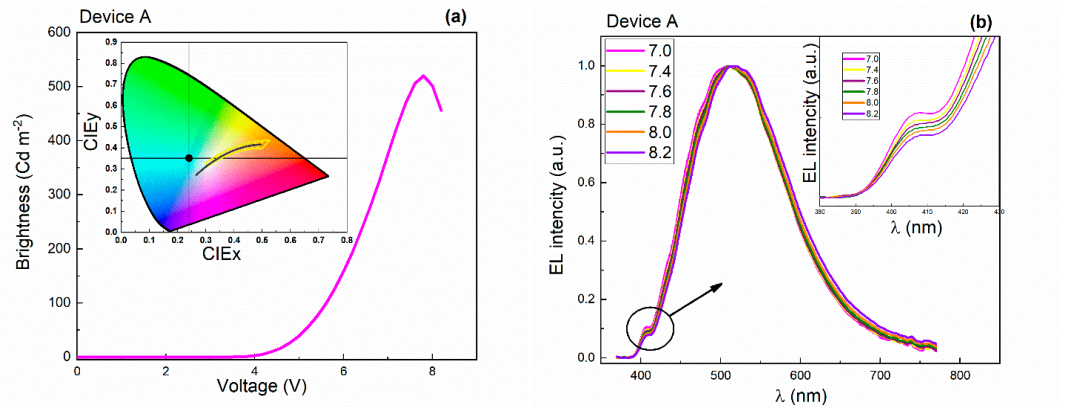


Figure S3. The brightness and CIE1931 chromaticity diagram (a) and EL spectra of the Device A at the different applied voltages (b)

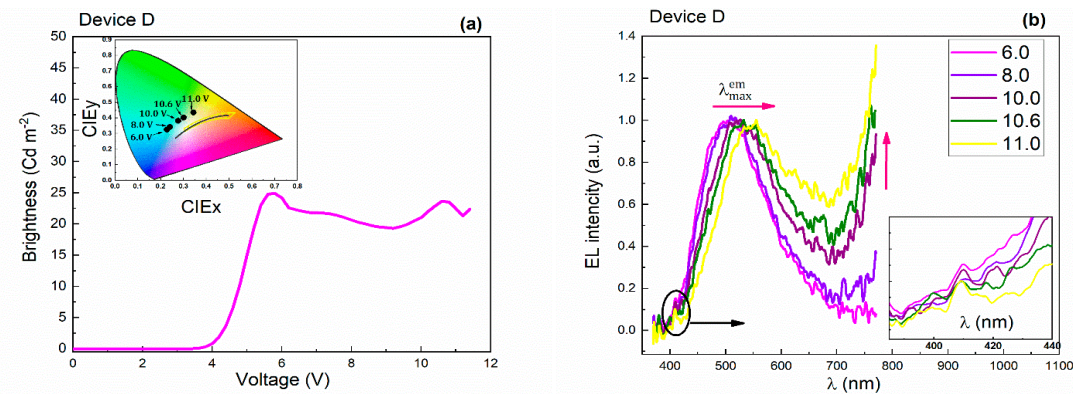


Figure S4. The brightness and CIE1931 chromaticity diagram (a) and EL spectra of the Device D at the different applied voltages (b)

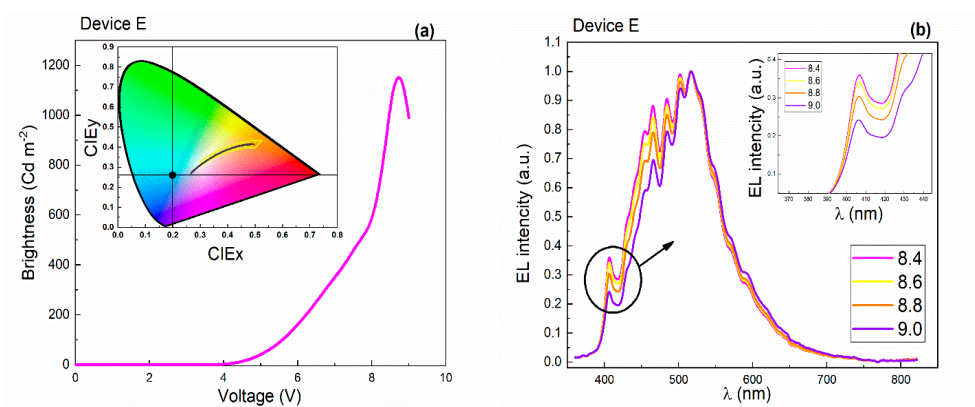


Figure S5. The brightness and CIE1931 chromaticity diagram (a) and EL spectra of the Device E at the different applied voltages (b)

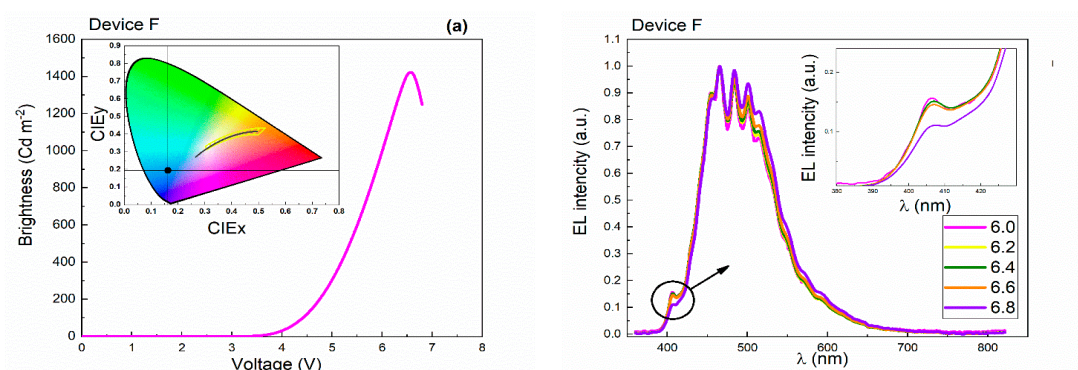


Figure S6. The brightness and CIE1931 chromaticity diagram (a) and EL spectra of the Device F at the different applied voltages (b)

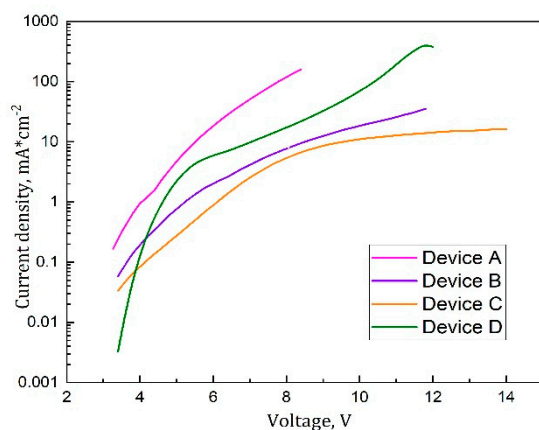


Figure S7. Current density – voltage plots for Devices A-D

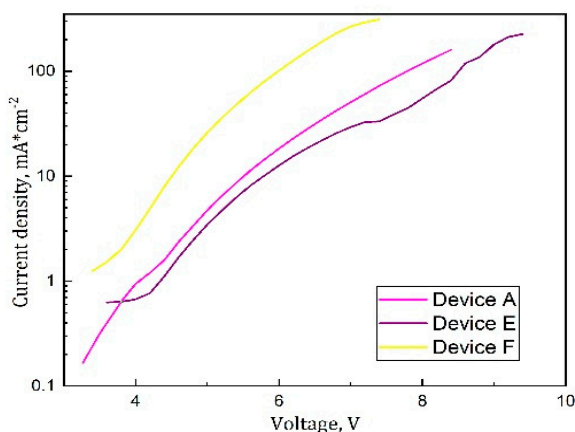


Figure S8. Current density – voltage plots for Devices A, E, F

Below are the cartesian coordinates for all the studied set of molecules optimized in THF solvent using DFT-B3LYP/6-31G(d,p) for ground state, DFT-CAM-B3LYP/6-31G(d,p) for the first singlet excited state, and PCM solvent model. All data is in Å.

Molecule 1

| S0 | | | | S1 | | | |
|----|--------------|-------------|-------------|----|--------------|-------------|-------------|
| C | 3.46703200 | -2.01667800 | 0.04994600 | C | 3.45262500 | 1.98140000 | -0.04402000 |
| C | 2.53848300 | -0.95018100 | 0.04116600 | C | 2.51570400 | 0.90082900 | -0.03918300 |
| C | 1.18124100 | -1.22401700 | -0.00482100 | C | 1.17776800 | 1.16318700 | 0.00651800 |
| C | 0.72988600 | -2.56235000 | -0.00230200 | C | 0.70318400 | 2.51617700 | 0.00752200 |
| C | 1.63782800 | -3.62465400 | 0.00954400 | C | 1.62690500 | 3.59474000 | 0.00675700 |
| C | 3.00070000 | -3.34942900 | 0.02863600 | C | 2.96667500 | 3.32595300 | -0.01474100 |
| C | 0.00000900 | -0.25084900 | -0.00004200 | C | -0.00001500 | 0.19106600 | -0.00002300 |
| C | -1.18125600 | -1.22398200 | 0.00476700 | C | -1.17775700 | 1.16323600 | -0.00655300 |
| C | -0.72993800 | -2.56232900 | 0.00221600 | C | -0.70311800 | 2.51620600 | -0.00753400 |
| C | -2.53849300 | -0.95011500 | -0.04120100 | C | -2.51570500 | 0.90093200 | 0.03914100 |
| C | -3.46706700 | -2.01658900 | -0.05000500 | C | -3.45258100 | 1.98154200 | 0.04399500 |
| C | -3.00076900 | -3.34935300 | -0.02874500 | C | -2.96657600 | 3.32607500 | 0.01473900 |
| C | -1.63790500 | -3.62461100 | -0.00966400 | C | -1.62679400 | 3.59480700 | -0.00675200 |
| C | 0.07479100 | 0.60858000 | 1.29310800 | C | 0.07560500 | -0.66401700 | -1.28826800 |
| C | -0.07474600 | 0.60846900 | -1.29328300 | C | -0.07566900 | -0.66402400 | 1.28821500 |
| C | -1.02148500 | 1.65757400 | 1.49327500 | C | -1.01173200 | -1.71588500 | -1.48859600 |
| C | -0.78231600 | 2.50534500 | 2.74697800 | C | -0.77298100 | -2.54992500 | -2.74514800 |
| C | -1.87233900 | 3.55486300 | 2.98084900 | C | -1.85287600 | -3.60215000 | -2.97983200 |
| C | -1.63745100 | 4.40686900 | 4.23187200 | C | -1.61835100 | -4.44035800 | -4.23390400 |
| C | -2.73184800 | 5.45307300 | 4.45699200 | C | -2.70303000 | -5.48921500 | -4.45932700 |
| C | 1.02153600 | 1.65744200 | -1.49351400 | C | 1.01162100 | -1.71594400 | 1.48853100 |
| C | 0.78246000 | 2.50503500 | -2.74735400 | C | 0.77284600 | -2.54997200 | 2.74508600 |
| C | 1.87247000 | 3.55455800 | -2.98126000 | C | 1.85268900 | -3.60225400 | 2.97975200 |
| C | 1.63768100 | 4.40638300 | -4.23242500 | C | 1.61814200 | -4.44044800 | 4.23382800 |
| C | 2.73206300 | 5.45259500 | -4.45757800 | C | 2.70276900 | -5.48936300 | 4.45923200 |
| C | 4.86149500 | -1.74495600 | 0.08501000 | C | 4.81929900 | 1.72971700 | -0.07956800 |
| C | -4.86152200 | -1.74482600 | -0.08504400 | C | -4.81926600 | 1.72991500 | 0.07953800 |
| C | 6.05370200 | -1.50138100 | 0.11456800 | C | 6.02194100 | 1.49735100 | -0.11074200 |
| C | -6.05372900 | -1.50123900 | -0.11456400 | C | -6.02191300 | 1.49758000 | 0.11071200 |
| C | 7.44617100 | -1.21909700 | 0.14904400 | C | 7.39839600 | 1.23284600 | -0.14605500 |
| C | -7.44620800 | -1.21899600 | -0.14895800 | C | -7.39835800 | 1.23301800 | 0.14604900 |
| C | 7.91182200 | 0.11101200 | 0.16248200 | C | 7.88209700 | -0.09416700 | -0.17482100 |
| C | 9.27317400 | 0.38189800 | 0.19705100 | C | 9.23743700 | -0.34698800 | -0.20871700 |
| C | 10.22282700 | -0.65477500 | 0.21856300 | C | 10.17683000 | 0.69721000 | -0.21796900 |
| C | 9.75285800 | -1.97989300 | 0.20413600 | C | 9.69326700 | 2.01566300 | -0.19006700 |
| C | 8.39377400 | -2.26202000 | 0.17071000 | C | 8.34115200 | 2.28487700 | -0.15400600 |
| C | -8.39377600 | -2.26194600 | -0.17083700 | C | -8.34115500 | 2.28501200 | 0.15403000 |
| C | -9.75286800 | -1.97985700 | -0.20418800 | C | -9.69325900 | 2.01574300 | 0.19011500 |
| C | -10.22288100 | -0.65475000 | -0.21832000 | C | -10.17676800 | 0.69727100 | 0.21801200 |
| C | -9.27326100 | 0.38195100 | -0.19658900 | C | -9.23733400 | -0.34688900 | 0.20872900 |
| C | -7.91190200 | 0.11110100 | -0.16209800 | C | -7.88200400 | -0.09401400 | 0.17480900 |
| C | 11.67324800 | -0.36035200 | 0.25558700 | C | 11.62516300 | 0.41828100 | -0.25574900 |
| C | -11.67331100 | -0.36036700 | -0.25526800 | C | -11.62508900 | 0.41828400 | 0.25581900 |
| C | 12.55733500 | -1.18296600 | 0.97418100 | C | 12.50666700 | 1.27850100 | -0.92343000 |
| C | 13.92281300 | -0.90617300 | 1.00898400 | C | 13.86937100 | 1.01611600 | -0.95867600 |

| | | | | | | | |
|---|--------------|-------------|-------------|---|--------------|-------------|-------------|
| C | 14.43396100 | 0.19976100 | 0.32645900 | C | 14.38305100 | -0.11246300 | -0.32721400 |
| C | 13.56676200 | 1.02603900 | -0.39145100 | C | 13.51966100 | -0.97610700 | 0.33979900 |
| C | 12.20135600 | 0.74883800 | -0.42666000 | C | 12.15690500 | -0.71397500 | 0.37517500 |
| C | -12.20146500 | 0.74860100 | 0.42730800 | C | -12.15679900 | -0.71398500 | -0.37510800 |
| C | -13.56687900 | 1.02576100 | 0.39217100 | C | -13.51954400 | -0.97617200 | -0.33970600 |
| C | -14.43404000 | 0.19966800 | -0.32599700 | C | -14.38295500 | -0.11257100 | 0.32733700 |
| C | -13.92284800 | -0.90604400 | -1.00884900 | C | -13.86930700 | 1.01602000 | 0.95880200 |
| C | -12.55736300 | -1.18280000 | -0.97411600 | C | -12.50661400 | 1.27846000 | 0.92353000 |
| H | 2.91166100 | 0.06679700 | 0.08082400 | H | 2.89910500 | -0.11183600 | -0.08203300 |
| H | 1.29000600 | -4.65364400 | 0.01022200 | H | 1.27187300 | 4.62006500 | 0.01746200 |
| H | 3.72310000 | -4.15904400 | 0.03680500 | H | 3.69029000 | 4.13392500 | -0.01690700 |
| H | -2.91165000 | 0.06687200 | -0.08081500 | H | -2.89914700 | -0.11171800 | 0.08197400 |
| H | -3.72319000 | -4.15894900 | -0.03694000 | H | -3.69015700 | 4.13407600 | 0.01691800 |
| H | -1.29010500 | -4.65360900 | -0.01036500 | H | -1.27172000 | 4.62011700 | -0.01744100 |
| H | 1.04936800 | 1.11207900 | 1.30495100 | H | 1.05233400 | -1.16146800 | -1.30333000 |
| H | 0.07933600 | -0.07627900 | 2.15056800 | H | 0.07546900 | 0.01966800 | -2.14560000 |
| H | -0.07926400 | -0.07647100 | -2.15067800 | H | -0.07549800 | 0.01965500 | 2.14555300 |
| H | -1.04932600 | 1.11196100 | -1.30519500 | H | -1.05242000 | -1.16143000 | 1.30327800 |
| H | -1.09824400 | 1.16709600 | 1.57752500 | H | -1.23270700 | -1.23270700 | -1.56483700 |
| H | -1.07815600 | 2.32078500 | 0.62033600 | H | -1.05938000 | -2.38538700 | -0.62106800 |
| H | 0.19382200 | 3.00554200 | 2.66644900 | H | 0.20612700 | -3.04293300 | -2.67344800 |
| H | -0.71664600 | 1.84623600 | 3.62468200 | H | -0.71680800 | -1.88497500 | -3.61756200 |
| H | -2.84819000 | 3.05376100 | 3.06115100 | H | -2.83173000 | -3.10844300 | -3.05165700 |
| H | -1.93876500 | 4.21232200 | 2.10137300 | H | -1.90993700 | -4.26563000 | -2.10582800 |
| H | -0.66178400 | 4.90630200 | 4.15055000 | H | -0.63985500 | -4.93242000 | -4.16110900 |
| H | -1.57132200 | 3.74859100 | 5.10943800 | H | -1.56157400 | -3.77622300 | -5.10594100 |
| H | -2.54043800 | 6.04797500 | 5.35723500 | H | -2.51307600 | -6.07621800 | -5.36324800 |
| H | -3.71335500 | 4.97705100 | 4.57250000 | H | -3.68722400 | -5.01995200 | -4.56617800 |
| H | -2.79722800 | 6.14339200 | 3.60696000 | H | -2.75887800 | -6.18474000 | -3.61466400 |
| H | 1.07813100 | 2.32077800 | -0.62066400 | H | 1.05922500 | -2.38544900 | 0.62100100 |
| H | 1.99830500 | 1.16695900 | -1.57761300 | H | 1.99147900 | -1.23281300 | 1.56475800 |
| H | 0.71689900 | 1.84580500 | -3.62497600 | H | 0.71672200 | -1.88501900 | 3.61750100 |
| H | -0.19370400 | 3.00520700 | -2.66698800 | H | -0.20628900 | -3.04292900 | 2.67340100 |
| H | 1.93878300 | 4.21214300 | -2.10186800 | H | 1.90970100 | -4.26573700 | 2.10574700 |
| H | 2.84834600 | 3.05347900 | -3.06139100 | H | 2.83157100 | -3.10859800 | 3.05155900 |
| H | 1.57166500 | 3.74798000 | -5.10990600 | H | 1.56141600 | -3.77631000 | 5.10586500 |
| H | 0.66198700 | 4.90579200 | -4.15127300 | H | 0.63961900 | -4.93245900 | 4.16105000 |
| H | 2.54072100 | 6.04736700 | -5.35792200 | H | 2.51280000 | -6.07635500 | 5.36315700 |
| H | 2.79733500 | 6.14303100 | -3.60763400 | H | 2.75856500 | -6.18489100 | 3.61456900 |
| H | 3.71359800 | 4.97659100 | -4.57292400 | H | 3.68699000 | -5.02015200 | 4.56606600 |
| H | 7.19355600 | 0.92456100 | 0.15527400 | H | 7.17268800 | -0.91458600 | -0.17962500 |
| H | 9.60740700 | 1.41406600 | 0.23322700 | H | 9.58137500 | -1.37482100 | -0.25604100 |
| H | 10.46459100 | -2.79947000 | 0.19411500 | H | 10.39633700 | 2.84163200 | -0.16969800 |
| H | 8.05033700 | -3.29131100 | 0.15132200 | H | 7.98851100 | 3.31001400 | -0.12166400 |
| H | -8.05030100 | -3.29122800 | -0.15167200 | H | -7.98855500 | 3.31016300 | 0.12169300 |
| H | -10.46457800 | -2.79945700 | -0.19435300 | H | -10.39636100 | 2.84168400 | 0.16976900 |
| H | -9.60753400 | 1.41411400 | -0.23251800 | H | -9.58123100 | -1.37473700 | 0.25604800 |
| H | -7.19365800 | 0.92466900 | -0.15471500 | H | -7.17256300 | -0.91440500 | 0.17959000 |
| H | 12.16737200 | -2.03018700 | 1.53026600 | H | 12.11665500 | 2.14762900 | -1.44305000 |
| H | 14.58728600 | -1.55073600 | 1.57741800 | H | 14.53234300 | 1.69233300 | -1.48930700 |
| H | 15.49804300 | 0.41561800 | 0.35374500 | H | 15.44844200 | -0.31744500 | -0.35480200 |
| H | 13.95485900 | 1.88415000 | -0.93286200 | H | 13.91011500 | -1.85507500 | 0.84312300 |
| H | 11.54009200 | 1.38289300 | -1.00957700 | H | 11.49881100 | -1.38146900 | 0.92183000 |
| H | -11.54022200 | 1.38250600 | 1.01041300 | H | -11.49869100 | -1.38144600 | -0.92178500 |
| H | -13.95501700 | 1.88369300 | 0.93383600 | H | -13.90997400 | -1.85514900 | -0.84303300 |
| H | -15.49813000 | 0.41549600 | -0.35323000 | H | -15.44833600 | -0.31759700 | 0.35494600 |
| H | -14.58729700 | -1.55045700 | -1.57748300 | H | -14.53229300 | 1.69220400 | 1.48945700 |
| H | -12.16736200 | -2.02985000 | -1.53043600 | H | -12.11662500 | 2.14759700 | 1.44315300 |

Molecule 2

| S0 | | | | S1 | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | 3.50072500 | -1.92009300 | 0.10333700 | C | 3.48862700 | -1.89703900 | 0.09964300 |
| C | 2.54654000 | -0.87631500 | 0.08595900 | C | 2.52349400 | -0.83959900 | 0.08485800 |
| C | 1.19714100 | -1.18143400 | 0.01119300 | C | 1.19417700 | -1.13361700 | 0.01087500 |
| C | 0.77657700 | -2.52960200 | -0.00693400 | C | 0.74995800 | -2.49904800 | -0.01108700 |
| C | 1.70956500 | -3.56972900 | 0.01401000 | C | 1.70289600 | -3.55472200 | -0.00018500 |
| C | 3.06511300 | -3.26283000 | 0.06186500 | C | 3.03441700 | -3.25269800 | 0.05063400 |
| C | -0.00655700 | -0.23585300 | 0.00120000 | C | -0.00722700 | -0.18988600 | 0.00249600 |
| C | -1.16514700 | -1.23587100 | -0.02726700 | C | -1.16203600 | -1.18980000 | -0.02399600 |
| C | -0.68273000 | -2.56326900 | -0.03219400 | C | -0.65310400 | -2.53260400 | -0.02469000 |
| C | -2.52707600 | -0.99224500 | -0.09910900 | C | -2.50376500 | -0.95853600 | -0.09543300 |
| C | -3.43205100 | -2.07847000 | -0.13642000 | C | -3.41730400 | -2.06045800 | -0.13009800 |
| C | -2.93496900 | -3.40016900 | -0.11718600 | C | -2.89896400 | -3.39353500 | -0.10273100 |
| C | -1.56667000 | -3.64491400 | -0.07245500 | C | -1.55453400 | -3.63234900 | -0.05462300 |
| C | 0.02193100 | 0.61196500 | 1.30381100 | C | 0.02168000 | 0.65432100 | 1.29970100 |
| C | -0.07541900 | 0.63480400 | -1.28460400 | C | -0.07766700 | 0.67657500 | -1.27822800 |
| C | -1.10147500 | 1.63440400 | 1.49047700 | C | -1.09336000 | 1.67932300 | 1.48666900 |
| C | -0.91063800 | 2.47297400 | 2.75859600 | C | -0.90413400 | 2.50337700 | 2.75815200 |
| C | -2.02930400 | 3.49519200 | 2.97757000 | C | -2.01312800 | 3.52810200 | 2.97839200 |

| | | | | | | | |
|---|--------------|-------------|-------------|---|--------------|-------------|-------------|
| C | -1.84415500 | 4.33809400 | 4.24305500 | C | -1.82903700 | 4.35618700 | 4.24753500 |
| C | -2.96740500 | 5.35655700 | 4.45272900 | C | -2.94291400 | 5.37717900 | 4.45805900 |
| C | 1.00077500 | 1.70981500 | -1.45336700 | C | 0.98778600 | 1.75604900 | -1.44706600 |
| C | 0.76548500 | 2.56683000 | -2.70150100 | C | 0.75390700 | 2.59747500 | -2.69959000 |
| C | 1.83667700 | 3.64189500 | -2.90433100 | C | 1.81297400 | 3.67705900 | -2.90292300 |
| C | 1.60536700 | 4.50345100 | -4.14947200 | C | 1.58285400 | 4.52280900 | -4.15274500 |
| C | 2.68103200 | 5.57500300 | -4.34353800 | C | 2.64672000 | 5.59893500 | -4.34760400 |
| C | 4.88789500 | -1.61681000 | 0.16625300 | C | 4.84850400 | -1.61295400 | 0.16251400 |
| C | -4.83148200 | -1.83753900 | -0.19744800 | C | -4.78884500 | -1.83939100 | -0.19183600 |
| C | 6.07438600 | -1.34932500 | 0.21864800 | C | 6.04481600 | -1.35423400 | 0.21682500 |
| C | -6.02804100 | -1.61914800 | -0.24872300 | C | -5.99528300 | -1.63249100 | -0.24565400 |
| C | 7.45979900 | -1.03727900 | 0.27900900 | C | 7.41615500 | -1.05898700 | 0.27726800 |
| C | -7.42610700 | -1.36959800 | -0.30801700 | C | -7.37831400 | -1.39789100 | -0.30601800 |
| C | 7.89861400 | 0.30498700 | 0.31337300 | C | 7.87110300 | 0.28021400 | 0.32132400 |
| C | 9.24833600 | 0.60828300 | 0.37184400 | C | 9.21566800 | 0.56607400 | 0.37986200 |
| C | 10.20574300 | -0.41938300 | 0.39803200 | C | 10.16138800 | -0.46953000 | 0.39698900 |
| C | 9.78889000 | -1.75706700 | 0.36430200 | C | 9.73397800 | -1.80046400 | 0.35425100 |
| C | 8.42989800 | -2.05501700 | 0.30562400 | C | 8.38074100 | -2.08557200 | 0.29543300 |
| C | -8.35091200 | -2.43622200 | -0.35722900 | C | -8.29876800 | -2.47186000 | -0.34751200 |
| C | -9.71249700 | -2.19159800 | -0.41474200 | C | -9.65315300 | -2.23707900 | -0.40634500 |
| C | -10.19662900 | -0.87292200 | -0.42523500 | C | -10.14584400 | -0.92402600 | -0.42626500 |
| C | -9.29384700 | 0.19803800 | -0.37683000 | C | -9.25404800 | 0.15252100 | -0.38596900 |
| C | -7.92573000 | -0.05510200 | -0.31904200 | C | -7.89186700 | -0.08619100 | -0.32694200 |
| O | 11.50345500 | -0.01721200 | 0.45614300 | O | 11.45539200 | -0.08317700 | 0.45550300 |
| O | -11.54872000 | -0.74013100 | -0.48351900 | O | -11.49071700 | -0.80162900 | -0.48475200 |
| C | -12.09348100 | 0.57651000 | -0.49833400 | C | -12.04786000 | 0.50210700 | -0.50768100 |
| C | 12.51565000 | -1.01975400 | 0.48632400 | C | 12.45729500 | -1.08641100 | 0.47549200 |
| H | 2.89430300 | 0.14898400 | 0.14143800 | H | 2.88058200 | 0.18207100 | 0.14322400 |
| H | 1.38662400 | -4.60676000 | -0.00068500 | H | 1.37435700 | -4.58868300 | -0.02623700 |
| H | 3.80569900 | -4.05585100 | 0.07710800 | H | 3.77724400 | -4.04327900 | 0.06094700 |
| H | -2.92175700 | 0.01665600 | -0.13783000 | H | -2.90925000 | 0.04569700 | -0.13749200 |
| H | -3.63810800 | -4.22615400 | -0.14749100 | H | -3.60314000 | -4.21842700 | -0.12763800 |
| H | -1.19631200 | -4.66613500 | -0.07538000 | H | -1.17707000 | -4.64981900 | -0.04539600 |
| H | 0.98468300 | 1.13653400 | 1.34171600 | H | 0.98651000 | 1.17324400 | 1.34099000 |
| H | 0.02329400 | -0.08136700 | 2.15447500 | H | 0.01849200 | -0.03780200 | 2.15028000 |
| H | -0.04800000 | -0.04132500 | -2.14856800 | H | -0.04395000 | 0.00172100 | -2.14191500 |
| H | -1.06067000 | 1.11661000 | -1.31082000 | H | -1.06576000 | 1.15057500 | -1.30848900 |
| H | -2.06873800 | 1.12160700 | 1.54648100 | H | -2.06342600 | 1.17325300 | 1.53326500 |
| H | -1.15287700 | 2.30625400 | 0.62380500 | H | -1.13555700 | 2.35811200 | 0.62602800 |
| H | 0.05565200 | 2.99559600 | 2.70678100 | H | 0.06496300 | 3.01914700 | 2.71637000 |
| H | -0.85092800 | 1.80560900 | 3.63047500 | H | -0.85405800 | 1.82941200 | 3.62402000 |
| H | -2.99518600 | 2.97144000 | 3.02870200 | H | -2.98189600 | 3.01152100 | 3.02006100 |
| H | -2.08953300 | 4.16097800 | 2.10391400 | H | -2.06392900 | 4.20075300 | 2.11100600 |
| H | -0.87854200 | 4.86043900 | 4.19087400 | H | -0.86069600 | 4.87134000 | 4.20485000 |
| H | -1.78407800 | 3.67159900 | 5.11483500 | H | -1.77838500 | 3.68298700 | 5.11297500 |
| H | -2.81145200 | 5.94553600 | 5.36365500 | H | -2.78894200 | 5.95745400 | 5.37311900 |
| H | -3.94019600 | 4.85705600 | 4.53927500 | H | -3.91830500 | 4.88424800 | 4.53499800 |
| H | -3.02820300 | 6.05472300 | 3.60878000 | H | -2.99409700 | 6.08140500 | 3.62032600 |
| H | 1.02742300 | 2.36391100 | -0.57213900 | H | 1.00280500 | 2.41741800 | -0.57208700 |
| H | 1.98936300 | 1.24166100 | -1.52532400 | H | 1.98000100 | 1.29670000 | -1.50849700 |
| H | 0.72926900 | 1.91669700 | -3.58759200 | H | 0.73015000 | 1.94054300 | -3.57957000 |
| H | -0.22242400 | 3.04526400 | -2.63274100 | H | -0.23776200 | 3.06680100 | -2.64224800 |
| H | 1.87388900 | 4.29025600 | -2.01640800 | H | 1.83783900 | 4.33248700 | -2.02134300 |
| H | 2.82425000 | 3.16255100 | -2.97319200 | H | 2.80436500 | 3.20710900 | -2.96078300 |
| H | 1.56833100 | 3.85427500 | -5.03549600 | H | 1.55824900 | 3.86674900 | -5.03237300 |
| H | 0.61805600 | 4.98129600 | -4.07954200 | H | 0.59186900 | 4.99121900 | -4.09389900 |
| H | 2.49266700 | 6.17625700 | -5.24021200 | H | 2.46040800 | 6.19082000 | -5.24821800 |
| H | 2.71706600 | 6.25656400 | -3.48472600 | H | 2.67013200 | 6.28669900 | -3.49419200 |
| H | 3.67426700 | 5.12110300 | -4.44716600 | H | 3.64350900 | 5.15382600 | -4.43914800 |
| H | 7.16431400 | 1.10386800 | 0.29342700 | H | 7.14455900 | 1.08536000 | 0.30822500 |
| H | 9.59032200 | 1.63784500 | 0.39855700 | H | 9.57103300 | 1.59015500 | 0.41378400 |
| H | 10.50824200 | -2.56651300 | 0.38295000 | H | 10.44718100 | -2.61475000 | 0.36621700 |
| H | 8.11065900 | -3.09198700 | 0.27965100 | H | 8.05175700 | -3.11852700 | 0.26231100 |
| H | -7.98382400 | -3.45746800 | -0.34956400 | H | -7.92385900 | -3.48943600 | -0.33243700 |
| H | -10.42684000 | -3.00761100 | -0.45275300 | H | -10.36395400 | -3.05555100 | -0.43846100 |
| H | -9.64312300 | 1.22322100 | -0.38349200 | H | -9.61322700 | 1.17361600 | -0.40007800 |
| H | -7.22942900 | 0.77659400 | -0.28157800 | H | -7.20221100 | 0.75032400 | -0.29568700 |
| H | -13.17550800 | 0.45038600 | -0.54705800 | H | -13.12767500 | 0.36631300 | -0.55509400 |
| H | -11.82963300 | 1.12617900 | 0.41294700 | H | -11.79001000 | 1.05946400 | 0.39909200 |
| H | -11.75052200 | 1.13867600 | -1.37497900 | H | -11.71184500 | 1.06159800 | -1.38715000 |
| H | 13.46414200 | -0.48383900 | 0.53343000 | H | 13.40924000 | -0.55908400 | 0.52468900 |
| H | 12.41325800 | -1.66138400 | 1.36949600 | H | 12.35311400 | -1.73342100 | 1.35292100 |
| H | 12.48933000 | -1.63855600 | -0.41842900 | H | 12.42534700 | -1.69694500 | -0.43316200 |

Molecule 3

| S0 | | | | S1 | | | |
|----|------------|-------------|-------------|----|------------|-------------|-------------|
| C | 3.61489300 | -1.36980500 | 0.05055500 | C | 3.60211300 | -1.35233300 | 0.05520300 |
| C | 2.53109800 | -0.46139200 | 0.05481400 | C | 2.50851400 | -0.43213000 | 0.07085500 |
| C | 1.23622300 | -0.93992600 | -0.05984900 | C | 1.22962700 | -0.89651800 | -0.03787300 |

| | | | | | | | |
|---|--------------|-------------|-------------|---|--------------|-------------|-------------|
| C | 1.00076100 | -2.33051900 | -0.13945900 | C | 0.97399700 | -2.30255700 | -0.12586200 |
| C | 2.06358300 | -3.23794000 | -0.14157800 | C | 2.05298800 | -3.22235200 | -0.14511200 |
| C | 3.36476500 | -2.75575100 | -0.05370700 | C | 3.33397400 | -2.75122600 | -0.06002800 |
| C | -0.08234100 | -0.16321200 | -0.06105200 | C | -0.08506200 | -0.11991800 | -0.02906000 |
| C | -1.09522000 | -1.30688900 | -0.14595200 | C | -1.09570100 | -1.26144800 | -0.10991700 |
| C | -0.44042500 | -2.55745100 | -0.19323300 | C | -0.41825000 | -2.52133800 | -0.16333900 |
| C | -2.47614800 | -1.24450700 | -0.22842700 | C | -2.45724100 | -1.20625100 | -0.18384500 |
| C | -3.22668200 | -2.43972500 | -0.31728400 | C | -3.21434500 | -2.41508300 | -0.27350100 |
| C | -2.55933300 | -3.68362100 | -0.34360200 | C | -2.52702800 | -3.66693900 | -0.30449600 |
| C | -1.17097300 | -3.74513200 | -0.28890900 | C | -1.16134100 | -3.72573100 | -0.25434700 |
| C | -0.18991600 | 0.63603900 | 1.26790000 | C | -0.18306600 | 0.67326700 | -1.29661900 |
| C | -0.24627700 | 0.73351100 | -1.32062900 | C | -0.25521000 | 0.77441300 | -1.28156200 |
| C | -1.45006500 | 1.48217900 | 1.46536600 | C | -1.43142700 | 1.52691200 | 1.50223800 |
| C | -1.39767500 | 2.30589100 | 2.75610900 | C | -1.36554500 | 2.33761700 | 2.79439500 |
| C | -2.66140100 | 3.13970800 | 2.98491300 | C | -2.61451300 | 3.18131700 | 3.03279400 |
| C | -2.62005100 | 3.96873500 | 4.27212000 | C | -2.55754000 | 3.99829800 | 4.32097600 |
| C | -3.88947100 | 4.79551900 | 4.49108700 | C | -3.81222700 | 4.83564500 | 4.54915600 |
| C | 0.67389200 | 1.95162900 | -1.42928900 | C | 0.65698800 | 1.99264200 | -1.39371400 |
| C | 0.35224600 | 2.80632200 | -2.65962600 | C | 0.33189100 | 2.83730000 | -2.62352800 |
| C | 1.26508200 | 4.02771400 | -2.79853200 | C | 1.23644700 | 4.05775600 | -2.76733000 |
| C | 0.94746400 | 4.88797300 | -4.02539700 | C | 0.91534700 | 4.90792800 | -3.99387000 |
| C | 1.86424900 | 6.10689600 | -4.15448200 | C | 1.82457500 | 6.12565900 | -4.12756000 |
| C | 4.94747900 | -0.88829100 | 0.15451500 | C | 4.91106900 | -0.89506400 | 0.15236100 |
| C | -4.64462200 | -2.37532600 | -0.37640000 | C | -4.60253900 | -2.36586400 | -0.32762200 |
| C | 6.08450200 | -0.46225200 | 0.24261300 | C | 6.06169700 | -0.48088600 | 0.23716000 |
| C | -5.85835500 | -2.29162100 | -0.41742200 | C | -5.82535300 | -2.29450800 | -0.36840300 |
| C | 7.41484900 | 0.02571800 | 0.34427700 | C | 7.37567400 | -0.00911700 | 0.33259900 |
| C | -7.27306000 | -2.16991100 | -0.45822900 | C | -7.22085400 | -2.19746200 | -0.41048900 |
| C | 8.52538900 | -0.88969500 | 0.36262800 | C | 8.49105600 | -0.92611700 | 0.32316200 |
| C | 9.85162200 | -0.36079100 | 0.46547100 | C | 9.80929400 | -0.40071600 | 0.42131400 |
| C | 10.03998400 | 1.04418300 | 0.54634600 | C | 10.00041500 | 0.99825600 | 0.52522000 |
| C | 8.96113000 | 1.90069500 | 0.52709500 | C | 8.92300300 | 1.85741800 | 0.53307100 |
| C | 7.64979700 | 1.39447300 | 0.42631300 | C | 7.61948200 | 1.36366000 | 0.43800900 |
| C | -8.06761500 | -3.29290200 | -0.66396500 | C | -8.00341500 | -3.34995400 | -0.52542300 |
| C | -9.47250200 | -3.18917400 | -0.70703500 | C | -9.39781100 | -3.27066200 | -0.56995800 |
| C | -10.08724800 | -1.96699100 | -0.54501300 | C | -10.03327000 | -2.04994300 | -0.50045700 |
| C | -9.31942700 | -0.79189100 | -0.33116000 | C | -9.28796800 | -0.85207200 | -0.38156200 |
| C | -7.89157000 | -0.88152300 | -0.28474400 | C | -7.86747800 | -0.90837700 | -0.33448100 |
| C | 8.35192000 | -2.29426300 | 0.28274000 | C | 8.31781000 | -2.32176800 | 0.22044800 |
| C | 9.43864000 | -3.14091500 | 0.30333800 | C | 9.40074200 | -3.16837000 | 0.21447000 |
| C | 10.75121200 | -2.62086100 | 0.40493900 | C | 10.70885400 | -2.65182600 | 0.31156900 |
| C | 10.95038500 | -1.26129100 | 0.48402700 | C | 10.90638700 | -1.29878900 | 0.41258800 |
| C | -9.93365300 | 0.47769700 | -0.15954900 | C | -9.92582000 | 0.41196000 | -0.30622100 |
| C | -9.17542500 | 1.60721900 | 0.04950800 | C | -9.19352400 | 1.56510800 | -0.18865400 |
| C | -7.76367900 | 1.51538400 | 0.09611200 | C | -7.78580200 | 1.50485900 | -0.14104700 |
| C | -7.13750400 | 0.29911700 | -0.06749500 | C | -7.13994600 | 0.29365900 | -0.21278500 |
| H | 2.73788000 | 0.59769600 | 0.15801300 | H | 2.72618400 | 0.62395700 | 0.17896300 |
| H | 1.88214400 | -4.30694400 | -0.20495300 | H | 1.86378400 | -4.28817600 | -0.22063300 |
| H | 4.20474500 | -3.44279200 | -0.05522900 | H | 4.17435900 | -3.43699000 | -0.07195000 |
| H | -3.00229900 | -0.29685000 | -0.23555000 | H | -2.99218600 | -0.26380900 | -0.18607500 |
| H | -3.14578100 | -4.59386100 | -0.41371400 | H | -3.11487700 | -4.57581400 | -0.37340800 |
| H | -0.66703600 | -4.70668500 | -0.32428200 | H | -0.65163100 | -4.68310700 | -0.28822400 |
| H | 0.68843600 | 1.28941900 | 1.33863100 | H | 0.70008900 | 1.31877000 | 1.36733700 |
| H | -0.10181600 | -0.07785800 | 2.09663500 | H | -0.09746700 | -0.04175300 | 2.12353700 |
| H | -0.10868200 | 0.09759400 | -2.20433400 | H | -0.11914000 | 0.14159900 | -2.16670300 |
| H | -1.28795300 | 1.07558900 | -1.35560900 | H | -1.29757500 | 1.11205300 | -1.31364400 |
| H | -2.33371800 | 0.83431300 | 1.49589700 | H | -2.32075800 | 0.88860500 | 1.53121100 |
| H | -1.58974900 | 2.16224400 | 0.61498200 | H | -1.56700900 | 2.21432900 | 0.65829400 |
| H | -0.52161900 | 2.97014900 | 2.72916400 | H | -0.48306800 | 2.99138500 | 2.76952800 |
| H | -1.24521300 | 1.63259400 | 3.61195400 | H | -1.21799200 | 1.65718000 | 3.64387000 |
| H | -3.53609400 | 2.47323100 | 3.01088900 | H | -3.49583200 | 2.52575400 | 3.05824000 |
| H | -2.81472400 | 3.81027600 | 2.12638700 | H | -2.76352300 | 3.85863800 | 2.18046400 |
| H | -1.74653200 | 4.63518000 | 4.24459300 | H | -1.67730700 | 4.65352900 | 4.29406100 |
| H | -2.46549000 | 3.29769700 | 5.12863000 | H | -2.40754500 | 3.32067200 | 5.17129500 |
| H | -3.83495500 | 5.37853200 | 5.41740900 | H | -3.74795700 | 5.41160800 | 5.47751200 |
| H | -4.77372500 | 4.14937700 | 4.55350500 | H | -4.70263300 | 4.20033000 | 4.61087400 |
| H | -4.05016800 | 5.49676200 | 3.66293000 | H | -3.96764800 | 5.54297600 | 3.72702900 |
| H | 0.58744700 | 2.57544200 | -0.53014300 | H | 0.56752500 | 2.61962900 | -0.49816500 |
| H | 1.71961100 | 1.62750800 | -1.48592300 | H | 1.70335300 | 1.67411100 | -1.44915400 |
| H | 0.43225700 | 2.18648000 | -3.56430500 | H | 0.41434600 | 2.21457900 | -3.52452700 |
| H | -0.69502400 | 3.13806900 | -2.60781800 | H | -0.71563100 | 3.16444300 | -2.57323000 |
| H | 1.18584000 | 4.64567000 | -1.89189100 | H | 1.15500800 | 4.67877700 | -1.86452600 |
| H | 2.31220100 | 3.69497100 | -2.84996800 | H | 2.28379700 | 3.72978300 | -2.81771400 |
| H | 1.02770400 | 4.26946800 | -4.93028200 | H | 0.99754300 | 4.28644600 | -4.89483300 |
| H | -0.09942000 | 5.21855500 | -3.97326400 | H | -0.13153400 | 5.23398300 | -3.94274700 |
| H | 1.61658000 | 6.70445200 | -5.03910300 | H | 1.57526300 | 6.71826600 | -5.01321200 |
| H | 1.77918200 | 6.75810200 | -3.27581100 | H | 1.73739000 | 6.77924300 | -3.25260000 |
| H | 2.91452800 | 5.80199500 | -4.23952300 | H | 2.87463600 | 5.82469100 | -4.21146800 |
| H | 11.05202600 | 1.43219700 | 0.62376000 | H | 11.01283600 | 1.38384000 | 0.59868700 |

| | | | | | | | |
|---|--------------|-------------|-------------|---|--------------|-------------|-------------|
| H | 9.11340100 | 2.97393400 | 0.58936600 | H | 9.08210200 | 2.92778000 | 0.61330200 |
| H | 6.80565800 | 2.07621400 | 0.41160500 | H | 6.77671000 | 2.04609800 | 0.44457200 |
| H | -7.59165500 | -4.25949500 | -0.79309200 | H | -7.51079100 | -4.31442800 | -0.58120000 |
| H | -10.06684700 | -4.08315500 | -0.86966900 | H | -9.97998200 | -4.18187500 | -0.66040900 |
| H | -11.17027900 | -1.88474100 | -0.57797500 | H | -11.11692900 | -1.99029900 | -0.53539100 |
| H | 7.34469000 | -2.69085200 | 0.20496300 | H | 7.31096200 | -2.71868000 | 0.14599800 |
| H | 9.28937500 | -4.21492400 | 0.24136300 | H | 9.24911300 | -4.23997900 | 0.13478300 |
| H | 11.59962900 | -3.29868500 | 0.42020200 | H | 11.55761800 | -3.32809500 | 0.30613000 |
| H | 11.95473800 | -0.85340700 | 0.56233000 | H | 11.91047700 | -0.89167100 | 0.48806500 |
| H | -11.01814200 | 0.53898800 | -0.19629700 | H | -11.01070000 | 0.44826000 | -0.34302000 |
| H | -9.65720700 | 2.57180200 | 0.17973800 | H | -9.69452600 | 2.52609800 | -0.13150100 |
| H | -7.17182000 | 2.41077300 | 0.26250000 | H | -7.21007600 | 2.41997400 | -0.04692700 |
| H | -6.05527300 | 0.22676800 | -0.03129400 | H | -6.05678700 | 0.24713400 | -0.17546900 |

Molecule 4

| S0 | | | | S1 | | | |
|----|--------------|-------------|-------------|----|--------------|-------------|-------------|
| C | -3.44252300 | -2.32989400 | -0.06864800 | C | -3.43125000 | -2.30642200 | -0.06239100 |
| C | -2.53033500 | -1.24922600 | -0.05213800 | C | -2.50912400 | -1.21140800 | -0.04830800 |
| C | -1.16905000 | -1.50176300 | -0.00491300 | C | -1.16770800 | -1.45361900 | -0.00146000 |
| C | -0.69611000 | -2.83260900 | -0.01424400 | C | -0.67146900 | -2.79828800 | -0.00803200 |
| C | -1.58746300 | -3.90880900 | -0.03381200 | C | -1.57848100 | -3.89052200 | -0.01827000 |
| C | -2.95455900 | -3.65505700 | -0.05383100 | C | -2.92245200 | -3.64346000 | -0.04112300 |
| C | -0.00340400 | -0.50976600 | -0.00162500 | C | -0.00488600 | -0.46302300 | 0.00059700 |
| C | 1.19352700 | -1.46370800 | -0.00998200 | C | 1.18851400 | -1.41620600 | -0.00986100 |
| C | 0.76349100 | -2.80904600 | -0.01626000 | C | 0.73605300 | -2.77540700 | -0.01980600 |
| C | 2.54611900 | -1.16813600 | 0.03970300 | C | 2.52278200 | -1.13194700 | 0.03917300 |
| C | 3.49239000 | -2.21916100 | 0.04308200 | C | 3.47730900 | -2.19539200 | 0.03880300 |
| C | 3.04708400 | -3.55901000 | 0.01292100 | C | 3.01379400 | -3.54564800 | 0.00144200 |
| C | 1.68886400 | -3.85620800 | -0.00959100 | C | 1.67754400 | -3.83695300 | -0.02352500 |
| C | -0.08965400 | 0.35598800 | -1.28977900 | C | -0.09182300 | 0.39929900 | -1.28197500 |
| C | 0.05488300 | 0.34313600 | 1.29665300 | C | 0.05469700 | 0.38498800 | 1.29426100 |
| C | 0.99050900 | 1.42297600 | -1.48240100 | C | 0.97941700 | 1.46904700 | -1.47432800 |
| C | 0.73926800 | 2.27504300 | -2.73080700 | C | 0.72875400 | 2.30856500 | -2.72488200 |
| C | 1.81323900 | 3.34260300 | -2.95726000 | C | 1.79290900 | 3.37842000 | -2.95169200 |
| C | 1.56611200 | 4.19881700 | -4.20303800 | C | 1.54630600 | 4.22210700 | -4.19975300 |
| C | 2.64441700 | 5.26315300 | -4.42074900 | C | 2.61533300 | 5.28856500 | -4.41727200 |
| C | -1.05802100 | 1.37388600 | 1.49985900 | C | -1.04862000 | 1.41937600 | 1.49824700 |
| C | -0.83733000 | 2.21642400 | 2.76046100 | C | -0.82812500 | 2.24697300 | 2.76235200 |
| C | -1.94440400 | 3.24749100 | 2.99632200 | C | -1.92430900 | 3.28163200 | 2.99965200 |
| C | -1.72890900 | 4.09426600 | 4.25437700 | C | -1.70866000 | 4.11333900 | 4.26141600 |
| C | -2.84057800 | 5.12172200 | 4.48123600 | C | -2.80977300 | 5.14442100 | 4.48920000 |
| C | -4.84088300 | -2.07958000 | -0.10471500 | C | -4.79959700 | -2.07553000 | -0.09884700 |
| C | 4.88241800 | -1.92603500 | 0.08124500 | C | 4.84196300 | -1.92079000 | 0.07673100 |
| C | -6.03559100 | -1.84739400 | -0.13490000 | C | -6.00638000 | -1.85655200 | -0.13061200 |
| C | 6.07024200 | -1.66136400 | 0.11322100 | C | 6.03923100 | -1.66720700 | 0.10948600 |
| C | -7.43378600 | -1.59490800 | -0.17001900 | C | -7.38386300 | -1.61414300 | -0.16611400 |
| C | 7.46141500 | -1.37196300 | 0.15014600 | C | 7.41449900 | -1.38807800 | 0.14604700 |
| C | -8.35765500 | -2.68853400 | -0.19381700 | C | -8.30939100 | -2.71090700 | -0.18331000 |
| C | -9.70942200 | -2.46508900 | -0.22789300 | C | -9.65074100 | -2.49242100 | -0.21786600 |
| C | -10.23701100 | -1.14167600 | -0.24090000 | C | -10.18399200 | -1.16813100 | -0.23824800 |
| C | -9.31718500 | -0.04089600 | -0.21706200 | C | -9.27127400 | -0.06902500 | -0.22122500 |
| C | -7.92646900 | -0.29609400 | -0.18186900 | C | -7.88880100 | -0.31287400 | -0.18556700 |
| C | 7.91985700 | -0.05892500 | 0.18431500 | C | 7.88407300 | -0.07557600 | 0.18259400 |
| C | 9.30096400 | 0.23285100 | 0.22141800 | C | 9.25897600 | 0.20447900 | 0.21910900 |
| C | 10.24957000 | -0.83986300 | 0.22373000 | C | 10.19857900 | -0.86661700 | 0.21902500 |
| C | 9.76039200 | -2.17431400 | 0.18807300 | C | 9.70355700 | -2.20024800 | 0.18136200 |
| C | 8.41349900 | -2.43719000 | 0.15261100 | C | 8.36573600 | -2.45681200 | 0.14629100 |
| C | 9.79080700 | 1.56955500 | 0.25724400 | C | 9.75729000 | 1.53865100 | 0.25685500 |
| C | 11.13586000 | 1.82798600 | 0.29334100 | C | 11.09641200 | 1.78725500 | 0.29210000 |
| C | 12.07486800 | 0.75836500 | 0.29574000 | C | 12.02643800 | 0.71381400 | 0.29190500 |
| C | 11.63861300 | -0.55248600 | 0.26124900 | C | 11.58340600 | -0.58958700 | 0.25580500 |
| C | -11.62354700 | -0.88482500 | -0.27627800 | C | -11.56345500 | -0.92071700 | -0.27405900 |
| C | -12.10508600 | 0.41382000 | -0.28821900 | C | -12.05210400 | 0.37210500 | -0.29299500 |
| C | -11.20011700 | 1.50828500 | -0.26445800 | C | -11.15686000 | 1.46917800 | -0.27608800 |
| C | -9.84326700 | 1.27598500 | -0.22990700 | C | -9.80575700 | 1.24529100 | -0.24127100 |
| O | -13.45959800 | 0.55698000 | -0.32306600 | O | -13.39983800 | 0.50604800 | -0.32748100 |
| O | 13.37765000 | 1.14809500 | 0.33383300 | O | 13.32546900 | 1.09146600 | 0.32911700 |
| C | 14.37430200 | 0.13061400 | 0.34056000 | C | 14.31216200 | 0.07458500 | 0.33286900 |
| C | -14.00427600 | 1.87321500 | -0.33829300 | C | -13.95416400 | 1.81049400 | -0.34915200 |
| H | -2.91932100 | -0.23800600 | -0.08697400 | H | -2.90771100 | -0.20432800 | -0.08561800 |
| H | -1.22369000 | -4.93233800 | -0.03962500 | H | -1.20763300 | -4.91043900 | -0.01369800 |
| H | -3.66384900 | -4.47615200 | -0.06785100 | H | -3.63261900 | -4.46335800 | -0.05039300 |
| H | 2.90249700 | -0.14537900 | 0.08600800 | H | 2.88848200 | -0.11290600 | 0.08827400 |
| H | 3.78234500 | -4.35704800 | 0.01699400 | H | 3.75004700 | -4.34228800 | 0.00008200 |
| H | 1.35795200 | -4.89075000 | -0.01574300 | H | 1.34051700 | -4.86835200 | -0.04031600 |
| H | -1.07193500 | 0.84437200 | -1.30020100 | H | -1.07613900 | 0.88172500 | -1.29548700 |
| H | -0.08238700 | -0.32387400 | -2.15119700 | H | -0.07995700 | -0.27882100 | -2.14366500 |
| H | 0.06762800 | -0.34663200 | 2.15009700 | H | 0.06206500 | -0.30421300 | 2.14717000 |
| H | 1.02158000 | 0.86146900 | 1.31420700 | H | 1.02396000 | 0.89670500 | 1.31568300 |

| | | | | | | | |
|---|--------------|-------------|-------------|---|--------------|-------------|-------------|
| H | 1.97469800 | 0.94804700 | -1.56892800 | H | 1.96644000 | 1.00125200 | -1.55336500 |
| H | 1.03641600 | 2.08133100 | -0.60515200 | H | 1.01663800 | 2.13290200 | -0.60191200 |
| H | -0.24446900 | 2.75975400 | -2.64785900 | H | -0.25762500 | 2.78646800 | -2.65012000 |
| H | 0.68423700 | 1.62063800 | -3.61275500 | H | 0.68270800 | 1.64917300 | -3.60211300 |
| H | 2.79670000 | 2.85704600 | -3.04002100 | H | 2.77901000 | 2.89985300 | -3.02673500 |
| H | 1.86904500 | 3.99543600 | -2.07360100 | H | 1.83995000 | 4.03637000 | -2.07290300 |
| H | 0.58280800 | 4.68265000 | -4.11931500 | H | 0.56057500 | 4.69905000 | -4.12378600 |
| H | 1.51070100 | 3.54515900 | -5.08478500 | H | 1.49961400 | 3.56350400 | -5.07657100 |
| H | 2.44449600 | 5.86069900 | -5.31739000 | H | 2.41696600 | 5.87916300 | -5.31704600 |
| H | 3.63321100 | 4.80303900 | -4.53847400 | H | 3.60641300 | 4.83474200 | -4.52708700 |
| H | 2.69859000 | 5.94903400 | -3.56634300 | H | 2.66062800 | 5.97876900 | -3.56761800 |
| H | -1.12130800 | 2.04234000 | 0.63135800 | H | -1.10218600 | 2.09497600 | 0.63575000 |
| H | -2.02747200 | 0.86795300 | 1.57651200 | H | -2.02153800 | 0.92122700 | 1.56593300 |
| H | -0.76568600 | 1.55231600 | 3.63391200 | H | -0.76672800 | 1.57614300 | 3.62990700 |
| H | 0.13142800 | 2.73196700 | 2.68799900 | H | 0.14411700 | 2.75461200 | 2.69957600 |
| H | -2.01666600 | 3.91002100 | 2.12110700 | H | -1.98650300 | 3.95108200 | 2.13053800 |
| H | -2.91280000 | 2.73089400 | 3.06825600 | H | -2.89624400 | 2.77321700 | 3.06241300 |
| H | -1.65687300 | 3.43097700 | 5.12768300 | H | -1.64671900 | 3.44330300 | 5.12856700 |
| H | -0.76074800 | 4.60935100 | 4.18142100 | H | -0.73711500 | 4.62021800 | 4.19768800 |
| H | -2.66289800 | 5.71328000 | 5.38648800 | H | -2.63320200 | 5.72709900 | 5.39862500 |
| H | -2.91257800 | 5.81683200 | 3.63564700 | H | -2.87144400 | 5.84562400 | 3.64963800 |
| H | -3.81507600 | 4.62965500 | 4.58857500 | H | -3.78750200 | 4.65994300 | 4.58719100 |
| H | -7.96596900 | -3.70058500 | -0.18431000 | H | -7.91438500 | -3.72093900 | -0.16812300 |
| H | -10.40095800 | -3.30308200 | -0.24571500 | H | -10.34127400 | -3.33032800 | -0.23064400 |
| H | -7.23517600 | 0.54139900 | -0.16391700 | H | -7.20103200 | 0.52674600 | -0.17279000 |
| H | 7.20567200 | 0.75935700 | 0.18269800 | H | 7.17444100 | 0.74581800 | 0.18280600 |
| H | 10.47472300 | -2.99329300 | 0.18953800 | H | 10.41578100 | -3.02005200 | 0.18118100 |
| H | 8.05209300 | -3.46012200 | 0.12581600 | H | 8.00009400 | -3.47753300 | 0.11788500 |
| H | 9.07802100 | 2.38961300 | 0.25569200 | H | 9.04895800 | 2.36159800 | 0.25712700 |
| H | 11.51782200 | 2.84338900 | 0.32098200 | H | 11.48649100 | 2.79878400 | 0.32108400 |
| H | 12.33782600 | -1.38038900 | 0.26204200 | H | 12.27756100 | -1.42106700 | 0.25469000 |
| H | -12.33040400 | -1.70878500 | -0.29480700 | H | -12.26743600 | -1.74640100 | -0.28748700 |
| H | -11.56814700 | 2.52683800 | -0.27325100 | H | -11.53087300 | 2.48489700 | -0.29037500 |
| H | -9.15409500 | 2.11593200 | -0.21186600 | H | -9.12073000 | 2.08773600 | -0.22835200 |
| H | 15.33252700 | 0.65003300 | 0.37374700 | H | 15.27350100 | 0.58607200 | 0.36558300 |
| H | 14.27487200 | -0.51490200 | 1.22144400 | H | 14.21102400 | -0.57119500 | 1.21186000 |
| H | 14.31967300 | -0.48301700 | -0.56663000 | H | 14.25356500 | -0.53667700 | -0.57421900 |
| H | -15.08695300 | 1.74485800 | -0.36647200 | H | -15.03493700 | 1.67517600 | -0.37582400 |
| H | -13.72787900 | 2.43179900 | 0.56383300 | H | -13.68226800 | 2.37541300 | 0.54884300 |
| H | -13.68108500 | 2.43037700 | -1.22562100 | H | -13.63683700 | 2.36501100 | -1.23868900 |